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Supporting Information

RNA Hydrolysis by Heterocyclic Amidines and Guanidines: Parameters Affecting Reactivity

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Supporting Information

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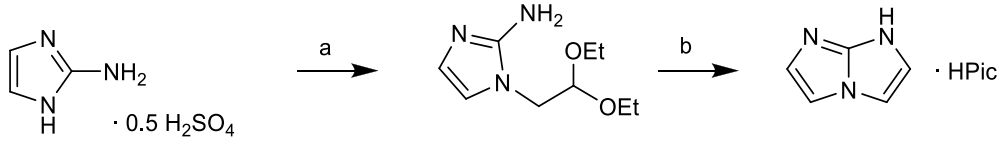
General

2-Aminobenzimidazole derivative **11**,[1] bislactam **23**,[2] as well as 2-aminoperimidine derivates **25**,[3] **26**,[3] and **27** [4] were prepared as described in the literature and not discussed here. New compounds are: **21**, **22**, **28**–**31** and the synthetic intermediates **38**, **39**, **41**–**43**, **45**, **46**, **51**, **55**, and **56**. All chemicals were reagent grade and used as purchased. All of the reactions except ester hydrolysis were performed under an argon atmosphere. Reactions were monitored by TLC using Merck TLC silica gel 60 F-254 aluminum sheets. Compounds were visualized by UV light (254 and 366 nm). Column chromatography was carried out on silica gel 60 (0.04 – 0.063 mm).

Melting points (uncorrected) were recorded on a Kofler system. ^{1}H and ^{13}C NMR spectra were recorded on a BRUKER DPX 250, a BRUKER AV 300 or a BRUKER AV 500 spectrometer. Chemical shifts are expressed in parts per million (ppm) relative to the nondeuterated solvent signal DMSO-d_5 (δ_H = 2.50, δ_C = 39.43) or $CHCl_3$ (δ_H = 7.26, δ_C = 77.00) as an internal reference. IR spectra were recorded with a Perkin Elmer 1600 Series FT-IR spectrometer (using a KBr pellet for solids) or a Perkin Elmer Spectrum Two FT-IR spectrometer equipped with a Perkin UATR Two unit. ESI mass spectroscopy was performed on a Fisons VG Platform II spectrometer or on a nano-ESI spectrometer (Perseptive Biosystems, Mariner). High-resolution mass spectra (HRMS) were obtained with a Thermo Scientific MALDI LTQ Orbitrap. Elemental analysis was carried out with a Vario MICRO cube apparatus. Preparative HPLC of 1*H*-imidazo[1,2-*a*]imidazol **18** was performed on a Waters pump 590 with a Beckman 163 variable wavelength detector. Analytical HPLC was performed on a JASCO PU-980 with a UV-975 UV/vis detector and a Varian 385-LC detector.

1*H*-Imidazo[1,2-*a*]imidazole 18



6 **32** **18**

a: Bromoacetaldehyde diethyl acetal, NaH, DMF, rt, 24 h, 33 %; b: HCl (2N), 100 °C, 6 h, 55 % as picrate salt.

1-(2,2-Diethoxyethyl)-2-aminoimidazole 32 [5]

To a suspension of 2-aminoimidazole hemisulfate **6** [6] (1.0 g, 7.57 mmol) in 10 mL of dry DMF and bromoacetaldehyde diethyl acetal (0.68 mL, 4.54 mmol) NaH (60 % dispersion in mineral oil; 450 mg, 11.3 mmol) was added in portions. The brown solution was stirred for 24 h at rt. The solvent was removed *in vacuo* and the crude product was purified by column chromatography (DCM/MeOH

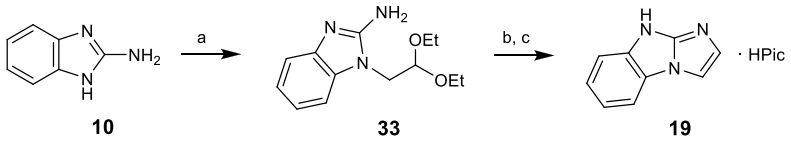
15/1), yielding 300 mg of the title compound as a brown oil (33 %). ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 6.61 (d, 1H, *J* = 1.4 Hz, *H*-C*5*), 6.51 (d, 1H, *J* = 1.4 Hz, *H*-C*4*), 4.59 (t, 1H, *J* = 5.3 Hz, acetal-*H*), 4.30 (br s, 2H, NH_2), 3.84 (d, 2H, *J* = 5.3 Hz, H_2C-N*1*), 3.80 - 3.68 (m, 2H, H_2C-O), 3.56 - 3.44 (m, 2H, H_2C-O), 1.20 (t, 6H, *J* = 7.0 Hz, CH_3). ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ = 149.0, 124.3, 116.0, 102.6, 64.0, 48.5, 15.3. IR (KBr): ṽ = 3399 (s), 3146 (m), 2977 (m), 1655 (m), 1560 (s), 1497 (m), 1381 (m), 1129 (m), 1064 (s), 702 (w).

Picrate and hydrochloride of 1*H*-imidazo[1,2-*a*]imidazole 18 [5,7]

32 (300 mg, 1.51 mmol) was dissolved in 12 mL of 2 N HCl and refluxed for 6 h. The solvent was removed *in vacuo* and the residue was taken up in 2 mL of MeOH. To this a solution of picric acid (60 % dispersion in H_2O, 576 mg, 1.51 mmol) in 5 mL MeOH was added and the precipitate was collected by filtration, yielding 280 mg of the picrate of **18** as dark yellow crystals (55 %). Mp: decomposition at 211.5 °C, ^{1}H-NMR (300 MHz, DMSO-d_6): δ = 13.11 (br s, 2H, N*H*), 8.58 (s, 2H, picrate), 7.64 (dd, 2H, *J* = 2.8 Hz, *J* = 0.7 Hz*, H*-C*3*, *H*-C*5*), 7.51 (dd, 2H, *J* = 2.8 Hz, *J* = 0.7 Hz, *H*-C*2* and *H*-C*6*). ^{13}C-NMR (75 MHz, DMSO-d_6): δ = 160.8, 141.9, 139.2, 125.2, 120.5, 108.8. Elemental analysis for $C_{13}H_8N_6O_7$ (336.22): calcd: C, 39.30; H, 2.40; N, 25.0; found: C, 39.25; H, 2.47; N, 25.14.
The picrate salt was converted into the corresponding hydrochloride using DOWEX ion exchange resin (Cl^--form).

Alternatively, the crude product was directly purified by HPLC, yielding the TFA salt of **18** as a slightly yellow solid. R_f = 0.22 (DCM/MeOH 9:1). Mp.: decomposition at 280 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 13.25 (br. s, 2H, N*H*), 7.64 (d, 2H, *J* = 2.0 Hz, *H*-C*3*, *H*-C*5*), 7.51 (d, 2H, *J* = 2.0 Hz, *H*-C*2* und *H*-C*6*). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 120.4, 108.6. IR (KBr): ṽ = 3140 (m), 3008 (m), 2958 (m), 2894 (m), 2741 (m), 1660 (s), 1413 (m), 1309 (w), 1205 (s), 1134 (s), 1088 (w), 963 (w), 916 (w), 864 (w), 833 (m), 815 (m) 760 (w), 722 (m), 688 (s), 590 (m). MS (ESI^+): m/z (%) = 107.5 (100) $[M+H]^+$, 214.7 (5) $[2M+H]^+$, calcd for $C_5H_5N_3$: 107.05. HRMS (MALDI) m/z = 108.05549 $[M+H]^+$, calcd for $C_5H_5N_3$+H^+: 108.05562. HPLC: analytical: ReproSil-Pur C18-AQ, 125 x 4.6, 5 µm, 0.1 % TFA (100 %), 0.8 mL/min, 220 nm, t_R = 7.00 min. Semi-preparative separation: ReproSil-Pur C18-AQ, 250 x 20, 10 µm, 0.1 % TFA/MeCN (995:5), 8.0 mL/min, 220 nm.
The TFA-salt was converted into the corresponding hydrochloride using DOWEX ion exchange resin (Cl^--form). Elemental analysis for $C_5H_5N_3 \cdot 1.5\ HCl \cdot 0.3\ H_2O$ (167.21): calcd: C, 35.92; H, 4.28; N, 25.13; found: C, 35.55; H, 4.37; N, 25.30.

9*H*-Imidazo[1,2-*a*]benzimidazole 19



10 **33** **19**

a: Bromoacetaldehyde diethyl acetal, NaH, DMF, 100 °C, 3 h, 39 %; b: HCl (2N), 100 °C, 3 h, c: picric acid, 61 %.

1-(2,2-Diethoxyethyl)-1*H*-benzo[*d*]imidazol-2-amine 33 [7]

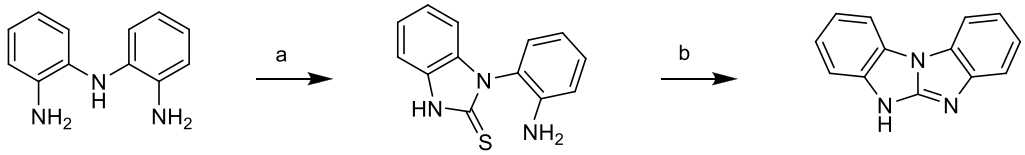
To a solution of 2-aminobenzimidazole **10** (1.0 g, 7.50 mmol) in 15 mL of dry DMF and bromoacetaldehyde diethyl acetal (1.13 mL, 7.50 mmol) NaH (60 % dispersion in mineral oil; 450 mg, 11.3 mmol) was added in portions. The solution was stirred at 100 °C for 3 h. The solvent was removed *in vacuo* and the crude product was purified by column chromatography (DCM/MeOH 20/1), yielding 730 mg of the title compound as an orange solid (39 %). Mp: 140-142 °C. ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 7.16 (d, 1H, *J* = 7.4 Hz*, H*-C7), 7.11 (d, 1H, *J* = 7.4 Hz*, H*-C4), 6.93 (dt, 1H, *J* = 7.4 Hz, *J* = 1.3 Hz*, H*-C5), 6.87 (dt, 1H, *J* = 7.4 Hz, *J* = 1.2 Hz*, H*-C6), 6.25 (br s, 2H, N*H*$_2$), 4.73 (t, 1H, *J* = 5.3 Hz, C*H*), 4.05 (d, 2H, *J* = 5.3 Hz*,* C*H*$_2$N), 3.63 (dq, 2H, *J* = 9.5 Hz, *J* = 7.1 Hz*,* OC*H*$_2$), 3.40 (dq, 2H, *J* = 9.5 Hz, *J* = 7.1 Hz*,* OC*H*$_2$), 1.01 (t, 6H, *J* = 7.0 Hz, C*H*$_3$). ^{13}C-NMR (125 MHz, DMSO-d_6): δ = 155.1, 142.5, 134.7, 120.2, 117.9, 114.6, 108.1, 100.2, 62.9, 45.0, 15.1. Elemental analysis for $C_{13}H_{19}N_3O_2$ (249.31): calcd: C, 62.63; H, 7.68; N, 16.85; found: C, 62.64; H, 7.67; N, 16.97.

Picrate and hydrochloride of 9*H*-imidazo[1,2-*a*]benzimidazole 19 [7]

33 (700 mg, 2.81 mmol) was dissolved in 20 mL of 2 N HCl and refluxed for 3 h. The solvent was removed *in vacuo* and the residue was taken up in MeOH. To this a solution of picric acid (60 % dispersion in H_2O, 1.08 g, 2.81 mmol) in MeOH was added and the precipitate was collected by filtration, yielding 660 mg of the picrate of **19** as light yellow crystals (61 %). R_f = 0.60 (DCM/MeOH 9:1). Mp: decomposition at 234.6 °C. ^{1}H-NMR (300 MHz, DMSO-d_6): δ = 8.58 (s, 2H, picric acid), 8.16 (d, 1H, *J* = 2.4 Hz), 8.07 - 8.04 (m, 1H), 7.68 - 7.65 (m, 1H), 7.61 (d, *J* = 2.4 Hz, 1H), 7.51 (td, 1H, *J* = 7.8 Hz, *J* = 1.4 Hz), 7.43 (td, 1H, *J* = 7.7 Hz, *J* = 1.3 Hz). ^{13}C-NMR (75 MHz, DMSO-d_6): δ = 142.5, 141.9, 134.5, 125.6, 125.2, 124.0, 122.5, 120.2, 113.6, 112.8, 109.1. Elemental analysis for $C_{15}H_{10}N_6O_7$ (386.28): calcd: C, 46.64; H, 2.60; N, 21.76; found: C, 46.66; H, 2.64; N, 22.15.

The picrate-salt was converted into the corresponding hydrochloride using DOWEX ion exchange resin (Cl^--form).

5*H*-Benzimidazo[1,2-*a*]benzimidazole 20



34 **35** **20**

a: TCDI, imidazole, MeCN, rt, 17.5 h, 69 %; b: Mukaiyama's reagent, DMF, rt, 7 days, 15 %.

1-(2-Aminophenyl)-2-mercaptobenzimidazole 35 [see also 8]

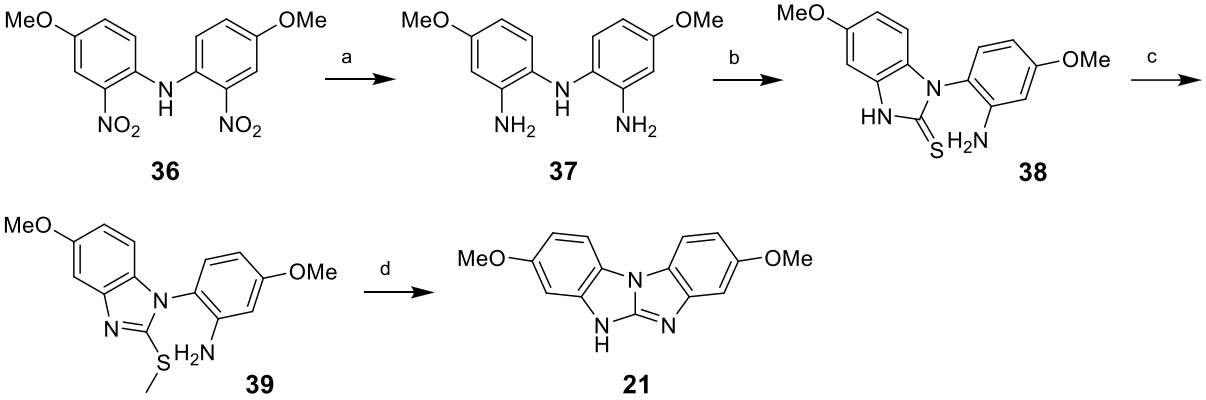
To a solution of bis-(2-aminophenyl)amine **34** (300 mg, 1.51 mmol), which was prepared as described in literature,[9] and imidazole (34 mg, 0.5 mmol) in 10 mL of dry MeCN, a solution of 1,1'-thiocarbonyl diimidazole (282 mg, 1.51 mmol) in 10 mL of dry MeCN was added dropwise at 0 °C. After stirring for 17.5 h, the precipitated solid was filtered off, washed with little MeCN and dried *in vacuo*. The filtrate was evaporated to dryness and the residue recrystallized from dry EtOH. The solid obtained by recrystallization and the precipitate filtered off were combined, yielding 252 mg of the colorless title compound (69 %). R_f = 0.61 (DCM/MeOH 9:1). Mp: 261 – 262 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 12.90 (br s, 1H, N*H*), 7.24 - 7.02 (m, 5H, Aryl-*H*), 6.90 (dd, 1H, *J* = 8.3 Hz, *J* = 1.3 Hz, Aryl-*H*), 6.72 - 6.64 (m, 2H, Aryl-*H*), 4.95 (br s, 2H, NH_2). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 168.8, 145.0, 133.4, 131.5, 129.7, 129.2, 122.9, 122.1, 119.6, 116.3, 116.2, 109.54, 109.50. IR (neat): ṽ = 3361 (w), 3304 (m), 3207 (m), 1634 (m), 1584 (w), 1506 (m), 1474 (m), 1462 (m), 1422 (s), 1378 (m), 1358 (m), 1344 (m), 1309 (s), 1268 (m), 1204 (m), 1179 (m), 1159 (m), 1139 (m), 749 (m), 734 (s), 629 (m), 620 (m), 586 (m), 570 (m), 524 (w). Elemental analysis for $C_{13}H_{11}N_3S$ (241.31): calcd: C, 64.70; H, 4.59; N, 17.41; S, 13.29; found: C, 64.88; H, 4.59; N, 17.58; S, 13.48.

5*H*-Benzimidazo[1,2-*a*]benzimidazole 20 [see also 10]

To a solution of thiourea **35** (100 mg, 0.41 mmol) in 1.7 mL of dry DMF, Mukaiyama's reagent (127 mg, 0.50 mmol) was added in several portions. The yellow solution was stirred at rt for one week. The solution was filtered and the solvent was removed *in vacuo*. The residue was purified by column chromatography (DCM/MeOH 98:2), yielding a colorless solid which was recrystallized from acetone. The product was obtained as colorless needles (13 mg, 15 %). R_f = 0.56 (DCM/MeOH 9:1). Mp: decomposition at 302 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 12.04 (br s, 1H, N*H*), 8.11 - 8.08 (m, 2H, Aryl-*H*), 7.52 - 7.48 (m, 2H, Aryl-*H*), 7.33 - 7.20 (m, 4H, Aryl-*H*). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 153.2, 141.0, 126.0, 122.7, 119.7, 114.4, 110.6. IR (neat): ṽ = 2981 (m), 2887 (w), 2630 (w), 1644 (m), 1588 (w), 1569 (m), 1495 (m), 1455 (m), 1429 (w), 1395 (m), 1285 (w), 1248 (w), 1221 (m), 1163 (m), 1147 (m), 1070 (m), 1006 (w), 961 (w), 868 (m), 841 (w), 736 (s), 620 (w), 605 (w), 534 (w). MS (ESI$^+$):

m/z (%) = 208.2 (100) $[M+H]^+$, calcd for $C_{13}H_9N_3$: 207.08. Elemental analysis for $C_{13}H_9N_3$ (207.23): calcd: C, 75.35; H, 4.38; N, 20.28; found: C, 75.15; H, 4.32; N, 20.05.

3,9-Dimethoxy-benzimidazo[1,2-*a*]benzimidazole 21



a: 10 bar H_2, Pd/C (10%), MeOH, 60 °C, 16 h, 96 %; b: TCDI, imidazole, MeCN, rt, 16 h, 57 %; c: MeI, AcOH, $MeNO_2$, 101 °C, 3 h, rt, overnight, 94 %; d: DMF, 153 °C, 3 days, 12 %.

Bis(4-methoxy-2-aminophenyl)amine 37 [11]

Bis(4-methoxy-2-nitrophenyl)amine **36** [11] (1.00 g, 3.13 mmol) was suspended in 15 mL of dry MeOH. After addition of Pd/C (100 mg), the reaction mixture was heated to 60 °C in an autoclave at 10 bar hydrogen pressure for 16 h, filtrated over celite and evaporated to dryness. The title compound was obtained as a brown solid (96 %). ^{1}H-NMR**:** (250 MHz, DMSO-d_6): δ = 6.40 (d, 2H, J = 8.6 Hz, Aryl-*H*), 6.28 (d, 2H, J = 2.8 Hz, Aryl-*H*), 6.04 (dd, 2H, J = 8.6 Hz, J = 2.8 Hz, Aryl-*H*), 5.56 (s, 1H, N*H*), 4.67 (s, 4H, NH_2) 3.61 (s, 6H, OCH_3).

1-(2-Amino-4-methoxyphenyl)-5-methoxy-1*H*-benzo[*d*]imidazole-2(3*H*)-thione 38

To a solution of amino compound **37** (530 mg, 2.04 mmol) and imidazole (41 mg, 0.61 mmol) in 20 mL of dry MeCN, a solution of thiocarbonyl diimidazole (545 mg, 2.04 mmol) was added slowly at 0 °C. The reaction mixture was stirred at rt for 16 h, evaporated to dryness and the residue was redissolved in DCM. The organic phase was washed with brine and dried over $MgSO_4$. After evaporation to dryness, the crude product was purified by column chromatography (cyclohexane/EtOAc 2:1), yielding 350 mg of the title compound as a colorless solid (57 %). Mp: 179 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 12.74 (s, 1H, N*H*), 6.92 (d, 1H, *J* = 8.7 Hz, Aryl-*H*), 6.71 (m, 2H, Aryl-*H*), 6.57 (d, 1H, *J* = 8.5 Hz, Aryl-*H*), 6.44 (s, 1H, *J* = 2.7 Hz, Aryl-*H*), 6.27 (dd, 1H, *J* = 8.7 Hz, *J* = 2.7 Hz, Aryl-*H*), 4.91 (s, 2H, NH_2), 3.76 (s, 3H, OCH_3), 3.74 (s, 3H, OCH_3). ^{13}C-NMR (125.8 MHz, DMSO-d_6): δ = 168.8, 160.3, 156.3, 146.1, 132.2, 130.1, 128.1, 113.3, 110.1, 109.4, 102.7, 100.5, 94.7,

55.7, 55.0. IR (neat): ṽ = 3351 (w), 3284 (w), 2926 (w), 1611 (w), 1593 (m), 1514 (s), 1463 (s), 1429 (s), 1360 (m), 1332 (m), 1287 (s), 1261 (m), 1224 (w), 1199 (s), 1156 (m), 1123 (w), 1109 (w), 1080 (w), 1025 (m), 950 (w), 851 (m), 788 (s), 729 (w), 704 (w), 655 (w), 621 (m), 571 (s), 540 (w), 480 (m), 456 (m), 405 (w). MS (ESI$^+$): m/z (%) = 302.1 $[M+H]^+$, calcd for $C_{15}H_{15}N_3O_2S$: 301.09. HRMS (MALDI) m/z = 302.09577 $[M+H]^+$, calcd for $C_{15}H_{15}N_3O_2S+H^+$: 302.09577.

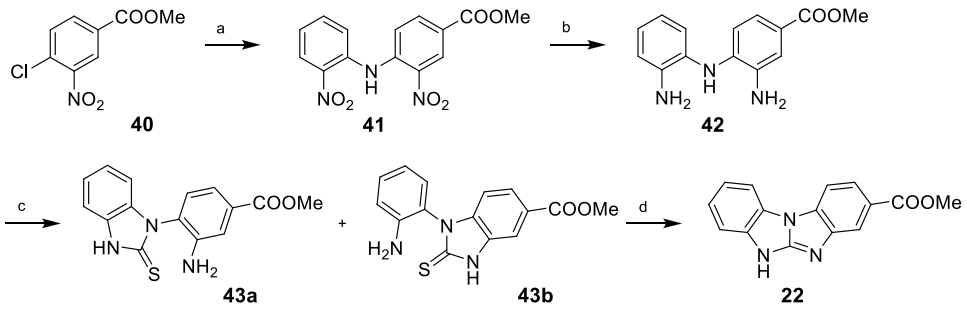
5-Methoxy-2-(5-methoxy-2-(methylthio)-1*H*-benzo[*d*]imidazole-1-yl) phenylamine 39

To a solution of thiourea **38** (307 mg, 1.01 mg) in 20 ml nitromethane, glacial acetic acid (0.23 mL, 4.04 mmol) and MeI (126 µL, 2.02 mmol) were added. The reaction mixture was refluxed for 3 h and then stirred at rt overnight. After evaporation of the solvent, the residue was dissolved in 50 mL DCM. The organic phase was washed with 50 mL of a saturated solution of $NaHCO_3$ and brine, dried over $MgSO_4$ and evaporated to dryness. Column chromatography (cyclohexane/EtOAc 2:1) yielded 300 mg of the product as a colorless solid (94 %). Mp: 187 °C. ^{1}H-NMR (500 MHz, DMSO-d_6): δ = 7.17 (d, 1H, *J* = 2.0 Hz, Aryl-*H*), 6.91 (d, 1H, *J* = 8.6 Hz, Aryl-*H*), 6.77 - 6.72 (m, 2H, Aryl-*H*), 6.44 (d, 1H, *J* = 2.8 Hz), 6.24 (dd, 1H, *J* = 8.7 Hz, *J* = 2.8 Hz), 4.95 (s, 2H, N*H*$_2$), 3.77 (s, 3H, OC*H*$_3$), 3.74 (s, 3H, OC*H*$_3$), 2.63 (s, 3H, SC*H*$_3$). ^{13}C-NMR (125.8 MHz, DMSO-d_6): δ = 160.8, 155.4, 154.1, 146.4, 144.2, 131.8, 129.8, 111.6, 110.3, 109.5, 102.7, 101.3, 100.1, 55.6, 55.0, 13.9. IR (neat): ṽ = 3395 (w), 3321 (m), 3210 (m), 3003 (w), 2949 (w), 2839 (w), 1627 (m), 1612 (m), 1578 (w), 1514 (s), 1485 (s), 1433 (m), 1420 (s), 1371 (w), 1303 (s), 1273 (m), 1241 (w), 1208 (m), 1193 (m), 1146 (s), 1107 (w), 1028 (s), 989 (w), 944 (w), 881(m), 839 (m), 826 (s), 795 (s),770 (w), 729 (w), 679 (w), 627 (m), 567 (m), 524 (w), 487 (w), 458 (w), 423 (w). MS (ESI$^+$): m/z (%) = 316.2 (100) $[M+H]^+$, calcd for $C_{16}H_{17}N_3O_2S$: 315.1. HRMS (MALDI) m/z = 316.11191 $[M+H]^+$, calcd for $C_{16}H_{17}N_3O_2S+H^+$: 316.11142.

3,9-Dimethoxy-benzimidazo[1,2-*a*]benzimidazole 21

The solution of **39** (300 mg, 0.95 mmol) in 15 mL dry DMF was refluxed for 3 days. The solvent was evaporated and the residue dried *in vacuo*. Column chromatography (cyclohexane/EtOAc 3:1) yielded 30 mg of the title compound as a colorless solid (12 %). Mp: decomposition at 275 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 11.93 (s, 1H, N*H*), 7.92 (d, 2H, *J* = 8.6 Hz, Aryl-*H*), 7.04 (d, 2H, *J* = 2.3 Hz, Aryl-*H*), 6.80 (dd, 2H, *J* = 8.6 Hz, *J* = 2.3 Hz Aryl-*H*), 3.82 (s, 6H, OC*H*$_3$). IR (neat): ṽ = 1638 (w), 1608 (w), 1580 (m), 1499 (m), 1468 (w), 1437 (w), 1420 (w), 1393 (m), 1315 (w), 1275 (s), 1189 (s), 1146 (s), 1126 (m), 1029 (s), 956 (m), 916 (s), 830 (m), 786 (s), 721 (w), 698 (w), 626 (w), 569 (s), 534 (m), 435 (w). MS (ESI$^+$): m/z (%) = 267.8 (100) $[M+H]^+$, calcd for $C_{15}H_{13}N_3O_2$: 267.1. HRMS (MALDI) m/z = 268.10849 $[M+H]^+$, calcd for $C_{15}H_{13}N_3O_2+H^+$: 268.10805.

Methyl benzimidazo[1,2-*a*]benzimidazole-3-carboxylate 22



a: 2-Nitroaniline, K_2CO_3, DMSO, 120 °C, 35 h, 46 %; b: 12 bar H_2, Pd/C (10%), EtOAc, rt, 19 h, 84 %; c: TCDI, imidazole, MeCN, rt, 72 h, 87 % of the product mixture; d: Mukaiyama's reagent, DMF, rt, 7 days, 16 %.

Methyl 4-(2-nitrophenylamino)-3-nitrobenzoate 41

The solution of 2-nitroaniline (1.28 g, 9.26 mmol), methyl 4-chloro-3-nitrobenzoate **40** [12] (2.00 g, 9.28 mmol) and K_2CO_3 in 30 mL DMSO was heated to 120 °C for 35 h. The dark solution was extracted with 60 mL DCM thrice. The combined organic phases were washed with 40 mL of brine four times, dried over Na_2SO_4 and evaporated to dryness. The residue was purified by column chromatography (*n*-hexane/EtOAc 9:1), yielding 1.35 g of the title compound as a yellow solid (46 %). R_f = 0.22 (*n*-hexane/EtOAc 3:1). Mp: 145 – 147 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 10.77 (br s, 1H, N*H*), 8.68 (d, 1H, *J* = 2.2 Hz, *H*-C*2*), 8.21 (dd, 1H, *J* = 8.5 Hz, *J* = 1.5 Hz, *H*-C*3'*), 8.07 (dd, 1 H, *J* = 8.8 Hz, *J* = 2.1 Hz, *H*-C*6*), 7.83 - 7.72 (m, 2H, *H*-C*5'*, *H*-C*6'*), 7.49 (d, 1H, *J* = 9.0 Hz, *H*-C*5*), 7.45 - 7.39 (m, 1H, *H*-C*4'*), 3.87 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 164.3, 142.2, 141.1, 135.3, 135.2, 135.0, 134.0, 127.7, 126.1, 125.1, 124.2, 120.8, 118.4, 52.3. IR (neat): ṽ = 3278 (w), 2924 (w), 2848 (w), 1719 (s), 1625 (m), 1605 (m), 1586 (m), 1506 (s), 1435 (m), 1341 (s), 1299 (s), 1263 (s), 1216 (s), 1148 (m), 1123 (m), 1071 (m), 975 (m), 919 (m), 882 (m), 837 (m), 782 (m), 755 (m), 738 (s), 674 (m), 516 (m). Elemental analysis for $C_{14}H_{11}N_3O_6$ (317.25): calcd: C, 53.00; H, 3.49; N, 13.24; found: C, 52.87; H, 3.59; N, 13.51.

Methyl 4-(2-aminophenylamino)-3-aminobenzoate 42

Nitro compound **41** (335 mg, 1.06 mmol) and Pd/C (33 mg) were suspended in 10 mL of dry EtOAc. The reaction mixture was stirred at rt in an autoclave at 12 bar hydrogen pressure for 19 h, filtrated over celite and evaporated to dryness. Column chromatography (*n*-hexane/EtOAc 3:1 → *n*-hexane/EtOAc 1:1) yielded 230 mg of diamine **42** as a brown solid (84 %). R_f = 0.27 (DCM/MeOH 98:2). Mp: 144 – 146 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 7.30 (d, 1H, *J* = 2.0 Hz, *H*-C*2*), 7.10 (dd, 1H, *J* = 8.2 Hz, *J* = 2.0 Hz, *H*-C*6*), 6.94 - 6.88 (m, 2 H, Aryl-*H*), 6.76 (dd, 1H, *J* = 8.6 Hz, *J* = 1.7 Hz, Aryl-*H*), 6.64 (br s, 1H, N*H*), 6.60 - 6.54 (m, 1H, Aryl-*H*), 6.31 (d, 1H, *J* = 8.2 Hz, *H*-C*5*), 4.95 (br s, 2H, NH_2), 4.73 (br s, 2H, NH_2), 3.73 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 166.6, 143.0, 137.4, 135.7,

126.1, 125.2, 125.1, 119.5, 119.0, 116.6, 115.2, 115.1, 112.0, 51.1. IR (neat): ṽ = 3371 (m), 2949 (w), 1684 (s), 1630 (m), 1591 (m), 1500 (m), 1448 (m), 1354 (w), 1292 (s), 1262 (s), 1223 (s), 1158 (m), 1082 (m), 987 (m), 917 (w), 890 (w), 849 (w), 809 (w), 763 (m), 740 (m), 714 (m), 489 (w), 459 (w). Elemental analysis for $C_{14}H_{15}N_3O_2$ (257.29): calcd: C, 65.35; H, 5.88; N, 16.33; found: C, 65.47; H, 6.15; N, 16.13.

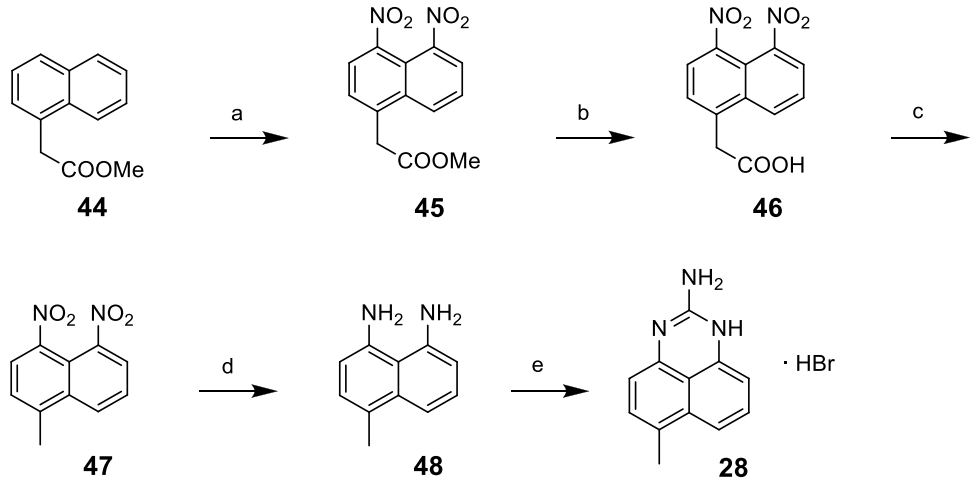
Mixture of methyl 3-amino-4-(1,2-dihydro-2-thioxobenzo[*d*]imidazol-3-yl)benzoate 43a and methyl 1-(2-aminophenyl)-2,3-dihydro-2-thioxo-1*H*-benzo[*d*]imidazole-5-carboxylate 43b

To a solution of diamine **42** (321 mg, 1.25 mmol) and imidazole (28 mg, 0.4 mmol) in 13 mL of dry MeCN, the solution of 1,1'-thiocarbonyl diimidazole (234 mg, 1.25 mmol) in 13 mL of dry MeCN was added dropwise at 0 °C. The brown solution was stirred for 72 h at rt. After evaporation of the solvent, column chromatography yielded 325 mg of a light brown solid (mixture of both constitutional isomers, altogether 87 %). R_f = 0.11 (DCM/MeOH 98:2). IR (neat): ṽ = 3327 (w), 3205 (w), 2949 (w), 1705 (s), 1623 (m), 1585 (m), 1505 (m), 1472 (m), 1429 (s), 1380 (m), 1359 (w), 1308 (s), 1244 (s), 1208 (s), 1151 (m), 1108 (m), 1089 (m), 991 (m), 886 (w), 762 (m), 739 (s), 644 (m), 624 (m). MS (ESI^-): m/z (%) = 297.9 (100) $[M-H]^-$, 148.6 (15) $[M-2H]^{2-}$, calcd for $C_{15}H_{13}N_3O_2S$: 299.07.

Methyl benzimidazo[1,2-*a*]benzimidazole-3-carboxylate 22

To a solution of the mixture of thioureas **43a** and **43b** (310 mg, 1.09 mmol) in 5.3 mL of dry DMF, Mukaiyama's reagent (335 mg, 1.31 mmol) was added in several portions. The yellow solution was stirred at rt for one week. The solvent was removed *in vacuo* and the residue was purified by column chromatography (DCM/MeOH 9:1 ⟶ DCM/MeOH 98:2). The product fractions were evaporated to dryness. The residue was washed with DCM several times and dried *in vacuo*. The title compound was obtained as a colorless solid (45 mg, 16 %). R_f = 0.59 (DCM/MeOH 9:1). Mp: 295 – 296 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 12.26 (br s, 1H, N*H*), 8.24 (br. d, 1H, *J* = 8.3 Hz, Aryl-*H*), 8.19 - 8.15 (m, 1H, Aryl-*H*), 8.09 (d, 1H, *J* =1.2 Hz, Aryl-*H*), 7.87 (dd, 1H, *J* = 8.3 Hz, *J* = 1.6 Hz, Aryl-*H*), 7.52 - 7.49 (m, 1H, Aryl-*H*), 7.39 - 7.25 (m, 2H, Aryl-*H*), 3.89 (s, 3H, OC*H*$_3$). ^{13}C-NMR (125.8 MHz, DMSO-d_6): δ = 166.6, 154.2, 143.8, 138.4, 129.8, 125.2, 123.8, 123.7, 120.9, 120.5, 116.7, 113.3, 111.2, 110.5, 52.0. IR (neat): ṽ = 2954 (w), 2675 (w), 1710 (s), 1657 (m), 1604 (m), 1576 (m), 1467 (m), 1449 (m), 1418 (m), 1284 (s), 1255 (m), 1237 (m), 1212 (m), 1166 (m), 1129 (m), 1103 (m), 1085 (m), 1070 (m), 983 (m), 892 (w), 881 (w), 869 (w), 761 (s), 741 (s), 729 (s), 616 (w), 543 (w). MS (ESI^+): m/z (%) = 265.9 (100) $[M+H]^+$, 531.5 (6) $[2M+H]^+$, calcd for $C_{15}H_{11}N_3O_2$: 265.09. HRMS (MALDI) m/z = 266.09323 $[M+H]^+$, calcd for $C_{15}H_{11}N_3O_2$+H^+: 266.09240. Elemental analysis for $C_{15}H_{11}N_3O_2 \cdot 0.5\ H_2O$ (274.28): calcd: C, 65.69; H, 4.41; N, 15.32; found: C, 65.65; H, 4.38; N, 15.46.

2-Amino-6-methyl-1*H*-perimidine hydrobromide 28



a: HNO_3/H_2SO_4, 0 °C, 10 min, 42%; b: 6 N HCl, 100 °C, 2 h 15 min, 89 %; c: NEt_3, acetone, rt, 3 h, 97 %; d: Et_3SiH, Pd/C (10 %), MeOH, rt, 18 min, 93 %; d: BrCN, DCM, 40 °C, 4.5 h, 84 %.

Methyl 2-(1,8-dinitronaphthalen-4-yl)acetate 45

To a solution of methyl 2-naphthalen-1-ylacetate **44** [13] (3.0 g, 15 mmol) in 6.6 mL conc. H_2SO_4 the mixture of 2.2 mL conc. HNO_3 and 2 mL conc. H_2SO_4 was added at 0 °C. The dark, viscous mixture was stirred at 0 °C for 10 min before it was poured on ice resulting in precipitation of an off-white solid. The precipitate was filtered off and washed with 10 mL of 2 M Na_2CO_3 four times followed by washing with 15 mL of a 1:1 mixture of *n*-hexane and Et_2O. The solid was dissolved in DCM and water was added. The organic phase was evaporated to dryness and the residue was recrystallized from toluene. Column chromatography (*n*-hexane/EtOAc 3:1 ⟶ *n*-hexane/EtOAc 1:1) yielded 1.84 g of the title compound as a colorless solid (42 %). R_f = 0.33 (*n*-hexane/EtOAc 1:1). Mp: 141 – 142 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 8.55 (dd, 1H, *J* = 8.5 Hz, *J* = 1.0 Hz, *H*-C*7* or C*5*), 8.51 - 8.44 (m, 2H, *H*-C*2*, *H*-C*5* or C*7*), 7.95 (dd, 1H, *J* = 8.6 Hz, *J* = 7.7 Hz, *H*-C*6*), 7.88 (d, 1H, *J* = 8.0 Hz, *H*-C*3*), 4.47 (s, 2H, CH_2), 3.65 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 170.4, 145.1, 144.0, 139.0, 133.4, 131.2, 129.1, 127.1, 127.0, 126.8, 115.5, 52.1, 38.0. IR (neat): ṽ = 3113 (w), 3080 (w), 2957 (w), 1734 (s),1631 (w), 1603 (w), 1576 (w), 1520 (s), 1431 (m), 1348 (s), 1325 (s), 1239 (m), 1192 (s), 1171 (s), 999 (w), 984 (m), 940 (w), 902 (w), 889 (w), 853 (w), 829 (m), 819 (m), 788 (w), 763 (m), 738 (m), 718 (m), 674 (w), 625 (w), 588 (w). Elemental analysis for $C_{13}H_{10}N_2O_6$ (290.23): calcd: C, 53.80; H, 3.47; N, 9.65; found: C, 53.80; H, 3.44; N, 9.59.

2-(1,8-Dinitronaphthalen-4-yl)acetic acid 46

Compound **45** (295 mg, 1.02 mmol) was suspended in 10 mL 6 N HCl and the mixture was refluxed for 2 h 15 min. The solvent was removed and the residue was washed with boiling DCM and dried *in*

vacuo. The free carboxylic acid **46** was obtained as an off-white solid (89 %). R_f = 0.64 (DCM/MeOH 9:1 + 1 % AcOH). Mp: 178 – 180 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 12.81 (br s, 1H, COO*H*), 8.55 (dd, 1H, *J* = 8.5 Hz, *J* = 1.1 Hz, *H*-C*7* or C*5*), 8.50 - 8.43 (m, 2 H, *H*-C*2*, *H*-C*5* or C*7*), 7.95 (dd, 1H, *J* = 8.5 Hz, *J* = 7.9 Hz, *H*-C*6*), 7.87 (d, 1 H, *J* = 7.9 Hz, *H*-C*3*), 4.36 (s, 2 H, CH_2). ^{13}C-NMR (125.8 MHz, DMSO-d_6): δ = 171.6, 145.1, 143.9, 140.0, 133.5, 131.3, 129.0, 127.1, 127.0, 126.9, 115.6, 38.6. IR (neat): ῦ = (2861 (w)), 1716 (m), 1525 (s), 1435 (w), 1417 (w), 1352 (s), 1254 (m), 1220 (m), 936 (w), 896 (m), 855 (m), 830 (m), 817 (s), 790 (m), 758 (m), 734 (s), 711 (m), 670 (m), 623 (m), 574 (w), 476 (w). MS (ESI$^-$): m/z (%) = 230.8 (100) $[M\text{-}NO_2]^-$, calcd for $C_{12}H_8N_2O_6$: 276.04.

4-Methyl-1,8-dinitronaphthalene 47 [14]

Carboxylic acid **46** (200 mg, 0.72 mmol) was dissolved in 7 mL acetone and NEt_3 was added (0.10 mL, 0.72 mmol). The reaction mixture was stirred at rt for 3 h. After evaporation of the solvent, column chromatography (*n*-hexane/EtOAc 3:1) yielded in 162 mg of the title compound as a colorless solid (97 %). R_f = 0.19 (*n*-hexane/EtOAc 3:1). Mp: 143 – 144 °C; Lit: 143 °C.[14] ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 8.63 (dd, 1H, *J* = 8.5 Hz, *J* = 1.1 Hz, *H*-C*5* or C*7*), 8.48 (dd, 1H, *J* = 7.8 Hz, *J* = 1.1 Hz, *H*-C*7* or C*5*), 8.39 (d, 1H, *J* = 7.8 Hz, *H*-C*2*), 7.94 (dd, 1H, *J* = 8.5 Hz, *J* = 7.7 Hz, *H*-C*6*), 7.77 (dd, 1H, *J* = 7.9 Hz, *J* = 1.0 Hz, *H*-C*3*), 2.85 (d, 3H, *J* = 0.5 Hz, CH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 145.1, 143.1, 142.9, 133.4, 131.1, 127.3, 126.9, 126.8, 126.8, 115.4, 19.8. IR (neat): ῦ = 2970 (w), 1521 (s), 1389 (w), 1341 (s), 1241 (w), 1201 (w), 887 (w), 841 (m), 821 (m), 769 (m), 760 (m), 737 (m), 651 (w), 636 (w), 622 (w), 586 (w), 560 (w), 534 (w), 484 (w). Elemental analysis for $C_{11}H_8N_2O_4$ (232.19): calcd: C, 56.90; H, 3.47; N, 12.06; found: C, 56.95; H, 3.42; N, 11.76.

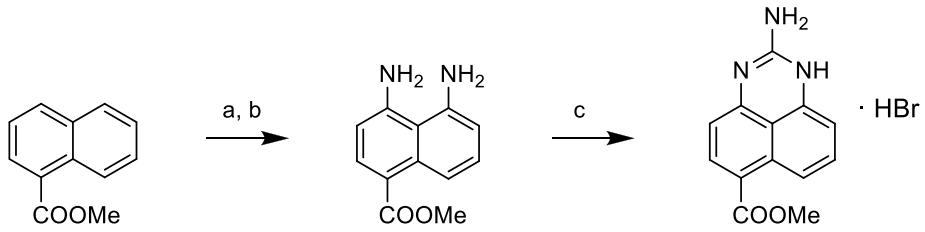
4-Methyl-1,8-diaminonaphthalene 48 [14]

To the suspension of dinitro compound **47** (277 mg, 1.19 mmol) and Pd/C (28 mg) in 10 mL of dry MeOH, Et_3SiH (1.54 mL, 9.54 mmol) was added dropwise. The reaction mixture was stirred at rt for 18 min, filtrated over celite and evaporated to dryness. The crude product was purified by column chromatography (*n*-hexane/EtOAc 3:1), yielding 290 mg of the pink title compound (93 %). R_f = 0.28 (*n*-hexane/EtOAc 3:1). Mp: 51 – 53 °C; Lit: 64 °C.[14] ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 7.12 (m, 1H, *H*-C*6*), 7.02 (dd, 1H, *J* = 8.3 Hz, *J* = 1.3 Hz, *H*-C*5* or C*7*), 6.93 (d, 1H, *J* = 7.4 Hz, *H*-C*2* or C*3*), 6.59 (dd, 1H, *J* = 7.3 Hz, *J* = 1.3 Hz, *H*-C*7* or C*5*), 6.51 (d, 1H, *J* = 7.5 Hz, *H*-C*3* or C*2*), 5.60 (br s, 2H, NH_2), 5.19 (br s, 2H, NH_2), 2.36 (s, 3H, CH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 146.7, 144.2, 135.1, 126.6, 126.0, 122.1, 116.0, 112.8, 110.1, 109.7, 19.3. IR (neat): ῦ = 3351 (w), 3300 (w), 2899 (w), 1584 (s), 1520 (w), 1459 (w), 1411 (m), 1351 (m), 1341 (w), 1292 (m), 1160 (m), 1029 (m), 870 (m), 815 (m), 777 (m), 747 (s), 638 (m), 620 (m). Elemental analysis for: $C_{11}H_{12}N_2$ (172.23): calcd: C, 76.71; H, 7.02; N, 16.27; found: C, 76.93; H, 7.06; N, 16.50.

2-Amino-6-methyl-1*H*-perimidine hydrobromide 28

Diamine **48** (150 mg, 0.87 mmol) was dissolved in 5 mL of dry DCM and BrCN was added (3.0 M solution in DCM; 0.35 mL, 1.05 mmol). The reaction mixture was refluxed for 4.5 h. The precipitated solid was filtered off, washed with acetone several times and dried *in vacuo*. 203 mg of the title compound were obtained as a grey solid (84 %). R_f = 0.25 (DCM/MeOH 9:1 + 1 % AcOH). Mp: 259 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 11.29 (br s, 2H, N*H*), 7.81 (br s, 2H, NH_2), 7.45 - 7.34 (m, 2H, *H*-C*8*, *H*-C*7*), 7.22 (dd, 1H, *J* = 7.6 Hz, *J* = 0.9 Hz, *H*-C*5*), 6.85 (dd, 1 H, *J* = 6.7 Hz, *J* = 1.5 Hz, *H*-C*9*), 6.24 (d, 1H, *J* = 7.6 Hz, *H*-C*4*), 2.41 (s, 3H, CH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 149.6, 133.0, 132.5, 130.7, 128.0, 128.0, 126.7, 117.3, 115.0, 106.7, 106.2, 18.1. IR (neat): ṽ = 3275 (w), 3163 (w), 2937 (m), 1668 (s), 1645 (s), 1576 (m), 1504 (m), 1484 (w), 1469 (m), 1439 (m), 1414 (w), 1385 (m), 1372 (m), 1318 (w), 1276 (m), 1160 (m), 1063 (m), 1022 (w), 820 (s), 806 (w), 756 (s), 714 (m), 686 (m), 587 (w), 564 (m). Elemental analysis for $C_{12}H_{11}N_3$ · HBr (278.15): calcd: C, 51.82; H, 4.35; N, 15.11; found: C, 51.76; H, 4.47; N, 15.21.

Methyl 2-amino-1*H*-perimidine-6-carboxylate hydrobromide 29



49 **50** **29**

a: HNO_3/H_2SO_4, 0 °C, 10 min; b: Et_3SiH, Pd/C (10%), MeOH, rt, 18 min, 16 % over 2 steps; c: BrCN, DCM (abs.), 40 °C, 20 h, 74 %.

Methyl 4,5-diaminonaphthalene-1-carboxylate 50

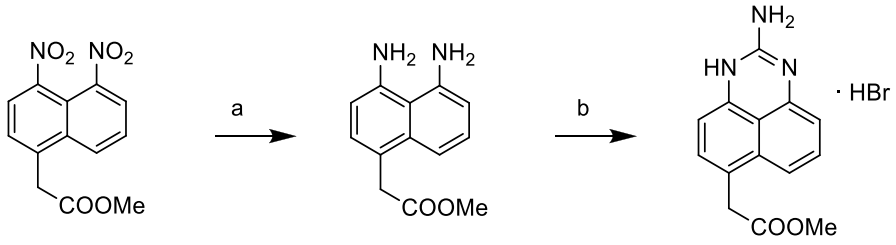
To a solution of methyl 1-naphthoic acid **49** [15] (3.70 g, 19.9 mmol) in 8.8 mL conc. H_2SO_4 the mixture of 2.9 mL conc. HNO_3 and 2.7 mL conc. H_2SO_4 was added at 0 °C. The dark, viscous mixture was stirred at 0 °C for 10 min before it was poured on ice resulting in precipitation of an off-white solid. The precipitate was filtered off and washed with 10 mL of 2 M Na_2CO_3 five times followed by washing with 40 mL of a 1:1 mixture of *n*-hexane and Et_2O. The crude product was recrystallized first from toluene, then from glacial acetic acid, yielding 1.63 g of an off-white solid, which was suspended in 10 mL of dry MeOH. After addition of Pd/C (163 mg), Et_3SiH (9.5 mL, 59 mmol) was added dropwise and the reaction mixture was stirred at rt for 18 min. The solution was filtered over celite and evaporated to dryness. Column chromatography (*n*-hexane/EtOAc 3:1) yielded 672 mg of a yellow

solid (16 %). R_f = 0.45 (*n*-hexane/EtOAc 1:1). Mp: 79 – 81 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 8.60 (dd, 1H, *J* = 8.7 Hz, *J* = 0.9 Hz, *H*-C*8*), 8.02 (d, 1H, *J* = 8.1 Hz, *H*-C*2*), 7.32 (dd, 1H, *J* = 8.7 Hz, *J* = 7.4 Hz, *H*-C*7*), 6.70 (dd, 1H, *J* = 7.3 Hz, *J* = 0.8 Hz, *H*-C*6*); 6.50 (d, 1H, *J* = 8.1 Hz, *H*-C*3*), 5.42 (br s, 2H, NH_2), 4.21 (br s, 2H, NH_2), 3.90 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ = 168.1, 150.4, 143.9, 135.7, 132.8, 128.0, 118.6, 116.3, 115.8, 113.6, 108.5, 51.5. IR (KBr): ṽ = 3407 (m), 3331 (m), 2928 (w), 1679 (m), 1628 (m), 1578 (s), 1522 (m), 1461 (w), 1430 (w), 1344 (w), 1258 (s), 1211 (m), 1183 (m), 1156 (m), 1111 (m), 962 (w), 867 (w), 812 (m), 756 (m), 660 (m), 623 (m), 568 (m). Elemental analysis for $C_{12}H_{12}N_2O_2$ (216.24): calcd: C, 66.65; H, 5.59; N, 12.96; found: C, 66.72; H, 5.70; N, 12.78.

Methyl 2-amino-1*H*-perimidine-6-carboxylate hydrobromide 29

Diamine **50** (720 mg, 3.33 mmol) was dissolved in 5 mL of dry DCM and BrCN was added (3.0 M solution in DCM; 1.3 mL, 4.0 mmol). The reaction mixture was refluxed for 20 h. The precipitated solid was filtered off, washed with acetone several times and dried *in vacuo*. 799 mg of the title compound were obtained as a grey solid (74 %). R_f = 0.24 (DCM/MeOH 9:1 + 1 % AcOH).Mp: 247 – 249 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 11.76 (br s, 2H, N*H*), 8.41 (dd, 1H, *J* = 8.8 Hz, *J* = 0.8 Hz, *H*-C*7*), 8.13 (d, 1H, *J* = 8.1 Hz, *H*-C*5*), 8.07 (br s, 2H, NH_2), 7.56 (dd, 1H, *J* = 8.8 Hz, *J* = 7.6 Hz, *H*-C*8*), 6.97 (dd, 1H, *J* = 7.6 Hz, *J* = 0.8 Hz, *H*-C*9*), 6.89 (d, 1H, *J* = 8.1 Hz, *H*-C*4*), 3.87 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 166.0, 149.4, 137.8, 133.8, 133.1, 132.0, 130.1, 118.6, 117.9, 115.3, 107.5, 105.8, 51.7. IR (neat): ṽ = 3114 (m), 1683 (s), 1641 (m), 1616 (m), 1579 (m), 1503 (m), 1463 (m), 1432 (m), 1367 (m), 1311 (w), 1245 (s), 1208 (m), 1187 (m), 1117 (m), 1065 (m), 1024 (m), 892 (w), 813 (m), 758 (s), 703 (m), 631 (w), 522 (w). MS (ESI$^+$): m/z (%) = 242.6 (100) $[M+H]^+$, calcd for $C_{13}H_{11}N_3O_2$: 241.09. Elemental analysis for $C_{13}H_{11}N_3O_2 \cdot HBr$ (322.16): calcd: C, 48.47; H, 3.75; N, 13.04; found: C, 48.58; H, 3.83; N, 13.05.

Methyl 2-(2-amino-1*H*-perimidin-7-yl)acetate hydrobromide 30



45 **51** **30**

a: Et_3SiH, Pd/C (10%), MeOH, rt, 15 min, 91 %; b: BrCN, DCM (abs.), 40 °C, 6.5 h, rt, 16 h, 76 %.

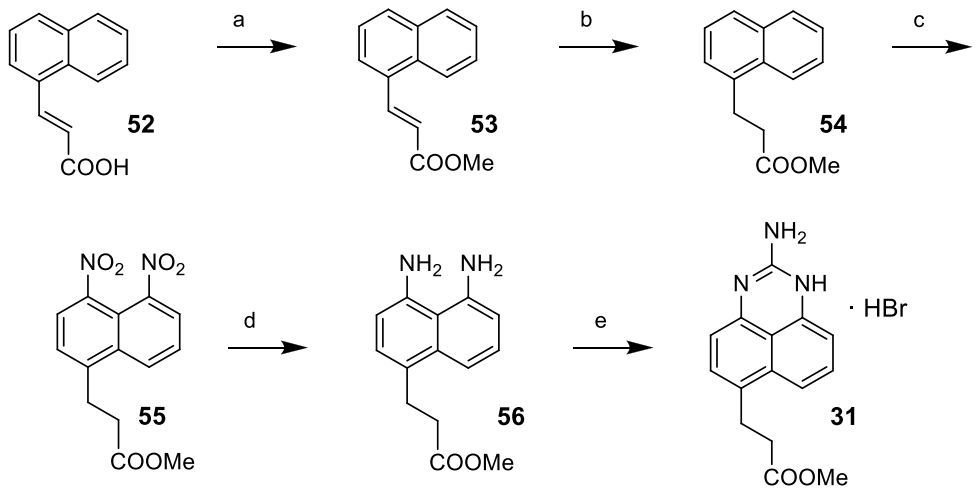
Methyl 2-(1,8-diaminonaphthalen-4-yl)acetate 51

To the suspension of dinitro compound **45** (352 mg, 1.21 mmol) and Pd/C (40 mg) in 5 mL of dry MeOH, Et_3SiH (2.0 mL, 12 mmol) was added dropwise. The reaction mixture was stirred at rt for 15 min, filtrated over celite and evaporated to dryness. The crude product was purified by column chromatography (*n*-hexane/EtOAc 3:1), yielding 255 mg of the pink title compound (91 %). R_f = 0.33 (*n*-hexane/EtOAc 1:1). Mp: 107 – 109 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 7.11 (dd, 1H, *J* = 8.4 Hz, *J* = 7.5 Hz, *H*-C*6*), 7.00 (d, 1H, *J* = 7.8 Hz, *H*-C*3*), 6.94 (dd, 1H, *J* = 8.5 Hz, *J* = 1.1 Hz, *H*-C*5*), 6.61 (dd, 1H, *J* = 7.5 Hz, *J* = 1.1 Hz, *H*-C*7*), 6.53 (d, 1H, *J* = 7.5 Hz, *H*-C*2*), 5.56 (br s, 2H, NH_2), 5.43 (br s, 2H, NH_2), 3.80 (s, 2H, CH_2), 3.56 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 172.2, 146.8, 145.7, 134.9, 128.4, 126.4, 119.0, 115.8, 112.6, 109.9, 109.4, 51.3, 38.4. IR (neat): ṽ = 3423 (w), 3389 (w), 3338 (w), 1726 (s), 1586 (s), 1434 (m), 1412 (m), 1355 (m), 1332 (m), 1240 (w), 1203 (m), 1161 (m), 996 (m), 889 (w), 867 (w), 826 (m), 810 (m), 747(s), 721 (m), 645 (m), 592 (m), 494 (w), 473 (w). Elemental analysis for $C_{13}H_{14}N_2O_2$ (230.26): calcd: C, 67.81; H, 6.13; N, 12.17; found: C, 67.64; H, 5.98; N, 12.05.

Methyl 2-(2-amino-1*H*-perimidin-7-yl)acetate hydrobromide 30

Diamine **51** (240 mg, 1.04 mmol) was dissolved in 7 mL of dry DCM and BrCN was added (3.0 M solution in DCM; 0.42 mL, 1.25 mmol). The reaction mixture was refluxed for 6.5 h and stirred at rt for further 16 h. The precipitated solid was filtered off, washed with acetone several times and dried *in vacuo*. 265 mg of the title compound were obtained as a grey solid (76 %). R_f = 0.26 (DCM/MeOH 9:1 + 1 % AcOH). Mp: 215 – 217 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 11.36 (br s, 2H, N*H*), 7.86 (br s, 2H, NH_2), 7.40 (dd, 1H, *J* = 8.5 Hz, *J* = 7.3 Hz, *H*-C*8*), 7.32 - 7.28 (m, 2H, *H*-C*5*, *H*-C*7*), 6.86 (dd, 1H, *J* = 7.3 Hz, *J* = 0.9 Hz, *H*-C*9*), 6.79 (d, 1H, *J* = 7.6 Hz, *H*-C*4*), 3.93 (s, 2H, CH_2), 3.59 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 171.3, 149.6, 133.1, 132.4, 132.0, 129.8, 128.4, 123.8, 117.1, 115.2, 106.8, 106.2, 51.6, 37.2. IR (neat): ṽ = 3280 (w), 3169 (w), 2905 (m), 2842 (m), 1733 (m), 1675 (s), 1645 (s), 1575 (m), 1507 (w), 1486 (w), 1451 (m), 1434 (m), 1377 (m), 1320 (m), 1266 (m), 1237 (m), 1206 (m), 1162 (s), 1142 (m), 1065 (w), 1002 (m), 837 (w), 816 (m), 763 (s), 702 (m). Elemental analysis for $C_{14}H_{13}N_3O_2 \cdot HBr$ (336.18): calcd: C, 50.02; H, 4.20; N, 12.50; found: C, 49.96; H, 4.12; N, 12.37.

Methyl 3-(2-amino-1*H*-perimidin-6-yl)propanoate hydrobromide 31



a: $SOCl_2$, MeOH (abs.), 0 °C - RT, 20 h, 97 %; b: 5 bar H_2, Pd/C (10%), EtOAc (abs.), 4 h, 97 %.; c: HNO_3/H_2SO_4, -5 °C, 5 min, 36 %; d: 4 bar H_2, Pd/C (10%), EtOAc, rt, 23 h, 97 %; e: BrCN, DCM (abs.), 40 °C, 4.5 h, rt, overnight, 40 %.

(*E*)-Methyl 3-(naphthalen-1-yl)acrylate 53

To a suspension of 3-(naphthalen-1-yl)acrylic acid **52** (1.00 g, 5.04 mmol) in 10 mL of dry MeOH, $SOCl_2$ (0.48 mL, 6.55 mmol) was added dropwise at 0 °C. The reaction mixture was stirred at rt for 20 h. The solvent was removed under reduced pressure. The residue was dissolved in 10 mL EtOH and washed with 10 mL saturated aqueous $NaHCO_3$. The combined organic phases were dried over Na_2SO_4 and evaporated to dryness, yielding 1.04 g of an orange oil (97 %). R_f = 0.23 (*n*-hexane/EtOAc 19:1). ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 8.46 (d, 1H, *J* = 15.8 Hz, =C*H*-Aryl), 8.22 (m, 1H, Aryl-*H*), 8.05 - 7.97 (m, 3H, Aryl-*H*), 7.68 - 7.54 (m, 3H, Aryl-*H*), 6.71 (d, 1H, *J* = 15.8 Hz, =C*H*-COOMe), 3.78 (s, 3H, OCH_3). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 166.3, 140.6, 133.2, 130.6, 130.5, 128.6, 127.1, 126.2, 125.5, 125.3, 122.8, 120.3, 51.4. IR (neat): ṽ = 2949 (w), 1710 (s), 1630 (m), 1511 (w), 1433 (m), 1347 (m), 1306 (m), 1266 (m), 1252 (m), 1239 (m), 1210 (w), 1191 (m), 1164 (s), 1087 (w), 1038 (w), 975 (m), 855 (w), 799 (m), 774 (s), 721 (m), 697 (w), 598 (m). Elemental analysis for $C_{14}H_{12}O_2 \cdot 0.1\ H_2O$ (214.05): calcd: C, 78.56; H, 5.74; found: C, 78.62; H, 5.70.

Methyl 3-(naphthalen-1-yl)propanoate 54 [16]

Compound **53** (1.02 g, 4.82 mmol) and Pd/C (112 mg) were suspended in 10 mL of dry EtOAc. The reaction mixture was stirred at rt in an autoclave at 5 bar hydrogen pressure for 4 h, filtrated over celite and evaporated to dryness, yielding 1.00 g of the title compound as a colorless oil (97 %). R_f = 0.22 (*n*-hexane/EtOAc 19:1). ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 8.08 - 8.04 (m, 1H, Aryl-*H*), 7.95 - 7.91 (m, 1H, Aryl-*H*), 7.80 (d, 1H, *J* = 7.3 Hz, Aryl-*H*), 7.60 - 7.49 (m, 2H, Aryl-*H*), 7.46 - 7.36 (m, 2H, Aryl-*H*),

3.60 (s, 3H, OC*H*$_3$), 3.33 (t, 2H, *J* = 7.3 Hz, C*H*$_2$-Aryl, overlaps with H_2O signal), 2.73 (t, 2 H, *J* = 7.3 Hz, C*H*$_2$-COOMe). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 172.5, 136.3, 133.3, 131.0, 128.5, 126.7, 126.0, 125.6, 125.5, 125.4, 123.2, 51.2, 34.2, 27.2. IR (neat): ṽ = 2950 (w), 1733 (s), 1598 (w), 1511 (w), 1435 (m), 1397 (w), 1366 (w), 1350 (w), 1296 (m), 1254 (m), 1195 (m), 1165 (m), 1056 (w), 1020 (w), 982 (w), 862 (w), 798 (m), 775 (s), 733 (w), 581 (w). Elemental analysis for $C_{14}H_{14}O_2$ (214.26): calcd: C, 78.48; H, 6.59; found: C, 78.44; H, 6.51.

Methyl 3-(1,8-dinitronaphthalen-4-yl)propanoate 55

To a solution of methyl ester **54** (2.70 g, 12.6 mmol) in 5.5 mL conc. H_2SO_4 the mixture of 1.9 mL conc. HNO_3 and 1.6 mL conc. H_2SO_4 was added at 0 °C. The dark, viscous mixture was stirred at -5 °C for 5 min before it was poured on ice resulting in precipitation of a light brown solid. 60 mL 2 M Na_2CO_3 and 100 mL EtOAc were added and the unsoluble solid was filtered off. The organic phase of the filtrate was separated and the aqueous phase was extracted with 50 mL EtOAc thrice. The combined organic phases were dried over Na_2SO_4 and evaporated to dryness. The residue was combined with the unsoluble solid isolated before, recrystallized from glacial acetic acid and purified by column chromatography (*n*-hexane/EtOAc 3:1 ⟶ *n*-hexane/EtOAc 1:1), yielding 1.39 g of a light yellow solid (36 %). R_f = 0.34 (*n*-hexane/EtOAc 1:1). Mp: 187 – 189 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 8.71 (dd, 1H, *J* = 8.7 Hz, *J* = 1.1 Hz, *H*-C*7*), 8.49 (dd, 1H, *J* = 7.6 Hz, *J* = 1.1 Hz, *H*-C*5*), 8.42 (d, 1 H, *J* = 7.9 Hz, *H*-C*2*), 7.95 (dd, 1 H, *J* = 8.7 Hz, *J* = 7.6 Hz, *H*-C*6*), 7.79 (d, 1H, *J* = 7.9 Hz, *H*-C*3*), 3.60 (s, 3H, OC*H*$_3$), 3.51 (t, 2H, *J* = 7.5 Hz, C*H*$_2$-Aryl), 2.82 (t, 2H, *J* = 7.5 Hz, C*H*$_2$-COOMe). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 172.0, 145.3, 144.9, 143.4, 132.7, 130.6, 127.1, 126.9, 126.8, 126.8, 115.6, 51.3, 33.7, 27.7. IR (neat): ṽ = 2923 (m), 2852 (w), 1736 (s), 1531 (s), 1435 (m), 1420 (w), 1346 (s), 1290 (m), 1189 (s), 1168 (s), 1086 (m), 975 (m), 905 (m), 881 (m), 850 (m), 822 (m), 789 (m), 780 (m), 770 (m), 757 (m), 734 (s), 714 (m), 654 (w), 630 (w). Elemental analysis for $C_{14}H_{12}N_2O_6$ (304.25): calcd: C, 55.27; H, 3.98; N, 9.21; found: C, 55.27; H, 4.04; N, 9.27.

Methyl 3-(1,8-diaminonaphthalen-4-yl)propanoate 56

Dinitro compound **55** (100 mg, 0.33 mmol) and Pd/C (23 mg) were suspended in 15 mL of dry EtOAc. The reaction mixture was stirred at rt in an autoclave at 4 bar hydrogen pressure for 23 h, filtrated over celite and evaporated to dryness. Column chromatography (*n*-hexane/EtOAc 3:1) yielded 68 mg of the title compound as a reddish brown viscous oil (97 %). R_f = 0.10 (*n*-hexane/EtOAc). ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 7.16 - 7.04 (m, 2H, *H*-C*6*, *H*-C*5*), 6.93 (d, 1H, *J* = 7.6 Hz, *H*-C*3*), 6.59 (dd, 1H, *J* = 7.0 Hz, *J* = 1.6 Hz, *H*-C*7*), 6.51 (d, 1 H, *J* = 7.6 Hz, *H*-C*2*), 5.58 (br s, 2H, N*H*$_2$), 5.30 (br s, 2H, N*H*$_2$), 3.58 (s, 3H, OC*H*$_3$), 3.04 (t, 2H, *J* = 7.5 Hz, C*H*$_2$-Aryl), 2.62 - 2.52 (m, 2 H, C*H*$_2$-COOMe, overlaps with DMSO). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 172.9, 147.0, 144.9, 134.2, 126.3, 126.2, 124.6, 116.0,

112.1, 109.8, 109.7, 51.2, 34.3, 27.9. IR (neat): ṽ = 3423 (w), 3337 (m), 2950 (m), 2871 (w), 1720 (s), 1588 (s), 1436 (m), 1418 (m), 1356 (m), 1301 (m), 1286 (m), 1265 (m), 1198 (m), 1163 (s), 1023 (w), 992 (w), 816 (m), 745 (s), 623 (m), 500 (w).

Methyl 3-(2-amino-1*H*-perimidin-6-yl)propanoate hydrobromide 31

Diamine **56** (50 mg, 0.2 mmol) was dissolved in 3 mL of dry DCM and BrCN was added (3.0 M solution in DCM; 0.08 mL, 0.25 mmol). The reaction mixture was refluxed for 4.5 h and stirred at rt overnight. The precipitated solid was filtered off, washed with acetone several times and dried *in vacuo*. 28 mg of the title compound were obtained as a colorless solid (40 %). R_f = 0.30 (DCM/MeOH 9:1 + 1 % AcOH). Mp: 195 – 197 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ = 11.33 (br s, 2H, N*H*), 7.83 (br s, 2H, NH_2), 7.43 - 7.41 (m, 2H, *H*-C*7*, *H*-C*8*), 7.22 (d, 1H, *J* = 7.8 Hz, *H*-C*5*), 6.85 (m, 1 H, *H*-C*9*), 6.76 (d, 1H, *J* = 7.6 Hz, *H*-C*4*), 3.58 (s, 3 H, OCH_3), 3.09 (t, 2 H, *J* = 7.3 Hz, CH_2-Aryl), 2.63 (t, 2 H, *J* = 7.3 Hz, CH_2-COOMe). ^{13}C-NMR (62.9 MHz, DMSO-d_6): δ = 172.5, 149.5, 133.2, 131.8, 131.3, 129.3, 128.3, 127.5, 116.7, 115.3, 106.7, 106.3, 51.2, 33.4, 26.7. IR (neat): ṽ = 3190 (m), 3050 (m), 1732 (m), 1668 (s), 1645 (s), 1589 (m), 1506 (m), 1469 (w), 1435 (m), 1372 (m), 1285 (m), 1225 (w), 1186 (m), 1161 (m), 1066 (w), 987 (w), 815 (m), 756 (m), 710 (w), 589 (w). Elemental analysis for $C_{15}H_{15}N_3O_2 \cdot HBr$ (350.21): calcd: C, 51.44; H, 4.60; N, 12.00; found: C, 51.23; H, 4.67; N, 11.84.

Cleavage and aggregation studies (analogous to experiments described in ref. 17 and 18)

General. All reagents were of the highest grades commercially available. Chemicals for polyacrylamide gel electrophoresis were purchased from Roth (Karlsruhe, Germany). Oligonucleotides were obtained from Biospring (Frankfurt, Germany).

Inactivation of RNases. All experimental steps were performed under sterile conditions. Plasticware, tubes and most solutions were treated with diethyl pyro-carbonate (DEPC). Solutions which are not compatible with DEPC treatment were prepared by mixing up molecular biology grade powdered reagents in DEPC-treated ultrapure water. All glassware was baked at 180 °C for six hours.

Purification of Cy-5-labelled oligonucleotides. The oligonucleotides were purified by denaturing PAGE (16 % monomer, 7 M urea). The bands of interest were excised, the gel fragments transferred to a nuclease-free tube and submerged with elution buffer (500 mM NaOAc, 0.1 % SDS, 2 mM EDTA). We routinely incubated the gel fragments under vigorous shaking overnight at room temperature. Quantum Prep Freeze'N'Squeeze spin columns (BioRad, Munich, Germany) were used to remove the gel fragments. After EtOH precipitation, the pellet was dissolved in 1 mL DEPC-treated H_2O and

desalted on a NAP-10 column. The pooled fractions were lyophilized to dryness, and the pellet was dissolved in DEPC-treated H_2O to give a concentration of approximately 0.5 µg/µL.

Polyacrylamide gel electrophoresis. The oligonucleotide fragments were separated by denaturing PAGE (16 % monomer, 8 M urea) on a DNA sequencing device (ALFexpress, GE Healthcare). Prior to electrophoresis, each sample was completed with 1.5 volumes of loading buffer (8 M urea, 20 mM EDTA and 0.2 % crocein orange in DEPC-treated H_2O) and 10 µL were loaded on the gel. Following running conditions were chosen: 1500 V (maximum), 60 mA (maximum), 25 W (constant), 60 °C, 2 s sampling interval and 400 min running time. For analyzing the electropherograms, the AlleleLinks 1.01 software package (Amersham Biosciences, Uppsala, Sweden/GE Healthcare) was used. The peak areas under the curves were added up, and the percentage of degraded RNA was calculated. Multiple cleavage reactions were disregarded in this system. All data were averaged over a minimum of two experiments.

RNA cleavage assay. 150 nM Cy5-labelled RNA **13**, **14** or **15** was incubated in a final volume of 10 µL with the indicated cleaver concentration (0.003 - 10 mM) in a 50 mM Tris-HCl buffer at pH 6.0, 7.0 or 8.0. All cleavage reactions were performed at 37 °C for 20 h.

FCS Measurements. Aggregation studies were carried out with a ConfoCor 2 (Carl Zeiss, Jena, Germany). As additional equipment, an Axiovert 200 M microscope containing a laser-adapted Zeiss C-Apochromat 40x /1.2 W corr H_2O-immersion objective was used. Fluctuation measurements, which are calculated in real time to give an autocorrelation curve, and further analysis, like determination of the average number and the diffusion time (at 24 °C) of the fluorescent particles in the confocal volume, were performed with the Fluorescence Correlation Microscope ConfoCor 2 Software version 3.2 SP1. Free Cy5 dye was used for calibration of the instrument (excitation source: He/Ne laser at 633 nm) and cover slips (24 x 60 mm, Roth, Karlsruhe, Germany) served as sample carriers. For comparison reasons, similar conditions as used for RNA-cleavage experiments were chosen.
To the mixture of an undegradable Cy5-labeled $T_{20}U$ probe **16** (19 nM) and an unlabeled DNA oligonucleotide **17** (131 nM) in 50 mM Tris-HCl buffer (pH 6.0, 7.0 or 8.0) the cleaver was added in the indicated concentration (0.003 - 10 mM). The incubation step (20 h, 37 °C) was omitted and the assay volume was increased to 30 µL. Each sample (30 µL droplet) was measured five times for 30 s.

Estimation of pK_a values

Spectrophotometric titrations were carried out with a solution of the cleavers (20 – 170 µM depending on the absorbance of the compound) in a 1:1 mixture of H_2O and MeOH. The solution was acidified with acetic acid and HCl. The pH (glass electrode) and the absorbance at an appropriate wavelength (282 – 408 nm, depending on the absorbance spectrum of the compound) were measured after each addition of 2 µL of a base (first 1 M TRIS, at pH values above 7.5 1 M NaOH). Extinction versus pH graphs resulted in sigmoidal curves which were fitted to a Boltzmann equation. Every titration was carried out at least twice. Please note that titrations were not carried out at constant ionic strength and no correction for MeOH was made. Thus, the results should be seen as approximations of sufficient accuracy for the discussion reported above, not as thermodynamically exact pK_a values.

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Additional computational details

Choice of tautomers

For some compounds several structures were obtained as local minima on the potential energy hypersurface. For compound **25** the rotamer with the methyl group in *trans* position to the imino nitrogen is 1.0 kJ mol^{-1} more stable at the AM1 level of theory than the *cis* rotamer, but less stable according to all other methods used. To allow for direct comparison between different methods, the *cis* rotamer as shown in Figure 6 was used also in discussions of the AM1 energetics. For compounds **27** – **31** the imino group can be in para position to the substituent or in the remote position. Both forms were considered, with the more stable variant being shown in Figure 6 and its values being included in this article.

Also for the imine structures different local minima were calculated. For the imino tautomers of compound **7** – **9**, **12** and **27** – **31** two different *E/Z*-isomers exist of which only one form is allowed by the proposed mechanism (see Figure 4 for an example of the allowed (*E*)-imine of compound **7**). Nevertheless both isomers where considered in the calculations. For compounds **7** and **12** AM1 favors the disallowed (*Z*)-isomer (by 4.0 and 6.7 kJ mol^{-1}) but all the other methods used favor the allowed (*E*)-isomer. For consistency also the AM1 energies in this article are from the (*E*)-isomer. For the imine tautomers of compounds **8** and **9** the allowed isomer is the more stable one in all methods used (AM1, B3LYP, RI-MP2 and RI-CCSD(T)). For the imine tautomers of compounds **27** – **31** the energy difference between *E*- and *Z*-isomer is small (≤ 1.0 kJ mol^{-1} for AM1, B3LYP and RI-MP2; no RI-CCSD(T) calculation was performed). If at all, the mechanistically forbidden isomer of **27** – **31** is favored at most by only 0.08 kJ mol^{-1} and their inclusion would therefore make almost no change for the energy differences. In the article only values derived by structural isomers that are allowed by the proposed mechanism are reported. For compound **9** also tautomers with multiple imines were considered in calculations, but as expected they are higher in energy than the single imine and therefore not included in this article. For compound **11** and **23** additionally the enol tautomers were considered but these are at least 9 kJ mol^{-1} less stable than the imine tautomer and thus not included in this article.

RI-B3LYP instead of B3LYP

Similar to calculations with B3LYP also calculations using RI-B3LYP were performed. The choice of B3LYP or RI-B3LYP affects absolute energies, but errors induced by the RI approximation essentially cancel out as expected when energy differences are calculated such that the effect on $\Delta_r G^\circ_{298}$ is small (the average of the absolute differences is 0.08 kJ mol^{-1} and for all structures the effect is < 0.7 kJ mol^{-1}).

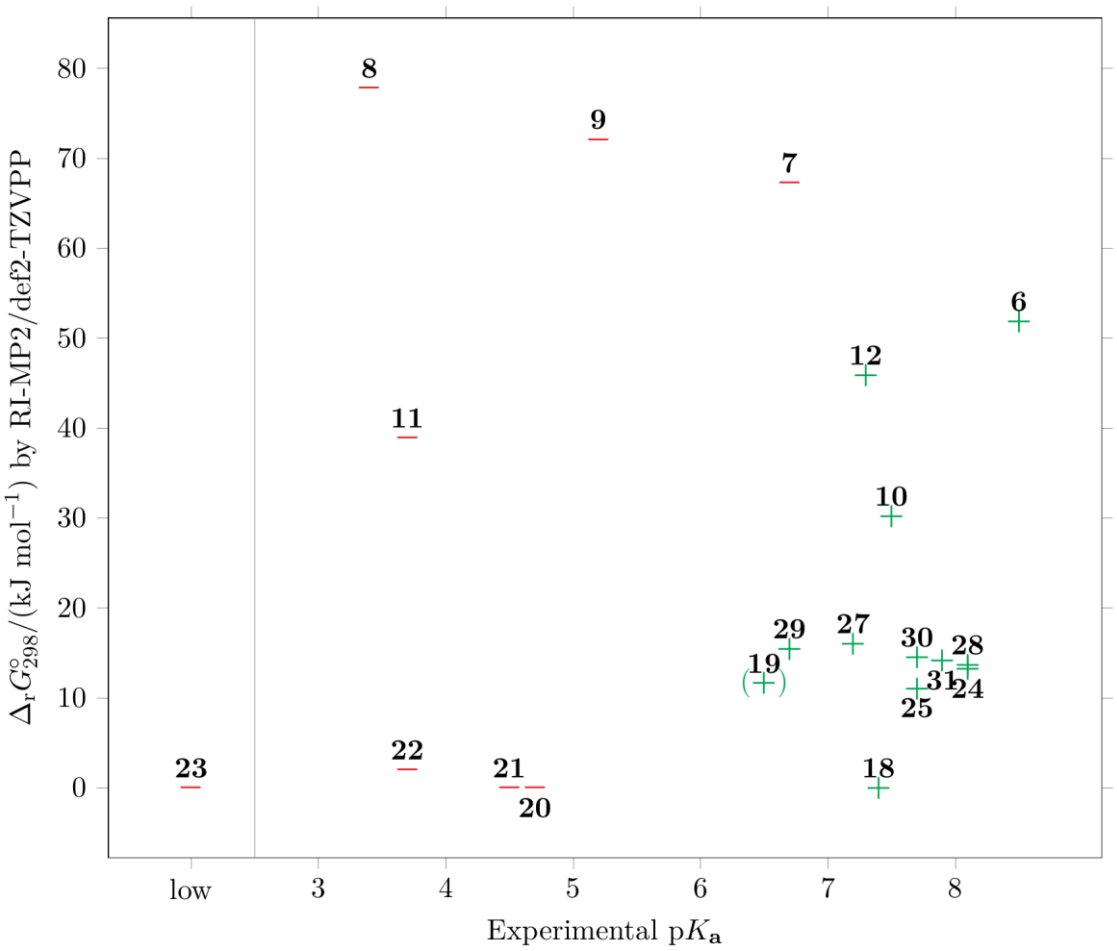

Figure S1. Variant of Figure 12 with $\Delta_r G^\circ_{298}$ from RI-MP2 instead of $\Delta_r H^\circ_{298}$ from AM1.

Energies of compounds and their tautomers

For pure electronic energies, see header of the xyz-coordinates.

Table S1. Calculated heat of formation $\Delta_f H^\circ_{298}$ and Gibbs free energies ΔG°_{298} for the various compounds by different methods.

Compound	σ [c]	$\Delta_f H^\circ_{298}$ / (kJ mol^{-1})	ΔG°_{298} / (kJ mol^{-1})			
		AM1	RI-B3LYP/ def2-TZVPP	B3LYP/ def2-TZVPP	RI-MP2/ def2-TZVPP	*E* RI-CCSD(T)/cc-pVTZ + Thermal of RI-MP2
6	1	219.83	-739007.29	-739006.49	-737740.02	-737898.10
6 Imine	1	260.44	-738971.42	-738970.56	-737688.16	-737852.71
7	1	137.62	-796875.75	-796874.90	-795432.73	-795632.32
7 Imine	1	208.66	-796818.32	-796817.44	-795365.46	-795573.57
8	2	197.02	-839049.57	-839048.83	-837577.45	-837766.41
8 Imine	1	262.10	-838979.43	-838978.62	-837499.62	-837696.04
9	6	270.11	-1171919.51	-1171918.44	-1169962.64	-1170187.42
9 Imine	1	333.50	-1171849.35	-1171848.95	-1169890.57	-1170117.13
10	1	287.82	-1142202.44	-1142201.33	-1140185.63	-1140438.58
10 Imine	1	303.52	-1142183.26	-1142182.17	-1140155.44	-1140412.19
11	1	179.88	-1642860.24	-1642858.94	-1640018.71	-1640369.57
11a	1	214.75	-1642832.17	-1642830.86	-1639979.82	-1640334.38
12	1	223.70	-1200050.46	-1200049.36	-1197865.57	-1198158.75
12 Imine	1	267.43	-1200012.88	-1200011.82	-1197819.71	-1198121.21
18 [a]	1	460.87	-938949.02	-938948.25	-937321.36	-937515.06
19	1	508.74	-1342149.13	-1342148.05	-1339777.09	-
19a	1	525.96	-1342139.87	-1342138.74	-1339765.46	-
20 [a]	1	572.03	-1745343.06	-1745341.65	-1742226.66	-
21 [a]	1	259.49	-2346482.57	-2346480.77	-2342425.69	-
22	1	223.40	-2343503.31	-2343501.67	-2339471.66	-
22a	1	226.18	-2343501.93	-2343500.28	-2339469.64	-
23 [a]	1	-147.32	-1540314.70	-1540313.48	-1537741.10	-1538065.29
24	1	312.62	-1545373.92	-1545372.57	-1542608.82	-1542961.82
24 Imine	1	333.09	-1545364.69	-1545363.36	-1542595.62	-1542950.75
25	1	326.71	-1648464.85	-1648463.37	-1645492.72	-1645892.21
25 Imine	1	330.53	-1648455.62	-1648454.15	-1645481.67	-1645882.00
26 [b]	1	348.36	-1751550.40	-1751548.83	-1748378.29	-
27	1	337.08	-8301980.36	-8301978.94	-8295401.26	-8295906.44
27 Imine	1	358.59	-8301967.76	-8301966.39	-8295385.25	-8295892.65
28	1	284.56	-1648492.98	-1648491.51	-1645533.84	-1645911.57
28 Imine	1	305.33	-1648483.48	-1648482.05	-1645520.17	-
29	1	-31.72	-2143529.26	-2143527.71	-2139846.16	-
29 Imine	1	-10.30	-2143516.87	-2143515.40	-2139830.70	-
30	1	-60.57	-2246628.34	-2246626.77	-2242753.73	-
30 Imine	1	-39.32	-2246617.81	-2246616.27	-2242739.19	-
31	1	-91.99	-2349745.15	-2349743.51	-2345669.34	-
31 Imine	1	-70.72	-2349735.14	-2349733.53	-2345655.20	-

[a] is equal to its tautomer. [b] no reasonable tautomer exists. [c] symmetry number used in the partition function for ΔG°_{298}.

Table S2. Calculated energy differences between the relevant tautomers by different methods.

Compound	$\Delta_r H^\circ_{298}$ / (kJ mol^{-1})	$\Delta_r G^\circ_{298}$ / (kJ mol^{-1})			
	AM1	RI-B3LYP/ def2-TZVPP	B3LYP/ def2-TZVPP	RI-MP2/ def2-TZVPP	*E* RI-CCSD(T)/cc-pVTZ + Thermal of RI-MP2
6	40.6	35.9	35.9	51.9	45.4
7	71.0	57.4	57.5	67.3	58.7
8	65.1	70.1	70.2	77.8	70.4
9	63.4	70.2	69.5	72.1	70.3
10	15.7	19.2	19.2	30.2	26.4
11	34.9	28.1	28.1	38.9	35.2
12	43.7	37.6	37.5	45.9	37.5
18 [a]	0.0	0.0	0.0	0.0	0.0
19	17.2	9.3	9.3	11.6	-
20 [a]	0.0	0.0	0.0	0.0	0.0
21 [a]	0.0	0.0	0.0	0.0	0.0
22	2.8	1.4	1.4	2.0	-
23 [a]	0.0	0.0	0.0	0.0	0.0
24	20.5	9.2	9.2	13.2	11.1
25	3.8	9.2	9.2	11.0	10.2
27	21.5	12.6	12.6	16.0	13.8
28	20.8	9.5	9.5	13.7	-
29	21.4	12.4	12.3	15.5	-
30	21.3	10.5	10.5	14.5	-
31	21.3	10.0	10.0	14.1	-

[a] is equal to its tautomer, energy differences are therefore 0.

xyz-Structures of compounds and their tautomers

All coordinates are given in Å.

Compound **6**

```
11
AM1 heat of formation 0.837269611779E-01 E_h
C    -1.413402    -0.764418     0.000000
C    -1.474363     0.644007     0.000000
N    -0.161740     1.095529    -0.000002
C     0.669147    -0.051224     0.000000
N    -0.095188    -1.191213     0.000001
N     2.086705     0.077647     0.000000
H    -2.240405    -1.473513    -0.000002
H    -2.324499     1.322573     0.000003
H     0.143861     2.032748     0.000007
H     2.462160    -0.362871     0.820128
H     2.462159    -0.362870    -0.820128
```

11
RI-B3LYP electronic energy -281.53262869877 E_h
C -1.3887451 -0.7355885 0.0076732
C -1.4634686 0.6234707 0.0013857
N -0.1437938 1.0573184 -0.0044521
C 0.6420189 -0.0564700 -0.0016906
N -0.0718908 -1.1539215 0.0139148
N 2.0290205 0.0172237 -0.0842267
H -2.2000265 -1.4434755 0.0201927
H -2.2911990 1.3090332 0.0139698
H 0.1718119 2.0043219 -0.1150364
H 2.4572365 0.6064939 0.6163550
H 2.4299956 -0.9091908 -0.0563423
11
B3LYP electronic energy -281.53228890772 E_h
C -1.3887392 -0.7355501 0.0076627
C -1.4633859 0.6235108 0.0013632
N -0.1437332 1.0572928 -0.0043699
C 0.6419657 -0.0565025 -0.0017093
N -0.0719187 -1.1539558 0.0138927
N 2.0289978 0.0172814 -0.0843545
H -2.2000974 -1.4435089 0.0202194
H -2.2910914 1.3092731 0.0141223
H 0.1720229 2.0043815 -0.1153801
H 2.4569495 0.6061759 0.6169307
H 2.4297505 -0.9093993 -0.0559704
11
RI-MP2 electronic energy -281.050500853986 E_h
C -1.3942602 -0.8600452 -0.0096324
C -1.4749959 0.5088918 -0.0454588
N -0.1666389 0.9415522 -0.0680939
C 0.6279387 -0.1623047 -0.0370984
N -0.0785493 -1.2724026 0.0033833
N 2.0193720 -0.0592864 -0.1207678
H -2.2034837 -1.5677947 0.0185796
H -2.3055924 1.1901157 -0.0468984
H 0.1522386 1.8866966 -0.1893751
H 2.4192474 0.3847235 0.6946992
H 2.4047237 -0.9901460 -0.1993372

Compound **6** Imine

11
AM1 heat of formation 0.991952372705E-01 E_h
C -1.413460 -0.662168 0.018628
C -1.388259 0.712232 0.010605
N -0.047660 1.174812 -0.086120
C 0.793160 -0.025942 -0.001845
N -0.096035 -1.178159 -0.084840
N 2.086948 -0.127460 0.008372
H -2.266848 -1.341911 0.021140
H -2.217143 1.421036 0.006268
H 0.205129 1.930728 0.512026
H 2.581554 0.737263 -0.024452
H 0.145894 -1.976194 0.458803
11
RI-B3LYP electronic energy -281.51758033775 E_h
C 1.4102893 -0.6557088 0.0000899
C 1.3961367 0.6882068 0.0000606
N 0.0565453 1.0857051 -0.0001616
C -0.7930746 -0.0170328 -0.0000534
N 0.0874977 -1.0862998 -0.0001303

N -2.0695494 -0.1300601 0.0000862
H 2.2382639 -1.3396012 0.0000968
H 2.2064728 1.3929211 0.0000433
H -0.2733246 2.0316580 0.0004254
H -2.5335636 0.7708043 0.0000951
H -0.2394121 -2.0339907 0.0001962
11
B3LYP electronic energy -281.51721405277 E_h
C 1.4102342 -0.6557163 0.0000963
C 1.3960977 0.6881904 0.0000661
N 0.0565467 1.0856839 -0.0001736
C -0.7930040 -0.0170046 -0.0000593
N 0.0874808 -1.0862712 -0.0001398
N -2.0694939 -0.1300941 0.0000938
H 2.2382021 -1.3397956 0.0001053
H 2.2064414 1.3930752 0.0000498
H -0.2734013 2.0317837 0.0004458
H -2.5334027 0.7709903 0.0001030
H -0.2395421 -2.0341014 0.0002147
11
RI-MP2 electronic energy -281.029119411236 E_h
C 1.2728599 -0.7234713 0.0000000
C 1.2579560 0.6285538 0.0000000
N -0.0782203 1.0176691 0.0000000
C -0.9248778 -0.0812928 0.0000000
N -0.0467712 -1.1467996 0.0000000
N -2.2072397 -0.2013929 0.0000000
H 2.1001629 -1.4068278 0.0000000
H 2.0667391 1.3337374 0.0000000
H -0.4123541 1.9625368 0.0000000
H -2.6500709 0.7106556 0.0000000
H -0.3781839 -2.0933682 0.0000000

Compound **7**

13
AM1 heat of formation 0.524156617509E-01 E_h
C -1.855511 -0.036092 -0.007513
C -1.080510 -1.208023 0.004372
N 0.259708 -1.233390 0.020169
C 0.916666 -0.025599 0.005797
C 0.202741 1.212630 0.007862
C -1.186859 1.188588 -0.002844
N 2.315719 -0.009755 -0.088370
H -2.950275 -0.090065 -0.018313
H -1.563296 -2.203123 0.007962
H 0.744212 2.167536 0.005608
H -1.753102 2.131953 -0.007781
H 2.776668 -0.872784 0.098984
H 2.738647 0.779473 0.344902
13
RI-B3LYP electronic energy -303.59020046869 E_h
C -1.8385453 -0.0701864 0.0049977
C -1.0453720 -1.2070147 0.0022383
N 0.2882930 -1.1851988 0.0009237
C 0.8991717 0.0023045 -0.0070596
C 0.1860477 1.2147135 -0.0051065
C -1.1937239 1.1661784 0.0034027
N 2.2768961 -0.0180837 -0.0630572
H -2.9162873 -0.1478764 0.0100037
H -1.4989486 -2.1926019 0.0060308
H 0.7127155 2.1601980 -0.0168636

H -1.7662632 2.0850354 0.0066369
H 2.6943009 -0.9058958 0.1633032
H 2.7726894 0.7881460 0.2749874
13
B3LYP electronic energy -303.58984609682 E_h
C -1.8385204 -0.0701335 0.0049718
C -1.0453886 -1.2069742 0.0022342
N 0.2882753 -1.1852498 0.0009590
C 0.8991011 0.0022687 -0.0070060
C 0.1861490 1.2147386 -0.0050376
C -1.1936124 1.1661958 0.0034046
N 2.2767963 -0.0181448 -0.0631631
H -2.9163770 -0.1477781 0.0099185
H -1.4990548 -2.1926380 0.0059488
H 0.7129760 2.1602320 -0.0169088
H -1.7662094 2.0851589 0.0065830
H 2.6942022 -0.9060181 0.1635675
H 2.7725904 0.7882331 0.2749177
13
RI-MP2 electronic energy -303.041413891314 E_h
C -1.8013621 -0.1988896 -0.0186507
C -1.0100522 -1.3387389 -0.0271312
N 0.3299056 -1.3180917 -0.0364741
C 0.9330635 -0.1257973 -0.0487094
C 0.2218439 1.0830269 -0.0453492
C -1.1616379 1.0399800 -0.0248607
N 2.3175897 -0.1392275 -0.1278305
H -2.8780316 -0.2793143 -0.0061676
H -1.4623786 -2.3226811 -0.0201797
H 0.7510651 2.0260288 -0.0644378
H -1.7325805 1.9584446 -0.0183963
H 2.7096927 -1.0285085 0.1387730
H 2.7828824 0.6437685 0.2994141

Compound **7** Imine
13
AM1 heat of formation 0.794739508213E-01 E_h
C -1.816897 0.006917 -0.000001
C -1.093871 1.170192 -0.000001
N 0.277671 1.191213 0.000004
C 1.035511 -0.009034 0.000000
C 0.240688 -1.256038 0.000000
C -1.113407 -1.239591 0.000001
N 2.338178 0.078695 -0.000002
H -2.912157 0.022245 -0.000006
H -1.579868 2.163721 -0.000004
H 0.809978 -2.195881 -0.000003
H -1.698522 -2.171916 0.000003
H 0.759127 2.062436 -0.000002
H 2.798352 -0.804634 -0.000002
13
RI-B3LYP electronic energy -303.56863495313 E_h
C -1.8198265 -0.0174801 0.0000002
C -1.0956914 -1.1645170 0.0000006
N 0.2619488 -1.1344274 0.0000005
C 1.0431915 0.0293464 -0.0000001
C 0.2525990 1.2476404 -0.0000005
C -1.1035549 1.2180220 -0.0000003
N 2.3190677 -0.1225597 -0.0000003
H -2.8976241 -0.0486139 0.0000003
H -1.5445979 -2.1475036 0.0000011

H 0.7910466 2.1855002 -0.0000009
H -1.6574539 2.1487101 -0.0000007
H 0.7910339 -1.9930907 0.0000008
H 2.7901737 0.7758366 -0.0000007
13
B3LYP electronic energy -303.56827215024 E_h
C -1.8198393 -0.0175062 0.0000092
C -1.0956191 -1.1645053 -0.0000012
N 0.2619597 -1.1343615 -0.0000120
C 1.0431473 0.0294199 -0.0000005
C 0.2526194 1.2476702 -0.0000094
C -1.1035463 1.2179426 -0.0000009
N 2.3190109 -0.1226292 0.0000132
H -2.8977488 -0.0486508 0.0000179
H -1.5444816 -2.1476528 -0.0000005
H 0.7911481 2.1855769 -0.0000167
H -1.6575554 2.1487148 -0.0000019
H 0.7911796 -1.9931402 -0.0000081
H 2.7900921 0.7759603 0.0000183
13
RI-MP2 electronic energy -303.015545932579 E_h
C -1.6775965 -0.0888878 0.0000000
C -0.9513881 -1.2397168 0.0000000
N 0.4063967 -1.2042659 0.0000000
C 1.1860050 -0.0487023 0.0000000
C 0.3998779 1.1669449 0.0000000
C -0.9627562 1.1432066 0.0000000
N 2.4687277 -0.2051560 0.0000000
H -2.7541372 -0.1261546 0.0000000
H -1.3973543 -2.2230280 0.0000000
H 0.9368880 2.1051595 0.0000000
H -1.5084688 2.0774670 0.0000000
H 0.9371260 -2.0630210 0.0000000
H 2.9166799 0.7061544 0.0000000

Compound **8**

12
AM1 heat of formation 0.750409692562E-01 E_h
C 1.837888 -0.000001 -0.016070
C 1.095722 -1.194613 0.000476
N -0.244226 -1.233648 0.020954
C -0.894667 -0.000002 0.010421
N -0.244225 1.233649 0.020955
C 1.095719 1.194614 0.000476
N -2.286847 0.000000 -0.076581
H 2.931218 0.000003 -0.035610
H 1.597717 -2.180100 0.002419
H 1.597720 2.180098 0.002421
H -2.753769 -0.846033 0.150840
H -2.753765 0.846041 0.150822
12
RI-B3LYP electronic energy -319.64219485987 E_h
C -0.0009834 -1.8088832 0.0000000
C 0.0027429 -1.0717248 1.1774664
N 0.0027429 0.2556286 1.1976572
C -0.0041457 0.8642985 0.0000000
N 0.0027429 0.2556286 -1.1976572
C 0.0027429 -1.0717248 -1.1774664
N -0.0430068 2.2232559 0.0000000
H -0.0008872 -2.8884730 0.0000000
H 0.0085522 -1.5642745 2.1445747

H 0.0085522 -1.5642745 -2.1445747
H 0.1221447 2.7018173 0.8663386
H 0.1221447 2.7018173 -0.8663386
12
B3LYP electronic energy -319.64186629077 E_h
C -0.0009442 -1.8088408 0.0000000
C 0.0027954 -1.0716719 1.1774564
N 0.0027954 0.2556726 1.1977245
C -0.0040747 0.8642320 0.0000000
N 0.0027954 0.2556726 -1.1977245
C 0.0027954 -1.0716719 -1.1774564
N -0.0428618 2.2230614 0.0000000
H -0.0008769 -2.8885375 0.0000000
H 0.0085443 -1.5642828 2.1446508
H 0.0085443 -1.5642828 -2.1446508
H 0.1206268 2.7019854 0.8665646
H 0.1206268 2.7019854 -0.8665646
12
RI-MP2 electronic energy -319.082639428603 E_h
C -0.0160579 -1.7232017 0.0000000
C -0.0166795 -0.9900879 1.1792615
N -0.0291314 0.3429802 1.1991346
C -0.0443353 0.9451561 0.0000000
N -0.0291314 0.3429802 -1.1991346
C -0.0166795 -0.9900879 -1.1792615
N -0.1235109 2.3111351 0.0000000
H -0.0069522 -2.8017376 0.0000000
H -0.0031564 -1.4801037 2.1451498
H -0.0031564 -1.4801037 -2.1451498
H 0.1443955 2.7615355 0.8568314
H 0.1443955 2.7615355 -0.8568314

Compound **8** Imine
12
AM1 heat of formation 0.998274890827E-01 E_h
C 1.801139 -0.022773 -0.000001
C 1.106030 1.159999 0.000004
N -0.262357 1.187530 -0.000008
C -1.013809 -0.041355 0.000001
N -0.278164 -1.281678 0.000011
C 1.024289 -1.241095 -0.000009
N -2.316917 0.059133 0.000001
H 2.893564 -0.057377 0.000021
H 1.610790 2.144375 0.000023
H 1.554564 -2.213529 -0.000026
H -0.754905 2.051404 -0.000018
H -2.807842 -0.808422 0.000002
12
RI-B3LYP electronic energy -319.61505506015 E_h
C -1.7896777 -0.0423387 -0.0000018
C -1.1151079 1.1372112 -0.0000050
N 0.2322595 1.1379111 -0.0000040
C 1.0116140 -0.0387984 0.0000017
N 0.3109605 -1.2414171 0.0000028
C -0.9871566 -1.2213312 0.0000016
N 2.2785425 0.0999895 0.0000051
H -2.8664603 -0.0828192 -0.0000026
H -1.5979249 2.1047241 -0.0000088
H -1.4800773 -2.1908832 0.0000031
H 0.7554467 1.9996986 -0.0000060
H 2.7186479 -0.8145624 0.0000086

12
B3LYP electronic energy -319.61472256024 E_h
C -1.7896924 -0.0422694 0.0000209
C -1.1149804 1.1372286 -0.0000008
N 0.2323176 1.1378483 -0.0000262
C 1.0115809 -0.0389025 -0.0000019
N 0.3109211 -1.2414657 -0.0000227
C -0.9872150 -1.2212229 -0.0000062
N 2.2785029 0.1000005 0.0000350
H -2.8665795 -0.0827010 0.0000388
H -1.5977341 2.1049157 -0.0000034
H -1.4802463 -2.1908458 -0.0000204
H 0.7556813 1.9997248 -0.0000322
H 2.7185295 -0.8147780 0.0000428
12
RI-MP2 electronic energy -319.051796387178 E_h
C -1.5789570 -0.1151084 0.0000000
C -0.9050787 1.0669681 0.0000000
N 0.4436056 1.0629162 0.0000000
C 1.2205648 -0.1037129 0.0000000
N 0.5281482 -1.3133308 0.0000000
C -0.7766965 -1.2912392 0.0000000
N 2.4935921 0.0375092 0.0000000
H -2.6545912 -0.1527070 0.0000000
H -1.3840164 2.0351334 0.0000000
H -1.2634349 -2.2614369 0.0000000
H 0.9678701 1.9246784 0.0000000
H 2.9089940 -0.8896701 0.0000000

Compound **9**
15
AM1 heat of formation 0.102879782206 E_h
N 0.089485 -1.420313 -0.028189
C 1.207082 -0.599062 -0.009294
N 1.185289 0.787654 -0.028191
C -0.084736 1.344892 -0.009296
N -1.274773 0.632660 -0.028212
C -1.122344 -0.745829 -0.009295
N -0.172046 2.730699 0.068090
N -2.278840 -1.514346 0.068106
N 2.450882 -1.216355 0.068085
H 0.646124 3.260282 -0.111703
H -1.050205 3.153410 -0.111740
H -3.146537 -1.070581 -0.111793
H -2.205824 -2.486201 -0.111774
H 2.500415 -2.189701 -0.111722
H 3.256031 -0.667204 -0.111786
15
RI-B3LYP electronic energy -446.44564688815 E_h
N 1.3727134 -0.1034857 0.0032828
C 0.5615022 -1.1673164 -0.0041482
N -0.7760240 -1.1369836 -0.0020475
C -1.2916123 0.0973950 0.0042177
N -0.5967930 1.2405187 -0.0020605
C 0.7301770 1.0699345 -0.0042105
N -2.6438453 0.1992855 0.0429905
N 1.4942731 2.1897319 -0.0357755
N 1.1490828 -2.3890127 -0.0355492
H -3.1856867 -0.6293768 -0.1196675
H -3.0554739 1.0997716 -0.1195710
H 1.0483032 3.0748309 0.1195412

H 2.4817427 2.0964116 0.1145056
H 2.1393997 -2.4448041 0.1145964
H 0.5754645 -3.1972904 0.1195576
15
B3LYP electronic energy -446.44513358600 E_h
N 1.2381602 -0.6018418 0.0033454
C 0.0920882 -1.2920002 -0.0040709
N -1.1402926 -0.7712680 -0.0020530
C -1.1648748 0.5662190 0.0041508
N -0.0979288 1.3731532 -0.0020608
C 1.0728795 0.7257456 -0.0040801
N -2.3844220 1.1590238 0.0427663
N 2.1956154 1.4853343 -0.0353668
N 0.1883047 -2.6441186 -0.0353120
H -3.1937128 0.5881854 -0.1189446
H -2.4354798 2.1480702 -0.1189240
H 2.1071572 2.4728522 0.1182518
H 3.0796985 1.0348828 0.1132517
H 1.0886635 -3.0611612 0.1130673
H -0.6429424 -3.1845956 0.1180663
15
RI-MP2 electronic energy -445.702324995676 E_h
N 1.3745777 -0.1036233 -0.0333495
C 0.5587522 -1.1629883 -0.0339566
N -0.7780087 -1.1390326 -0.0148247
C -1.2872114 0.0970291 0.0014837
N -0.5984618 1.2427832 -0.0148521
C 0.7267864 1.0660705 -0.0339869
N -2.6407891 0.1990710 0.0783986
N 1.4913710 2.1878036 -0.0922701
N 1.1465419 -2.3866640 -0.0921808
H -3.1637199 -0.6253559 -0.1541951
H -3.0341563 1.0926023 -0.1542025
H 1.0411180 3.0513821 0.1492042
H 2.4653872 2.0788111 0.1226679
H 2.1258915 -2.4249053 0.1227536
H 0.5719214 -3.1729834 0.1493102

Compound **9** Imine
15
AM1 heat of formation 0.127025217911 E_h
N 0.067816 -1.378132 -0.055535
C 1.178173 -0.611541 -0.011113
N 1.148192 0.787350 -0.044208
C -0.131734 1.458095 -0.005148
N -1.311563 0.665104 -0.020448
C -1.170414 -0.675512 -0.013879
N -0.093495 2.765096 0.027321
N -2.311318 -1.470757 0.081148
N 2.433373 -1.239595 0.103166
H 1.973223 1.327242 0.087972
H -0.984584 3.211451 0.030134
H -3.185486 -1.037800 -0.101930
H -2.222455 -2.432352 -0.144639
H 2.427311 -2.228814 -0.018685
H 3.204807 -0.769444 -0.312111
15
RI-B3LYP electronic energy -446.41686828006 E_h
N -0.2033045 -1.3387704 0.0059478
C -1.1949959 -0.4874502 -0.0040961
N -1.0026131 0.8469592 -0.0032900

C 0.2998737 1.4120000 0.0031021
N 1.3343672 0.5179355 0.0080217
C 1.0424872 -0.7621665 -0.0003986
N 0.3529176 2.6868992 0.0018915
N 2.0627235 -1.6497706 -0.0224233
N -2.4732565 -0.9521609 -0.0511007
H -1.7640596 1.5051675 -0.0532975
H 1.3240263 2.9824801 0.0028121
H 3.0027100 -1.3097008 0.0595369
H 1.8635673 -2.6280234 0.0666857
H -2.5768864 -1.9393702 0.1101804
H -3.2293873 -0.3624963 0.2491103
15
B3LYP electronic energy -446.41637053630 E_h
N -0.2030508 -1.3389036 0.0059650
C -1.1948350 -0.4877016 -0.0039889
N -1.0026967 0.8466689 -0.0027414
C 0.2996435 1.4120125 0.0031000
N 1.3343168 0.5182601 0.0077070
C 1.0426071 -0.7619580 -0.0000730
N 0.3522291 2.6869529 0.0015659
N 2.0628130 -1.6491343 -0.0195138
N -2.4730183 -0.9525438 -0.0515784
H -1.7643992 1.5047686 -0.0528033
H 1.3234795 2.9826432 0.0021544
H 3.0038276 -1.3092917 0.0511409
H 1.8642839 -2.6286325 0.0566799
H -2.5765661 -1.9398492 0.1100496
H -3.2292708 -0.3628569 0.2487194
15
RI-MP2 electronic energy -445.672544644013 E_h
N -0.1267896 -1.2480306 -0.0406804
C -1.1119889 -0.3903633 -0.0436658
N -0.9216782 0.9414051 -0.0344513
C 0.3710609 1.5070485 -0.0218872
N 1.4141356 0.6170345 -0.0235586
C 1.1164026 -0.6594562 -0.0474133
N 0.4225666 2.7859818 -0.0118368
N 2.1353723 -1.5503824 -0.1054895
N -2.3962402 -0.8458347 -0.1043775
H -1.6868071 1.5949928 -0.0949409
H 1.4021445 3.0560709 -0.0098452
H 3.0591241 -1.2028260 0.0747349
H 1.9224181 -2.5099605 0.0915698
H -2.4817382 -1.8298785 0.0857490
H -3.1179824 -0.2658013 0.2860927

Compound **10**
17
AM1 heat of formation 0.109624887522 E_h
C -2.573675 -0.714008 -0.004934
C -2.578947 0.688700 -0.011410
C -1.398182 1.423515 -0.005200
C -0.197877 0.710704 0.001436
C -0.179740 -0.740974 0.005234
C -1.390496 -1.443084 0.005485
N 1.141857 1.130074 0.066379
C 1.920880 -0.077934 0.001227
N 1.151360 -1.203147 0.017985
N 3.326421 -0.030262 -0.107158
H -3.535044 -1.249762 -0.007853

H -3.542022 1.220899 -0.021921
H -1.411661 2.521147 -0.004359
H -1.397392 -2.542078 0.014892
H 1.458104 2.002065 -0.271686
H 3.739306 0.627804 0.522115
H 3.739459 -0.938244 -0.022651
17
RI-B3LYP electronic energy -435.14489352350 E_h
C -2.5470014 -0.7224766 0.0014942
C -2.5664811 0.6771156 -0.0016918
C -1.3854196 1.4149284 0.0016255
C -0.1990240 0.6984412 0.0005278
C -0.1597539 -0.7119973 0.0003991
C -1.3510815 -1.4320360 0.0036885
N 1.1368778 1.0850186 0.0136081
C 1.8802837 -0.0732547 -0.0013049
N 1.1562256 -1.1577313 0.0082031
N 3.2559384 -0.0349091 -0.0808391
H -3.4849614 -1.2621287 0.0019397
H -3.5153881 1.1966550 -0.0054073
H -1.4024432 2.4971908 0.0027480
H -1.3362065 -2.5134967 0.0066887
H 1.4908453 2.0115082 -0.1444897
H 3.7101704 0.6677805 0.4822055
H 3.6655577 -0.9484798 0.0410806
17
B3LYP electronic energy -435.14442826482 E_h
C -2.5469164 -0.7224640 0.0014998
C -2.5663645 0.6771402 -0.0016869
C -1.3853573 1.4150087 0.0015926
C -0.1990409 0.6984164 0.0005570
C -0.1597651 -0.7120139 0.0004182
C -1.3510551 -1.4320913 0.0036903
N 1.1368202 1.0849519 0.0135370
C 1.8802176 -0.0732482 -0.0012903
N 1.1562087 -1.1577660 0.0082170
N 3.2559069 -0.0347926 -0.0810337
H -3.4850255 -1.2620978 0.0019536
H -3.5154131 1.1966856 -0.0054180
H -1.4023056 2.4973600 0.0026970
H -1.3361541 -2.5136441 0.0066851
H 1.4909290 2.0116159 -0.1440369
H 3.7098555 0.6674542 0.4830795
H 3.6652537 -0.9486148 0.0413144
17
RI-MP2 electronic energy -434.377106790712 E_h
C -2.4442968 -0.8078145 -0.0125342
C -2.4641330 0.5974280 -0.0199275
C -1.2872495 1.3400349 -0.0216381
C -0.0971910 0.6190669 -0.0255453
C -0.0567685 -0.7923294 -0.0216496
C -1.2490131 -1.5177838 -0.0119149
N 1.2310470 1.0039642 -0.0176925
C 1.9752014 -0.1489897 -0.0279694
N 1.2556708 -1.2438354 -0.0145348
N 3.3553209 -0.0971402 -0.1168454
H -3.3824708 -1.3454181 -0.0075429
H -3.4142656 1.1135190 -0.0223685
H -1.3045116 2.4214977 -0.0236342
H -1.2308499 -2.5987077 -0.0050805
H 1.5882591 1.9302065 -0.1748345
H 3.7812155 0.5483917 0.5310747

H 3.7440353 -1.0220899 -0.0073622

Compound **10** Imine

17
AM1 heat of formation 0.115602786662 E_h
C -2.553278 0.686918 -0.018282
C -2.549129 -0.703234 -0.024426
C -1.350460 -1.431624 -0.011394
C -0.158688 -0.723059 0.007973
C -0.163559 0.720651 0.020982
C -1.359956 1.423255 0.004601
N 1.186748 -1.187879 -0.057141
C 2.027211 0.018666 0.006620
N 1.171570 1.193648 0.133876
N 3.319036 0.103193 -0.067507
H -3.510602 1.229687 -0.031481
H -3.502943 -1.251765 -0.040909
H -1.363582 -2.530034 -0.021663
H -1.379965 2.521474 0.014467
H 1.425856 -1.904207 0.595279
H 3.804777 -0.767193 -0.091202
H 1.432137 1.989868 -0.405527
17
RI-B3LYP electronic energy -435.13675625830 E_h
C -2.5456649 -0.6876733 -0.0000075
C -2.5419504 0.7029706 -0.0000014
C -1.3416119 1.4218189 0.0000054
C -0.1622583 0.7021213 0.0000046
C -0.1650553 -0.7044767 -0.0000026
C -1.3510015 -1.4151669 -0.0000079
N 1.1721109 1.0928098 0.0000138
C 2.0231037 -0.0135968 0.0000023
N 1.1618236 -1.1027597 -0.0000011
N 3.2945536 -0.1117540 -0.0000027
H -3.4872424 -1.2197575 -0.0000121
H -3.4800134 1.2410905 -0.0000013
H -1.3409017 2.5037895 0.0000115
H -1.3576612 -2.4969325 -0.0000129
H 1.5075386 2.0378235 -0.0000046
H 3.7522556 0.7925537 0.0000039
H 1.5132393 -2.0426233 -0.0000123
17
B3LYP electronic energy -435.13630139823 E_h
C -2.5455567 -0.6876913 0.0000264
C -2.5418523 0.7029590 0.0000302
C -1.3415760 1.4218843 0.0000001
C -0.1622796 0.7021284 -0.0000254
C -0.1650634 -0.7044667 -0.0000259
C -1.3509378 -1.4152340 -0.0000042
N 1.1720579 1.0927776 -0.0000516
C 2.0230311 -0.0135727 -0.0000042
N 1.1617720 -1.1027052 -0.0000463
N 3.2944903 -0.1118052 0.0000605
H -3.4872653 -1.2197917 0.0000497
H -3.4800594 1.2410756 0.0000559
H -1.3408427 2.5039440 0.0000022
H -1.3575354 -2.4970892 -0.0000041
H 1.5075447 2.0378943 0.0000650
H 3.7520807 0.7927297 0.0000780
H 1.5132449 -2.0426753 0.0000327
17

RI-MP2 electronic energy -434.364052692215 E_h

C	-2.3461807	-0.7314687	0.0000000
C	-2.3420204	0.6652808	0.0000000
C	-1.1439234	1.3852268	0.0000000
C	0.0375771	0.6599787	0.0000000
C	0.0347543	-0.7452841	0.0000000
C	-1.1538065	-1.4603676	0.0000000
N	1.3676123	1.0486150	0.0000000
C	2.2169841	-0.0548443	0.0000000
N	1.3575195	-1.1416740	0.0000000
N	3.4935600	-0.1592233	0.0000000
H	-3.2885052	-1.2608149	0.0000000
H	-3.2806479	1.2010556	0.0000000
H	-1.1404093	2.4665705	0.0000000
H	-1.1583507	-2.5415620	0.0000000
H	1.7043861	1.9939307	0.0000000
H	3.9303230	0.7560915	0.0000000
H	1.7111276	-2.0815106	0.0000000

Compound **11**

23

AM1 heat of formation 0.685132316743E-01 E_h

C	-3.796861	-0.308789	0.010995
C	-3.440912	1.047856	-0.001922
C	-2.110963	1.453970	-0.021412
C	-1.134783	0.456129	-0.022030
C	-1.490340	-0.954043	-0.005066
C	-2.841672	-1.318280	0.006917
N	0.266169	0.503442	-0.094305
C	0.702256	-0.865898	-0.019742
N	-0.327958	-1.755833	-0.005697
C	1.149163	1.581868	0.232327
C	2.587525	1.293041	-0.200368
C	3.029352	-0.142823	-0.016226
N	2.071596	-1.155181	0.008494
O	4.227858	-0.455067	0.078445
H	-4.863831	-0.579003	0.023704
H	-4.234347	1.810480	0.003094
H	-1.840052	2.517691	-0.037917
H	-3.131895	-2.378621	0.011909
H	1.127869	1.776116	1.345525
H	0.781924	2.513610	-0.285857
H	3.281901	1.950320	0.386478
H	2.719388	1.534962	-1.289854
H	2.350934	-2.110205	0.075080

23

RI-B3LYP electronic energy -625.87754092215 E_h

C	3.7616703	-0.3320194	0.0531996
C	3.4244848	1.0264750	0.0057794
C	2.0966806	1.4415786	-0.0322571
C	1.1299516	0.4465377	-0.0225359
C	1.4523641	-0.9285741	0.0180002
C	2.7867645	-1.3223603	0.0604538
N	-0.2597326	0.4865082	-0.0369133
C	-0.6660945	-0.8211552	-0.0341765
N	0.2939025	-1.6980022	0.0104895
C	-1.1712286	1.5931942	-0.2584216
C	-2.5325627	1.2465935	0.3481199
C	-3.0182577	-0.1622666	0.0345529
N	-2.0170180	-1.1017882	-0.0985529
O	-4.1888634	-0.4604988	-0.0477806

H 4.8057524 -0.6140716 0.0832364
H 4.2108975 1.7692068 -0.0025116
H 1.8419592 2.4924174 -0.0710799
H 3.0464961 -2.3715277 0.0956924
H -1.2648726 1.7912231 -1.3311288
H -0.7653872 2.4899086 0.2083027
H -3.2996411 1.9405911 0.0126735
H -2.4793359 1.3187345 1.4383060
H -2.2876583 -2.0675380 -0.2126974
23
B3LYP electronic energy -625.87700417235 E_h
C 3.7615659 -0.3320241 0.0528200
C 3.4243697 1.0264800 0.0055862
C 2.0965951 1.4416618 -0.0320782
C 1.1299513 0.4465534 -0.0222293
C 1.4523438 -0.9285446 0.0180864
C 2.7867275 -1.3224035 0.0602287
N -0.2597216 0.4865530 -0.0362272
C -0.6660551 -0.8210767 -0.0337903
N 0.2939010 -1.6979968 0.0106243
C -1.1712356 1.5930233 -0.2585393
C -2.5325175 1.2465464 0.3479662
C -3.0182139 -0.1622574 0.0343925
N -2.0169311 -1.1017033 -0.0983551
O -4.1887906 -0.4605148 -0.0482279
H 4.8057872 -0.6140544 0.0825728
H 4.2109351 1.7692314 -0.0028610
H 1.8418043 2.4925819 -0.0707930
H 3.0464622 -2.3716669 0.0953268
H -1.2647742 1.7904310 -1.3314401
H -0.7655720 2.4901350 0.2077043
H -3.2996068 1.9407016 0.0126798
H -2.4791589 1.3186307 1.4382290
H -2.2874763 -2.0675944 -0.2125474
23
RI-MP2 electronic energy -624.795830568950 E_h
C 3.5372714 -0.5940563 0.0656714
C 3.1951810 0.7685215 -0.0001655
C 1.8685644 1.1835892 -0.0546131
C 0.9053764 0.1781002 -0.0442695
C 1.2289465 -1.1983404 0.0144960
C 2.5676686 -1.5897231 0.0748971
N -0.4746828 0.2146464 -0.0726771
C -0.8826983 -1.0882913 -0.0575712
N 0.0784788 -1.9753168 0.0065293
C -1.3878249 1.3141890 -0.2946116
C -2.7105973 0.9686554 0.3762486
C -3.2226285 -0.4133647 0.0213983
N -2.2348227 -1.3596300 -0.1406572
O -4.4035347 -0.6891485 -0.0743545
H 4.5818778 -0.8696711 0.1089300
H 3.9812653 1.5108484 -0.0102346
H 1.6084823 2.2321156 -0.1077263
H 2.8297019 -2.6373750 0.1244029
H -1.5223914 1.4751128 -1.3667935
H -0.9625388 2.2181939 0.1364021
H -3.4869034 1.6818438 0.1139422
H -2.5798678 0.9888714 1.4600276
H -2.5143238 -2.3197703 -0.2792716

Compound **11a** (energetically higher in energy tautomer)

23
AM1 heat of formation 0.817955468077E-01 E_h
C -3.776171 -0.250866 0.097211
C -3.400243 1.089677 0.045287
C -2.057151 1.472421 -0.045057
C -1.097120 0.468677 -0.079761
C -1.488432 -0.926360 -0.023272
C -2.829089 -1.280679 0.062389
N 0.305568 0.514332 -0.238833
C 0.793875 -0.842815 -0.090040
N -0.327433 -1.730840 -0.132012
C 1.178908 1.567421 0.210666
C 2.637596 1.269606 -0.143842
C 3.036815 -0.191013 0.027720
N 2.059748 -1.212547 0.006591
O 4.233420 -0.483003 0.167049
H -4.843028 -0.513214 0.166109
H -4.174262 1.871875 0.073922
H -1.775301 2.533125 -0.092452
H -3.141486 -2.333420 0.097280
H 1.087167 1.713286 1.326915
H 0.854321 2.524159 -0.288361
H 3.299809 1.906699 0.497253
H 2.833952 1.539677 -1.215694
H -0.267640 -2.631204 0.280601
23
RI-B3LYP electronic energy -625.86626496804 E_h
C 3.7546755 -0.2723077 0.0214884
C 3.3854398 1.0698706 -0.0382487
C 2.0429672 1.4524292 -0.0625917
C 1.0920772 0.4469202 -0.0242779
C 1.4660504 -0.9080312 0.0297392
C 2.7959390 -1.2864830 0.0562057
N -0.2977828 0.4784059 -0.0218467
C -0.7974866 -0.8015983 -0.0083310
N 0.2855221 -1.6392993 0.0455408
C -1.2059502 1.6020012 -0.1824228
C -2.5638305 1.2058621 0.3974632
C -3.0096609 -0.2129756 -0.0023066
N -2.0349454 -1.1904660 -0.0664640
O -4.1847606 -0.4496200 -0.1883476
H 4.8030477 -0.5364765 0.0394127
H 4.1516277 1.8323694 -0.0677048
H 1.7621927 2.4952514 -0.1120052
H 3.0850843 -2.3277583 0.0997304
H -1.2916558 1.8510843 -1.2450232
H -0.7938328 2.4701777 0.3318097
H -3.3345155 1.9064306 0.0859213
H -2.5166142 1.2297305 1.4900165
H 0.1818689 -2.6384590 0.0637046
23
B3LYP electronic energy -625.86572324139 E_h
C 3.7545409 -0.2723266 0.0212099
C 3.3853092 1.0698622 -0.0385133
C 2.0428805 1.4525043 -0.0626172
C 1.0920465 0.4469618 -0.0241239
C 1.4660170 -0.9079763 0.0298448
C 2.7958682 -1.2865251 0.0561174
N -0.2977799 0.4784406 -0.0213637
C -0.7974573 -0.8015463 -0.0080417
N 0.2855247 -1.6391959 0.0457801
C -1.2060166 1.6018776 -0.1823976

C -2.5637090 1.2056946 0.3977069
C -3.0095477 -0.2129673 -0.0024545
N -2.0348943 -1.1905101 -0.0664308
O -4.1845933 -0.4494994 -0.1889941
H 4.8030468 -0.5364798 0.0389554
H 4.1516459 1.8323769 -0.0681596
H 1.7620622 2.4954094 -0.1120597
H 3.0849816 -2.3278981 0.0996261
H -1.2918493 1.8505185 -1.2451617
H -0.7939957 2.4704046 0.3314337
H -3.3344943 1.9065112 0.0867827
H -2.5160345 1.2291391 1.4903309
H 0.1818387 -2.6384820 0.0639208
23
RI-MP2 electronic energy -624.780492910904 E_h
C 3.4488243 -0.5194591 0.0054072
C 3.0762356 0.8279630 -0.0650379
C 1.7349234 1.2103329 -0.0969571
C 0.7869939 0.1958251 -0.0561674
C 1.1606448 -1.1587013 0.0076447
C 2.4954233 -1.5374901 0.0434762
N -0.5956779 0.2255924 -0.0578112
C -1.0978762 -1.0500858 -0.0431144
N -0.0158339 -1.8860106 0.0242088
C -1.5015565 1.3424166 -0.2304652
C -2.8271585 0.9434168 0.4005257
C -3.2942001 -0.4431810 -0.0514306
N -2.3378942 -1.4441239 -0.1175349
O -4.4731823 -0.6510420 -0.2784922
H 4.4977445 -0.7785390 0.0292707
H 3.8430834 1.5888416 -0.0972086
H 1.4479956 2.2508847 -0.1545813
H 2.7856463 -2.5775645 0.0951276
H -1.6189510 1.5543762 -1.2960532
H -1.0761341 2.2201134 0.2528291
H -3.6061155 1.6601223 0.1577687
H -2.7107535 0.9122836 1.4857709
H -0.1221814 -2.8859713 0.0428245

Compound **12**

19
AM1 heat of formation 0.852011310597E-01 E_h
C 2.914367 0.347772 0.008149
C 2.649866 -1.042088 0.000460
C 1.363374 -1.518543 -0.007302
C 0.254084 -0.608463 -0.007840
C 0.533895 0.792185 -0.000732
C 1.875795 1.246306 0.007523
N -1.026976 -1.109621 -0.023515
C -2.052495 -0.235889 -0.004255
C -1.848451 1.203376 -0.007863
C -0.571474 1.689448 -0.003910
N -3.368823 -0.712102 0.095425
H 3.957816 0.694558 0.015273
H 3.498480 -1.743424 0.001907
H 1.163495 -2.601379 -0.011534
H 2.066144 2.330228 0.014258
H -2.716525 1.876174 -0.001276
H -0.377179 2.773219 -0.002528
H -3.495640 -1.687187 -0.066336
H -4.039764 -0.134744 -0.358515

19
RI-B3LYP electronic energy -457.19447760640 E_h
C -2.9051869 0.3256184 0.0031512
C -2.6196575 -1.0550192 0.0008687
C -1.3220007 -1.5061393 -0.0011773
C -0.2429371 -0.5921463 -0.0014949
C -0.5334496 0.8031813 0.0009937
C -1.8769986 1.2364198 0.0033809
N 1.0296332 -1.0725795 0.0024632
C 2.0284226 -0.2192835 -0.0049530
C 1.8424016 1.1973616 -0.0057131
C 0.5734649 1.6899310 0.0008674
N 3.3049860 -0.7340901 -0.0585672
H -3.9331297 0.6629641 0.0044965
H -3.4353375 -1.7668279 0.0005160
H -1.0907594 -2.5627424 -0.0030753
H -2.0846501 2.3000141 0.0049249
H 2.7013377 1.8557847 -0.0183121
H 0.3986216 2.7592703 0.0023628
H 3.3771275 -1.7172559 0.1462064
H 4.0601028 -0.1640623 0.2800679
19
B3LYP electronic energy -457.19401675293 E_h
C -2.9051138 0.3256518 0.0031347
C -2.6195943 -1.0549790 0.0008582
C -1.3219537 -1.5061567 -0.0011723
C -0.2429438 -0.5921621 -0.0014753
C -0.5334404 0.8031329 0.0009934
C -1.8769273 1.2364631 0.0033585
N 1.0296224 -1.0726653 0.0025416
C 2.0283321 -0.2192907 -0.0048908
C 1.8423788 1.1973354 -0.0056628
C 0.5734519 1.6899022 0.0008820
N 3.3048961 -0.7340115 -0.0587122
H -3.9331838 0.6630034 0.0044547
H -3.4354016 -1.7668208 0.0004736
H -1.0906895 -2.5628502 -0.0031116
H -2.0845248 2.3001608 0.0048789
H 2.7014597 1.8557176 -0.0184114
H 0.3985250 2.7593157 0.0023210
H 3.3770495 -1.7172851 0.1462446
H 4.0599992 -0.1638862 0.2801904
19
RI-MP2 electronic energy -456.362546608142 E_h
C -2.8631822 0.2469997 -0.0097732
C -2.5808281 -1.1336234 -0.0158171
C -1.2762545 -1.5813567 -0.0230493
C -0.2026218 -0.6652777 -0.0253853
C -0.4926200 0.7292175 -0.0190725
C -1.8351754 1.1654717 -0.0111724
N 1.0701960 -1.1565258 -0.0247352
C 2.0658619 -0.2945199 -0.0346893
C 1.8804950 1.1169501 -0.0363860
C 0.6090594 1.6190107 -0.0216731
N 3.3507501 -0.8057398 -0.1087685
H -3.8902142 0.5859211 -0.0042874
H -3.3938023 -1.8471440 -0.0150173
H -1.0403560 -2.6369817 -0.0279229
H -2.0424290 2.2286993 -0.0069367
H 2.7405113 1.7732431 -0.0549028
H 0.4358769 2.6882493 -0.0187948
H 3.3970885 -1.7832356 0.1329249

H 4.0676442 -0.2493579 0.3254589

Compound **12** Imine

19
AM1 heat of formation 0.101860103067 E_h
C 2.887135 0.396803 0.000015
C 2.654914 -0.985060 -0.000006
C 1.366903 -1.490937 -0.000017
C 0.256121 -0.604849 -0.000005
C 0.497271 0.797692 -0.000001
C 1.815892 1.275773 0.000015
N -1.037681 -1.099995 0.000007
C -2.172522 -0.258341 0.000004
C -1.895137 1.197798 -0.000011
C -0.639697 1.685519 -0.000015
N -3.356015 -0.808594 0.000014
H 3.918093 0.777855 0.000033
H 3.510209 -1.678576 -0.000016
H 1.204142 -2.579015 -0.000037
H 1.988837 2.363111 0.000026
H -2.773885 1.859077 -0.000020
H -0.442057 2.769366 -0.000036
H -1.170372 -2.087139 0.000023
H -4.104383 -0.150953 0.000012
19
RI-B3LYP electronic energy -457.18049168945 E_h
C 2.8880448 0.3831978 -0.0000094
C 2.6410518 -0.9922691 -0.0000072
C 1.3460663 -1.4810059 0.0000047
C 0.2645462 -0.5920517 0.0000114
C 0.5008929 0.8004355 0.0000102
C 1.8218137 1.2649129 0.0000014
N -1.0332739 -1.0426049 0.0000106
C -2.1743150 -0.2484799 0.0000045
C -1.9037490 1.1844990 0.0000035
C -0.6473312 1.6702188 0.0000092
N -3.3142672 -0.8393946 -0.0000240
H 3.9037454 0.7536398 -0.0000203
H 3.4696562 -1.6882855 -0.0000163
H 1.1620877 -2.5483057 0.0000041
H 1.9972898 2.3337625 -0.0000023
H -2.7603687 1.8447494 -0.0000069
H -0.4787158 2.7407788 0.0000044
H -1.2120941 -2.0355540 0.0000053
H -4.0709362 -0.1635325 -0.0000444
19
B3LYP electronic energy -457.18005031964 E_h
C -2.8879705 0.3831968 0.0000203
C -2.6409351 -0.9922691 0.0000110
C -1.3459731 -1.4810584 -0.0000158
C -0.2645484 -0.5920337 -0.0000254
C -0.5008750 0.8004347 -0.0000222
C -1.8217678 1.2649384 -0.0000026
N 1.0332153 -1.0425606 -0.0000211
C 2.1742155 -0.2484727 0.0000134
C 1.9037183 1.1844733 0.0000014
C 0.6473043 1.6702153 -0.0000194
N 3.3141637 -0.8394260 0.0000413
H -3.9038046 0.7536190 0.0000451
H -3.4696462 -1.6883478 0.0000283
H -1.1619002 -2.5484372 -0.0000194

H -1.9972256 2.3338850 0.0000049
H 2.7604734 1.8446923 0.0000141
H 0.4786074 2.7408511 -0.0000249
H 1.2120489 -2.0356417 -0.0000092
H 4.0707841 -0.1632624 0.0000555
19
RI-MP2 electronic energy -456.344683394416 E_h
C 2.7607960 0.3129559 0.0000000
C 2.5157866 -1.0650635 0.0000000
C 1.2165969 -1.5511850 0.0000000
C 0.1364621 -0.6605486 0.0000000
C 0.3736130 0.7287857 0.0000000
C 1.6945901 1.1985691 0.0000000
N -1.1607056 -1.1132656 0.0000000
C -2.2970443 -0.3240475 0.0000000
C -2.0299421 1.1067779 0.0000000
C -0.7701474 1.6008779 0.0000000
N -3.4434407 -0.9174190 0.0000000
H 3.7760247 0.6833519 0.0000000
H 3.3427115 -1.7619098 0.0000000
H 1.0295391 -2.6178328 0.0000000
H 1.8661064 2.2677863 0.0000000
H -2.8862106 1.7673443 0.0000000
H -0.6054943 2.6716281 0.0000000
H -1.3382693 -2.1077067 0.0000000
H -4.1809719 -0.2190986 0.0000000

Compound **18**
13
AM1 heat of formation 0.175534930487 E_h
C 2.117312 -0.114525 -0.000671
N 1.286897 -1.238059 -0.001989
C 0.032467 -0.710989 0.007466
N 0.057797 0.744728 0.010310
C 1.396309 1.103200 0.003972
N -1.314164 -1.129067 -0.081777
C -2.085242 0.060682 0.008351
C -1.268287 1.188645 0.004633
H 3.201195 -0.232648 -0.000413
H 1.733508 2.135869 -0.006543
H -1.596554 -1.964058 0.373815
H -3.174733 0.010036 0.004952
H -1.532481 2.245504 -0.000119
13
RI-B3LYP electronic energy -357.69703621067 E_h
C -2.0770732 -0.1004938 0.0000004
N -1.2509780 -1.2070093 -0.0000008
C -0.0539932 -0.6731487 -0.0000018
N -0.0456773 0.6990071 -0.0000004
C -1.3790811 1.0842465 0.0000023
N 1.2535540 -1.0801558 0.0000011
C 2.0602395 0.0494891 -0.0000007
C 1.2691166 1.1538946 0.0000021
H -3.1484447 -0.2156310 -0.0000005
H -1.6934734 2.1110683 0.0000028
H 1.5595427 -2.0345421 -0.0000175
H 3.1321605 -0.0213493 -0.0000021
H 1.5366728 2.1936337 0.0000041
13
B3LYP electronic energy -357.69671910168 E_h
C -2.0770065 -0.1005117 0.0000110

N -1.2509586 -1.2070168 0.0000010
C -0.0539909 -0.6730876 -0.0000133
N -0.0456474 0.6990450 -0.0000164
C -1.3790505 1.0842489 0.0000001
N 1.2534799 -1.0801432 0.0000020
C 2.0601586 0.0494336 0.0000100
C 1.2691304 1.1539010 0.0000013
H -3.1484785 -0.2156932 0.0000234
H -1.6934216 2.1111514 0.0000038
H 1.5594653 -2.0346950 -0.0000208
H 3.1321834 -0.0215790 0.0000214
H 1.5366873 2.1937156 0.0000107
13
RI-MP2 electronic energy -357.077398249371 E_h
C -2.1643838 -0.2571017 0.0000000
N -1.3454889 -1.3652387 0.0000000
C -0.1431244 -0.8238194 0.0000000
N -0.1358619 0.5507918 0.0000000
C -1.4604552 0.9363599 0.0000000
N 1.1646778 -1.2274782 0.0000000
C 1.9678231 -0.1065260 0.0000000
C 1.1735344 1.0076346 0.0000000
H -3.2354694 -0.3670104 0.0000000
H -1.7721776 1.9637181 0.0000000
H 1.4709130 -2.1824518 0.0000000
H 3.0395945 -0.1759113 0.0000000
H 1.4404183 2.0470331 0.0000000

Compound **19**

19
AM1 heat of formation 0.193769708793 E_h
C -0.815199 0.880515 -0.001380
N 0.347381 1.712842 -0.099319
C 1.441496 0.800075 0.002526
N 0.954821 -0.572746 0.011800
C -0.444063 -0.528919 -0.000005
N 2.794949 0.845960 -0.001260
C 3.182117 -0.501713 0.003374
C 2.079757 -1.383026 0.005785
C -1.415401 -1.522162 -0.001101
C -2.756007 -1.123191 0.002067
C -3.116798 0.222834 0.005704
C -2.157455 1.240792 0.002750
H 0.391210 2.510343 0.499661
H 4.239332 -0.767538 0.005246
H 2.027599 -2.468920 -0.001580
H -1.144252 -2.586759 -0.007532
H -3.540183 -1.895656 -0.000273
H -4.182756 0.497928 0.009432
H -2.461681 2.296983 -0.001834
19
RI-B3LYP electronic energy -511.31098157030 E_h
C -0.8025145 -0.8638153 -0.0000032
N 0.3640217 -1.6184700 -0.0000149
C 1.4364014 -0.7563450 0.0000018
N 0.9523470 0.5287200 -0.0000057
C -0.4393134 0.5040192 -0.0000065
N 2.7377683 -0.8386784 0.0000112
C 3.1337043 0.4913539 0.0000087
C 2.0703362 1.3554694 -0.0000047
C -1.3969615 1.5038201 -0.0000057

C -2.7356165 1.1181832 0.0000012
C -3.0970615 -0.2302900 0.0000046
C -2.1372108 -1.2397685 0.0000009
H 0.4349222 -2.6185849 0.0000710
H 4.1788369 0.7519495 0.0000153
H 2.0084203 2.4273946 -0.0000116
H -1.1154986 2.5477083 -0.0000076
H -3.5058711 1.8770575 0.0000039
H -4.1444637 -0.4999368 0.0000099
H -2.4258874 -2.2823518 0.0000022
19
B3LYP electronic energy -511.31053274709 E_h
C -0.8025257 -0.8637565 0.0000123
N 0.3639796 -1.6183527 -0.0000155
C 1.4363449 -0.7562803 0.0000018
N 0.9523236 0.5287813 0.0000252
C -0.4393227 0.5040641 0.0000189
N 2.7377169 -0.8387511 -0.0000246
C 3.1336826 0.4912382 -0.0000174
C 2.0703834 1.3554380 0.0000113
C -1.3969618 1.5038809 -0.0000001
C -2.7355678 1.1181479 -0.0000166
C -3.0969746 -0.2303501 -0.0000051
C -2.1371736 -1.2398403 0.0000104
H 0.4348998 -2.6185811 0.0000721
H 4.1789433 0.7517688 -0.0000329
H 2.0084590 2.4274450 0.0000239
H -1.1154744 2.5478668 -0.0000085
H -3.5059931 1.8770251 -0.0000388
H -4.1445084 -0.4999875 -0.0000150
H -2.4257760 -2.2825306 0.0000103
19
RI-MP2 electronic energy -510.406993228543 E_h
C -0.5610266 -0.9807085 0.0000000
N 0.5983182 -1.7324981 0.0000000
C 1.6716707 -0.8714129 0.0000000
N 1.1864251 0.4144932 0.0000000
C -0.2005061 0.3873172 0.0000000
N 2.9812405 -0.9549477 0.0000000
C 3.3668314 0.3746030 0.0000000
C 2.2919473 1.2424519 0.0000000
C -1.1559794 1.3957611 0.0000000
C -2.4933463 1.0096463 0.0000000
C -2.8567412 -0.3448092 0.0000000
C -1.9013913 -1.3572873 0.0000000
H 0.6682958 -2.7335492 0.0000000
H 4.4093047 0.6426507 0.0000000
H 2.2233687 2.3140099 0.0000000
H -0.8687453 2.4377778 0.0000000
H -3.2644299 1.7667499 0.0000000
H -3.9043941 -0.6111613 0.0000000
H -2.1908424 -2.3990868 0.0000000

Compound **19a** (energetically higher in energy tautomer)
19
AM1 heat of formation 0.200329460051 E_h
C 0.816625 -0.906686 0.000395
N -0.344672 -1.717072 -0.002089
C -1.354745 -0.818586 0.000269
N -0.902931 0.574125 -0.003108
C 0.486191 0.520404 0.002978

N -2.766391 -0.814946 -0.082026
C -3.149607 0.555723 0.014103
C -2.037491 1.388823 0.007375
C 1.480868 1.501129 -0.000320
C 2.802321 1.074020 0.001260
C 3.135782 -0.289764 0.002897
C 2.166660 -1.283011 0.002279
H -3.278015 -1.518859 0.396836
H -4.205924 0.826247 0.015345
H -1.974957 2.477171 0.009071
H 1.227271 2.569251 -0.003354
H 3.608863 1.822488 0.001248
H 4.198666 -0.575949 0.003292
H 2.442440 -2.347401 0.000717
19
RI-B3LYP electronic energy -511.30774457711 E_h
C 0.7904844 -0.8888225 -0.0000058
N -0.3540228 -1.6784226 -0.0000013
C -1.3115046 -0.7902633 0.0000005
N -0.9105697 0.5312142 -0.0000034
C 0.4786658 0.5008631 -0.0000075
N -2.6770128 -0.7796241 0.0000057
C -3.1115426 0.5454131 0.0000074
C -2.0286364 1.3594496 0.0000053
C 1.4492226 1.4917507 -0.0000089
C 2.7752226 1.0761348 -0.0000027
C 3.1059922 -0.2867918 0.0000020
C 2.1313494 -1.2749074 -0.0000015
H -3.2552373 -1.5986648 0.0000412
H -4.1558580 0.7964524 0.0000107
H -1.9717570 2.4315042 0.0000042
H 1.1918806 2.5427325 -0.0000099
H 3.5639566 1.8163258 0.0000005
H 4.1496720 -0.5731886 0.0000087
H 2.3930600 -2.3242914 0.0000035
19
B3LYP electronic energy -511.30727498908 E_h
C 0.7904730 -0.8888102 0.0000080
N -0.3539973 -1.6784025 -0.0000063
C -1.3114636 -0.7901943 -0.0000117
N -0.9105526 0.5312637 0.0000032
C 0.4786788 0.5008622 0.0000069
N -2.6769153 -0.7796360 -0.0000276
C -3.1114713 0.5453383 0.0000044
C -2.0286221 1.3594482 0.0000219
C 1.4491644 1.4918152 -0.0000090
C 2.7751257 1.0761232 -0.0000141
C 3.1058941 -0.2868138 0.0000038
C 2.1313144 -1.2749593 0.0000166
H -3.2551585 -1.5988585 0.0000252
H -4.1559383 0.7962391 0.0000096
H -1.9716882 2.4315825 0.0000421
H 1.1917566 2.5428843 -0.0000231
H 3.5640134 1.8163355 -0.0000321
H 4.1497103 -0.5731827 0.0000062
H 2.3930003 -2.3244341 0.0000263
19
RI-MP2 electronic energy -510.403364236995 E_h
C 0.6659474 -1.0461329 -0.0003089
N -0.4688570 -1.8427887 -0.0002299
C -1.4285968 -0.9432902 -0.0000915
N -1.0257680 0.3773087 -0.0001594

C	0.3554716	0.3454640	-0.0003021
N	-2.7936066	-0.9272153	0.0001439
C	-3.2255037	0.3888246	0.0001628
C	-2.1344781	1.2094541	-0.0000683
C	1.3245357	1.3456356	-0.0001392
C	2.6489204	0.9278376	0.0001552
C	2.9831452	-0.4402470	0.0001793
C	2.0118288	-1.4315089	-0.0000897
H	-3.3735206	-1.7459816	0.0002730
H	-4.2689249	0.6428401	0.0003553
H	-2.0733771	2.2810510	-0.0001826
H	1.0629968	2.3950792	-0.0002802
H	3.4380176	1.6669008	0.0003730
H	4.0270921	-0.7229597	0.0004048
H	2.2746772	-2.4802714	-0.0001955

Compound **20**

25

AM1 heat of formation 0.217874394844 E_h

C	2.124446	-0.858320	-0.002323
N	1.282391	-2.001936	-0.000410
C	0.039237	-1.485782	-0.003466
N	0.018087	-0.019527	-0.013103
C	1.348601	0.382447	-0.004970
N	-1.293753	-1.986236	0.096713
C	-2.125191	-0.820831	0.002806
C	-1.316265	0.391384	-0.000167
C	1.970991	1.632016	-0.000617
C	3.361065	1.655158	0.001555
C	4.118000	0.474521	0.000708
C	3.521381	-0.780535	-0.001355
C	-3.510251	-0.728558	-0.000137
C	-4.089276	0.546273	-0.004209
C	-3.312081	1.701627	-0.003068
C	-1.913551	1.645434	-0.001277
H	-1.517029	-2.761107	-0.491373
H	1.384411	2.560143	0.001002
H	3.880752	2.625307	0.004235
H	5.216328	0.546574	0.002925
H	4.127205	-1.698264	-0.000037
H	-4.140549	-1.629027	0.006039
H	-5.186815	0.630051	-0.006614
H	-3.802953	2.687005	-0.001858
H	-1.311060	2.564192	0.002404

25

RI-B3LYP electronic energy -664.92312450640 E_h

C	-2.0852238	-0.8429428	0.0000059
N	-1.2513251	-1.9628755	0.0000178
C	-0.0632142	-1.4381530	0.0000041
N	-0.0143017	-0.0543821	-0.0000074
C	-1.3400484	0.3682255	-0.0000025
N	1.2268492	-1.8994065	-0.0000136
C	2.0936376	-0.8072948	0.0000044
C	1.3105503	0.3701291	-0.0000019
C	-1.9400938	1.6175850	-0.0000110
C	-3.3313486	1.6499536	-0.0000155
C	-4.0829543	0.4690429	-0.0000073
C	-3.4757666	-0.7814014	0.0000045
C	3.4759272	-0.7404997	0.0000072
C	4.0652758	0.5239694	0.0000064
C	3.2923701	1.6838060	0.0000013

C 1.8987573 1.6227988 -0.0000046
H 1.4817354 -2.8695374 0.0001142
H -1.3612070 2.5307723 -0.0000203
H -3.8387206 2.6052125 -0.0000259
H -5.1631776 0.5330300 -0.0000119
H -4.0596009 -1.6916956 0.0000108
H 4.0812372 -1.6370483 0.0000093
H 5.1438778 0.6022171 0.0000101
H 3.7789073 2.6494396 -0.0000004
H 1.3011800 2.5229468 -0.0000100
25
B3LYP electronic energy -664.92253837489 E_h
C -2.0851899 -0.8429260 0.0000138
N -1.2513009 -1.9628353 -0.0000068
C -0.0632058 -1.4380035 -0.0000830
N -0.0143007 -0.0542537 -0.0001328
C -1.3401051 0.3682760 -0.0000750
N 1.2268139 -1.8992684 -0.0001055
C 2.0936140 -0.8072537 -0.0000376
C 1.3105746 0.3701961 -0.0000786
C -1.9401096 1.6176464 -0.0000876
C -3.3313580 1.6498693 0.0000137
C -4.0829026 0.4689141 0.0001203
C -3.4757284 -0.7815134 0.0001162
C 3.4758966 -0.7406334 0.0000609
C 4.0652304 0.5238184 0.0001313
C 3.2923852 1.6837049 0.0000857
C 1.8987836 1.6228577 -0.0000228
H 1.4816524 -2.8695334 0.0001228
H -1.3611989 2.5309152 -0.0001697
H -3.8389187 2.6051701 0.0000126
H -5.1632469 0.5329142 0.0002047
H -4.0595221 -1.6919306 0.0001942
H 4.0811576 -1.6373168 0.0000952
H 5.1439557 0.6020817 0.0002217
H 3.7791173 2.6493791 0.0001426
H 1.3012064 2.5231045 -0.0000512
25
RI-MP2 electronic energy -663.735382679243 E_h
C -2.1249320 -1.0507278 0.0000000
N -1.3050937 -2.1768187 0.0000000
C -0.1095415 -1.6459508 0.0000000
N -0.0609708 -0.2632956 0.0000000
C -1.3765785 0.1605128 0.0000000
N 1.1825001 -2.1032011 0.0000000
C 2.0411795 -1.0138578 0.0000000
C 1.2571140 0.1624644 0.0000000
C -1.9676981 1.4204779 0.0000000
C -3.3579375 1.4544229 0.0000000
C -4.1184016 0.2717074 0.0000000
C -3.5199724 -0.9826973 0.0000000
C 3.4290364 -0.9416652 0.0000000
C 4.0087009 0.3260780 0.0000000
C 3.2282524 1.4890437 0.0000000
C 1.8361000 1.4249606 0.0000000
H 1.4408604 -3.0734616 0.0000000
H -1.3817672 2.3288457 0.0000000
H -3.8635200 2.4100730 0.0000000
H -5.1974378 0.3433515 0.0000000
H -4.1075048 -1.8902163 0.0000000
H 4.0376333 -1.8353378 0.0000000
H 5.0862063 0.4113914 0.0000000

H 3.7136879 2.4545517 0.0000000
H 1.2300846 2.3193491 0.0000000

Compound **21**

33
AM1 heat of formation 0.988359445982E-01 E_h
C -2.183502 0.835504 -0.004465
N -1.435676 2.040762 -0.002397
C -0.153434 1.621116 -0.003189
N -0.018072 0.165901 -0.012972
C -1.313981 -0.339101 -0.005794
N 1.134762 2.224956 0.097952
C 2.057147 1.133061 0.005173
C 1.345509 -0.140989 0.002353
C -1.836525 -1.635080 -0.001950
C -3.213945 -1.779741 -0.001581
C -4.062198 -0.645569 -0.003884
C -3.572514 0.659678 -0.005698
C 3.440737 1.161883 -0.000720
C 4.117880 -0.079013 -0.003768
C 3.438313 -1.300759 -0.000193
C 2.039427 -1.341269 0.002790
O -5.410119 -0.961988 -0.005091
O 5.494665 0.043649 -0.015324
C -6.312501 0.137220 0.009733
C 6.236822 -1.170198 0.006292
H 1.298728 3.029605 -0.467795
H -1.176822 -2.513522 0.000618
H -3.671907 -2.779636 0.000681
H -4.235467 1.535233 -0.005601
H 4.013426 2.099243 0.003798
H 3.991057 -2.250980 0.002063
H 1.511411 -2.305408 0.007626
H -7.319104 -0.352902 0.014547
H -6.184700 0.765277 -0.905367
H -6.169922 0.753626 0.930514
H 7.301057 -0.821695 0.005050
H 6.021178 -1.780562 -0.904147
H 6.014182 -1.753358 0.932660
33
RI-B3LYP electronic energy -893.94242538001 E_h
C -2.1447374 0.8048972 0.0000307
N -1.4019352 1.9850448 0.0000325
C -0.1742309 1.5521514 0.0000452
N -0.0185185 0.1818700 0.0000559
C -1.3100966 -0.3406818 0.0000523
N 1.0763383 2.1174739 0.0000420
C 2.0269025 1.1000507 0.0000341
C 1.3382851 -0.1369874 0.0000482
C -1.8276144 -1.6275743 0.0000540
C -3.2071165 -1.7637832 0.0000254
C -4.0501947 -0.6379493 -0.0000069
C -3.5321317 0.6543727 -0.0000018
C 3.4051695 1.1533723 0.0000042
C 4.1083106 -0.0587423 -0.0000163
C 3.4330292 -1.2823280 0.0000031
C 2.0352737 -1.3268499 0.0000370
O -5.3878824 -0.9225014 -0.0000489
O 5.4668549 0.0659552 -0.0000642
C -6.3061935 0.1548698 -0.0001021
C 6.2590400 -1.1093762 -0.0001082

H 1.2523043 3.1048855 0.0000284
H -1.1914660 -2.5018577 0.0000713
H -3.6648084 -2.7428921 0.0000205
H -4.1608032 1.5312397 -0.0000268
H 3.9515321 2.0860394 -0.0000136
H 3.9811555 -2.2112523 -0.0000131
H 1.5228833 -2.2781553 0.0000454
H -7.2966749 -0.2936906 -0.0001359
H -6.1928578 0.7791992 -0.8911600
H -6.1929314 0.7792271 0.8909457
H 7.2927192 -0.7732326 -0.0001513
H 6.0768638 -1.7152480 -0.8919987
H 6.0769433 -1.7152636 0.8917879
33
B3LYP electronic energy -893.94166469231 E_h
C -2.1447078 0.8048705 -0.0000616
N -1.4019198 1.9850041 -0.0000529
C -0.1742161 1.5520168 -0.0001366
N -0.0184987 0.1817512 -0.0002139
C -1.3101261 -0.3407315 -0.0001590
N 1.0763083 2.1173555 -0.0001102
C 2.0268668 1.1000381 -0.0000969
C 1.3383175 -0.1370254 -0.0001690
C -1.8276167 -1.6276314 -0.0001643
C -3.2071045 -1.7637792 -0.0000586
C -4.0500622 -0.6378976 0.0000481
C -3.5321038 0.6544112 0.0000403
C 3.4051174 1.1534637 0.0000026
C 4.1081867 -0.0586191 0.0000413
C 3.4330684 -1.2822698 -0.0000344
C 2.0353454 -1.3268658 -0.0001411
O -5.3877243 -0.9224608 0.0001596
O 5.4667104 0.0660405 0.0001595
C -6.3059013 0.1549583 0.0003049
C 6.2586696 -1.1093720 0.0003047
H 1.2522081 3.1049016 -0.0000085
H -1.1913952 -2.5019762 -0.0002424
H -3.6649884 -2.7428919 -0.0000484
H -4.1608418 1.5312972 0.0001225
H 3.9515173 2.0861565 0.0000706
H 3.9813785 -2.2111978 -0.0000032
H 1.5229072 -2.2782556 -0.0001910
H -7.2965079 -0.2936113 0.0004035
H -6.1928343 0.7794032 -0.8908030
H -6.1926279 0.7793394 0.8914311
H 7.2925088 -0.7733406 0.0004180
H 6.0766904 -1.7153564 -0.8916484
H 6.0764683 -1.7152815 0.8922633
33
RI-MP2 electronic energy -892.398183686765 E_h
C -2.1780840 0.9732229 -0.0004468
N -1.4546067 2.1629378 -0.0003743
C -0.2179110 1.7319099 -0.0003808
N -0.0569972 0.3603744 -0.0004385
C -1.3339905 -0.1677130 -0.0005593
N 1.0329910 2.2966108 -0.0002309
C 1.9787960 1.2824171 -0.0001390
C 1.2927005 0.0454831 -0.0002320
C -1.8347141 -1.4678287 -0.0005705
C -3.2132946 -1.6094099 -0.0003285
C -4.0693989 -0.4886544 -0.0000978
C -3.5681231 0.8094857 -0.0002726

C	3.3626557	1.3321220	0.0000821
C	4.0589541	0.1196138	0.0001333
C	3.3803787	-1.1089134	-0.0000110
C	1.9844560	-1.1545926	-0.0001252
O	-5.4024716	-0.7938106	0.0004065
O	5.4180073	0.2389389	0.0003361
C	-6.2919346	0.3074599	0.0007114
C	6.1596678	-0.9687621	0.0004229
H	1.2098413	3.2848250	-0.0002540
H	-1.1883861	-2.3341960	-0.0007630
H	-3.6673836	-2.5901083	-0.0003304
H	-4.2036210	1.6811756	-0.0003393
H	3.9130452	2.2622793	0.0002297
H	3.9282085	-2.0374880	-0.0000700
H	1.4655767	-2.1022512	-0.0000876
H	-7.2910007	-0.1151013	0.0010740
H	-6.1570299	0.9246934	-0.8890380
H	-6.1563953	0.9247165	0.8903482
H	7.2036111	-0.6752056	0.0006030
H	5.9483736	-1.5620902	-0.8902105
H	5.9480794	-1.5621408	0.8909527

Compound **22**

31

AM1 heat of formation 0.850890367974E-01 E_h

C	-3.576451	-0.814398	-0.003502
N	-2.764606	-1.993322	-0.096442
C	-1.423887	-1.517215	0.004720
N	-1.419812	-0.048197	0.014562
C	-2.749161	0.384473	0.000784
N	-0.189907	-2.052760	0.001321
C	0.670370	-0.921925	0.003672
C	-0.087177	0.331486	0.005994
C	-3.324907	1.648221	0.001981
C	-4.722499	1.727195	0.002347
C	-5.518097	0.584330	0.002130
C	-4.960117	-0.699830	-0.001770
C	2.066550	-0.872155	0.002795
C	2.685797	0.378828	0.001124
C	1.943070	1.577926	-0.000405
C	0.556075	1.572815	0.001414
C	4.150736	0.490695	-0.000410
O	4.834798	1.519323	-0.001767
O	4.811706	-0.711287	0.000530
C	6.238688	-0.651735	-0.003039
H	-3.002888	-2.768252	0.485712
H	-2.707681	2.557336	-0.000568
H	-5.197323	2.720530	0.001048
H	-6.614341	0.685927	0.003331
H	-5.604949	-1.590062	-0.008916
H	2.664618	-1.797940	0.001633
H	2.490653	2.535902	-0.003129
H	-0.015747	2.510457	-0.000682
H	6.545870	-1.726485	-0.003269
H	6.600248	-0.121539	0.910574
H	6.595836	-0.122468	-0.918926

31

RI-B3LYP electronic energy -892.78628620215 E_h

C	3.5324855	-0.8017603	0.0000410
N	2.6840461	-1.9090722	-0.0000474
C	1.3871445	-1.4710576	-0.0001345

N 1.4123992 -0.0840803 -0.0001193
C 2.7317284 0.3626760 -0.0000110
N 0.2081878 -2.0140336 -0.0001941
C -0.6427617 -0.9068609 -0.0002029
C 0.0849611 0.3157730 -0.0001613
C 3.2982805 1.6249749 0.0000651
C 4.6904707 1.7085232 0.0002090
C 5.4817404 0.5610245 0.0002716
C 4.9135780 -0.7128199 0.0001851
C -2.0303034 -0.8714704 -0.0001880
C -2.6651861 0.3728601 -0.0001336
C -1.9232510 1.5669817 -0.0001220
C -0.5370852 1.5563947 -0.0001329
C -4.1473754 0.4939848 -0.0000039
O -4.7520730 1.5413189 0.0000953
O -4.7683663 -0.7058025 0.0000374
C -6.2012891 -0.6661130 0.0002962
H 2.9558955 -2.8747357 -0.0000428
H 2.6861689 2.5152650 0.0000217
H 5.1613714 2.6817728 0.0002765
H 6.5588867 0.6568480 0.0003907
H 5.5334324 -1.5992756 0.0002365
H -2.6012351 -1.7872692 -0.0001891
H -2.4630727 2.5025534 -0.0000802
H 0.0249074 2.4797099 -0.0001062
H -6.5226737 -1.7036693 0.0003250
H -6.5708749 -0.1518188 -0.8857232
H -6.5705441 -0.1518730 0.8864858
31
B3LYP electronic energy -892.78557484972 E_h
C 3.5324553 -0.8017201 0.0000253
N 2.6839996 -1.9089319 0.0000874
C 1.3871476 -1.4709097 0.0000909
N 1.4123900 -0.0839492 0.0001176
C 2.7317522 0.3627454 0.0000515
N 0.2081982 -2.0139914 0.0000472
C -0.6427389 -0.9068467 0.0000396
C 0.0849016 0.3158193 0.0000859
C 3.2982994 1.6250373 -0.0000180
C 4.6904808 1.7084319 -0.0001167
C 5.4816875 0.5608823 -0.0001398
C 4.9135432 -0.7129466 -0.0000633
C -2.0302742 -0.8715541 -0.0000100
C -2.6651273 0.3727520 0.0000026
C -1.9233025 1.5669316 0.0000622
C -0.5371523 1.5564363 0.0001027
C -4.1472925 0.4938686 -0.0000196
O -4.7520360 1.5411743 0.0000869
O -4.7683434 -0.7058756 -0.0001614
C -6.2012163 -0.6659223 -0.0001543
H 2.9557902 -2.8747341 -0.0000244
H 2.6861725 2.5154195 -0.0000055
H 5.1615736 2.6817258 -0.0001823
H 6.5589573 0.6567221 -0.0002199
H 5.5333606 -1.5995318 -0.0000840
H -2.6012127 -1.7874211 -0.0000518
H -2.4633229 2.5025088 0.0000779
H 0.0248785 2.4798278 0.0001491
H -6.5228078 -1.7035399 -0.0002675
H -6.5707280 -0.1515474 -0.8862686
H -6.5707232 -0.1517418 0.8860749
31

RI-MP2 electronic energy -891.250595768904 E_h

C	3.4939502	-0.8869033	-0.0001464
N	2.6552810	-1.9928983	-0.0001639
C	1.3566197	-1.5603809	-0.0007054
N	1.3783428	-0.1764974	-0.0009198
C	2.6888709	0.2744233	-0.0006078
N	0.1704665	-2.1144254	-0.0008846
C	-0.6690756	-1.0057525	-0.0010616
C	0.0567190	0.2214393	-0.0012213
C	3.2431780	1.5478533	-0.0003920
C	4.6337341	1.6373968	0.0005218
C	5.4356973	0.4890660	0.0011189
C	4.8801052	-0.7893083	0.0005048
C	-2.0628671	-0.9711191	-0.0004483
C	-2.6866249	0.2756701	-0.0000492
C	-1.9485895	1.4769555	-0.0001717
C	-0.5619877	1.4685501	-0.0009110
C	-4.1655808	0.3993167	0.0003336
O	-4.7721911	1.4503200	0.0006701
O	-4.7792824	-0.8029039	0.0002747
C	-6.2100354	-0.7215300	0.0006529
H	2.9316582	-2.9583635	0.0001988
H	2.6207592	2.4308904	-0.0009192
H	5.1011620	2.6116889	0.0007431
H	6.5113688	0.5945546	0.0022618
H	5.5052775	-1.6713991	0.0002947
H	-2.6384393	-1.8844135	-0.0002470
H	-2.4948337	2.4091268	0.0003661
H	0.0037350	2.3896118	-0.0013202
H	-6.5575893	-1.7477655	0.0005642
H	-6.5601393	-0.1964495	-0.8837040
H	-6.5596893	-0.1967533	0.8853679

Compound **22a** (energetically higher in energy tautomer)

31

AM1 heat of formation 0.861460407725E-01 E_h

C	3.579552	-0.837614	-0.003678
N	2.767207	-2.004460	0.002592
C	1.512007	-1.523954	0.001691
N	1.450828	-0.054830	-0.009645
C	2.772339	0.381986	-0.006722
N	0.193060	-2.058646	0.106291
C	-0.668348	-0.914110	0.011235
C	0.110849	0.319682	0.004709
C	3.360691	1.646995	-0.006403
C	4.750568	1.706324	-0.007827
C	5.537487	0.546272	-0.008237
C	4.973410	-0.724605	-0.006313
C	-2.053202	-0.862009	0.012828
C	-2.667520	0.402468	0.005282
C	-1.915987	1.583801	0.003691
C	-0.519424	1.559488	0.003328
C	-4.132764	0.517098	0.001559
O	-4.812032	1.548084	0.015596
O	-4.794854	-0.683435	-0.023045
C	-6.222531	-0.621241	-0.021008
H	-0.012219	-2.838595	-0.482601
H	2.750723	2.560047	-0.005109
H	5.244265	2.690118	-0.008430
H	6.633801	0.646210	-0.008917
H	5.603031	-1.626322	-0.004646

H -2.667657 -1.776195 0.023282
H -2.444648 2.552884 0.003948
H 0.059100 2.493937 0.005182
H -6.531150 -1.695419 -0.038703
H -6.580782 -0.075601 -0.926779
H -6.579811 -0.106205 0.902887
31
RI-B3LYP electronic energy -892.78574288025 E_h
C 3.5285666 -0.8258300 0.0000144
N 2.7225898 -1.9677806 -0.0000050
C 1.5226367 -1.4759039 -0.0000324
N 1.4380569 -0.0902281 -0.0000280
C 2.7542754 0.3658042 0.0000059
N 0.2447876 -1.9681236 -0.0000590
C -0.6480851 -0.8966364 -0.0000651
C 0.1088204 0.2998000 -0.0000474
C 3.3218800 1.6298471 0.0000295
C 4.7118895 1.6967218 0.0000625
C 5.4923299 0.5349504 0.0000732
C 4.9167210 -0.7304840 0.0000497
C -2.0270625 -0.8668775 -0.0000692
C -2.6547485 0.3869006 -0.0000482
C -1.9008490 1.5659443 -0.0000421
C -0.5113645 1.5390419 -0.0000429
C -4.1360961 0.5156466 -0.0000015
O -4.7334413 1.5657837 0.0000527
O -4.7598122 -0.6827492 -0.0000063
C -6.1944334 -0.6386536 0.0000893
H 0.0123412 -2.9440314 -0.0000609
H 2.7204777 2.5282686 0.0000209
H 5.1952767 2.6642257 0.0000805
H 6.5705595 0.6258083 0.0001007
H 5.5229003 -1.6259364 0.0000599
H -2.6139422 -1.7730900 -0.0000704
H -2.4282227 2.5085930 -0.0000233
H 0.0620797 2.4544410 -0.0000287
H -6.5189732 -1.6750558 0.0000877
H -6.5607566 -0.1230804 -0.8862161
H -6.5606351 -0.1231211 0.8864686
31
B3LYP electronic energy -892.78502908742 E_h
C 3.5285298 -0.8258022 -0.0000710
N 2.7225680 -1.9677387 -0.0000151
C 1.5226257 -1.4757608 0.0001195
N 1.4380466 -0.0901028 0.0001729
C 2.7543240 0.3658642 0.0000498
N 0.2448212 -1.9680004 0.0001883
C -0.6480672 -0.8966235 0.0001992
C 0.1087927 0.2998446 0.0001988
C 3.3218796 1.6299204 0.0000257
C 4.7118850 1.6966598 -0.0001415
C 5.4922737 0.5348467 -0.0002768
C 4.9166816 -0.7305751 -0.0002378
C -2.0270351 -0.8669985 0.0001578
C -2.6546959 0.3867535 0.0001023
C -1.9008981 1.5658566 0.0001200
C -0.5114372 1.5390628 0.0001721
C -4.1360100 0.5155115 -0.0000371
O -4.7333719 1.5656384 -0.0001382
O -4.7598242 -0.6828165 -0.0000739
C -6.1943948 -0.6384090 -0.0002814
H 0.0124551 -2.9440560 0.0000990

H 2.7204429 2.5284191 0.0001307
H 5.1954426 2.6642173 -0.0001705
H 6.5706247 0.6257239 -0.0004131
H 5.5228338 -1.6261460 -0.0003411
H -2.6139163 -1.7732853 0.0001345
H -2.4284747 2.5085090 0.0000692
H 0.0620244 2.4545528 0.0001659
H -6.5191734 -1.6748606 -0.0003306
H -6.5606019 -0.1228288 -0.8867427
H -6.5608613 -0.1228323 0.8860748
31
RI-MP2 electronic energy -891.249846503623 E_h
C 3.5663346 -0.9107325 0.0002429
N 2.7765173 -2.0597913 -0.0000289
C 1.5684313 -1.5626612 -0.0003103
N 1.4817550 -0.1800231 -0.0002222
C 2.7859343 0.2793440 0.0000006
N 0.2883683 -2.0542136 -0.0003816
C -0.5978684 -0.9900185 -0.0003153
C 0.1549331 0.2085612 -0.0002623
C 3.3422300 1.5549472 -0.0001377
C 4.7310850 1.6258345 -0.0001355
C 5.5230631 0.4642253 0.0004261
C 4.9586474 -0.8060225 0.0004223
C -1.9847023 -0.9626078 -0.0002522
C -2.6002152 0.2927120 -0.0000702
C -1.8513727 1.4802810 -0.0000591
C -0.4619502 1.4539700 -0.0001685
C -4.0794330 0.4227215 0.0001389
O -4.6790615 1.4762609 0.0003440
O -4.6944390 -0.7785165 0.0000618
C -6.1268645 -0.6944880 0.0002548
H 0.0545711 -3.0309844 -0.0004726
H 2.7324132 2.4474070 -0.0001467
H 5.2106255 2.5947570 -0.0007709
H 6.5997322 0.5648014 0.0010813
H 5.5702384 -1.6974240 0.0004248
H -2.5753212 -1.8665478 -0.0003927
H -2.3854947 2.4192965 0.0000286
H 0.1166065 2.3663751 -0.0001997
H -6.4764097 -1.7198894 0.0001895
H -6.4742906 -0.1686925 -0.8844557
H -6.4740636 -0.1688815 0.8851666

Compound **23**

21
AM1 heat of formation -0.561095253040E-01 E_h
C 2.495837 0.859395 -0.320021
C 2.417136 -0.628430 -0.027022
N 1.155799 -1.251903 0.028321
C 0.050772 -0.510820 0.006652
N 0.018266 0.910917 -0.127511
C 1.260402 1.600701 0.176082
N -1.185549 -1.193706 0.065422
C -2.423852 -0.561210 -0.043982
C -2.454976 0.936705 -0.215534
C -1.182415 1.607157 0.285498
O 3.451526 -1.293454 0.123751
O -3.452799 -1.254077 -0.008125
H 3.405106 1.293019 0.170050
H 1.211061 2.611513 -0.320904

H -1.160905 -2.193292 0.118322
H -3.336688 1.345311 0.344416
H -2.609907 1.146986 -1.308169
H -1.226909 1.692690 1.411590
H -1.130553 2.652640 -0.134357
H 1.351661 1.769611 1.289796
H 2.610281 0.983614 -1.429410
21
RI-B3LYP electronic energy -586.80701694626 E_h
C -2.4198463 0.8212119 0.4700208
C -2.3847341 -0.6419108 0.0347436
N -1.1288990 -1.2174789 -0.0834034
C -0.0721170 -0.4639260 -0.0515324
N -0.0249604 0.8946128 0.0056665
C -1.2890256 1.6050977 -0.1787389
N 1.1480030 -1.1237781 -0.0893183
C 2.4083690 -0.5781871 0.0672885
C 2.4116584 0.9204468 0.2742325
C 1.2044710 1.5878979 -0.3692593
O -3.4018310 -1.2725282 -0.1486769
O 3.4016766 -1.2673036 0.0634679
H -3.3884089 1.2450162 0.2148585
H -1.1896333 2.5958722 0.2659489
H 1.0779319 -2.1302142 -0.1527724
H 3.3447325 1.3158075 -0.1219613
H 2.4105561 1.0963840 1.3534911
H 1.3139739 1.6052128 -1.4613432
H 1.1205782 2.6217256 -0.0357621
H -1.4839670 1.7416885 -1.2505618
H -2.3161864 0.8498879 1.5586313
21
B3LYP electronic energy -586.80651093656 E_h
C -2.4194937 0.8210853 0.4705782
C -2.3846561 -0.6418106 0.0347360
N -1.1288727 -1.2175571 -0.0833076
C -0.0721359 -0.4639729 -0.0513704
N -0.0249580 0.8945491 0.0059525
C -1.2889928 1.6048745 -0.1786515
N 1.1480107 -1.1236672 -0.0892242
C 2.4083258 -0.5780255 0.0673792
C 2.4113626 0.9205875 0.2741275
C 1.2042916 1.5874816 -0.3699209
O -3.4017898 -1.2721789 -0.1492601
O 3.4016673 -1.2670801 0.0635945
H -3.3882525 1.2451883 0.2164396
H -1.1896873 2.5959602 0.2655081
H 1.0780150 -2.1302353 -0.1526083
H 3.3446184 1.3161843 -0.1215568
H 2.4095528 1.0967061 1.3534407
H 1.3138007 1.6035973 -1.4621161
H 1.1204749 2.6217618 -0.0375805
H -1.4841991 1.7409282 -1.2505990
H -2.3148120 0.8493875 1.5591841
21
RI-MP2 electronic energy -585.828323579720 E_h
C -2.4299858 0.3366887 0.4807838
C -2.4179258 -1.1021721 -0.0010077
N -1.1646200 -1.7005929 -0.1211163
C -0.1109153 -0.9420976 -0.0634163
N -0.0584920 0.4153721 0.0384573
C -1.3163338 1.1100583 -0.1950652
N 1.1095986 -1.5939015 -0.1207217

C	2.3664504	-1.0468070	0.0551953
C	2.3561918	0.4428181	0.2765840
C	1.1592043	1.0849496	-0.3951367
O	-3.4425562	-1.7150500	-0.2281585
O	3.3674546	-1.7344043	0.0457739
H	-3.4028213	0.7720560	0.2710680
H	-1.2263645	2.1160957	0.2113971
H	1.0428691	-2.5998928	-0.2009389
H	3.2942555	0.8455478	-0.0961727
H	2.3122826	0.6146028	1.3532725
H	1.2567768	1.0352975	-1.4857431
H	1.0777481	2.1327778	-0.1130985
H	-1.5046743	1.1906582	-1.2724227
H	-2.2681428	0.3379957	1.5604664

Compound **24**

23

AM1 heat of formation 0.119069415797 E_h

C	0.372130	-2.448898	0.010778
C	1.779655	-2.427194	0.000992
C	2.483872	-1.244341	-0.008918
C	1.798334	-0.002723	-0.006015
C	0.386774	-0.011548	0.014055
C	-0.342858	-1.251345	0.015733
C	2.478338	1.246496	-0.021949
C	1.770680	2.422756	-0.023426
C	0.359268	2.435088	-0.005667
C	-0.337362	1.231457	0.023873
N	-1.737088	1.182946	0.103372
C	-2.381104	-0.080827	0.003221
N	-1.744523	-1.252316	0.020970
N	-3.799148	-0.047563	-0.144820
H	-0.154073	-3.414790	0.012543
H	2.317724	-3.388210	-0.000608
H	3.583229	-1.241571	-0.018248
H	3.577690	1.247179	-0.034786
H	2.298475	3.388982	-0.039612
H	-0.166471	3.399839	-0.011111
H	-2.238747	2.007731	-0.136516
H	-4.249058	0.565740	0.502395
H	-4.209820	-0.959902	-0.146766

23

RI-B3LYP electronic energy -588.74865470828 E_h

C	0.3328427	-2.4279885	-0.0038031
C	1.7375526	-2.4313093	-0.0041647
C	2.4636848	-1.2624564	0.0005185
C	1.8019045	-0.0114239	0.0040658
C	0.3793860	-0.0109846	0.0072241
C	-0.3593663	-1.2301264	0.0026648
C	2.4749676	1.2381559	0.0009062
C	1.7657289	2.4131265	-0.0021429
C	0.3568226	2.4215432	0.0011018
C	-0.3181609	1.2203429	0.0062382
N	-1.7128926	1.1352302	0.0059221
C	-2.3516349	-0.0808820	-0.0020323
N	-1.7519199	-1.2199429	0.0174925
N	-3.7295572	-0.0205438	-0.0772003
H	-0.2261318	-3.3534141	-0.0064872
H	2.2579234	-3.3809978	-0.0077494
H	3.5457901	-1.2867587	0.0014463
H	3.5572113	1.2521903	-0.0017018

H 2.2923439 3.3587965 -0.0067028
H -0.1856889 3.3587228 -0.0008313
H -2.2471233 1.9703984 -0.1654155
H -4.1798500 0.7142520 0.4460716
H -4.1562520 -0.9243781 0.0544123
23
B3LYP electronic energy -588.74808639139 E_h
C 0.3328894 -2.4279823 -0.0037927
C 1.7375929 -2.4311630 -0.0041991
C 2.4637427 -1.2623153 0.0004914
C 1.8018527 -0.0113638 0.0040679
C 0.3793678 -0.0109990 0.0072707
C -0.3593105 -1.2301388 0.0027110
C 2.4748965 1.2382064 0.0008865
C 1.7655373 2.4131082 -0.0021739
C 0.3566355 2.4215539 0.0010783
C -0.3181830 1.2202906 0.0063014
N -1.7128592 1.1351099 0.0060118
C -2.3515341 -0.0809654 -0.0019943
N -1.7518726 -1.2200485 0.0175891
N -3.7294481 -0.0205325 -0.0774762
H -0.2261086 -3.3534980 -0.0065293
H 2.2580565 -3.3809371 -0.0078483
H 3.5459343 -1.2865425 0.0013715
H 3.5572221 1.2522543 -0.0017506
H 2.2921666 3.3589086 -0.0067734
H -0.1860220 3.3587547 -0.0008636
H -2.2472452 1.9703376 -0.1653184
H -4.1795839 0.7141447 0.4463806
H -4.1560827 -0.9245141 0.0545758
23
RI-MP2 electronic energy -587.695046760437 E_h
C 0.2549047 -2.4870256 -0.0130095
C 1.6604309 -2.4966069 -0.0143413
C 2.3855606 -1.3217349 -0.0105416
C 1.7233902 -0.0728824 -0.0073716
C 0.2983034 -0.0728351 -0.0008548
C -0.4385833 -1.2879833 -0.0070048
C 2.3982632 1.1716485 -0.0123593
C 1.6889924 2.3539732 -0.0149169
C 0.2809498 2.3591121 -0.0061887
C -0.3983412 1.1568735 0.0001494
N -1.7909024 1.0736088 0.0089661
C -2.4247721 -0.1424683 -0.0154567
N -1.8355469 -1.2900287 0.0055398
N -3.8048788 -0.0657793 -0.1107692
H -0.3099299 -3.4091272 -0.0162747
H 2.1812131 -3.4451988 -0.0173626
H 3.4679516 -1.3434444 -0.0100244
H 3.4806839 1.1833199 -0.0177813
H 2.2171906 3.2979657 -0.0212869
H -0.2649758 3.2940875 -0.0056374
H -2.3260614 1.8953823 -0.2202177
H -4.2264669 0.6266212 0.4893564
H -4.2173758 -0.9774778 0.0173877

Compound **24** Imine

23
AM1 heat of formation 0.126865660712 E_h
C -0.356511 2.441814 0.000886
C -1.765315 2.419319 -0.026224

C -2.465273 1.236777 -0.029326
C -1.775932 -0.005025 -0.011283
C -0.364041 -0.001515 0.006972
C 0.354029 1.242592 0.027389
C -2.459512 -1.250628 -0.008824
C -1.754500 -2.429611 0.010622
C -0.344928 -2.445037 0.019699
C 0.359574 -1.242835 0.008447
N 1.751835 -1.203589 -0.029979
C 2.491353 0.017045 -0.001198
N 1.745224 1.220362 0.116415
N 3.798557 0.107442 -0.072050
H 0.162518 3.410767 0.007384
H -2.301361 3.381278 -0.043900
H -3.564488 1.229780 -0.046612
H -3.558839 -1.248597 -0.020625
H -2.286128 -3.394088 0.017317
H 0.178257 -3.411401 0.030369
H 2.250477 -2.055428 0.078082
H 4.292720 -0.755480 -0.115058
H 2.243860 2.076285 0.009376
23
RI-B3LYP electronic energy -588.74497079539 E_h
C -0.3505382 -2.4223756 -0.0000045
C -1.7574685 -2.4087864 0.0000046
C -2.4667328 -1.2327392 0.0000085
C -1.7874764 0.0103776 0.0000048
C -0.3661013 0.0006224 -0.0000043
C 0.3417318 -1.2285268 -0.0000093
C -2.4494406 1.2634659 0.0000098
C -1.7260781 2.4301902 0.0000070
C -0.3183039 2.4236261 -0.0000023
C 0.3549857 1.2202616 -0.0000082
N 1.7460985 1.1473135 -0.0000226
C 2.4888881 -0.0221694 0.0000009
N 1.7270160 -1.1732039 -0.0000242
N 3.7628557 -0.1220155 0.0000290
H 0.1857013 -3.3626984 -0.0000084
H -2.2855370 -3.3536288 0.0000079
H -3.5486086 -1.2424256 0.0000147
H -3.5311527 1.2873832 0.0000162
H -2.2414603 3.3819541 0.0000112
H 0.2305595 3.3570319 -0.0000057
H 2.2684163 2.0062196 0.0000114
H 4.2237317 0.7811887 0.0000338
H 2.2657639 -2.0233603 0.0000019
23
B3LYP electronic energy -588.74441711083 E_h
C -0.3504485 -2.4223947 -0.0000279
C -1.7573748 -2.4086980 0.0000138
C -2.4667217 -1.2326943 0.0000435
C -1.7874262 0.0103791 0.0000218
C -0.3660847 0.0006219 -0.0000198
C 0.3417158 -1.2285068 -0.0000407
C -2.4494338 1.2634224 0.0000419
C -1.7259783 2.4300954 0.0000108
C -0.3182137 2.4236399 -0.0000301
C 0.3549676 1.2202384 -0.0000410
N 1.7460194 1.1472791 -0.0000693
C 2.4887731 -0.0221522 0.0000080
N 1.7269354 -1.1731567 -0.0000713
N 3.7627424 -0.1220616 0.0001190

H 0.1858785 -3.3627692 -0.0000493
H -2.2854948 -3.3536537 0.0000260
H -3.5486801 -1.2423647 0.0000776
H -3.5312280 1.2873288 0.0000757
H -2.2414060 3.3819764 0.0000211
H 0.2307250 3.3571014 -0.0000532
H 2.2684029 2.0062871 0.0000123
H 4.2235072 0.7813719 0.0001550
H 2.2657657 -2.0234104 0.0000039
23
RI-MP2 electronic energy -587.688542610608 E_h
C -0.2107964 -2.4508607 0.0000000
C -1.6178198 -2.4425615 0.0000000
C -2.3270951 -1.2603795 0.0000000
C -1.6465953 -0.0207306 0.0000000
C -0.2235530 -0.0310328 0.0000000
C 0.4845058 -1.2559536 0.0000000
C -2.3092706 1.2289272 0.0000000
C -1.5853425 2.4019046 0.0000000
C -0.1778641 2.3896262 0.0000000
C 0.4979561 1.1846687 0.0000000
N 1.8877299 1.1131821 0.0000000
C 2.6285767 -0.0535389 0.0000000
N 1.8685704 -1.2020233 0.0000000
N 3.9070926 -0.1589025 0.0000000
H 0.3292981 -3.3890142 0.0000000
H -2.1460964 -3.3865148 0.0000000
H -3.4092019 -1.2679531 0.0000000
H -3.3912380 1.2512725 0.0000000
H -2.1007853 3.3528600 0.0000000
H 0.3752364 3.3205168 0.0000000
H 2.4110708 1.9724638 0.0000000
H 4.3462676 0.7559725 0.0000000
H 2.4093537 -2.0519289 0.0000000

Compound **25**

26
AM1 heat of formation 0.124437767620 E_h
C 0.338556 2.427672 0.033334
C 1.730392 2.636162 0.005259
C 2.618353 1.584420 -0.022017
C 2.144907 0.247537 -0.018406
C 0.751204 0.026108 0.020322
C -0.171331 1.129239 0.039127
C 3.018694 -0.874260 -0.051519
C 2.511537 -2.149956 -0.051143
C 1.121491 -2.392039 -0.014309
C 0.238603 -1.317773 0.032362
N -1.148189 -1.496812 0.131334
C -1.995183 -0.355011 0.048078
N -1.554497 0.902433 0.060082
N -3.392269 -0.645639 -0.074096
H -3.685101 -1.346990 0.579915
C -4.304333 0.466474 -0.129443
H -0.338089 3.294631 0.048892
H 2.104247 3.672156 0.003464
H 3.703103 1.761485 -0.045823
H 4.103200 -0.696160 -0.078938
H 3.189221 -3.017310 -0.080684
H 0.759643 -3.429389 -0.018530
H -1.511135 -2.394235 -0.097013

H -4.045957 1.120120 -1.004123
H -4.296728 1.097624 0.800023
H -5.335064 0.046761 -0.278304
26
RI-B3LYP electronic energy -628.03930165769 E_h
C 0.3084859 2.4033294 -0.0087554
C 1.6941921 2.6321937 -0.0041841
C 2.5989092 1.5952513 0.0037473
C 2.1462297 0.2543931 0.0066571
C 0.7421100 0.0259280 0.0055637
C -0.1836973 1.1097215 -0.0035711
C 3.0112831 -0.8708375 0.0068381
C 2.4992602 -2.1442371 0.0030627
C 1.1101135 -2.3783358 0.0027201
C 0.2500995 -1.3011070 0.0049981
N -1.1383529 -1.4420264 0.0044811
C -1.9704979 -0.3425333 -0.0141211
N -1.5560265 0.8785650 0.0027392
N -3.3106818 -0.6314788 -0.0775142
H -3.5849976 -1.5160377 0.3165733
C -4.2918311 0.4371656 0.0307674
H -0.3914480 3.2273635 -0.0145427
H 2.0552282 3.6532294 -0.0069516
H 3.6630588 1.7930522 0.0077496
H 4.0818002 -0.7111315 0.0075775
H 3.1705945 -2.9934011 0.0010618
H 0.7251248 -3.3905678 0.0013924
H -1.5265039 -2.3550801 -0.1627994
H -4.1105557 1.1778323 -0.7441044
H -4.2532457 0.9462690 0.9973265
H -5.2815707 0.0074610 -0.1135608
26
B3LYP electronic energy -628.03866848475 E_h
C 0.3085680 2.4033427 -0.0088949
C 1.6942970 2.6320283 -0.0042328
C 2.5990000 1.5950735 0.0038206
C 2.1461621 0.2542927 0.0067419
C 0.7420622 0.0259472 0.0055425
C -0.1836481 1.1097698 -0.0036652
C 3.0111613 -0.8709519 0.0070107
C 2.4989902 -2.1442921 0.0031800
C 1.1098442 -2.3783809 0.0026871
C 0.2500172 -1.3010407 0.0049713
N -1.1383976 -1.4418381 0.0042521
C -1.9704281 -0.3423696 -0.0142863
N -1.5560113 0.8787285 0.0026887
N -3.3106252 -0.6315789 -0.0780165
H -3.5844555 -1.5154796 0.3183626
C -4.2915612 0.4371496 0.0312288
H -0.3913682 3.2274933 -0.0147326
H 2.0554361 3.6531539 -0.0070216
H 3.6632490 1.7927902 0.0079156
H 4.0817639 -0.7112737 0.0078532
H 3.1703437 -2.9935939 0.0012294
H 0.7246789 -3.3906454 0.0013248
H -1.5267233 -2.3549201 -0.1632482
H -4.1081956 1.1796653 -0.7414725
H -4.2549938 0.9439489 0.9991692
H -5.2812849 0.0082682 -0.1164728
26
RI-MP2 electronic energy -626.907617065980 E_h
C 0.4299839 2.3930903 -0.0108751

C	1.8150673	2.6320701	-0.0071770
C	2.7220638	1.5911444	-0.0024761
C	2.2720659	0.2510925	-0.0018551
C	0.8660069	0.0188442	0.0017895
C	-0.0596949	1.0970069	-0.0079151
C	3.1411761	-0.8663555	-0.0065422
C	2.6338113	-2.1484160	-0.0116653
C	1.2454963	-2.3827292	-0.0045107
C	0.3780743	-1.3077720	0.0024737
N	-1.0082710	-1.4545226	0.0160109
C	-1.8363531	-0.3553322	-0.0246355
N	-1.4383773	0.8739044	-0.0054807
N	-3.1762602	-0.6590091	-0.1138420
H	-3.4360404	-1.4907283	0.3930035
C	-4.1213164	0.4397380	0.0052103
H	-0.2775677	3.2109360	-0.0164797
H	2.1741350	3.6529585	-0.0078541
H	3.7864654	1.7889951	0.0006488
H	4.2110346	-0.7013548	-0.0095048
H	3.3087020	-2.9938407	-0.0181531
H	0.8595172	-3.3943610	-0.0038808
H	-1.3967499	-2.3506515	-0.2303449
H	-3.9355243	1.1541218	-0.7897164
H	-4.0331939	0.9646469	0.9567293
H	-5.1242509	0.0365238	-0.1029573

Compound **25** Imine

26

AM1 heat of formation 0.125891102266 E_h

C	-1.078186	-2.403797	-0.003011
C	-2.468927	-2.180088	-0.042495
C	-2.992837	-0.909663	-0.047797
C	-2.133443	0.220898	-0.019579
C	-0.736803	0.015642	0.011111
C	-0.203823	-1.318394	0.033841
C	-2.631851	1.551474	-0.019053
C	-1.765735	2.617534	0.010374
C	-0.368571	2.431470	0.031764
C	0.156784	1.140839	0.022859
N	1.529406	0.902809	-0.003881
C	2.083535	-0.407856	0.029255
N	1.175296	-1.494607	0.135891
N	3.370980	-0.693112	-0.028061
C	4.358103	0.328994	-0.083363
H	1.548371	-2.412468	0.031661
H	-0.702912	-3.436916	0.004802
H	-3.136756	-3.055514	-0.068141
H	-4.079567	-0.745752	-0.074698
H	-3.720008	1.706696	-0.040482
H	-2.154165	3.648058	0.015566
H	0.287360	3.312991	0.050002
H	2.146659	1.672919	0.108575
H	4.268881	0.980885	-0.995801
H	5.350064	-0.197051	-0.123656
H	4.352832	0.998206	0.821097

26

RI-B3LYP electronic energy -628.03540962234 E_h

C	-1.0911828	-2.3814241	-0.0000025
C	-2.4785544	-2.1501344	-0.0000118
C	-2.9978142	-0.8784926	-0.0000116
C	-2.1340573	0.2441464	0.0000009

C -0.7309923 0.0153590 0.0000106
C -0.2207493 -1.3093935 0.0000064
C -2.5946027 1.5845225 0.0000015
C -1.7004535 2.6261156 0.0000132
C -0.3106410 2.4024249 0.0000234
C 0.1688399 1.1096914 0.0000207
N 1.5332572 0.8255432 0.0000227
C 2.0835443 -0.4435617 0.0000018
N 1.1540316 -1.4686050 0.0000060
N 3.3258329 -0.7319625 -0.0000256
C 4.2922116 0.3437584 -0.0000365
H 1.5585278 -2.3902112 -0.0000111
H -0.7072136 -3.3935685 -0.0000057
H -3.1464481 -3.0019741 -0.0000212
H -4.0681543 -0.7206402 -0.0000209
H -3.6597455 1.7748104 -0.0000076
H -2.0632481 3.6458708 0.0000133
H 0.3759411 3.2397235 0.0000302
H 2.1785468 1.5956425 0.0000247
H 4.2155262 0.9884323 -0.8877617
H 5.2954643 -0.0793050 -0.0001416
H 4.2156624 0.9883180 0.8877825
26
B3LYP electronic energy -628.03477933197 E_h
C -1.0911029 -2.3814490 0.0000154
C -2.4784453 -2.1500173 -0.0000384
C -2.9977662 -0.8783968 -0.0000710
C -2.1339560 0.2441715 -0.0000376
C -0.7309280 0.0153577 0.0000122
C -0.2207459 -1.3093823 0.0000359
C -2.5945232 1.5845147 -0.0000436
C -1.7002834 2.6260344 0.0000104
C -0.3104684 2.4024174 0.0000580
C 0.1688823 1.1096590 0.0000513
N 1.5332329 0.8254868 0.0000836
C 2.0834369 -0.4435829 0.0000281
N 1.1539753 -1.4685797 0.0000875
N 3.3257056 -0.7321207 -0.0000510
C 4.2917882 0.3438092 -0.0001010
H 1.5585627 -2.3902771 0.0000229
H -0.7070843 -3.3936715 0.0000440
H -3.1464311 -3.0019399 -0.0000553
H -4.0681828 -0.7204980 -0.0001121
H -3.6597439 1.7748212 -0.0000827
H -2.0630855 3.6459188 0.0000156
H 0.3762312 3.2397345 0.0000982
H 2.1786397 1.5956353 0.0000591
H 4.2149363 0.9885537 -0.8878854
H 5.2952564 -0.0790021 -0.0002718
H 4.2151746 0.9884070 0.8878092
26
RI-MP2 electronic energy -626.901611650849 E_h
C -1.1895107 -2.4758891 -0.0000159
C -2.5768137 -2.2435580 -0.0000051
C -3.0892556 -0.9635299 -0.0000020
C -2.2196545 0.1514415 -0.0000215
C -0.8159351 -0.0844114 -0.0000146
C -0.3108540 -1.4074658 0.0000093
C -2.6757140 1.4904863 0.0000314
C -1.7758579 2.5346881 0.0000602
C -0.3882589 2.2994666 -0.0000373
C 0.0879994 1.0026705 -0.0000001

N	1.4502190	0.7144089	-0.0000017
C	1.9915478	-0.5543289	0.0000071
N	1.0619729	-1.5742266	0.0000431
N	3.2395825	-0.8466845	0.0000424
C	4.1588923	0.2730940	0.0000383
H	1.4647251	-2.4976198	-0.0000858
H	-0.8061790	-3.4883043	-0.0000983
H	-3.2485187	-3.0915288	-0.0000129
H	-4.1587231	-0.7985296	0.0000549
H	-3.7406100	1.6835065	0.0000959
H	-2.1346199	3.5551287	0.0002042
H	0.3059243	3.1305695	-0.0002904
H	2.1012253	1.4811249	-0.0001077
H	4.0459969	0.9075967	-0.8871650
H	5.1763576	-0.1056638	-0.0000062
H	4.0460620	0.9075582	0.8872777

Compound **26**

29

AM1 heat of formation 0.132684907841 E_h

C	0.836590	2.444459	-0.107392
C	2.241698	2.528836	-0.132074
C	3.033991	1.403890	-0.087277
C	2.445990	0.115004	-0.016242
C	1.037744	0.017791	0.004184
C	0.216035	1.197621	-0.038462
C	3.218478	-1.077931	0.033751
C	2.601577	-2.302752	0.102926
C	1.195959	-2.422366	0.125382
C	0.408894	-1.275528	0.072122
N	-0.987893	-1.324934	0.064762
C	-1.725967	-0.119926	0.067524
N	-1.183321	1.089632	-0.011498
N	-3.168185	-0.309550	0.168387
C	-3.777344	-0.511690	-1.131205
C	-3.834042	0.698298	0.967931
H	0.238193	3.366653	-0.142568
H	2.705000	3.526486	-0.187822
H	4.130339	1.484362	-0.106417
H	4.314601	-0.996442	0.016502
H	3.201990	-3.224977	0.143255
H	0.744427	-3.422130	0.183565
H	-1.443408	-2.195796	0.208805
H	-3.239481	-1.332438	-1.673269
H	-3.767355	0.411454	-1.771776
H	-4.842438	-0.823016	-0.964545
H	-3.288434	0.823183	1.938973
H	-4.871774	0.324115	1.175471
H	-3.903480	1.698273	0.461263

29

RI-B3LYP electronic energy -667.32763451976 E_h

C	-0.9751405	2.4276334	0.0027826
C	-2.3785531	2.4390323	0.0246711
C	-3.1145582	1.2751807	0.0305121
C	-2.4603854	0.0209998	0.0146357
C	-1.0378653	0.0129882	-0.0087372
C	-0.2871093	1.2244212	-0.0140676
C	-3.1383612	-1.2261569	0.0198637
C	-2.4334420	-2.4039070	0.0039542
C	-1.0249186	-2.4182354	-0.0179113
C	-0.3449756	-1.2185565	-0.0239579

N 1.0486763 -1.1448535 -0.0432630
C 1.7106423 0.0638484 -0.0597239
N 1.0993169 1.2062761 -0.0305229
N 3.0819101 0.0103457 -0.1260398
C 3.8014489 -1.2252643 0.1211753
C 3.8303504 1.2514200 0.0211459
H -0.4120061 3.3506449 -0.0005631
H -2.8923960 3.3924015 0.0371115
H -4.1963028 1.3073416 0.0475707
H -4.2205728 -1.2363545 0.0365808
H -2.9639195 -3.3475407 0.0080272
H -0.4865412 -3.3579044 -0.0303568
H 1.5638102 -2.0055134 -0.0721946
H 3.5056269 -2.0138664 -0.5751970
H 3.6813052 -1.5953833 1.1469014
H 4.8606222 -1.0463588 -0.0461267
H 3.2605872 2.0660978 -0.4114673
H 4.7822217 1.1525627 -0.4999721
H 4.0254462 1.4910722 1.0724097
29
B3LYP electronic energy -667.32692339123 E_h
C -0.9752347 2.4276606 0.0028112
C -2.3786375 2.4388250 0.0249142
C -3.1145965 1.2749421 0.0308100
C -2.4602264 0.0208888 0.0147568
C -1.0377459 0.0130360 -0.0088534
C -0.2871253 1.2245160 -0.0141998
C -3.1381266 -1.2262864 0.0200546
C -2.4330423 -2.4039381 0.0039756
C -1.0245311 -2.4182178 -0.0181522
C -0.3448167 -1.2184484 -0.0242495
N 1.0487665 -1.1446233 -0.0438833
C 1.7105729 0.0640691 -0.0601183
N 1.0993073 1.2065212 -0.0307817
N 3.0817733 0.0103788 -0.1265405
C 3.8006232 -1.2253061 0.1222495
C 3.8303589 1.2512505 0.0210644
H -0.4121708 3.3508204 -0.0005024
H -2.8926189 3.3922521 0.0375059
H -4.1964275 1.3069604 0.0480635
H -4.2204159 -1.2365400 0.0369765
H -2.9634883 -3.3477271 0.0081252
H -0.4859466 -3.3578749 -0.0307121
H 1.5641197 -2.0053034 -0.0726009
H 3.5080661 -2.0132517 -0.5764415
H 3.6763192 -1.5967824 1.1470635
H 4.8605249 -1.0457852 -0.0403031
H 3.2603457 2.0661756 -0.4109674
H 4.7820564 1.1527024 -0.5006004
H 4.0258734 1.4904691 1.0724522
29
RI-MP2 electronic energy -666.120350128752 E_h
C -1.2209982 2.4691605 0.0315492
C -2.6249089 2.4925879 0.0822560
C -3.3643519 1.3260493 0.0720900
C -2.7163512 0.0715303 0.0128264
C -1.2922770 0.0586773 -0.0361328
C -0.5387185 1.2631929 -0.0280032
C -3.4022163 -1.1670221 -0.0033462
C -2.7036296 -2.3544637 -0.0631648
C -1.2964661 -2.3711263 -0.1070944
C -0.6061618 -1.1742662 -0.0920914

N	0.7847726	-1.1068454	-0.1246680
C	1.4443769	0.0996451	-0.1495567
N	0.8532811	1.2523611	-0.0729751
N	2.8143890	0.0322809	-0.2787834
C	3.5076375	-1.1381195	0.2296816
C	3.5234058	1.2909513	-0.1077629
H	-0.6474200	3.3859846	0.0388808
H	-3.1344201	3.4463281	0.1284300
H	-4.4457372	1.3596044	0.1114094
H	-4.4841795	-1.1704708	0.0318415
H	-3.2401895	-3.2937617	-0.0762782
H	-0.7595154	-3.3104941	-0.1515333
H	1.2959760	-1.9567697	-0.2852939
H	3.2378600	-2.0387637	-0.3204492
H	3.3295276	-1.3055870	1.2964181
H	4.5726638	-0.9906762	0.0761372
H	3.0319992	2.0603777	-0.6910612
H	4.5428868	1.1553297	-0.4601136
H	3.5387647	1.6143053	0.9367880

Compound **27**

23

AM1 heat of formation 0.128387357259 E_h

C	0.259950	-2.223004	0.015835
C	-1.100011	-1.876432	0.010370
C	-1.516122	-0.558482	0.001908
C	-0.560908	0.496268	0.001014
C	0.811083	0.150330	0.016179
C	1.234851	-1.224391	0.017521
C	-0.911501	1.874788	-0.013876
C	0.058696	2.846542	-0.017979
C	1.430005	2.521283	-0.004258
C	1.812581	1.184222	0.022467
N	3.161314	0.805534	0.091305
C	3.492221	-0.570912	0.000328
N	2.593224	-1.558746	0.021291
N	4.873779	-0.877384	-0.147461
Br	-3.357638	-0.199954	-0.006460
H	0.545552	-3.285569	0.017153
H	-1.840828	-2.694060	0.011312
H	-1.975459	2.156825	-0.023761
H	-0.225011	3.910694	-0.033200
H	2.173581	3.330254	-0.011160
H	3.845205	1.494780	-0.124207
H	5.062385	-1.859424	-0.129501
H	5.468615	-0.362197	0.466465

23

RI-B3LYP electronic energy -3162.19098296693 E_h

C	0.2868432	-2.2032439	-0.0055735
C	-1.0751108	-1.8712384	-0.0062689
C	-1.4867340	-0.5603505	-0.0013386
C	-0.5571340	0.5111692	0.0025018
C	0.8239232	0.1517798	0.0057600
C	1.2483704	-1.2094591	0.0014888
C	-0.8927566	1.8884711	-0.0000826
C	0.0909745	2.8461727	-0.0024480
C	1.4544555	2.5041017	0.0008018
C	1.8058314	1.1720752	0.0052972
N	3.1361845	0.7476485	0.0043179
C	3.4608154	-0.5856637	-0.0008567
N	2.5976818	-1.5417375	0.0175332

N 4.8090333 -0.8665707 -0.0727922
Br -3.3695311 -0.2002504 0.0014027
H 0.5990452 -3.2379438 -0.0083529
H -1.8131298 -2.6609954 -0.0101170
H -1.9330002 2.1762329 -0.0023718
H -0.1850574 3.8925805 -0.0064276
H 2.2150213 3.2747755 -0.0005899
H 3.8577866 1.4302648 -0.1560913
H 5.0043184 -1.8464127 0.0604658
H 5.4314373 -0.2580045 0.4352889
23
B3LYP electronic energy -3162.19039455900 E_h
C 0.2868231 -2.2032544 -0.0055658
C -1.0751179 -1.8712535 -0.0062761
C -1.4866676 -0.5603520 -0.0013463
C -0.5570881 0.5111662 0.0025080
C 0.8239097 0.1517429 0.0057898
C 1.2483200 -1.2094682 0.0015196
C -0.8927473 1.8884422 -0.0001042
C 0.0910493 2.8460823 -0.0024812
C 1.4545395 2.5040579 0.0007863
C 1.8057865 1.1720285 0.0053563
N 3.1360820 0.7475875 0.0044323
C 3.4606760 -0.5856681 -0.0008223
N 2.5976198 -1.5417990 0.0176100
N 4.8089234 -0.8664405 -0.0730638
Br -3.3694686 -0.2001989 0.0013964
H 0.5991065 -3.2380279 -0.0083893
H -1.8132423 -2.6610296 -0.0101625
H -1.9330749 2.1762345 -0.0024187
H -0.1849814 3.8926165 -0.0065028
H 2.2152264 3.2747360 -0.0006005
H 3.8578247 1.4302210 -0.1560886
H 5.0041566 -1.8464082 0.0605788
H 5.4311102 -0.2579570 0.4356733
23
RI-MP2 electronic energy -3159.684831082283 E_h
C -0.8202878 -2.3550423 -0.0149559
C -2.1847577 -2.0296774 -0.0161082
C -2.5939186 -0.7112419 -0.0115931
C -1.6629661 0.3565705 -0.0083717
C -0.2801043 -0.0043916 -0.0023862
C 0.1435079 -1.3611216 -0.0085198
C -2.0046071 1.7289650 -0.0125787
C -1.0193287 2.6941776 -0.0146814
C 0.3430756 2.3492356 -0.0065054
C 0.6998723 1.0151277 -0.0012130
N 2.0285015 0.5934251 0.0053784
C 2.3491016 -0.7388955 -0.0145549
N 1.4948632 -1.7057427 0.0058684
N 3.7043831 -1.0032236 -0.1066492
Br -4.4498034 -0.3396642 -0.0085047
H -0.5013390 -3.3882180 -0.0184316
H -2.9263419 -2.8162656 -0.0193582
H -3.0465867 2.0129131 -0.0172502
H -1.2971615 3.7394704 -0.0201909
H 1.1058461 3.1175447 -0.0056445
H 2.7483753 1.2633414 -0.2123015
H 3.8836158 -1.9873320 0.0236153
H 4.2860605 -0.4299546 0.4849369

Compound **27** Imine

23
AM1 heat of formation 0.136579722579 E_h
C -0.261180 -2.223405 -0.000007
C 1.098262 -1.869613 -0.000001
C 1.505022 -0.551352 -0.000001
C 0.541100 0.498892 -0.000005
C -0.831185 0.152651 -0.000006
C -1.236905 -1.225961 -0.000014
C 0.890188 1.876032 -0.000009
C -0.082279 2.847283 -0.000012
C -1.451004 2.519971 -0.000008
C -1.836342 1.180578 -0.000001
N -3.178164 0.807764 0.000025
C -3.607869 -0.551206 0.000005
N -2.589825 -1.540146 -0.000045
N -4.856478 -0.953325 0.000032
Br 3.343528 -0.181135 0.000008
H -0.534063 -3.288488 -0.000007
H 1.841196 -2.685426 0.000002
H 1.953620 2.160153 -0.000012
H 0.201317 3.911810 -0.000016
H -2.195946 3.328032 -0.000008
H -3.868629 1.521084 -0.000023
H -2.870773 -2.495333 -0.000011
H -5.545784 -0.235373 0.000054
23
RI-B3LYP electronic energy -3162.18605448158 E_h
C -0.2813742 -2.2048899 0.0000020
C 1.0807695 -1.8634833 -0.0000013
C 1.4835054 -0.5524874 -0.0000032
C 0.5433798 0.5123019 -0.0000022
C -0.8366940 0.1512065 0.0000013
C -1.2361944 -1.2099227 0.0000034
C 0.8743285 1.8883789 -0.0000042
C -0.1155572 2.8402961 -0.0000030
C -1.4761258 2.4917323 0.0000004
C -1.8329419 1.1599582 0.0000028
N -3.1652867 0.7561133 0.0000073
C -3.6092432 -0.5558028 0.0000097
N -2.5921426 -1.4892882 0.0000068
N -4.8208527 -0.9588267 0.0000145
Br 3.3623220 -0.1816985 -0.0000074
H -0.5733472 -3.2468183 0.0000034
H 1.8202592 -2.6513684 -0.0000022
H 1.9131073 2.1803536 -0.0000068
H 0.1541477 3.8882982 -0.0000048
H -2.2375853 3.2614386 0.0000013
H -3.8762454 1.4669115 0.0000082
H -2.9095827 -2.4445429 0.0000097
H -5.4871632 -0.1945403 0.0000167
23
B3LYP electronic energy -3162.18547972729 E_h
C -0.2813878 -2.2049069 0.0000522
C 1.0807477 -1.8634996 0.0000348
C 1.4834205 -0.5524950 -0.0000045
C 0.5433403 0.5123120 -0.0000073
C -0.8366784 0.1512039 0.0000169
C -1.2361425 -1.2099045 0.0000270
C 0.8743431 1.8883558 -0.0000237
C -0.1156186 2.8402018 0.0000096

C -1.4762003 2.4917106 0.0000476
C -1.8328942 1.1599344 0.0000417
N -3.1651805 0.7560768 0.0000675
C -3.6091000 -0.5557792 0.0000090
N -2.5920356 -1.4892402 0.0000045
N -4.8206896 -0.9588689 -0.0000351
Br 3.3622484 -0.1816683 -0.0000470
H -0.5734819 -3.2469007 0.0000755
H 1.8203414 -2.6514136 0.0000509
H 1.9132003 2.1803755 -0.0000510
H 0.1540861 3.8883322 0.0000060
H -2.2377577 3.2614389 0.0000782
H -3.8762235 1.4669620 0.0000566
H -2.9095289 -2.4446159 -0.0000233
H -5.4869678 -0.1943596 -0.0000252
23
RI-MP2 electronic energy -3159.677246984180 E_h
C 0.7554001 -2.3348701 0.0000000
C 2.1190126 -1.9991767 0.0000000
C 2.5198936 -0.6801481 0.0000000
C 1.5780823 0.3792723 0.0000000
C 0.1971553 0.0167277 0.0000000
C -0.2034807 -1.3402847 0.0000000
C 1.9135752 1.7518854 0.0000000
C 0.9219403 2.7100109 0.0000000
C -0.4375405 2.3559435 0.0000000
C -0.7977562 1.0220034 0.0000000
N -2.1294077 0.6205436 0.0000000
C -2.5725876 -0.6883016 0.0000000
N -1.5586822 -1.6202275 0.0000000
N -3.7878693 -1.0969093 0.0000000
Br 4.3724288 -0.2980420 0.0000000
H 0.4589329 -3.3758799 0.0000000
H 2.8620449 -2.7839926 0.0000000
H 2.9540196 2.0406024 0.0000000
H 1.1917331 3.7573659 0.0000000
H -1.2021048 3.1226334 0.0000000
H -2.8412061 1.3317566 0.0000000
H -1.8785208 -2.5756274 0.0000000
H -4.4350628 -0.3152851 0.0000000

Compound **28**

26
AM1 heat of formation 0.108384787801 E_h
C 0.406283 -2.314600 0.013648
C 1.792273 -2.082089 0.006247
C 2.324829 -0.806584 -0.003344
C 1.450690 0.319373 -0.002411
C 0.056254 0.095008 0.015870
C -0.480885 -1.239466 0.016892
C 1.923430 1.661671 -0.018656
C 1.043231 2.714913 -0.022171
C -0.352218 2.509607 -0.005856
C -0.851712 1.211861 0.024298
N -2.228017 0.951379 0.103464
C -2.673609 -0.394802 0.001458
N -1.865765 -1.454816 0.019616
N -4.080582 -0.576610 -0.148480
C 3.792088 -0.604149 -0.013335
H 0.032529 -3.349298 0.014969
H 2.465384 -2.954730 0.006198

H 3.008449 1.841210 -0.030267
H 1.416776 3.750593 -0.038836
H -1.021647 3.380779 -0.012682
H -2.848187 1.690669 -0.138311
H -4.617439 -0.043695 0.503797
H -4.346911 -1.541073 -0.154631
H 4.334773 -1.581362 -0.008981
H 4.111757 -0.021598 0.887122
H 4.101130 -0.035623 -0.926405
26
RI-B3LYP electronic energy -628.05053220613 E_h
C 0.3844190 -2.2889110 -0.0041749
C 1.7699534 -2.0620001 -0.0047351
C 2.3255189 -0.7991622 0.0001359
C 1.4503740 0.3271071 0.0038199
C 0.0451031 0.0970999 0.0070960
C -0.4931398 -1.2235024 0.0025120
C 1.9025684 1.6738567 0.0008100
C 1.0085648 2.7170022 -0.0023411
C -0.3797321 2.4947592 0.0008863
C -0.8452676 1.1973174 0.0061188
N -2.2077327 0.8894730 0.0060023
C -2.6446349 -0.4130112 -0.0018552
N -1.8694170 -1.4391227 0.0179252
N -4.0159311 -0.5723743 -0.0777996
C 3.8184967 -0.6128257 0.0011958
H -0.0122402 -3.2947671 -0.0068851
H 2.4317561 -2.9204223 -0.0086232
H 2.9627222 1.8811281 -0.0016032
H 1.3745149 3.7357507 -0.0068661
H -1.0706815 3.3285790 -0.0008818
H -2.8680381 1.6283289 -0.1681366
H -4.5739802 0.0747865 0.4577195
H -4.2907773 -1.5338309 0.0512626
H 4.3261153 -1.5767781 -0.0008519
H 4.1590607 -0.0594835 0.8809199
H 4.1597707 -0.0555021 -0.8757600
26
B3LYP electronic energy -628.04990918220 E_h
C 0.3844269 -2.2889135 -0.0041614
C 1.7699529 -2.0620038 -0.0047367
C 2.3254428 -0.7991516 0.0001316
C 1.4503109 0.3270886 0.0038294
C 0.0450982 0.0970627 0.0071302
C -0.4931086 -1.2235097 0.0025479
C 1.9025541 1.6737919 0.0007802
C 1.0085065 2.7168947 -0.0023872
C -0.3798048 2.4947221 0.0008703
C -0.8452344 1.1972726 0.0061897
N -2.2076466 0.8894215 0.0061437
C -2.6445184 -0.4130129 -0.0018285
N -1.8693831 -1.4391770 0.0179829
N -4.0158273 -0.5722329 -0.0780854
C 3.8183531 -0.6126462 0.0011695
H -0.0123058 -3.2948426 -0.0069232
H 2.4318035 -2.9205036 -0.0086686
H 2.9628103 1.8810263 -0.0016694
H 1.3744832 3.7357609 -0.0069645
H -1.0708532 3.3285749 -0.0008844
H -2.8680914 1.6283238 -0.1680415
H -4.5736718 0.0748601 0.4580090
H -4.2906277 -1.5338141 0.0514359

H 4.3261033 -1.5766354 -0.0007948
H 4.1588844 -0.0591118 0.8808814
H 4.1595885 -0.0552897 -0.8758773
26
RI-MP2 electronic energy -626.923409495434 E_h
C 0.1198532 -2.3360117 -0.0126487
C 1.5063788 -2.1151164 -0.0138501
C 2.0575170 -0.8446596 -0.0096865
C 1.1859349 0.2782112 -0.0066311
C -0.2221923 0.0488133 -0.0001884
C -0.7593499 -1.2672498 -0.0067316
C 1.6447218 1.6188942 -0.0113992
C 0.7504597 2.6703153 -0.0140566
C -0.6374838 2.4473415 -0.0053302
C -1.1094986 1.1486715 0.0009623
N -2.4701019 0.8441942 0.0100721
C -2.9032438 -0.4571014 -0.0142820
N -2.1374182 -1.4944575 0.0059502
N -4.2790118 -0.6002204 -0.1091356
C 3.5445143 -0.6476729 -0.0091314
H -0.2847030 -3.3390139 -0.0161784
H 2.1721380 -2.9701147 -0.0169838
H 2.7064982 1.8210720 -0.0165457
H 1.1193535 3.6873535 -0.0203001
H -1.3297856 3.2798180 -0.0044457
H -3.1290566 1.5709063 -0.2178085
H -4.8024678 0.0106685 0.4995225
H -4.5395849 -1.5668883 0.0159965
H 4.0548540 -1.6086544 -0.0094835
H 3.8705952 -0.0898916 0.8701138
H 3.8710797 -0.0892072 -0.8878002

Compound **28** Imine
26
AM1 heat of formation 0.116295805175 E_h
C -0.408437 -2.307239 -0.010352
C -1.793934 -2.063456 0.015990
C -2.312953 -0.785109 0.019050
C -1.426664 0.333989 0.002500
C -0.032645 0.104142 -0.012933
C 0.482412 -1.236592 -0.036048
C -1.892749 1.677050 -0.001462
C -1.006500 2.726526 -0.018908
C 0.386004 2.513748 -0.023060
C 0.883164 1.212269 -0.009209
N 2.251395 0.951409 0.040052
C 2.787604 -0.370896 0.007248
N 1.859608 -1.437644 -0.131916
N 4.062738 -0.669010 0.091850
C -3.778064 -0.567650 0.040672
H -0.050143 -3.346659 -0.017647
H -2.471670 -2.932301 0.033001
H -2.976676 1.863050 0.007216
H -1.376040 3.763965 -0.027443
H 1.059964 3.381719 -0.031274
H 2.878766 1.712564 -0.075402
H 4.687508 0.104019 0.144837
H 2.212436 -2.362131 -0.012930
H -4.330100 -1.539519 0.057477
H -4.101122 0.003049 -0.866140
H -4.072534 0.018257 0.947483

26
RI-B3LYP electronic energy -628.04668920675 E_h
C -0.4014313 -2.2838771 -0.0000136
C -1.7866182 -2.0400359 -0.0000066
C -2.3251355 -0.7727281 0.0000029
C -1.4337652 0.3428392 0.0000049
C -0.0306627 0.1025255 -0.0000055
C 0.4753470 -1.2225000 -0.0000138
C -1.8727489 1.6914684 0.0000154
C -0.9657799 2.7238015 0.0000140
C 0.4188655 2.4865928 0.0000024
C 0.8813740 1.1870641 -0.0000067
N 2.2423070 0.8910843 -0.0000171
C 2.7894543 -0.3817752 -0.0000022
N 1.8525672 -1.3929440 -0.0000233
N 4.0318528 -0.6826293 0.0000248
C -3.8161055 -0.5686638 0.0000115
H -0.0296740 -3.3006349 -0.0000203
H -2.4548739 -2.8927359 -0.0000081
H -2.9304039 1.9094511 0.0000241
H -1.3193782 3.7468307 0.0000218
H 1.1158263 3.3153105 0.0000012
H 2.8948294 1.6557670 0.0000069
H 4.6297167 0.1363568 0.0000339
H 2.2450000 -2.3196789 -0.0000071
H -4.3344411 -1.5268089 -0.0000103
H -4.1502283 -0.0103304 -0.8785555
H -4.1502235 -0.0103732 0.8786077
26
B3LYP electronic energy -628.04608061837 E_h
C -0.4013616 -2.2838980 -0.0000397
C -1.7865472 -2.0400778 -0.0000123
C -2.3250179 -0.7727675 0.0000152
C -1.4337081 0.3428064 0.0000086
C -0.0306600 0.1025202 -0.0000249
C 0.4753320 -1.2224729 -0.0000431
C -1.8727841 1.6913717 0.0000350
C -0.9657736 2.7236672 0.0000158
C 0.4188893 2.4865847 -0.0000228
C 0.8813247 1.1870521 -0.0000391
N 2.2421983 0.8910925 -0.0000653
C 2.7893232 -0.3817125 0.0000124
N 1.8524919 -1.3928722 -0.0000594
N 4.0317143 -0.6826204 0.0001198
C -3.8159140 -0.5685539 0.0000454
H -0.0294718 -3.3007082 -0.0000569
H -2.4548421 -2.8928672 -0.0000094
H -2.9305404 1.9093110 0.0000667
H -1.3194113 3.7468125 0.0000338
H 1.1159039 3.3153653 -0.0000391
H 2.8947976 1.6558680 0.0000133
H 4.6295011 0.1366126 0.0001500
H 2.2450093 -2.3197122 0.0000154
H -4.3343814 -1.5267355 0.0000210
H -4.1500187 -0.0101034 -0.8785498
H -4.1499932 -0.0101601 0.8786864
26
RI-MP2 electronic energy -626.916649335703 E_h
C -0.0786640 -2.3154679 -0.0001191
C -1.4641154 -2.0767693 -0.0000337
C -1.9989284 -0.8016258 -0.0000177
C -1.1106553 0.3090750 -0.0000547

C	0.2943932	0.0693338	-0.0000547
C	0.8014040	-1.2511708	-0.0000722
C	-1.5549710	1.6531006	-0.0000077
C	-0.6475164	2.6925567	0.0000134
C	0.7370616	2.4521318	-0.0000998
C	1.2043447	1.1512751	-0.0000617
N	2.5641977	0.8581770	-0.0000691
C	3.1106766	-0.4115137	0.0000497
N	2.1767285	-1.4217121	-0.0000922
N	4.3567665	-0.7177115	0.0003216
C	-3.4838728	-0.5876855	0.0000959
H	0.2986640	-3.3302723	-0.0003124
H	-2.1360696	-2.9263301	0.0000561
H	-2.6142767	1.8665131	0.0000086
H	-1.0023876	3.7145199	0.0001863
H	1.4360274	3.2791770	-0.0003386
H	3.2173517	1.6234528	-0.0000603
H	4.9345495	0.1165570	0.0004286
H	2.5722862	-2.3481101	-0.0001412
H	-4.0042382	-1.5432472	0.0001412
H	-3.8044451	-0.0271322	-0.8790916
H	-3.8043110	-0.0271213	0.8793254

Compound **29**

29

AM1 heat of formation -0.120813129364E-01 E_h

C	0.144611	-2.160958	-0.085336
C	-1.180750	-1.713073	-0.088432
C	-1.505751	-0.362551	-0.060373
C	-0.470257	0.618157	-0.021165
C	0.872659	0.166266	-0.021738
C	1.193019	-1.236132	-0.050908
C	-0.709359	2.018688	0.024585
C	0.334512	2.911041	0.068502
C	1.675757	2.480993	0.067139
C	1.951194	1.118542	0.013632
N	3.268314	0.638040	-0.037709
C	3.493335	-0.758117	0.012267
N	2.518471	-1.674064	-0.047369
N	4.840927	-1.178307	0.165776
C	-2.920359	0.025716	-0.078165
O	-3.448830	1.117882	-0.312238
O	-3.775536	-1.016245	0.204245
C	-5.170703	-0.717380	0.190145
H	0.352715	-3.241068	-0.107725
H	-1.990149	-2.464271	-0.112654
H	-1.749018	2.386324	0.019562
H	0.132680	3.993337	0.105901
H	2.480608	3.228091	0.104673
H	4.001944	1.272226	0.182271
H	5.495011	-0.673297	-0.392723
H	4.958586	-2.169164	0.104277
H	-5.651584	-1.694635	0.441611
H	-5.474991	-0.359234	-0.822673
H	-5.402304	0.061764	0.955617

29

RI-B3LYP electronic energy -816.60986397981 E_h

C	-0.1414206	-2.1296409	-0.0038756
C	1.1756481	-1.6813098	-0.0039259
C	1.5191889	-0.3339054	0.0010824
C	0.4705529	0.6501492	0.0023204

C -0.8764636 0.1747371 0.0040256
C -1.1861440 -1.2182475 0.0017087
C 0.6655685 2.0556901 -0.0019796
C -0.4066885 2.9170987 -0.0062882
C -1.7311325 2.4560379 -0.0037757
C -1.9510445 1.0972988 0.0014634
N -3.2395582 0.5546854 -0.0012296
C -3.4442791 -0.7956217 -0.0004222
N -2.4929651 -1.6706860 0.0177002
N -4.7550814 -1.2078573 -0.0655555
C 2.9490910 0.0458528 0.0065386
O 3.3993734 1.1719453 0.0259203
O 3.7727510 -1.0363184 -0.0126468
C 5.1740805 -0.7477776 -0.0067288
H -0.3693372 -3.1861004 -0.0053993
H 1.9703910 -2.4114565 -0.0064256
H 1.6703391 2.4405256 -0.0029166
H -0.2250267 3.9842192 -0.0113147
H -2.5614351 3.1513120 -0.0066305
H -4.0195627 1.1752998 -0.1398367
H -5.4457402 -0.6459914 0.4054156
H -4.8602689 -2.1992883 0.0802293
H 5.6713311 -1.7137849 -0.0236982
H 5.4514604 -0.1932043 0.8890170
H 5.4523451 -0.1617096 -0.8818921
29
B3LYP electronic energy -816.60915921265 E_h
C -0.1414669 -2.1296919 -0.0038923
C 1.1755915 -1.6813772 -0.0039599
C 1.5191298 -0.3339842 0.0010677
C 0.4705243 0.6500713 0.0023360
C -0.8764500 0.1746836 0.0040509
C -1.1861411 -1.2182568 0.0017242
C 0.6656328 2.0555659 -0.0019534
C -0.4066267 2.9169682 -0.0062715
C -1.7311040 2.4560081 -0.0037737
C -1.9509624 1.0972810 0.0015165
N -3.2394359 0.5547083 -0.0011553
C -3.4441781 -0.7955328 -0.0003878
N -2.4929557 -1.6706941 0.0177749
N -4.7550199 -1.2076130 -0.0657970
C 2.9489769 0.0457854 0.0064936
O 3.3992695 1.1718759 0.0257420
O 3.7727028 -1.0363309 -0.0125607
C 5.1739375 -0.7475003 -0.0066704
H -0.3694971 -3.1862190 -0.0054744
H 1.9704589 -2.4115312 -0.0065181
H 1.6705373 2.4402666 -0.0028830
H -0.2249247 3.9842008 -0.0113149
H -2.5614870 3.1513162 -0.0066355
H -4.0195677 1.1753637 -0.1398054
H -5.4454779 -0.6457228 0.4057479
H -4.8601844 -2.1991464 0.0804140
H 5.6714254 -1.7135244 -0.0235602
H 5.4513833 -0.1928192 0.8890908
H 5.4522561 -0.1614750 -0.8819491
29
RI-MP2 electronic energy -815.207780340274 E_h
C -0.2081924 -2.1599875 0.0595908
C 1.1184649 -1.7232852 0.0681995
C 1.4524799 -0.3759154 0.0617499
C 0.4189954 0.6107126 0.0316806

C -0.9314296 0.1418526 0.0150276
C -1.2471893 -1.2447280 0.0351943
C 0.6327762 2.0109219 -0.0127598
C -0.4339162 2.8856543 -0.0625454
C -1.7611777 2.4295439 -0.0666516
C -1.9980053 1.0711783 -0.0287458
N -3.2876929 0.5388534 -0.0387158
C -3.4966270 -0.8102188 -0.0175621
N -2.5614654 -1.7007406 0.0436415
N -4.8194939 -1.1981562 -0.1160473
C 2.8825734 0.0080231 0.1166777
O 3.3240879 1.0969112 0.4274543
O 3.6926566 -1.0238504 -0.2208461
C 5.0880971 -0.7133162 -0.1326064
H -0.4473637 -3.2141567 0.0775000
H 1.9151960 -2.4519265 0.0907528
H 1.6422583 2.3863488 0.0021825
H -0.2436421 3.9499474 -0.0976807
H -2.5877508 3.1281545 -0.1006214
H -4.0578142 1.1446159 -0.2719375
H -5.4657879 -0.6509585 0.4308019
H -4.9157232 -2.1879535 0.0516042
H 5.6036711 -1.6242538 -0.4131872
H 5.3504962 -0.4190023 0.8800015
H 5.3415190 0.0957317 -0.8121518

Compound **29** Imine

29
AM1 heat of formation -0.392379762309E-02 E_h
C 0.145407 -2.162112 -0.074215
C -1.178770 -1.706425 -0.083361
C -1.492707 -0.355943 -0.063243
C -0.448938 0.619331 -0.022450
C 0.893764 0.166277 -0.006769
C 1.194599 -1.238711 -0.036452
C -0.686054 2.018817 0.010482
C 0.360465 2.909771 0.053720
C 1.698699 2.476626 0.067856
C 1.976224 1.111231 0.038510
N 3.285814 0.635537 0.056086
C 3.609766 -0.750382 0.016780
N 2.516080 -1.656825 -0.028621
N 4.821599 -1.251406 0.022021
C -2.905007 0.041505 -0.089690
O -3.426477 1.130010 -0.352477
O -3.764961 -0.988415 0.220311
C -5.158910 -0.682874 0.199650
H 0.339942 -3.244007 -0.096172
H -1.990921 -2.454791 -0.107640
H -1.724429 2.389491 -0.006055
H 0.159775 3.992907 0.077293
H 2.505132 3.222582 0.101894
H 4.028912 1.293878 0.070761
H 5.566485 -0.592002 0.053399
H 2.722862 -2.631123 -0.047315
H -5.644265 -1.650807 0.477218
H -5.462191 -0.349962 -0.822033
H -5.385469 0.117278 0.944673
29
RI-B3LYP electronic energy -816.60500506100 E_h
C -0.1356490 -2.1299735 0.0001107

C 1.1805302 -1.6714554 0.0000994
C 1.5118603 -0.3246548 0.0000782
C 0.4552006 0.6520727 0.0000222
C -0.8904744 0.1743372 0.0000007
C -1.1730048 -1.2164369 0.0000659
C 0.6457629 2.0565391 -0.0000644
C -0.4328179 2.9097088 -0.0001612
C -1.7541515 2.4412156 -0.0001693
C -1.9797307 1.0824732 -0.0000888
N -3.2720288 0.5587602 -0.0001002
C -3.5941550 -0.7840913 -0.0000043
N -2.4903561 -1.6183174 0.0000835
N -4.7590776 -1.3062499 0.0000072
C 2.9426607 0.0633011 0.0001916
O 3.3853139 1.1912238 0.0008648
O 3.7684893 -1.0152273 -0.0005358
C 5.1703416 -0.7226846 -0.0003220
H -0.3427547 -3.1921491 0.0001621
H 1.9780607 -2.3980749 0.0001369
H 1.6484058 2.4461423 -0.0000249
H -0.2590058 3.9781007 -0.0002285
H -2.5852575 3.1353664 -0.0002400
H -4.0430026 1.2041230 -0.0001634
H -5.4985176 -0.6124186 -0.0000627
H -2.7167626 -2.5996048 0.0001371
H 5.6696587 -1.6875590 -0.0009672
H 5.4453649 -0.1522745 0.8858942
H 5.4453845 -0.1510809 -0.8857614
29
B3LYP electronic energy -816.60431775244 E_h
C -0.1357118 -2.1300269 -0.0002326
C 1.1804576 -1.6715220 -0.0001998
C 1.5117848 -0.3247312 -0.0001419
C 0.4551722 0.6520171 -0.0000548
C -0.8904622 0.1743213 -0.0000238
C -1.1729925 -1.2164160 -0.0001432
C 0.6458456 2.0564325 0.0000861
C -0.4327568 2.9095759 0.0002538
C -1.7541242 2.4412029 0.0002746
C -1.9796568 1.0824714 0.0001348
N -3.2719093 0.5588050 0.0001608
C -3.5940367 -0.7839834 -0.0000092
N -2.4902905 -1.6182195 -0.0001727
N -4.7589411 -1.3061893 -0.0000281
C 2.9425271 0.0632225 -0.0002576
O 3.3851971 1.1911400 -0.0011904
O 3.7684165 -1.0152561 0.0008049
C 5.1701724 -0.7224383 0.0005634
H -0.3429690 -3.1922625 -0.0003262
H 1.9781183 -2.3981490 -0.0002586
H 1.6486198 2.4459153 0.0000225
H -0.2589174 3.9780850 0.0003649
H -2.5852856 3.1354093 0.0004001
H -4.0429635 1.2042574 0.0002852
H -5.4983496 -0.6120977 0.0000988
H -2.7167665 -2.5996241 -0.0002733
H 5.6697252 -1.6873297 0.0015500
H 5.4452426 -0.1505145 0.8858930
H 5.4453115 -0.1522882 -0.8858901
29
RI-MP2 electronic energy -815.200672670351 E_h
C -0.2586427 -2.1533802 0.0733910

C	1.0658980	-1.7062100	0.0843719
C	1.3896225	-0.3587021	0.0735447
C	0.3475949	0.6192507	0.0404674
C	-1.0002485	0.1491688	0.0170035
C	-1.2920445	-1.2364348	0.0427336
C	0.5567906	2.0193713	-0.0006395
C	-0.5156878	2.8858379	-0.0497027
C	-1.8394819	2.4203185	-0.0622565
C	-2.0806035	1.0618732	-0.0283347
N	-3.3757906	0.5492530	-0.0444419
C	-3.7069330	-0.7883896	-0.0123604
N	-2.6141820	-1.6288170	0.0332115
N	-4.8796786	-1.3065706	-0.0212474
C	2.8188007	0.0331556	0.1286832
O	3.2537522	1.1213702	0.4486959
O	3.6313056	-0.9919611	-0.2191884
C	5.0267054	-0.6776195	-0.1299480
H	-0.4750107	-3.2136663	0.0937129
H	1.8649973	-2.4317881	0.1097840
H	1.5643733	2.3990926	0.0198321
H	-0.3343824	3.9517823	-0.0802918
H	-2.6671982	3.1176065	-0.0980586
H	-4.1431197	1.1992061	-0.0798685
H	-5.5951910	-0.5876126	-0.0548223
H	-2.8506206	-2.6083507	0.0529239
H	5.5445709	-1.5844486	-0.4190527
H	5.2886350	-0.3912764	0.8849364
H	5.2757691	0.1379409	-0.8030787

Compound **30**

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AM1 heat of formation -0.230706870107E-01 E_h

C	0.230485	-1.935022	-0.197534
C	-1.016016	-1.285666	-0.291097
C	-1.128372	0.087261	-0.267415
C	0.050757	0.892798	-0.161117
C	1.308131	0.254732	-0.064903
C	1.393604	-1.181258	-0.090313
C	0.021629	2.311262	-0.154191
C	1.185623	3.038581	-0.039163
C	2.438848	2.412919	0.075059
C	2.520353	1.019988	0.063788
N	3.762362	0.381629	0.174174
C	3.796170	-0.951847	0.175610
N	2.661053	-1.776428	-0.044082
N	5.022066	-1.630134	0.435124
C	-2.440345	0.783706	-0.356301
C	-3.634480	-0.118286	-0.275308
O	-3.992056	-1.028005	-1.026427
O	-4.444764	0.185891	0.786585
C	-5.633103	-0.590827	0.935307
H	0.258792	-3.033607	-0.216811
H	-1.914560	-1.918775	-0.393733
H	-0.941880	2.832690	-0.247370
H	1.146167	4.139495	-0.034712
H	3.346409	3.026720	0.172330
H	2.708535	-2.748754	0.159211
H	5.800681	-1.007752	0.519891
H	5.203789	-2.379271	-0.199548
H	-2.515760	1.545513	0.470122
H	-2.508100	1.327139	-1.340787

H -6.117156 -0.162655 1.847271
H -5.369593 -1.666288 1.078339
H -6.280844 -0.473064 0.033500
32
RI-B3LYP electronic energy -855.90334910337 E_h
C 0.1575646 -1.8788873 -0.2785898
C -1.0676744 -1.1921244 -0.3655503
C -1.1532055 0.1786445 -0.2964355
C 0.0476729 0.9429731 -0.1431580
C 1.2907177 0.2529985 -0.0533212
C 1.3185221 -1.1603396 -0.1214728
C 0.0834230 2.3576723 -0.0781492
C 1.2800237 3.0228497 0.0773556
C 2.4982945 2.3386134 0.1745871
C 2.5208428 0.9561051 0.1088475
N 3.7314851 0.2750571 0.1854744
C 3.7117158 -1.0120859 0.1399234
N 2.5748255 -1.7622929 -0.0200649
N 4.8788029 -1.7318558 0.2989658
C -2.4777748 0.9150015 -0.3931981
C -3.6917542 0.0176794 -0.3262168
O -4.1770189 -0.5703487 -1.2599872
O -4.1833822 -0.0542989 0.9280374
C -5.3313798 -0.8981371 1.1063832
H 0.1783347 -2.9597852 -0.3377054
H -1.9653313 -1.7787127 -0.5075092
H -0.8313770 2.9264351 -0.1552683
H 1.2809178 4.1047130 0.1243756
H 3.4314136 2.8707316 0.2961052
H 2.6226581 -2.7605143 0.0966522
H 5.6960470 -1.1421961 0.2755884
H 4.9738655 -2.5717923 -0.2502604
H -2.5483682 1.6473772 0.4116713
H -2.5328456 1.4563501 -1.3414185
H -5.5854144 -0.8277583 2.1598016
H -5.0955393 -1.9270131 0.8383484
H -6.1588771 -0.5527930 0.4885576
32
B3LYP electronic energy -855.90257917724 E_h
C 0.1569046 -1.8785574 -0.2776379
C -1.0681594 -1.1914171 -0.3640309
C -1.1532035 0.1793526 -0.2948895
C 0.0479181 0.9433285 -0.1420933
C 1.2907562 0.2530292 -0.0528707
C 1.3180944 -1.1602944 -0.1211006
C 0.0839557 2.3579779 -0.0768973
C 1.2808367 3.0227737 0.0781147
C 2.4990026 2.3382658 0.1746897
C 2.5211033 0.9557723 0.1088027
N 3.7316283 0.2744317 0.1847828
C 3.7113641 -1.0127020 0.1392120
N 2.5742427 -1.7625502 -0.0202875
N 4.8782260 -1.7329257 0.2979335
C -2.4774938 0.9162126 -0.3908409
C -3.6917200 0.0190942 -0.3265963
O -4.1773669 -0.5658276 -1.2620959
O -4.1831076 -0.0567869 0.9275194
C -5.3311309 -0.9010240 1.1032416
H 0.1773969 -2.9595575 -0.3366957
H -1.9661320 -1.7778376 -0.5055214
H -0.8308412 2.9269848 -0.1535279
H 1.2820505 4.1047466 0.1252826

H 3.4324022 2.8701497 0.2958668
H 2.6219616 -2.7609271 0.0962990
H 5.6956961 -1.1433309 0.2737766
H 4.9727563 -2.5726470 -0.2519842
H -2.5483247 1.6467995 0.4157072
H -2.5317747 1.4598295 -1.3378320
H -5.5849233 -0.8342069 2.1570692
H -5.0956061 -1.9291453 0.8316912
H -6.1589142 -0.5535037 0.4868602
32
RI-MP2 electronic energy -854.428922311891 E_h
C 0.2226970 -1.8290444 -0.3305040
C -0.9896274 -1.1244581 -0.4302961
C -1.0415278 0.2557843 -0.3717659
C 0.1668798 0.9934540 -0.2183790
C 1.3989721 0.2813138 -0.1123564
C 1.4009878 -1.1304625 -0.1693989
C 0.2222227 2.4064786 -0.1683253
C 1.4308656 3.0577332 -0.0093424
C 2.6347435 2.3471020 0.1063442
C 2.6356255 0.9622872 0.0553592
N 3.8426037 0.2685156 0.1535780
C 3.7861300 -1.0206077 0.1205438
N 2.6430389 -1.7536724 -0.0575578
N 4.9300783 -1.7760399 0.3163137
C -2.3441709 1.0132708 -0.4856559
C -3.5329514 0.0992535 -0.3940134
O -4.0862165 -0.4337914 -1.3298288
O -3.8981813 -0.0883274 0.8906824
C -4.9862539 -1.0070011 1.0604364
H 0.2294447 -2.9105793 -0.3811228
H -1.9012148 -1.6906295 -0.5722581
H -0.6850696 2.9861173 -0.2624722
H 1.4500610 4.1392095 0.0255059
H 3.5786376 2.8594699 0.2318094
H 2.6734146 -2.7435302 0.1255518
H 5.7491552 -1.1874652 0.2978554
H 5.0197435 -2.5683083 -0.3012512
H -2.4064645 1.7501407 0.3145919
H -2.3936475 1.5328381 -1.4433576
H -5.1639950 -1.0514189 2.1280484
H -4.7171903 -1.9867581 0.6747085
H -5.8687904 -0.6508742 0.5365569

Compound **30** Imine

32
AM1 heat of formation -0.149761366810E-01 E_h
C 0.222268 -1.949115 0.200709
C -1.015804 -1.288916 0.300379
C -1.116348 0.085896 0.262975
C 0.069268 0.877774 0.148232
C 1.319713 0.225598 0.051290
C 1.394123 -1.209453 0.063040
C 0.047022 2.298623 0.135519
C 1.212433 3.019106 0.023258
C 2.464219 2.384474 -0.075117
C 2.531735 0.991547 -0.053000
N 3.755446 0.328100 -0.095849
C 3.854223 -1.085155 -0.182887
N 2.635747 -1.821339 -0.083982
N 5.044581 -1.611774 -0.346260

C -2.422444 0.793654 0.350184
C -3.624482 -0.098869 0.279553
O -3.982471 -1.005600 1.034054
O -4.441207 0.212225 -0.775067
C -5.637837 -0.554042 -0.913015
H 0.240756 -3.047947 0.230808
H -1.919625 -1.912239 0.418351
H -0.914956 2.824121 0.220770
H 1.182417 4.120247 0.010611
H 3.372164 2.998061 -0.161269
H 4.584107 0.856446 -0.258002
H 5.081210 -2.606034 -0.374036
H 2.690142 -2.808266 0.012755
H -2.483675 1.345278 1.330556
H -2.494667 1.549341 -0.482135
H -6.126143 -0.121374 -1.820589
H -6.276232 -0.430528 -0.005344
H -5.385014 -1.631734 -1.058459
32
RI-B3LYP electronic energy -855.89910529477 E_h
C -0.1620910 -1.8849992 -0.2834763
C 1.0595318 -1.1956816 -0.3820030
C 1.1449606 0.1756300 -0.3124804
C -0.0569956 0.9327412 -0.1510165
C -1.2944845 0.2352252 -0.0502212
C -1.3306808 -1.1796012 -0.1152893
C -0.0943209 2.3489952 -0.0927204
C -1.2883940 3.0128132 0.0625218
C -2.5068525 2.3255879 0.1691028
C -2.5115530 0.9461962 0.1123896
N -3.6827661 0.2125453 0.2080417
C -3.7834603 -1.1631974 0.1536807
N -2.5694411 -1.8074982 -0.0089164
N -4.9363893 -1.7047420 0.2533927
C 2.4687889 0.9123541 -0.4231182
C 3.6830062 0.0168163 -0.3270896
O 4.1653878 -0.6023002 -1.2419172
O 4.1751780 -0.0127533 0.9277293
C 5.3235159 -0.8508673 1.1342487
H -0.1764323 -2.9659444 -0.3431480
H 1.9566749 -1.7806533 -0.5329521
H 0.8193076 2.9180152 -0.1753155
H -1.2950775 4.0943811 0.1035089
H -3.4344929 2.8696574 0.2919707
H -4.5638346 0.6852719 0.3235596
H -4.8969247 -2.7166081 0.2010329
H -2.5994181 -2.8111737 -0.0575928
H 2.5281668 1.4276651 -1.3853714
H 2.5369786 1.6647548 0.3625979
H 5.5781247 -0.7442088 2.1843785
H 6.1502679 -0.5269318 0.5041245
H 5.0864830 -1.8880092 0.9019107
32
B3LYP electronic energy -855.89834987987 E_h
C -0.1614726 -1.8847459 -0.2813050
C 1.0600008 -1.1950343 -0.3788666
C 1.1448565 0.1762966 -0.3096500
C -0.0574505 0.9330348 -0.1494343
C -1.2947431 0.2351852 -0.0496276
C -1.3304020 -1.1796410 -0.1144037
C -0.0951186 2.3492483 -0.0912985
C -1.2895679 3.0126931 0.0627087

C -2.5079752 2.3252098 0.1682279
C -2.5121221 0.9458193 0.1117200
N -3.6831265 0.2118448 0.2064154
C -3.7833178 -1.1639032 0.1522988
N -2.5690151 -1.8078537 -0.0090438
N -4.9361920 -1.7057365 0.2511153
C 2.4683526 0.9136883 -0.4188477
C 3.6829147 0.0182473 -0.3271027
O 4.1643810 -0.5979543 -1.2443531
O 4.1766537 -0.0150100 0.9270088
C 5.3254450 -0.8534096 1.1293461
H -0.1754425 -2.9658027 -0.3406561
H 1.9575363 -1.7798530 -0.5288376
H 0.8185433 2.9185007 -0.1731123
H -1.2966052 4.0943849 0.1035438
H -3.4359900 2.8690291 0.2901361
H -4.5645691 0.6843587 0.3210548
H -4.8961236 -2.7177463 0.1989988
H -2.5986714 -2.8116754 -0.0574915
H 2.5266743 1.4325314 -1.3792973
H 2.5369177 1.6633820 0.3695071
H 5.5814440 -0.7499805 2.1795801
H 6.1514523 -0.5273143 0.4992023
H 5.0884917 -1.8900145 0.8941250
32
RI-MP2 electronic energy -854.421977158719 E_h
C -0.0811682 -1.8470901 -0.2597089
C 1.1272398 -1.1394432 -0.3769821
C 1.1768666 0.2409228 -0.3250857
C -0.0339364 0.9715088 -0.1667521
C -1.2578711 0.2503758 -0.0467356
C -1.2671915 -1.1620094 -0.0924583
C -0.0922361 2.3852608 -0.1284535
C -1.3010000 3.0329508 0.0255456
C -2.5035546 2.3187698 0.1509390
C -2.4852784 0.9364609 0.1138221
N -3.6403386 0.1826366 0.2287703
C -3.7129062 -1.1924869 0.1935164
N -2.4900783 -1.8136084 0.0321946
N -4.8606084 -1.7534330 0.3089927
C 2.4773538 0.9995588 -0.4571119
C 3.6676494 0.0887501 -0.3454029
O 4.2237391 -0.4594993 -1.2705835
O 4.0281984 -0.0748600 0.9431474
C 5.1176251 -0.9885402 1.1340061
H -0.0798318 -2.9290731 -0.3034639
H 2.0385334 -1.7044273 -0.5251779
H 0.8127370 2.9668032 -0.2277378
H -1.3284063 4.1140904 0.0511247
H -3.4424629 2.8435653 0.2725226
H -4.5318989 0.6375896 0.3433011
H -4.7766382 -2.7639131 0.2674218
H -2.5013575 -2.8190864 -0.0035949
H 2.5255836 1.4967988 -1.4264180
H 2.5402080 1.7532794 0.3267941
H 5.2911832 -1.0127664 2.2028791
H 6.0011930 -0.6400602 0.6068836
H 4.8514166 -1.9755444 0.7653690

Compound **31**
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AM1 heat of formation -0.350363104335E-01 E_h
C 0.949338 -2.097141 -0.015964
C -0.355542 -1.573559 -0.010319
C -0.606390 -0.215519 -0.000980
C 0.493099 0.697728 0.000152
C 1.807023 0.179555 -0.016258
C 2.046743 -1.239243 -0.017549
C 0.322629 2.110539 0.016679
C 1.409826 2.949412 0.021769
C 2.727693 2.449127 0.006967
C 2.934715 1.073867 -0.022803
N 4.222856 0.523505 -0.098642
C 4.369724 -0.886290 0.000626
N 3.352065 -1.747906 -0.019399
N 5.703107 -1.367167 0.151549
C -1.983101 0.347707 0.007186
C -3.085684 -0.689943 -0.003017
C -4.430924 -0.033318 0.000564
O -4.720787 1.164393 0.000380
O -5.455454 -0.943164 0.004011
C -6.782278 -0.416404 0.007035
H 1.090939 -3.188235 -0.017331
H -1.186879 -2.296846 -0.011644
H -0.694998 2.528482 0.027244
H 1.266806 4.041271 0.038558
H 3.569509 3.155228 0.014819
H 4.987978 1.113858 0.137256
H 6.348263 -0.952722 -0.488182
H 5.758071 -2.366097 0.149556
H -2.111987 1.017519 -0.888706
H -2.109186 0.997160 0.918299
H -3.016124 -1.339432 -0.916386
H -3.018175 -1.355376 0.898917
H -7.429035 -1.327986 0.009617
H -6.948765 0.201746 -0.907721
H -6.943911 0.203474 0.921494
35
RI-B3LYP electronic energy -895.20515480425 E_h
C -0.9724261 -2.0711869 -0.0044158
C 0.3303314 -1.5447880 -0.0054400
C 0.5961825 -0.1908741 -0.0009000
C -0.5119792 0.7138450 0.0027730
C -1.8310314 0.1783594 0.0065832
C -2.0642071 -1.2289425 0.0024296
C -0.3727800 2.1277355 -0.0005734
C -1.4772183 2.9454256 -0.0034252
C -2.7805418 2.4206537 0.0004553
C -2.9444707 1.0522466 0.0059399
N -4.2045051 0.4494470 0.0064045
C -4.3416958 -0.9169637 -0.0009492
N -3.3574515 -1.7451476 0.0184233
N -5.6426472 -1.3774784 -0.0758779
C 1.9989408 0.3742894 -0.0000459
C 3.1279558 -0.6485720 -0.0013150
C 4.4972644 -0.0067192 0.0012738
O 4.7279870 1.1758055 0.0060010
O 5.4650648 -0.9485132 -0.0022388
C 6.8161557 -0.4623823 0.0000074
H -1.1347525 -3.1401598 -0.0068315
H 1.1504112 -2.2499666 -0.0093988
H 0.6116565 2.5712035 -0.0033728
H -1.3459811 4.0198495 -0.0081816

H -3.6400167 3.0794038 -0.0010309
H -5.0123202 1.0239557 -0.1658128
H -6.3321554 -0.8685224 0.4555086
H -5.6978456 -2.3757307 0.0542930
H 2.1274209 1.0287371 0.8668337
H 2.1275894 1.0309243 -0.8652978
H 3.0759300 -1.3086319 0.8681169
H 3.0774215 -1.3050668 -0.8734865
H 7.4457804 -1.3472471 -0.0033943
H 7.0057020 0.1376654 0.8887899
H 7.0060908 0.1447414 -0.8838682
35
B3LYP electronic energy -895.20434135091 E_h
C 0.9723485 -2.0711933 0.0053545
C -0.3303959 -1.5447838 0.0065117
C -0.5961641 -0.1908745 0.0016282
C 0.5119677 0.7137964 -0.0025264
C 1.8309498 0.1783134 -0.0065473
C 2.0640949 -1.2289553 -0.0020456
C 0.3726776 2.1276403 0.0005528
C 1.4771307 2.9452993 0.0029117
C 2.7804824 2.4206053 -0.0012271
C 2.9443356 1.0522094 -0.0064765
N 4.2043189 0.4494251 -0.0071767
C 4.3415020 -0.9169250 0.0006077
N 3.3573314 -1.7452010 -0.0182790
N 5.6425203 -1.3772681 0.0755796
C -1.9987990 0.3743834 0.0008633
C -3.1277528 -0.6483971 0.0018579
C -4.4970557 -0.0066908 -0.0006014
O -4.7279547 1.1758105 -0.0026407
O -5.4647654 -0.9485534 -0.0002639
C -6.8157998 -0.4624335 -0.0023408
H 1.1347397 -3.1402588 0.0081059
H -1.1505674 -2.2500094 0.0108628
H -0.6118878 2.5710345 0.0035837
H 1.3458850 4.0198405 0.0075027
H 3.6400604 3.0793696 -0.0001548
H 5.0123311 1.0239969 0.1646766
H 6.3316242 -0.8685035 -0.4567944
H 5.6976114 -2.3756737 -0.0547477
H -2.1272150 1.0290653 -0.8658991
H -2.1275215 1.0309635 0.8661856
H -3.0755343 -1.3084738 -0.8675798
H -3.0771923 -1.3050180 0.8740004
H -7.4454992 -1.3473923 -0.0018672
H -7.0047492 0.1400330 -0.8897224
H -7.0066498 0.1423127 0.8830804
35
RI-MP2 electronic energy -893.653422563106 E_h
C -1.1780499 -2.0959575 -0.0114206
C 0.1278236 -1.5781679 -0.0133169
C 0.3887497 -0.2170836 -0.0092464
C -0.7127968 0.6862869 -0.0056871
C -2.0359203 0.1533179 0.0013098
C -2.2710906 -1.2486557 -0.0046860
C -0.5623669 2.0956344 -0.0105472
C -1.6673667 2.9232631 -0.0123421
C -2.9715952 2.4004708 -0.0029640
C -3.1446086 1.0296746 0.0032063
N -4.4044387 0.4326151 0.0122868
C -4.5405360 -0.9315875 -0.0100247

N	-3.5643202	-1.7744275	0.0097918
N	-5.8503517	-1.3752746	-0.1027726
C	1.7829384	0.3484892	-0.0088156
C	2.8910399	-0.6866944	-0.0080318
C	4.2533676	-0.0457540	-0.0049458
O	4.4809180	1.1429617	0.0018399
O	5.2210822	-0.9866447	-0.0103872
C	6.5534143	-0.4552234	-0.0070279
H	-1.3508253	-3.1636381	-0.0147816
H	0.9502701	-2.2805385	-0.0170860
H	0.4262331	2.5318189	-0.0162049
H	-1.5309876	3.9964676	-0.0185310
H	-3.8305426	3.0596428	-0.0014927
H	-5.2078807	0.9969615	-0.2118847
H	-6.4965799	-0.8929351	0.5032734
H	-5.8915859	-2.3752995	0.0244728
H	1.9110385	0.9993141	0.8591280
H	1.9117380	0.9986837	-0.8772110
H	2.8317591	-1.3392173	0.8640892
H	2.8347953	-1.3380345	-0.8811493
H	7.2093086	-1.3173205	-0.0121370
H	6.7185898	0.1481149	0.8811352
H	6.7187776	0.1587372	-0.8878389

Compound **31** Imine

35

AM1 heat of formation -0.269363135511E-01 E_h

C	0.956168	-2.100697	0.028577
C	-0.348967	-1.573540	0.015972
C	-0.593695	-0.216999	0.012170
C	0.511177	0.693394	0.014255
C	1.826611	0.177510	0.016790
C	2.051613	-1.241611	0.039228
C	0.339348	2.104449	0.015861
C	1.427018	2.944677	0.018806
C	2.743156	2.445306	0.011095
C	2.954952	1.067933	0.000246
N	4.237698	0.526380	-0.054708
C	4.486926	-0.878122	-0.022788
N	3.356044	-1.726618	0.114181
N	5.670975	-1.437004	-0.107048
C	-1.968152	0.351926	0.004831
C	-3.074616	-0.681719	-0.002358
C	-4.417224	-0.019489	-0.009902
O	-4.701180	1.179561	-0.005800
O	-5.445198	-0.925004	-0.023040
C	-6.769980	-0.392674	-0.030594
H	1.087844	-3.192297	0.036536
H	-1.180341	-2.296758	0.010430
H	-0.678110	2.522854	0.016877
H	1.282034	4.036609	0.025027
H	3.584752	3.152088	0.008500
H	5.012027	1.141221	0.038202
H	6.444086	-0.812659	-0.163539
H	3.507314	-2.706077	0.010957
H	-2.088282	1.012717	-0.898888
H	-2.098385	1.010869	0.908537
H	-3.003411	-1.338975	-0.909944
H	-3.014484	-1.339652	0.905580
H	-7.420290	-1.301681	-0.040667
H	-6.924156	0.231928	-0.943114

H -6.938593 0.221983 0.886114
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RI-B3LYP electronic energy -895.20113707343 E_h
C -0.9727203 -2.0752662 -0.0000335
C 0.3305035 -1.5435169 -0.0000273
C 0.5902715 -0.1911761 -0.0000070
C -0.5236284 0.7091452 0.0000129
C -1.8429797 0.1753589 0.0000078
C -2.0555977 -1.2273982 -0.0000173
C -0.3856653 2.1207801 0.0000380
C -1.4934202 2.9345069 0.0000588
C -2.7944542 2.4070952 0.0000542
C -2.9667500 1.0386946 0.0000277
N -4.2329770 0.4585908 0.0000200
C -4.4956944 -0.9013882 -0.0000078
N -3.3637755 -1.6884831 -0.0000237
N -5.6445347 -1.4615992 -0.0000189
C 1.9917671 0.3779088 -0.0000078
C 3.1231073 -0.6424141 -0.0000078
C 4.4903317 0.0050978 -0.0000679
O 4.7142107 1.1888338 -0.0003286
O 5.4610736 -0.9323652 0.0001938
C 6.8109933 -0.4412277 0.0001198
H -1.1177830 -3.1480662 -0.0000514
H 1.1502434 -2.2483569 -0.0000394
H 0.5977622 2.5656995 0.0000405
H -1.3659629 4.0093301 0.0000790
H -3.6530077 3.0669340 0.0000706
H -5.0335558 1.0665709 0.0000322
H -6.4041841 -0.7899720 -0.0000060
H -3.5485890 -2.6777895 -0.0000442
H 2.1185371 1.0330083 0.8662138
H 2.1185401 1.0330107 -0.8662256
H 3.0743480 -1.3003320 0.8712357
H 3.0743111 -1.3003524 -0.8712374
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H 6.9980511 0.1631414 0.8863909
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B3LYP electronic energy -895.20033757352 E_h
C -0.9726354 -2.0752792 0.0003692
C 0.3305715 -1.5435137 0.0004982
C 0.5902414 -0.1911722 0.0004496
C -0.5236133 0.7091207 0.0002916
C -1.8429008 0.1753486 0.0001199
C -2.0554706 -1.2273780 0.0001604
C -0.3855385 2.1207080 0.0002827
C -1.4933325 2.9343738 0.0000766
C -2.7943979 2.4070574 -0.0001333
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C -4.4954748 -0.9013397 -0.0003032
N -3.3635926 -1.6884197 -0.0000135
N -5.6442831 -1.4616208 -0.0005317
C 1.9916030 0.3780058 0.0005422
C 3.1228747 -0.6422370 0.0001385
C 4.4900886 0.0051223 -0.0001160
O 4.7141547 1.1888217 -0.0002433
O 5.4607358 -0.9324109 -0.0002257
C 6.8106017 -0.4412963 -0.0005726
H -1.1177828 -3.1481612 0.0004121
H 1.1504189 -2.2483909 0.0006305

H 0.5980120 2.5655733 0.0004443
H -1.3658834 4.0093187 0.0000711
H -3.6530246 3.0669343 -0.0003086
H -5.0334713 1.0666281 -0.0005120
H -6.4039189 -0.7897454 -0.0007255
H -3.5484481 -2.6778506 -0.0000281
H 2.1184328 1.0329480 0.8669229
H 2.1183219 1.0334445 -0.8654700
H 3.0742084 -1.3003841 0.8712632
H 3.0737792 -1.3000889 -0.8711909
H 7.4431663 -1.3241026 -0.0006124
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RI-MP2 electronic energy -893.646538884530 E_h
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C -0.7706057 0.6852263 -0.0002759
C -2.0930192 0.1539227 -0.0001104
C -2.3093136 -1.2440687 -0.0001939
C -0.6232420 2.0934964 -0.0002235
C -1.7316102 2.9157795 0.0000312
C -3.0332228 2.3875620 0.0002104
C -3.2126775 1.0171219 0.0001503
N -4.4793267 0.4419669 0.0003545
C -4.7439554 -0.9144397 0.0002965
N -3.6162409 -1.7029602 -0.0000225
N -5.8960159 -1.4791387 0.0005135
C 1.7300022 0.3574353 -0.0004223
C 2.8399445 -0.6758673 -0.0002489
C 4.2006623 -0.0305250 -0.0001888
O 4.4229353 1.1591254 -0.0008501
O 5.1705641 -0.9681634 0.0006871
C 6.5019137 -0.4330544 0.0007527
H -1.3763627 -3.1678661 -0.0006457
H 0.9038826 -2.2740776 -0.0006327
H 0.3641507 2.5318047 -0.0004042
H -1.6009749 3.9896481 0.0001193
H -3.8920103 3.0471221 0.0003740
H -5.2798026 1.0515112 0.0005512
H -6.6386001 -0.7874847 0.0007392
H -3.8057106 -2.6923441 -0.0000757
H 1.8574229 1.0074074 0.8679479
H 1.8575578 1.0072867 -0.8688600
H 2.7840211 -1.3274311 0.8727999
H 2.7841920 -1.3275042 -0.8732637
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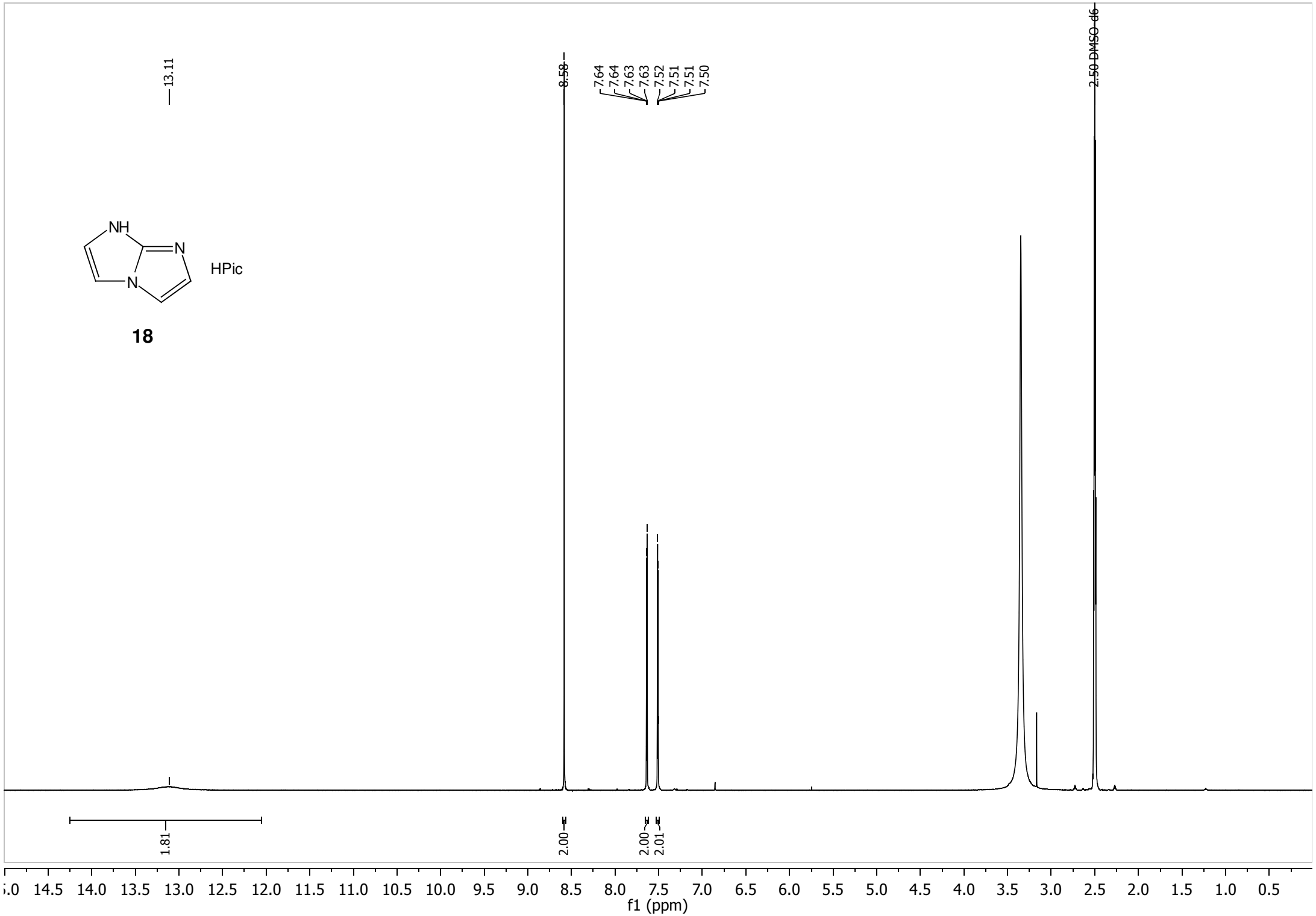
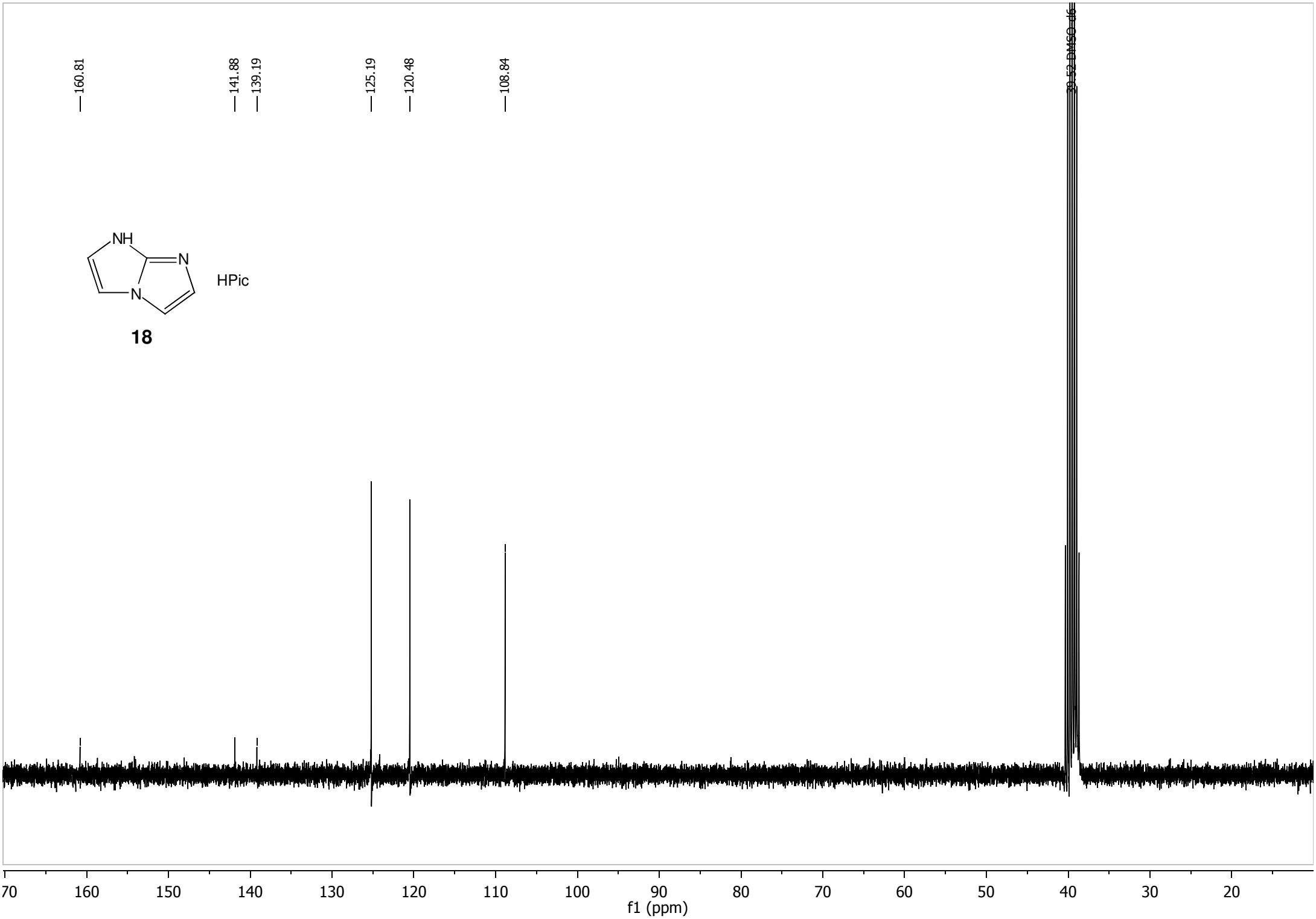

13.11
8.58
7.64
7.64
7.63
7.63
7.52
7.51
7.51
7.50
2.50 DMSO-d6
NH
N
N
HPic
18
1.81
2.00
2.00
2.01
f1 (ppm)


160.81
141.88
139.19
125.19
120.48
108.84
39.52 DMSO-d6
NH
N
N
HPic
18
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

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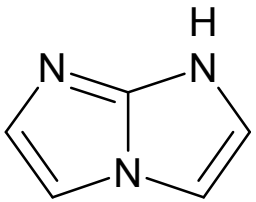
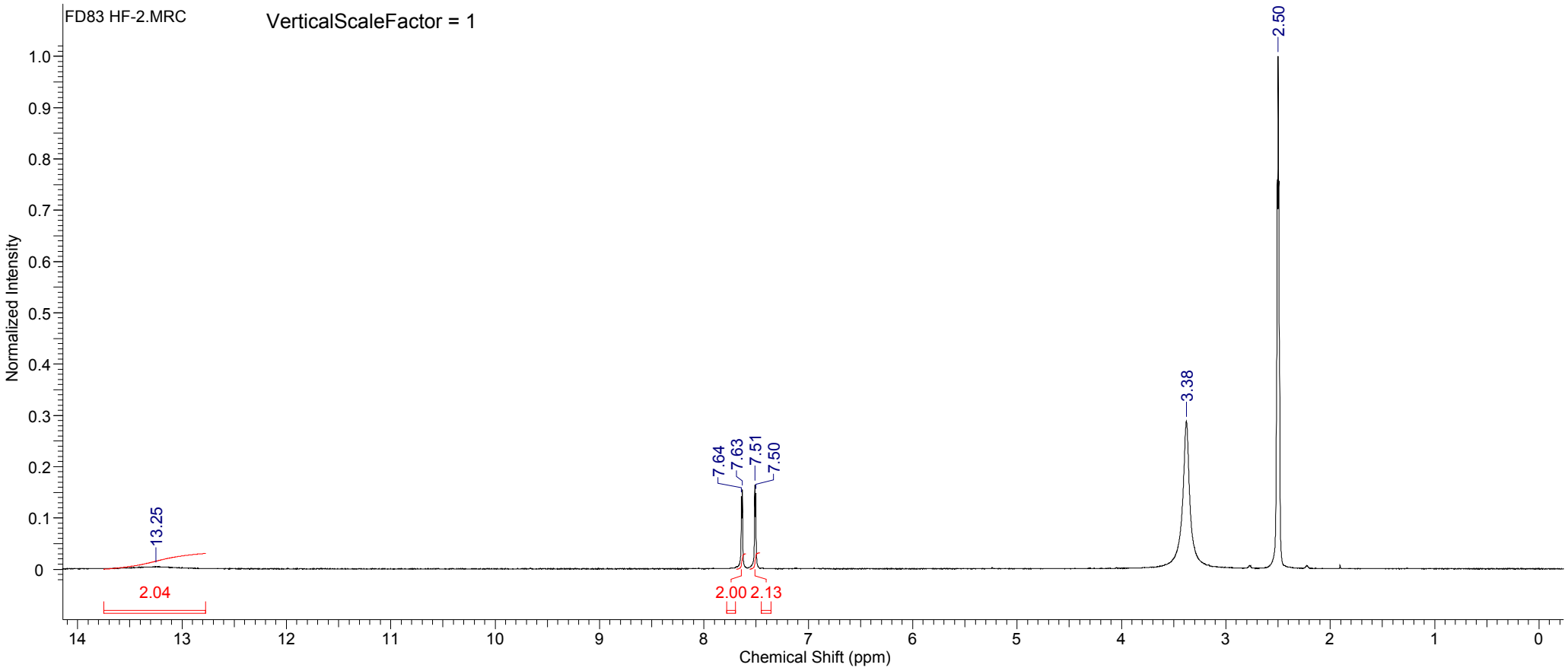
Compound 18

Acquisition Time (sec)	3.1261	***Date***	15 Feb 2012 09:54:40				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD54 - 97\FD83\FD83 HF-2.MRC					***Frequency (MHz)***	250.13
Nucleus	1H	***Origin***	Bruker	***Original Points Count***	32768	***Points Count***	65536
Pulse Sequence	ZG30	***Spectrum Offset (Hz)***	2504.2529	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10482.18



· TFA



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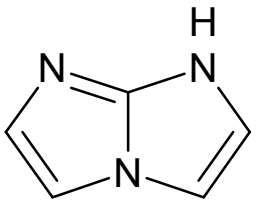
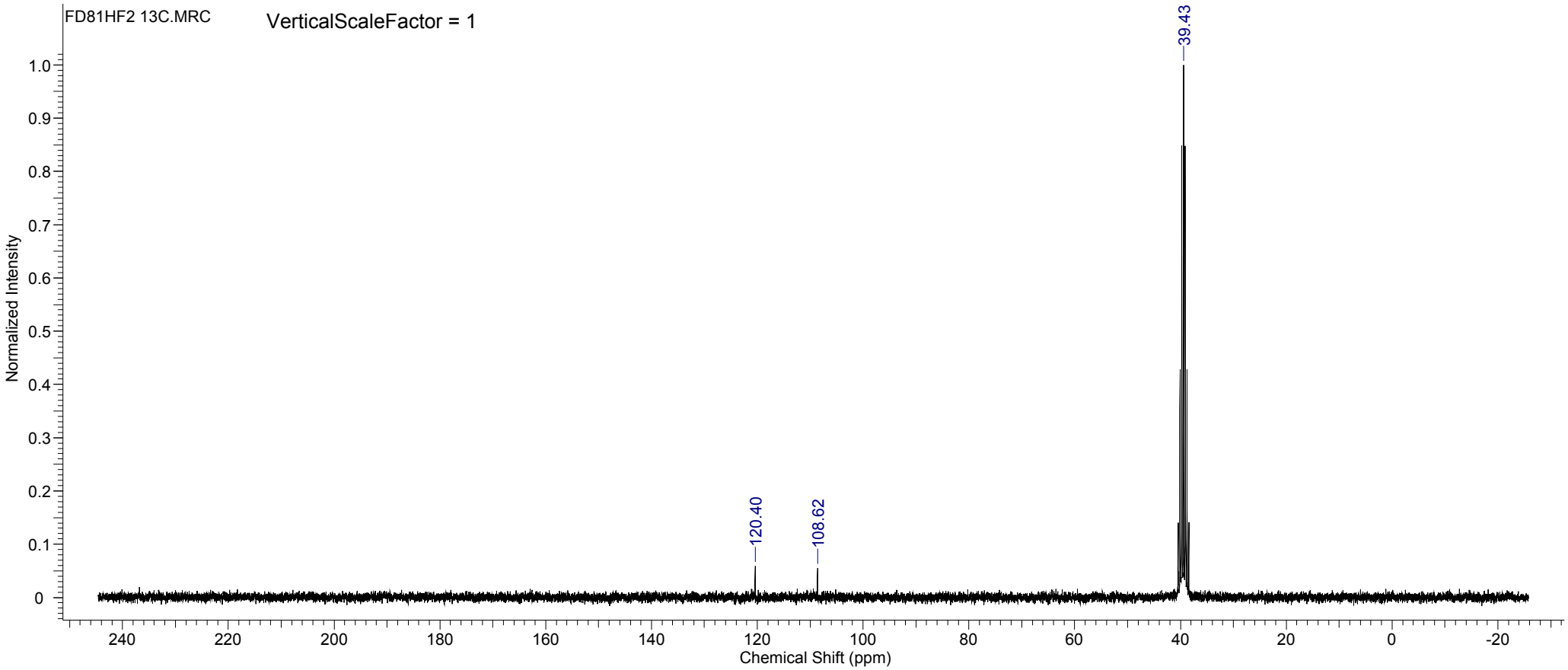
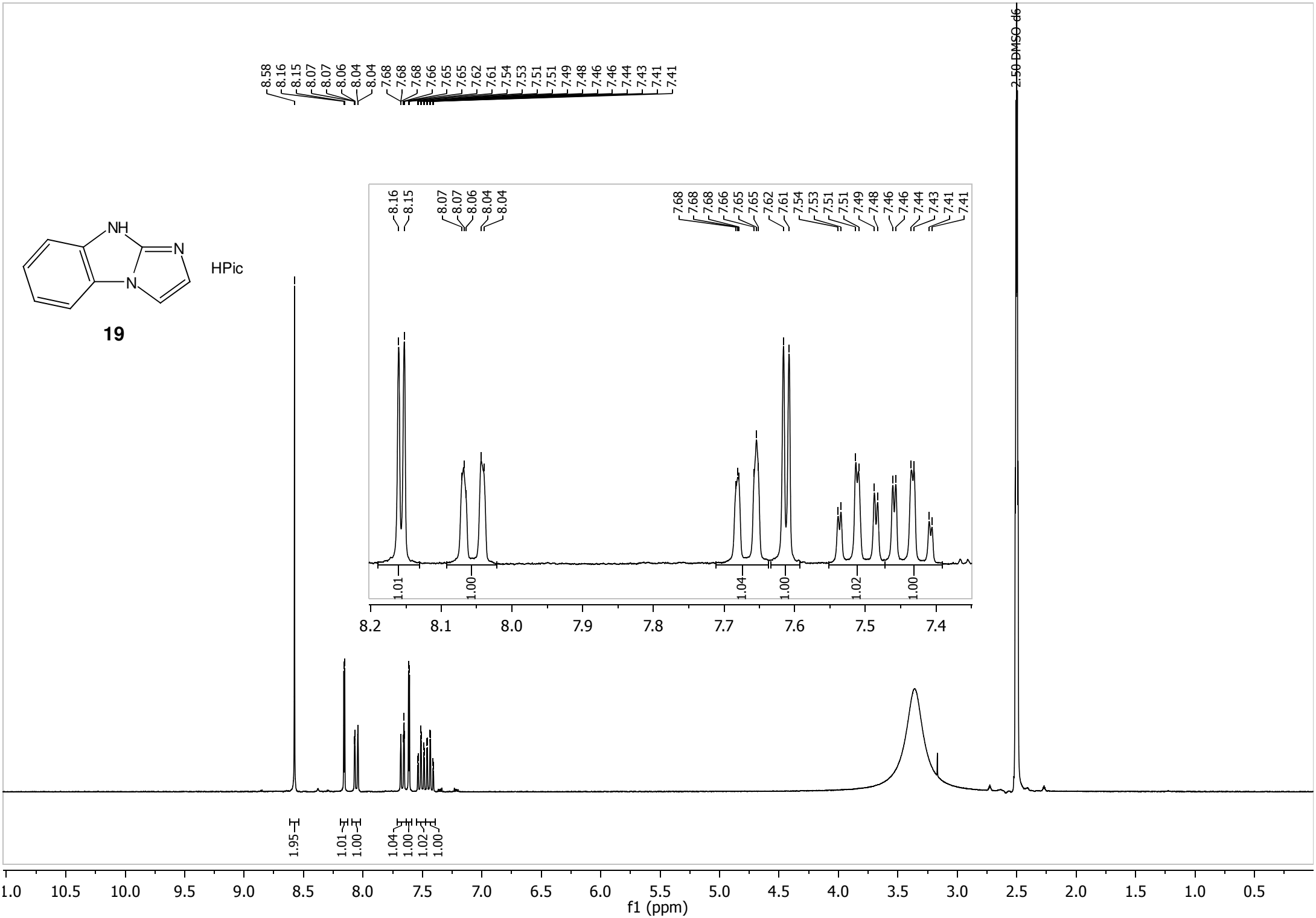
Compound 18

Acquisition Time (sec)	1.4451	***Date***	15 Feb 2012 09:54:38				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD54 - 97\FD83\FD81HF2 13C.MRC					***Frequency (MHz)***	62.90
Nucleus	13C	***Origin***	Bruker	***Original Points Count***	24576	***Points Count***	65536
Pulse Sequence	ZGPG30	***Spectrum Offset (Hz)***	6882.2896	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	17006.80



· TFA

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8.16
8.15
8.07
8.07
8.06
8.04
8.04
7.68
7.68
7.68
7.66
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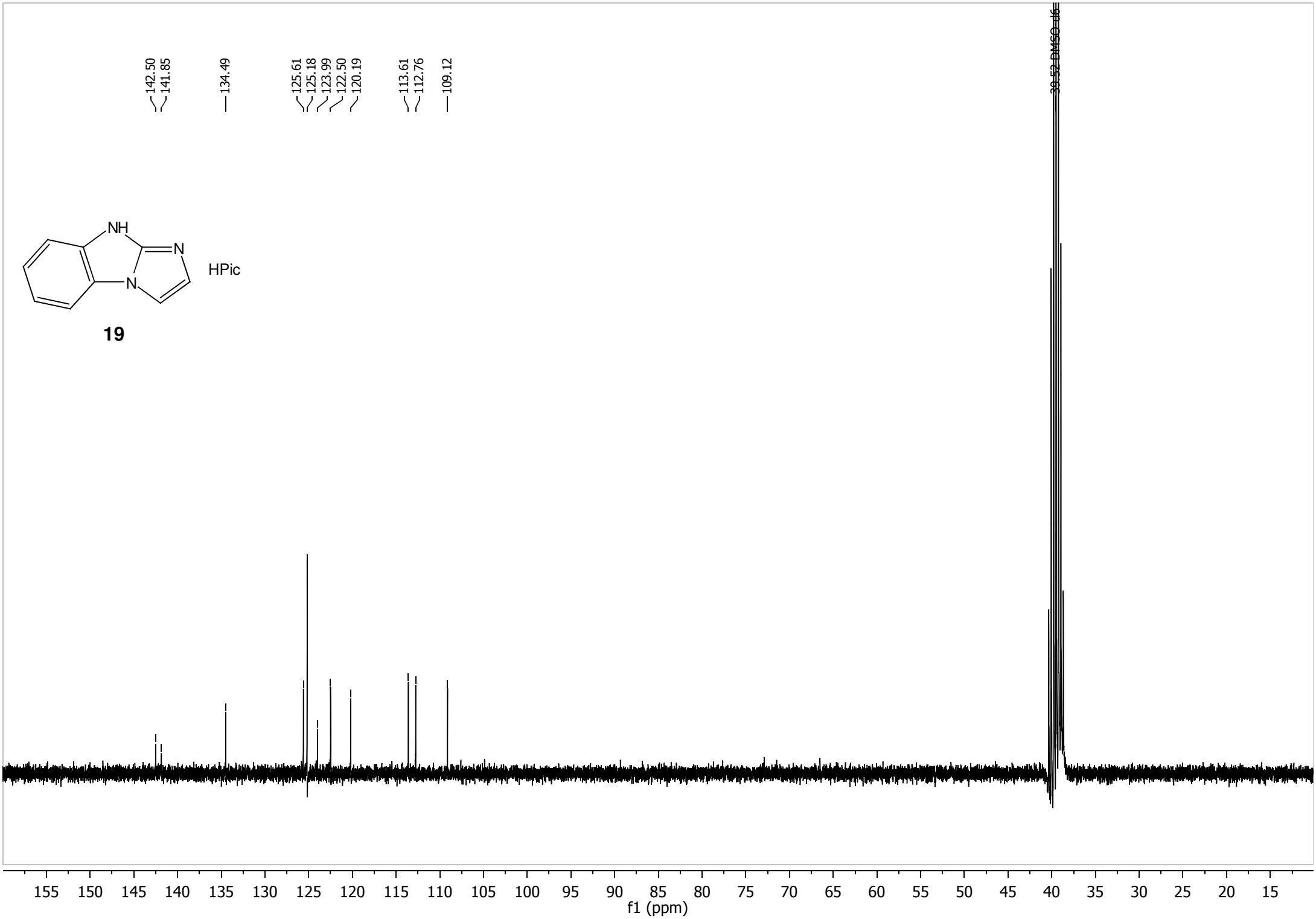
7.65
7.62
7.61
7.54
7.53
7.51
7.51
7.49
7.48
7.46
7.46
7.44
7.43
7.41
7.41
2.50 DMSO-d6
NH
N
N
HPic
19
1.95
1.01
1.00
1.04
1.00
1.02
1.00
f1 (ppm)


142.50
141.85
134.49
125.61
125.18
123.99
122.50
120.19
113.61
112.76
109.12
39.52 DMSO-d6
NH
N
N
HPic
19
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

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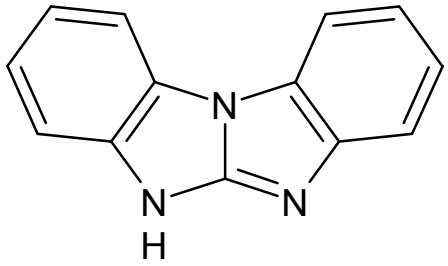
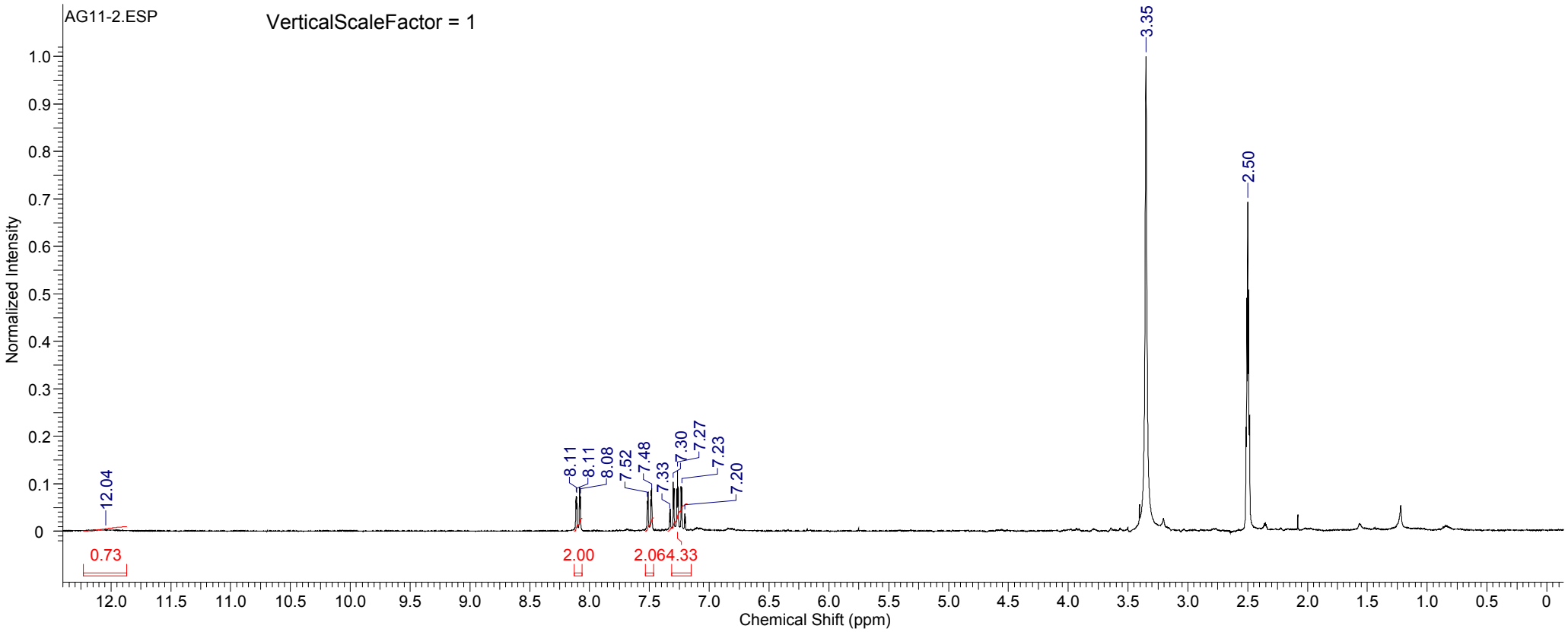
Compound 20

AG11-2

Acquisition Time (sec)	3.9998	***Comment***	AG11-2	***Date***	13 May 2013 17:38:40			***Date Stamp***	13 May 2013 17:38:40
File Name	C:\USERS\RIKE\DESKTOP\ALEX\NMR\AG11-2\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	19959	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	406.40	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1497.8323	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						



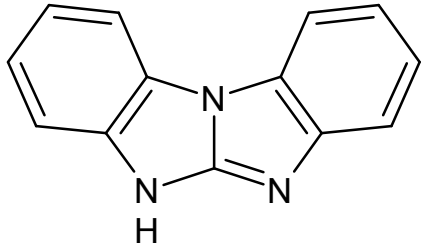


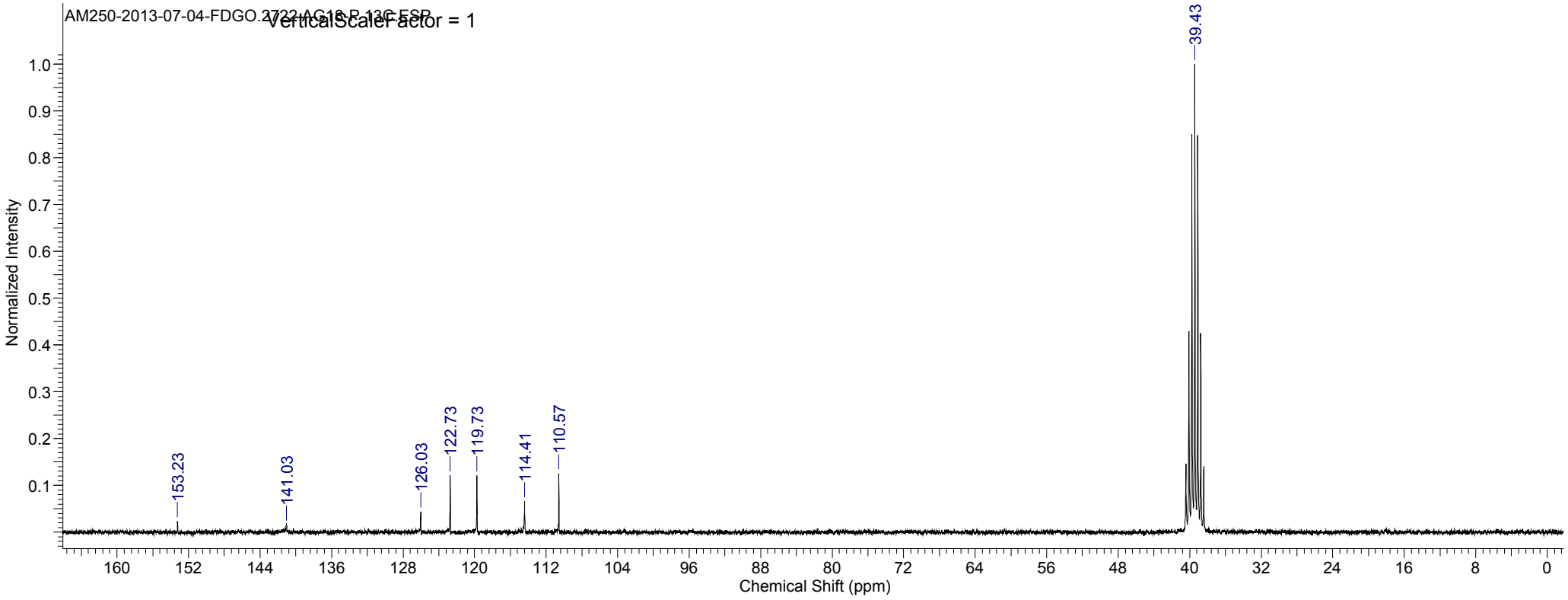
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 20

AG18-P

Acquisition Time (sec)	1.0420	***Comment***	AG18-P	***Date***	05 Jul 2013 01:55:44		
Date Stamp	05 Jul 2013 01:55:44						
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR AK-PRAKTIS\NMR AG01 - 18\AG18\AM250-2013-07-04-FDGO.2722 AG18-P 13C\1\PDATA\1\1R						
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	4096	***Origin***	spect
Original Points Count	16384	***Owner***	service	***Points Count***	131072	***Pulse Sequence***	zgpg30
Receiver Gain	11585.20	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6252.8521
Spectrum Type	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000		

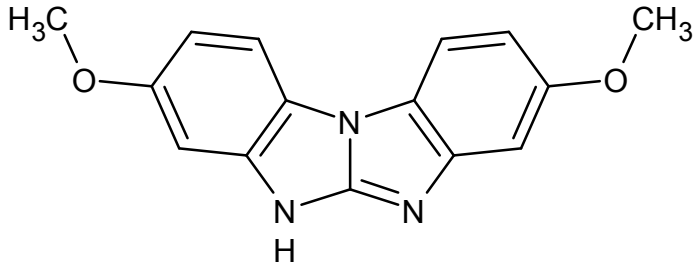


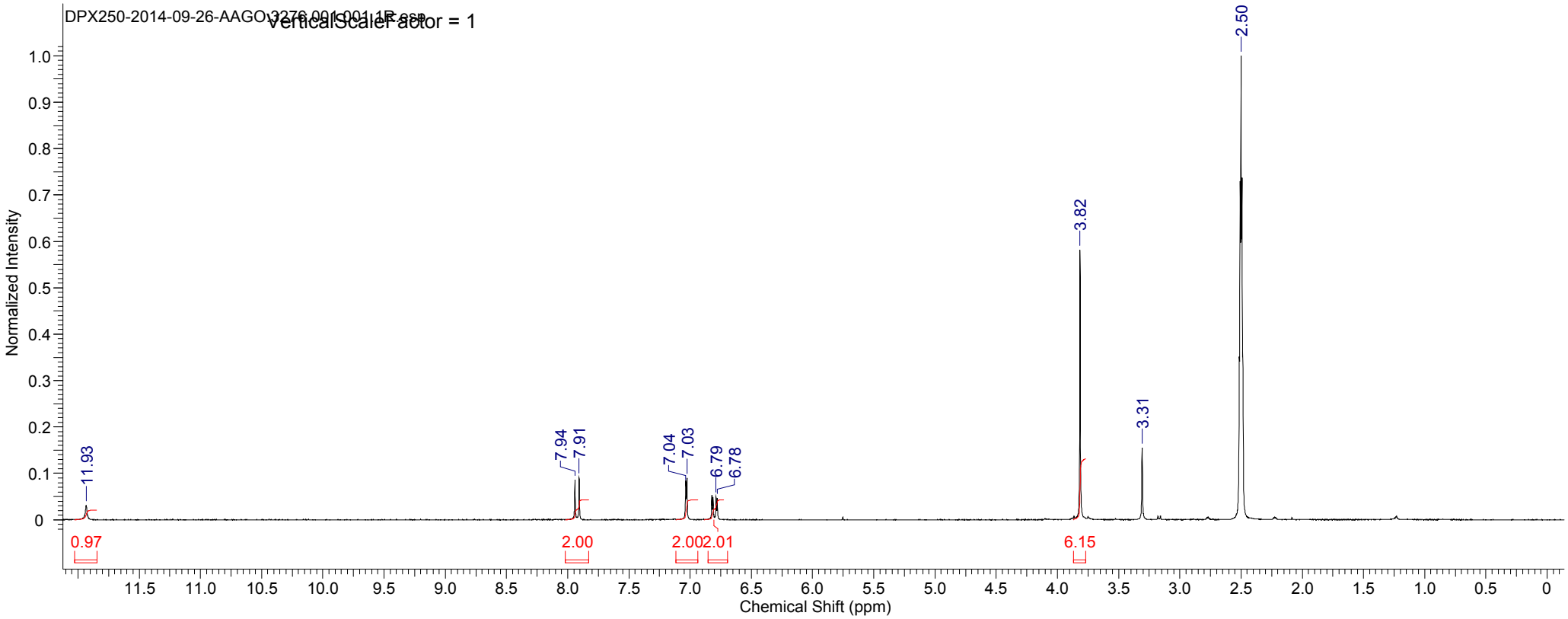


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 21

Acquisition Time (sec)	5.5394	***Comment***	AA7-XX	***Date***	26 Sep 2014 17:02:24		
Date Stamp	26 Sep 2014 17:02:24						
File Name	C:\USERS\RIKE\DATEN RIKE\WRT\AP\SPEKTREN ABDULLAH\ENDPRODUKT\NMR\DPX250-2014-09-26-AAGO.3276\1\PDATA\1\1R						
Frequency (MHz)	250.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Original Points Count	28672	***Owner***	service	***Points Count***	131072	***Pulse Sequence***	zg30_ns
Receiver Gain	912.30	***SW(cyclical) (Hz)***	5175.98	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1541.4249
Spectrum Type	STANDARD	***Sweep Width (Hz)***	5175.94	***Temperature (degree C)***	27.160		

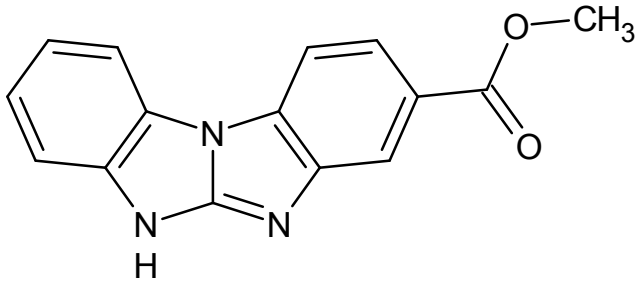


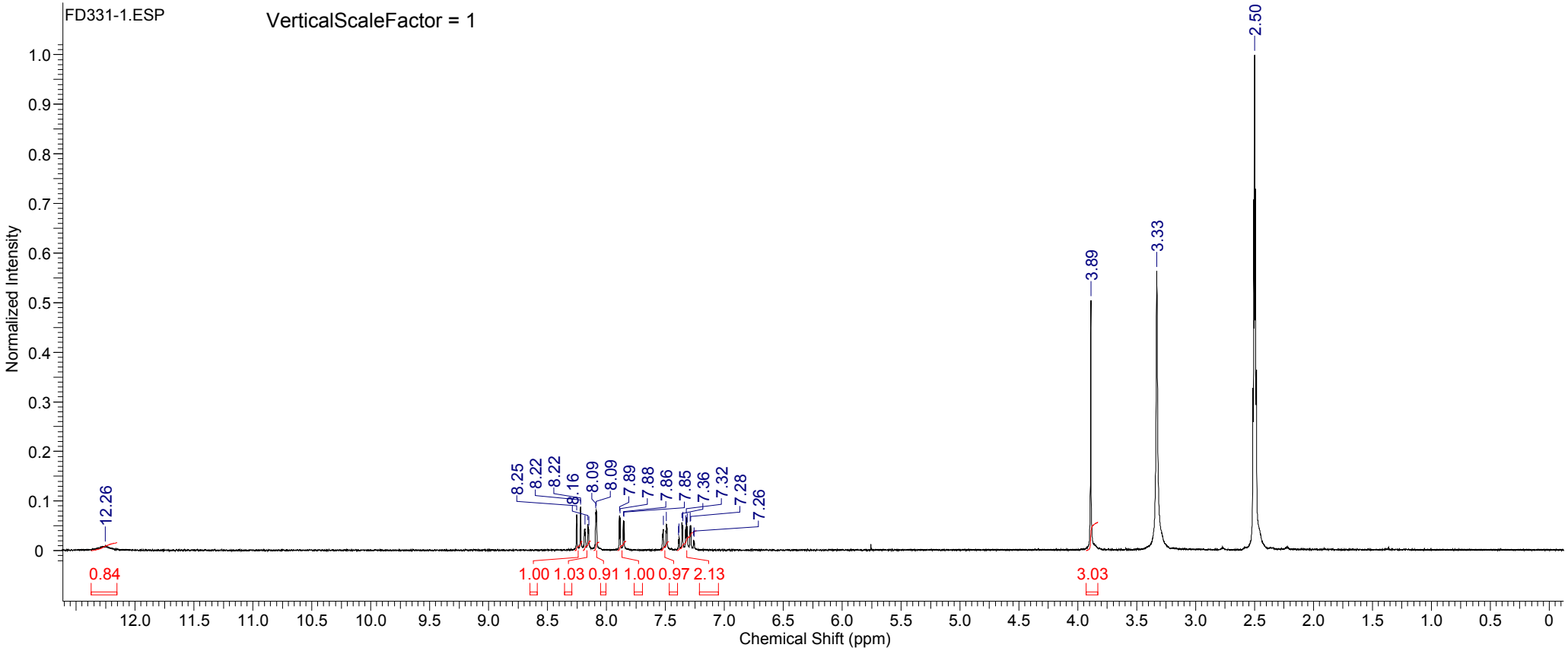


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 22

Acquisition Time (sec)	3.9999	***Comment***	FD331-1	***Date***	14 Aug 2013 23:30:40			***Date Stamp***	14 Aug 2013 23:30:40
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD331-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	17985	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30_ns
Receiver Gain	256.00	***SW(cyclical) (Hz)***	4496.40	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1254.2698	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.27	***Temperature (degree C)***	27.000						





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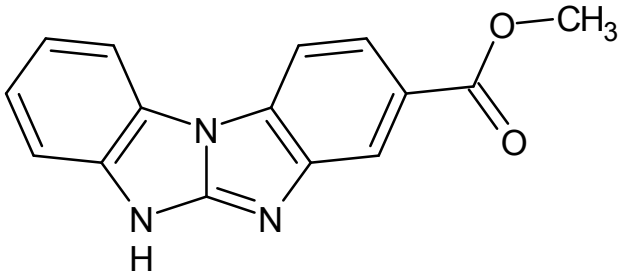
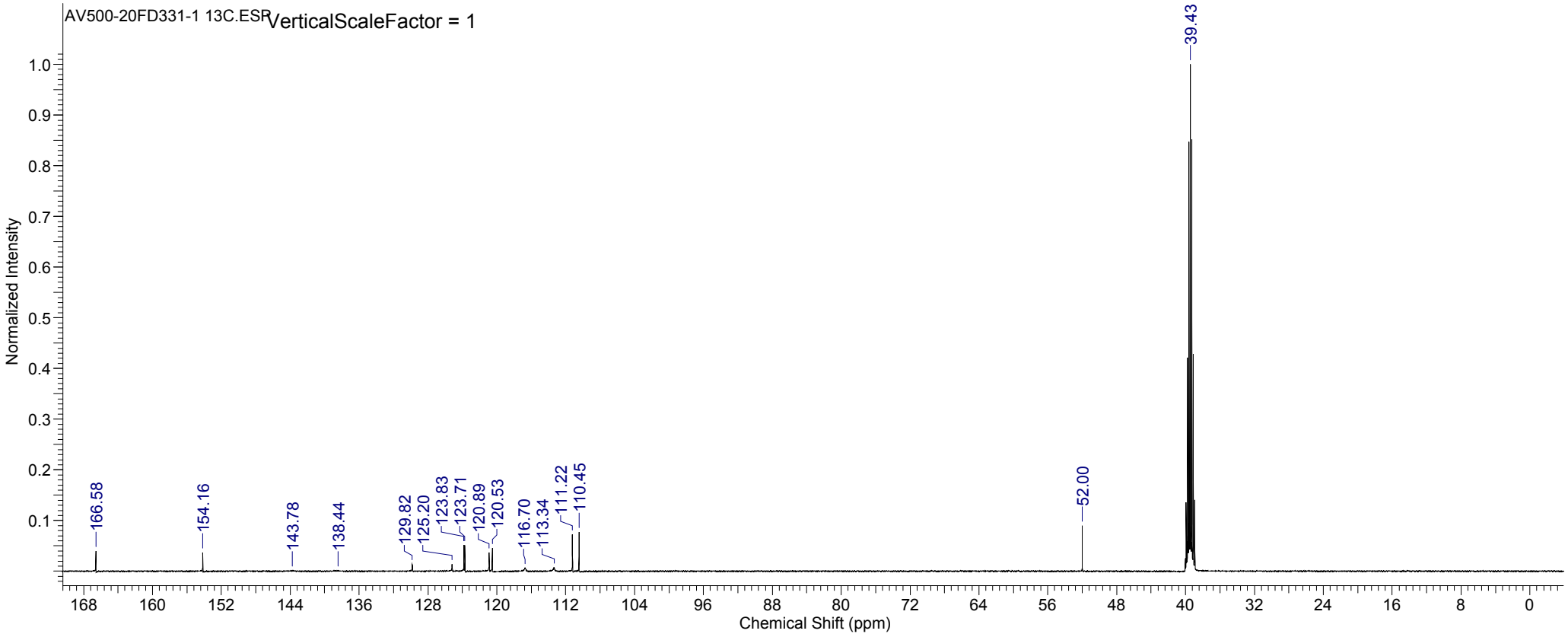
Compound 22

Acquisition Time (sec)	1.0457	***Comment***	FD331-1	***Date***	20 Aug 2013 13:16:16		
Date Stamp	20 Aug 2013 13:16:16			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\AV500-2013-08-20-FDGO.1048 FD331-1 13C\1\PDATA\1\1R		
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	2048	***Origin***	spect
Original Points Count	32678	***Owner***	service	***Points Count***	65536	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	12431.8789
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.52	***Temperature (degree C)***	25.002		

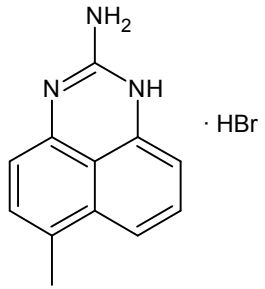


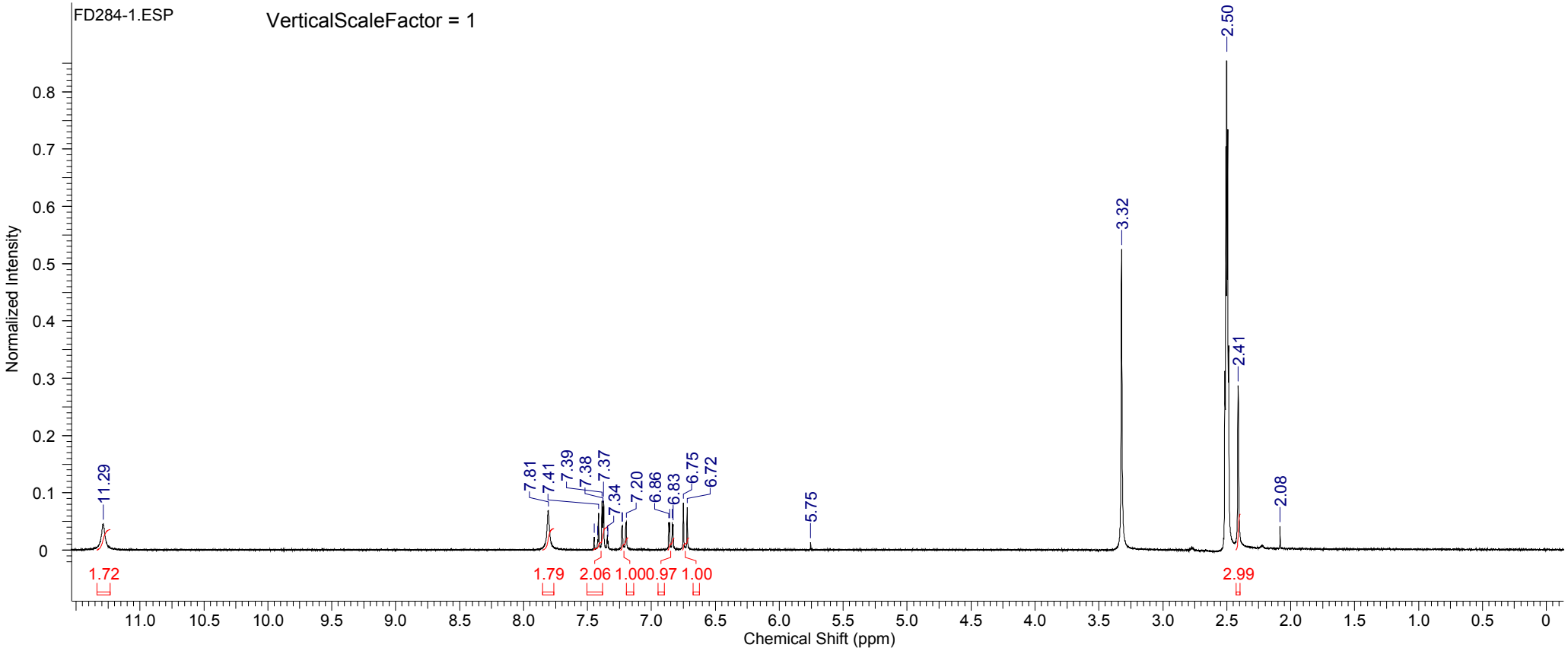


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 28

Acquisition Time (sec)	5.1302	***Comment***	FD284-1	***Date***	28 Sep 2012 15:47:44			***Date Stamp***	28 Sep 2012 15:47:44
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD284-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	25600	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	812.70	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4247	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						

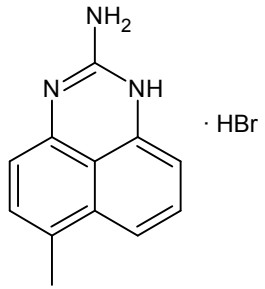


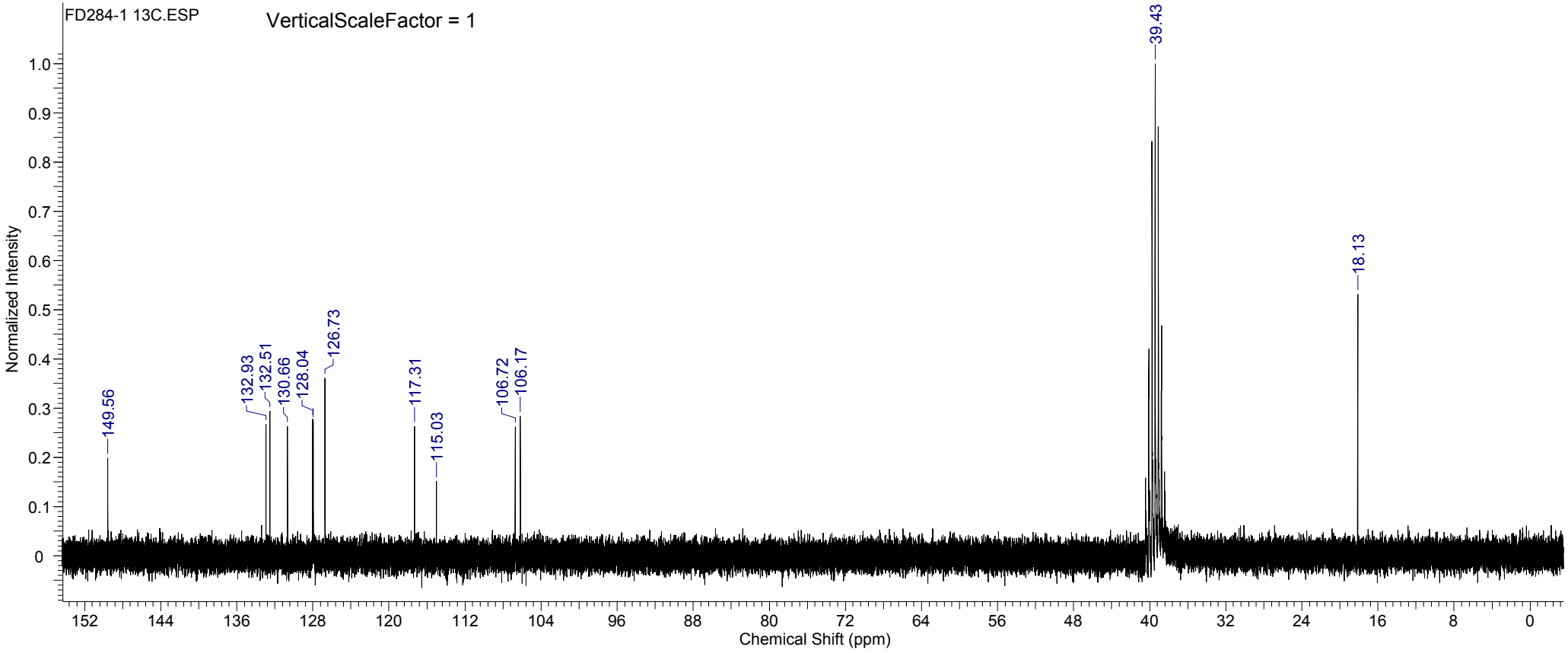


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 28

Acquisition Time (sec)	4.5588	***Comment***	FD284-1	***Date***	30 Sep 2012 23:41:20				
Date Stamp	30 Sep 2012 23:41:20			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD284-1 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1520	***Origin***	spect	***Original Points Count***	71680
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6564.2656	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000

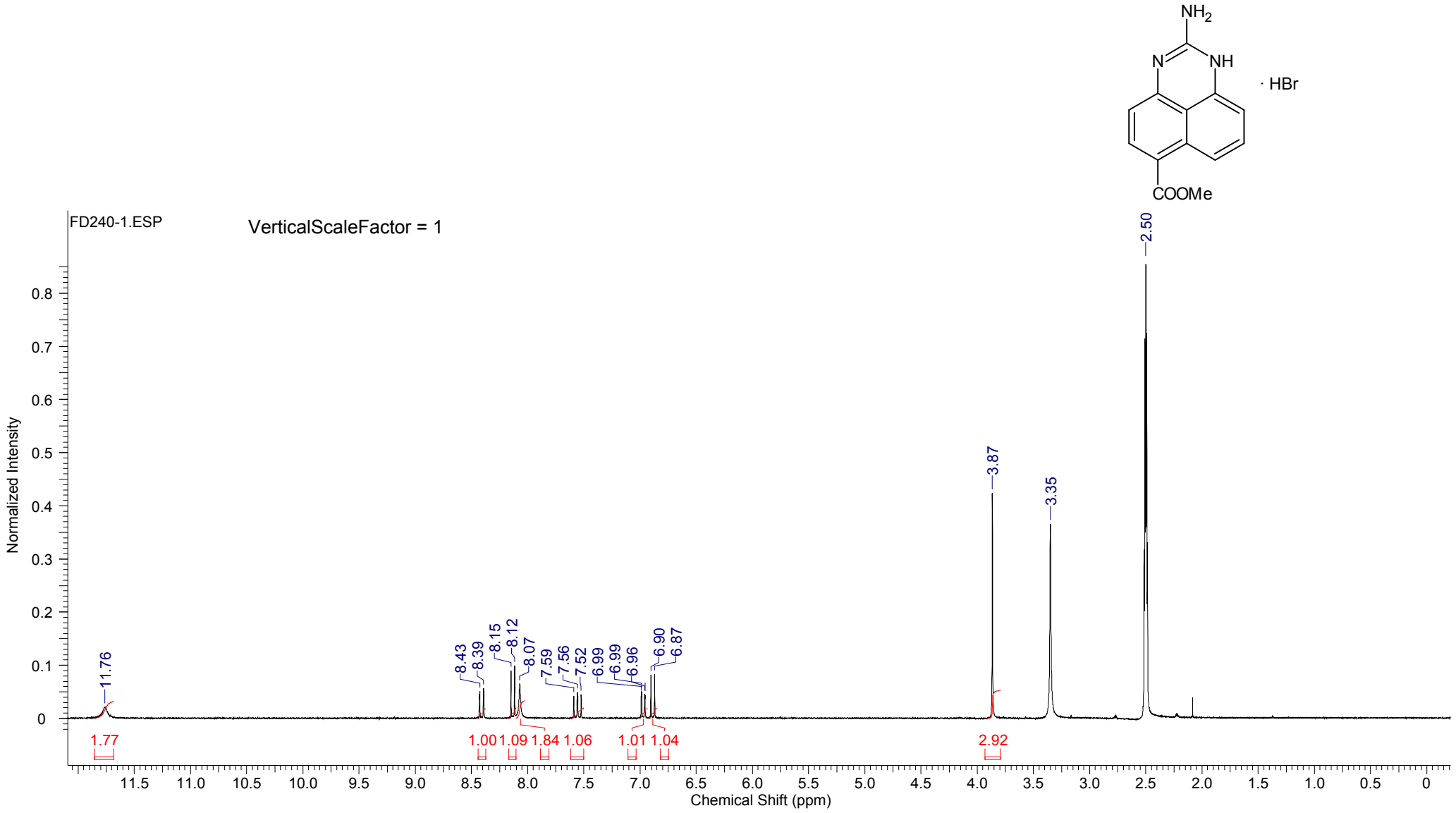




This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 29

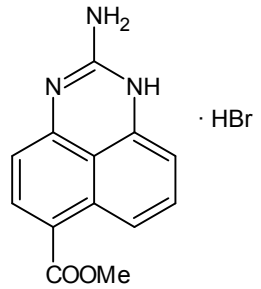
Acquisition Time (sec)	6.1563	***Comment***	FD240-1	***Date***	21 Mar 2012 12:58:56			***Date Stamp***	21 Mar 2012 12:58:56
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD240-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	30720	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zgvar
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1754.1251	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						

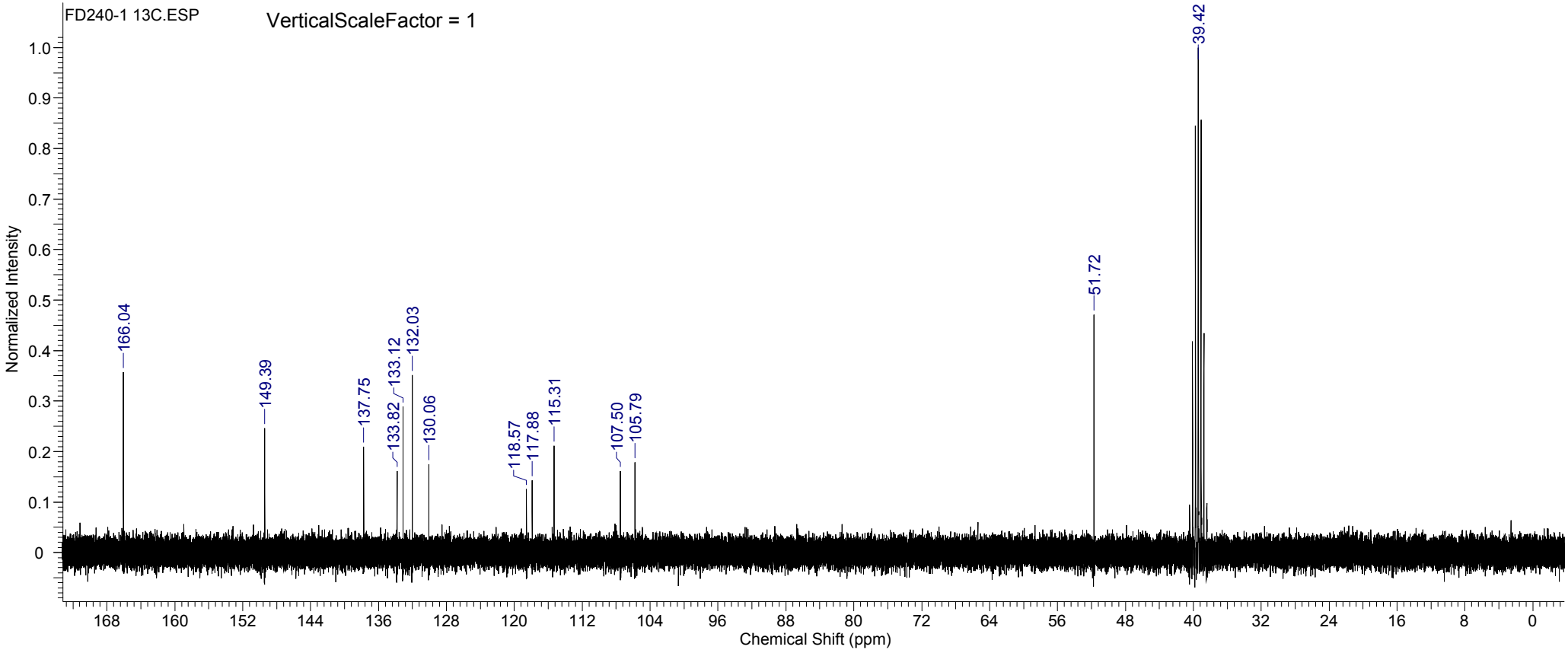


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 29

Acquisition Time (sec)	4.4286	***Comment***	FD240-1	***Date***	24 Mar 2012 12:41:52				
Date Stamp	24 Mar 2012 12:41:52			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD240-1 13C\1\FID			***Frequency (MHz)***	62.90
Nucleus	13C	***Number of Transients***	1200	***Origin***	spect	***Original Points Count***	69632	***Owner***	service
Points Count	131072	***Pulse Sequence***	zgpgvar	***Receiver Gain***	7298.20	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	6566.0649	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000		

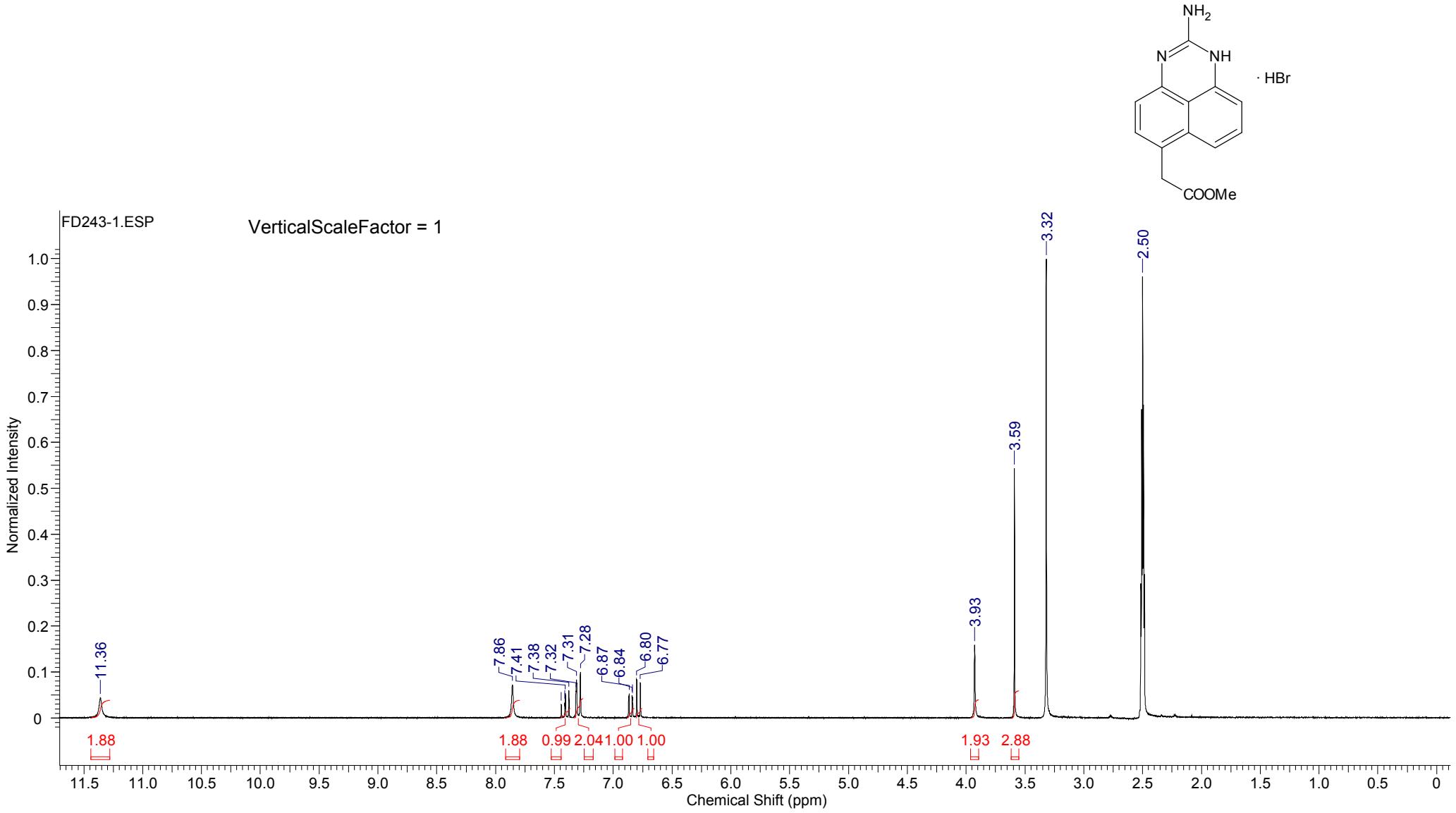




This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 30

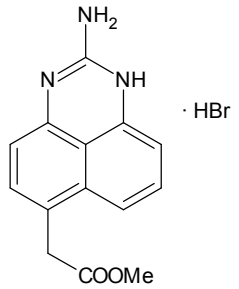
Acquisition Time (sec)	6.1563	***Comment***	FD243-1	***Date***	28 Mar 2012 15:56:16			***Date Stamp***	28 Mar 2012 15:56:16
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD243-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	30720	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zgvar
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4247	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						

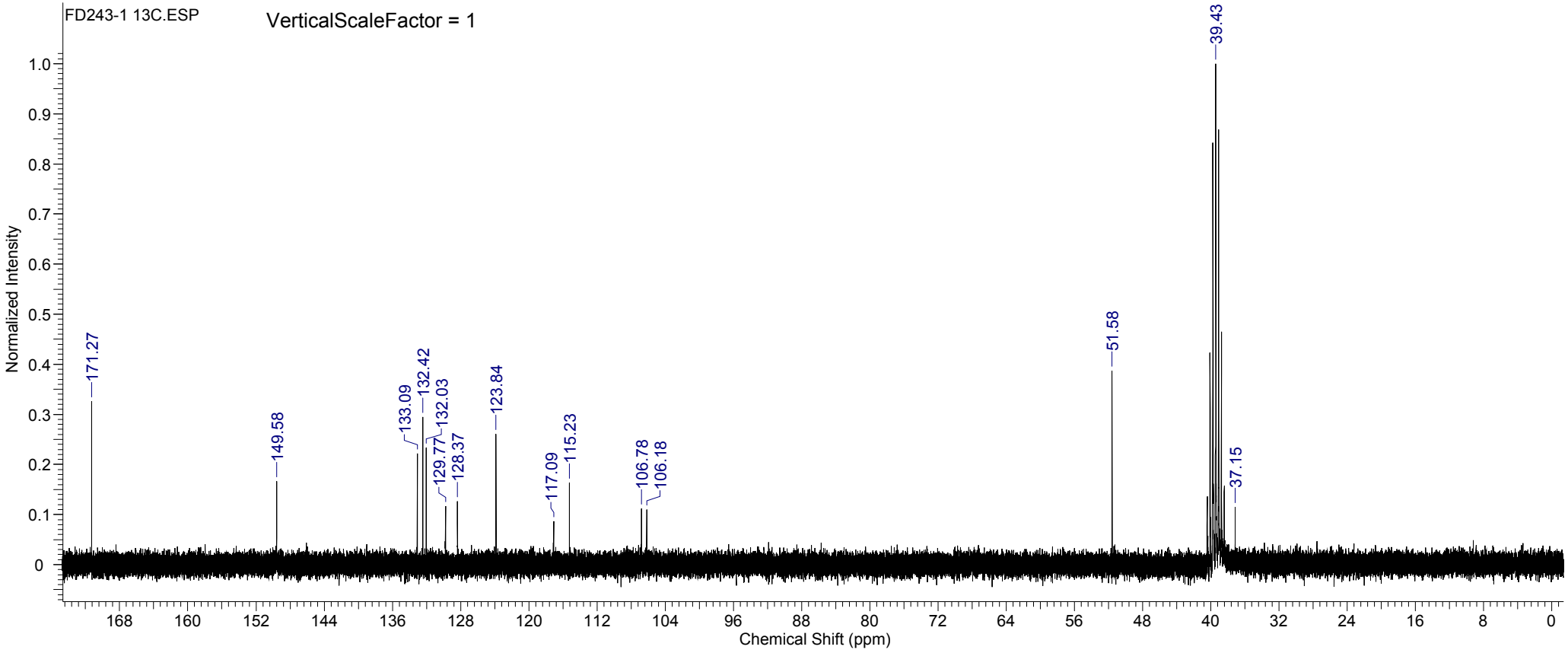


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 30

Acquisition Time (sec)	4.6891	***Comment***	FD243-1	***Date***	30 Mar 2012 22:58:40				
Date Stamp	30 Mar 2012 22:58:40			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD243-1 13C\1\FID			***Frequency (MHz)***	62.90
Nucleus	13C	***Number of Transients***	1440	***Origin***	spect	***Original Points Count***	73728	***Owner***	service
Points Count	131072	***Pulse Sequence***	zgpgvar	***Receiver Gain***	11585.20	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	6564.2656	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000		

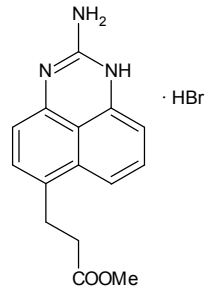


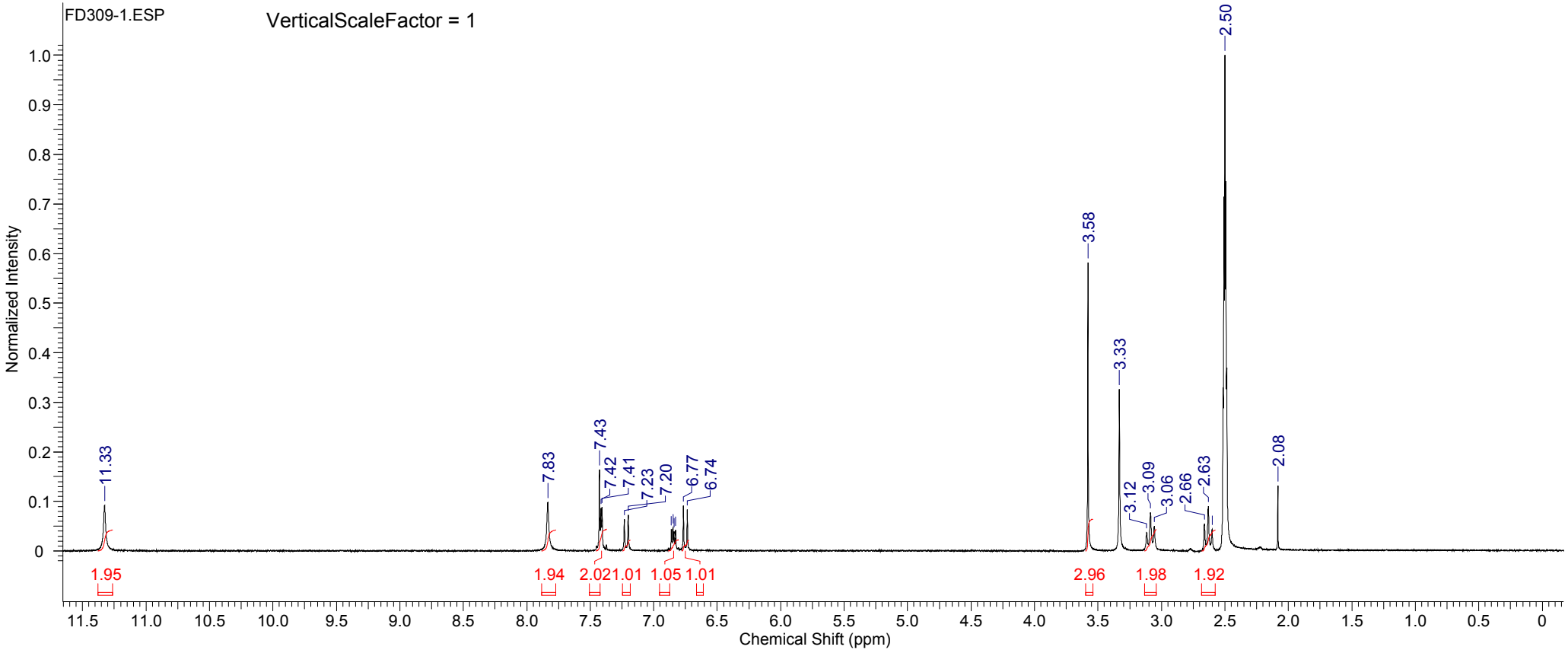


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 31

Acquisition Time (sec)	4.5146	***Comment***	FD309-1	***Date***	05 Mar 2013 14:47:44			***Date Stamp***	05 Mar 2013 14:47:44
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD309-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	22528	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.5770	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						

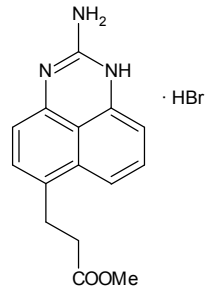


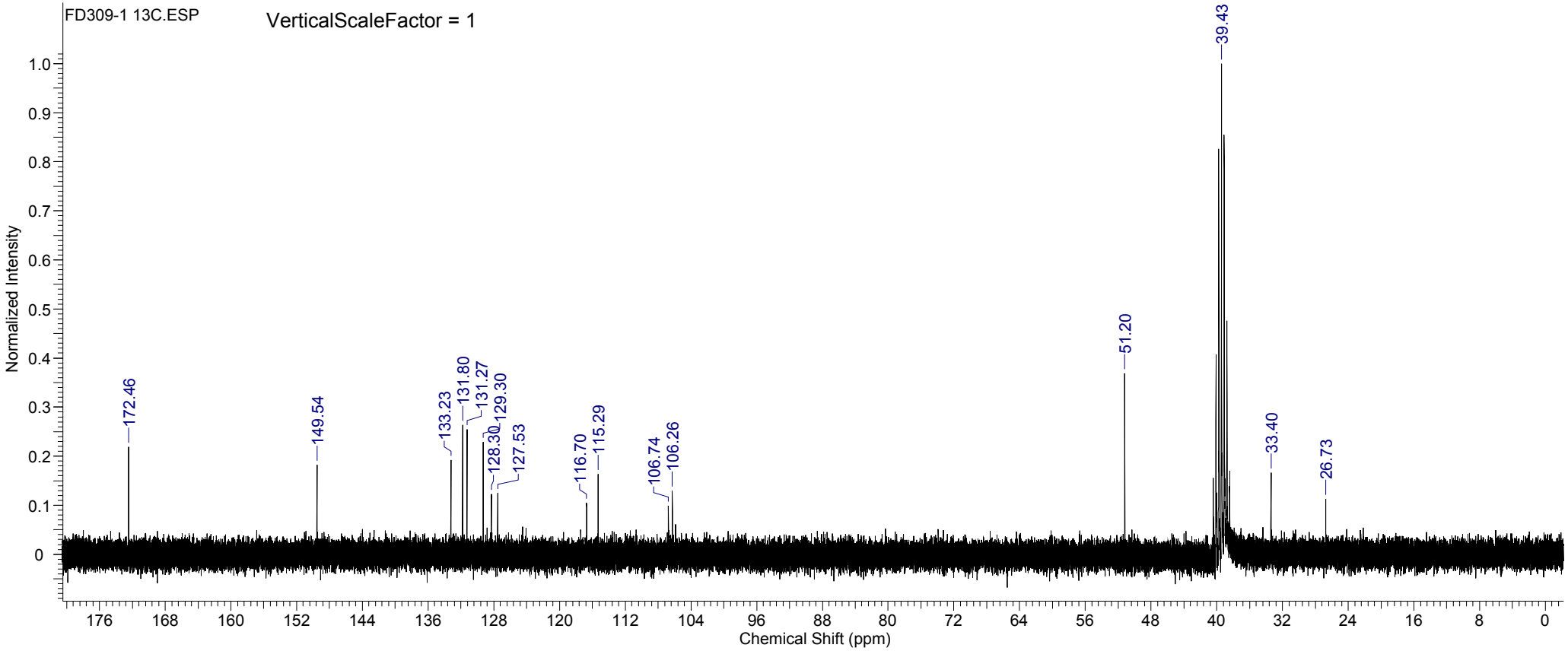


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 31

Acquisition Time (sec)	4.8845	***Comment***	FD309-1	***Date***	08 Mar 2013 03:01:36				
Date Stamp	08 Mar 2013 03:01:36			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD309-1 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1400	***Origin***	spect	***Original Points Count***	76800
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6565.2256	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000

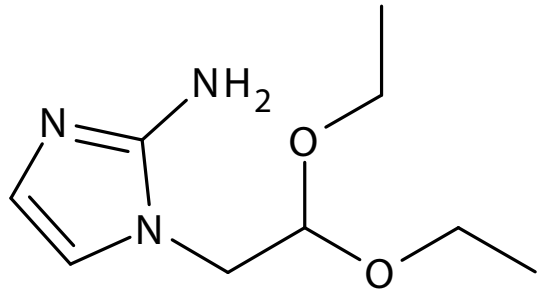


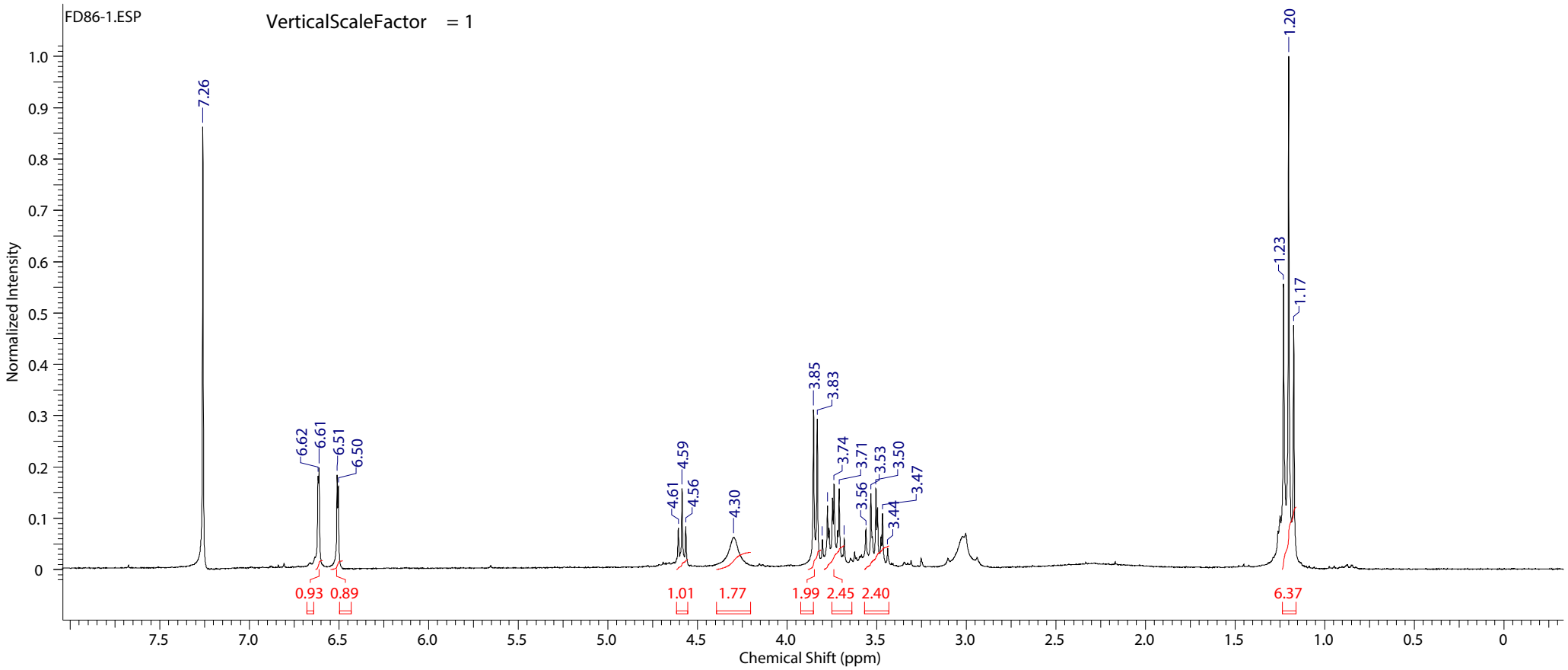


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 32

Acquisition Time (sec)	3.1261	Date	15 Feb 2012 09:55:18				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD54 - 97\FD86\FD86-1.MRC				Frequency (MHz)	250.13	Nucleus 1H
Origin	Bruker	Original Points Count	32768	Points Count 65536	Pulse Sequence	ZG30	Spectrum Offset (Hz) 2488.5195
Spectrum Type	STANDARD	Sweep Width (Hz)	10482.18				

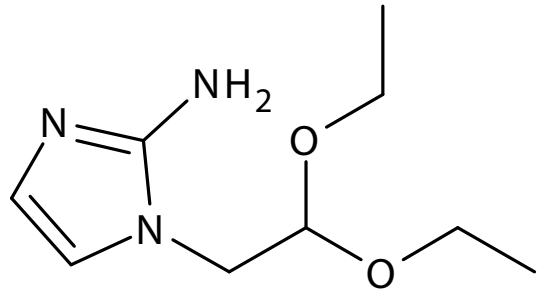


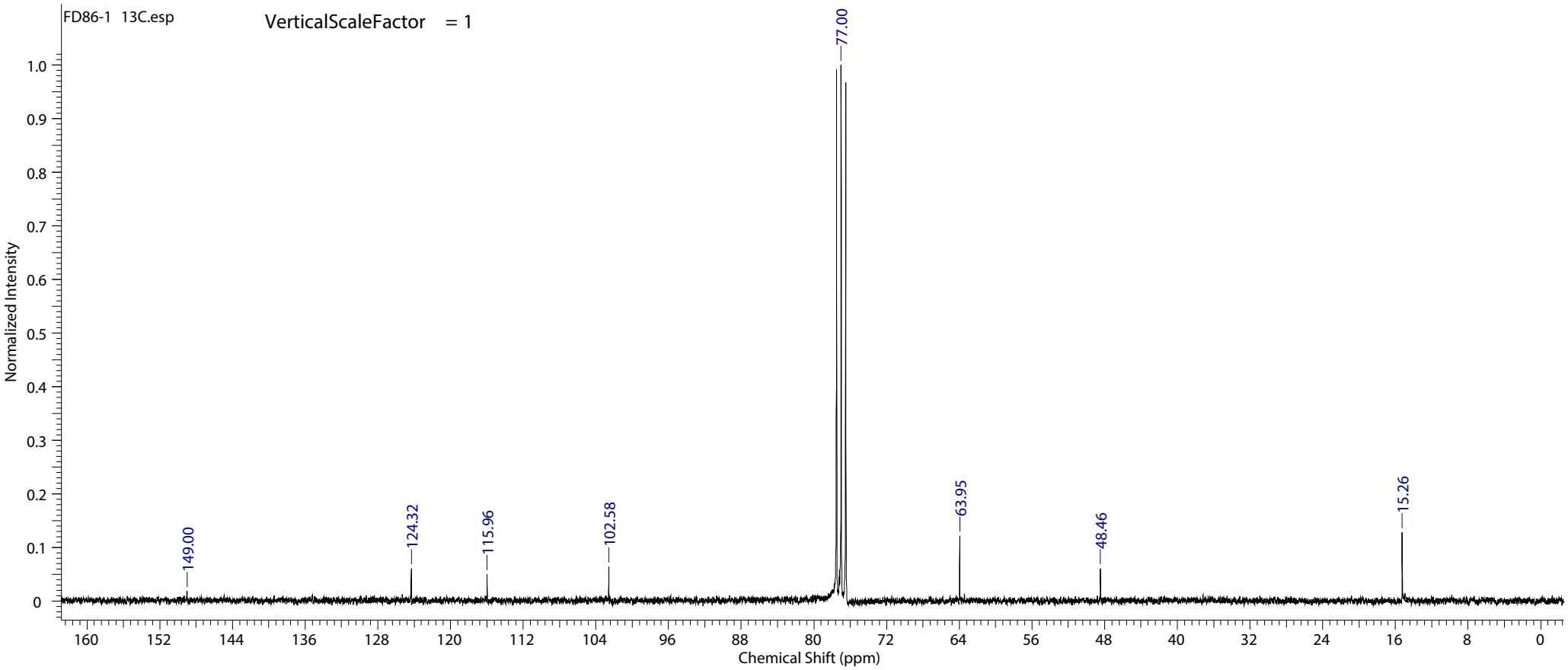


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 32

Acquisition Time (sec)	1.3849	Date	15 Feb 2012 09:55:18				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD54 - 97\FD86\FD86-1 13C.MRC					Frequency (MHz)	62.90
Nucleus	13C	Origin	Bruker	Original Points Count	23552	Points Count	65536
Pulse Sequence	ZGPG30	Spectrum Offset (Hz)	6918.8745	Spectrum Type	STANDARD	Sweep Width (Hz)	17006.80



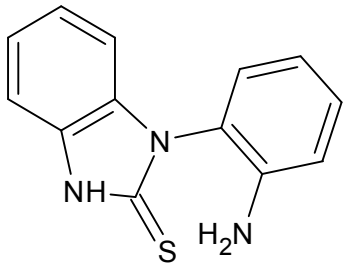


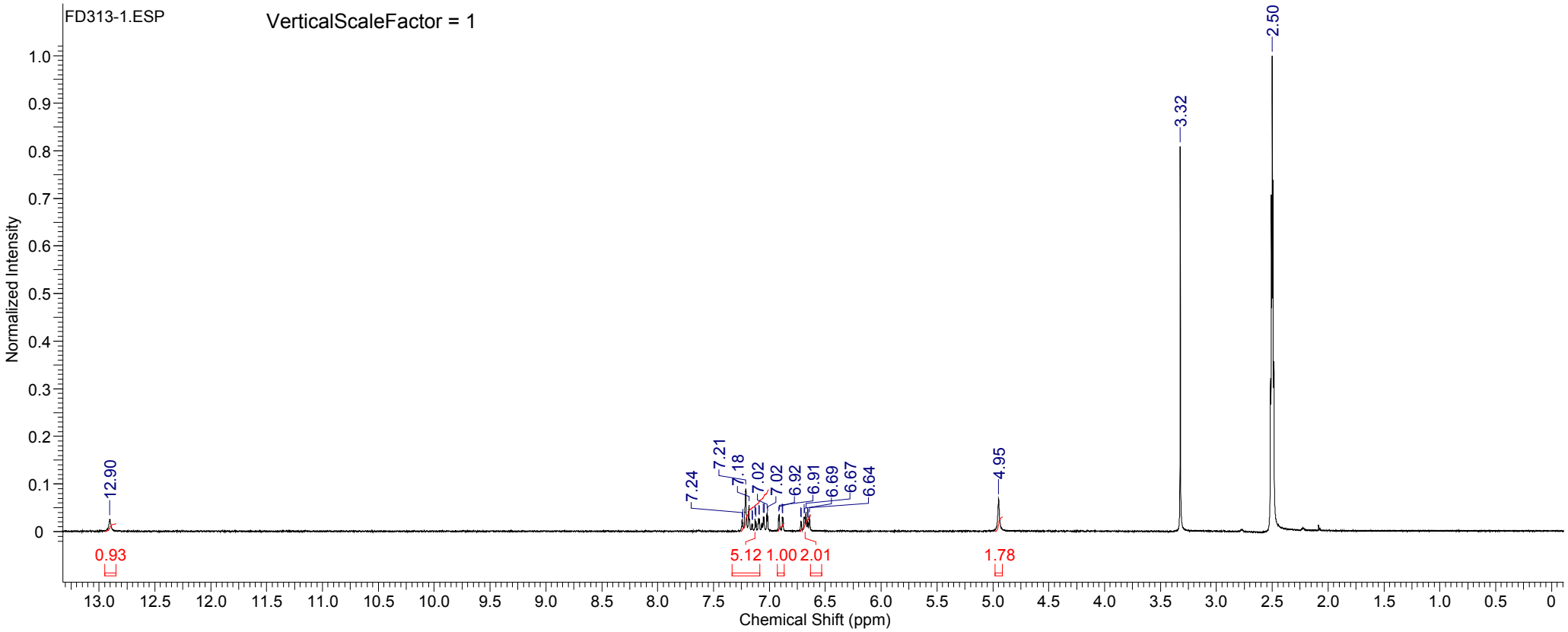
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 35

FD313-1

Acquisition Time (sec)	4.5146	***Comment***	FD313-1	***Date***	20 Mar 2013 12:48:16			***Date Stamp***	20 Mar 2013 12:48:16
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD313-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	22528	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	645.10	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1754.1251	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						



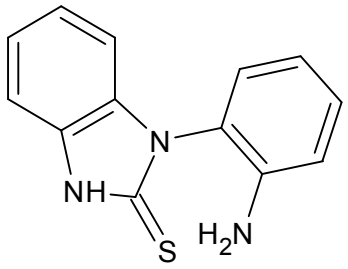


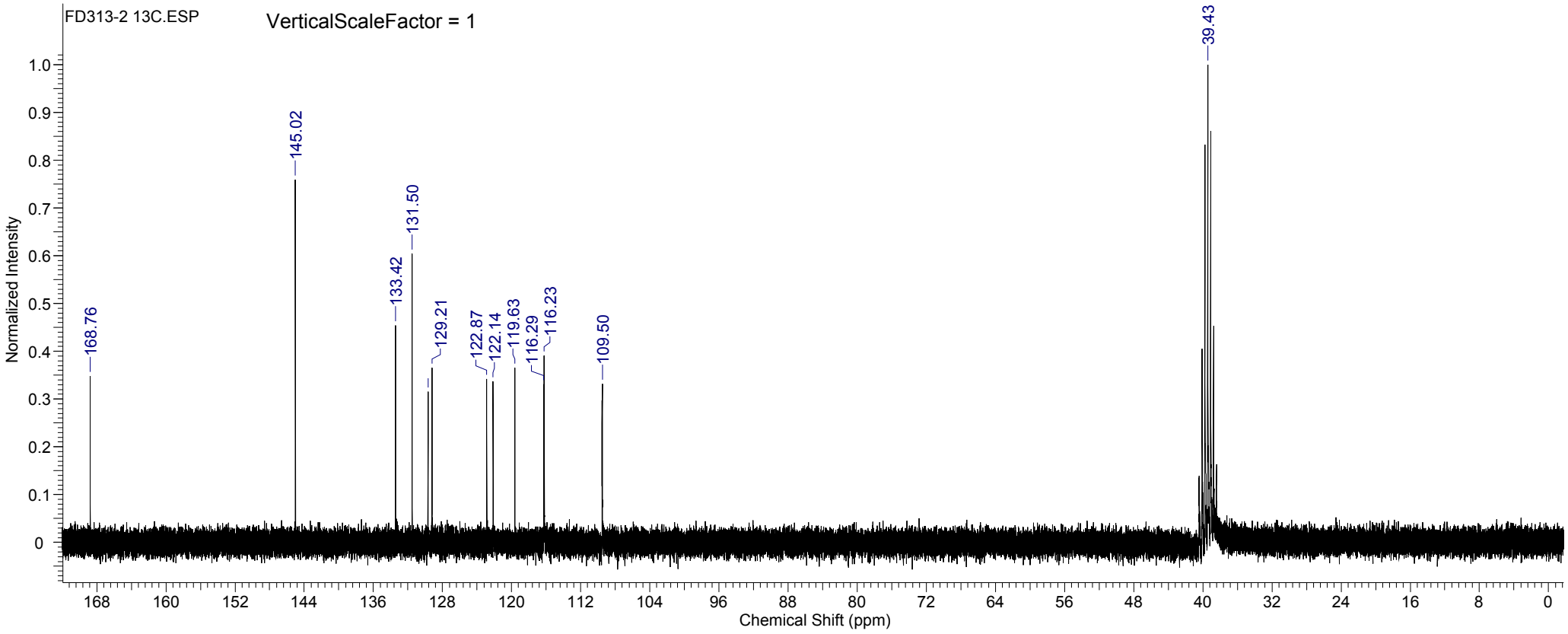
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 35

FD313-2

Acquisition Time (sec)	4.8845	***Comment***	FD313-2	***Date***	25 Mar 2013 21:16:00				
Date Stamp	25 Mar 2013 21:16:00			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD313-2 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1400	***Origin***	spect	***Original Points Count***	76800
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6568.1045	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000

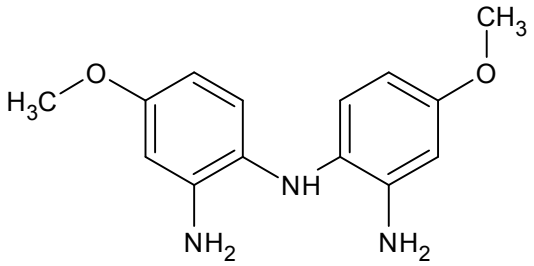


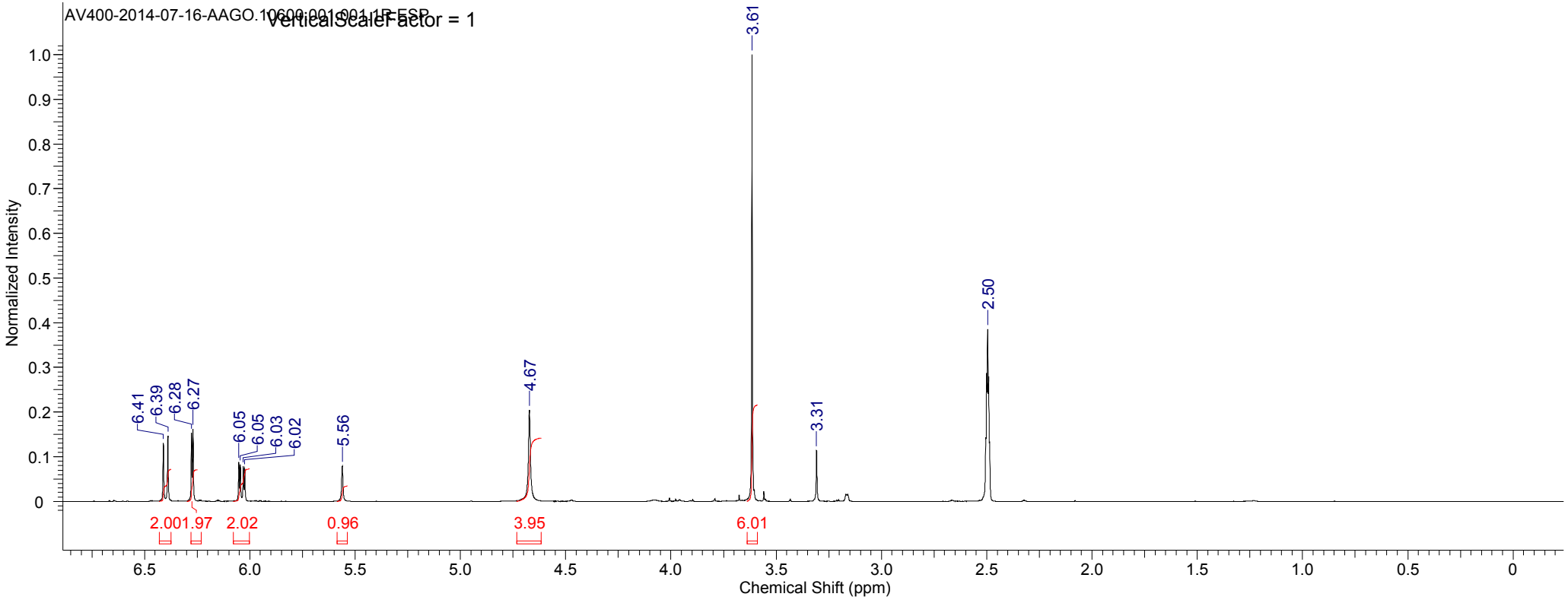


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 37

Acquisition Time (sec)	4.0894						
Comment	Goethe-UniversitÃ¤t Frankfurt NMR Service Abteilung Spektrometer AV400 HH003200 Probenkopf BBI Z-Grad Z862701 0065 Arbeitskreis AK Goebel AA5						
Date	16 Jul 2014 15:11:28	***Date Stamp***	16 Jul 2014 15:11:28				
File Name	C:\USERS\PLAM\DESKTOP\ABDULLAH\AV400-2014-07-16-AAGO.10600\1\PDATA\1\1R					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	80	***Origin***	spect	***Original Points Count***	32768
Owner	service	***Points Count***	65536	***Pulse Sequence***	zg30	***Receiver Gain***	322.50
SW(cyclical) (Hz)	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2392.6284	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.70	***Temperature (degree C)***	24.996				

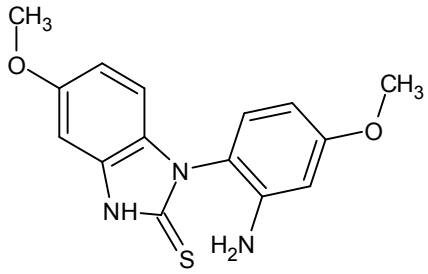


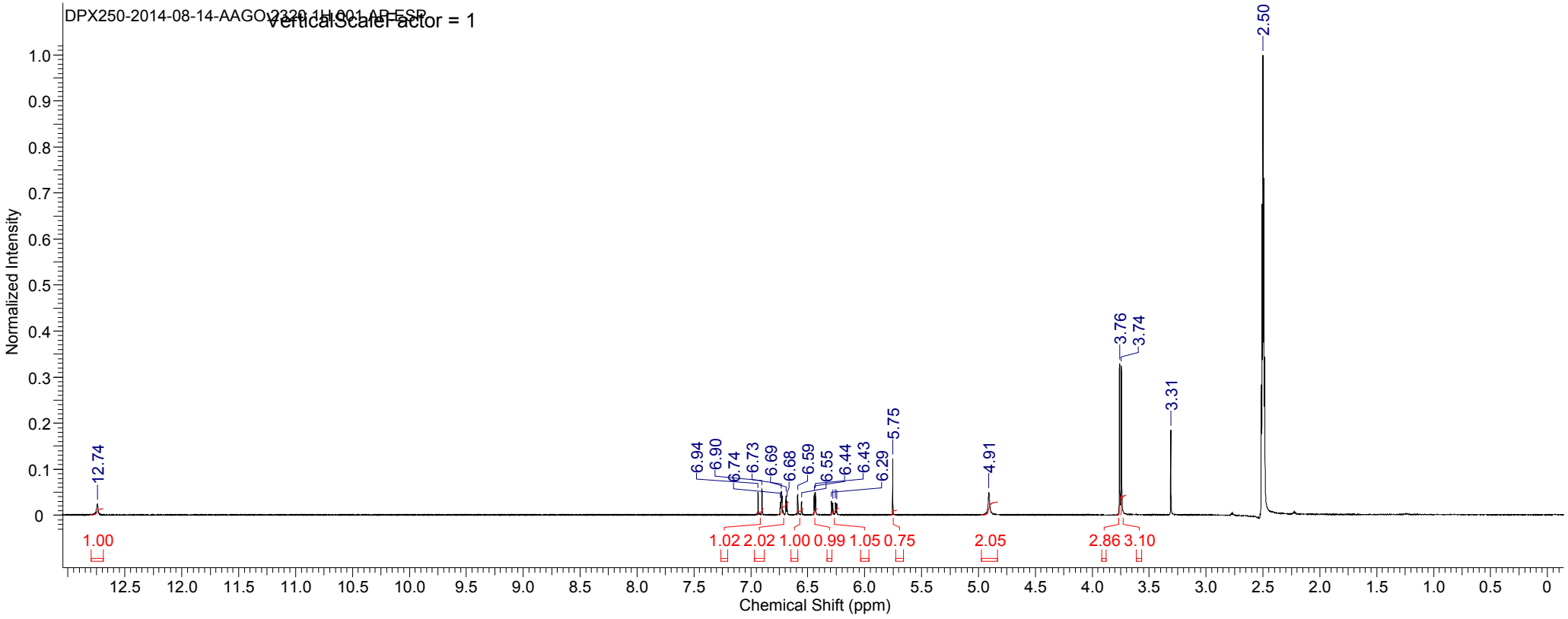


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 38

Acquisition Time (sec)	3.9998	***Comment***	AA6-SI	***Date***	14 Aug 2014 19:14:40		
Date Stamp	14 Aug 2014 19:14:40						
File Name	C:\USERS\RIKE\DATEN RIKE\WRT\AP\SPEKTREN ABDULLAH\THIOHARNSTOFF\NMR\DPX250-2014-08-14-AAGO.2320 1H\1\FID						
Frequency (MHz)	250.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Original Points Count	20703	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30_ns
Receiver Gain	724.10	***SW(cyclical) (Hz)***	5175.98	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1541.2472
Spectrum Type	STANDARD	***Sweep Width (Hz)***	5175.83	***Temperature (degree C)***	26.160		





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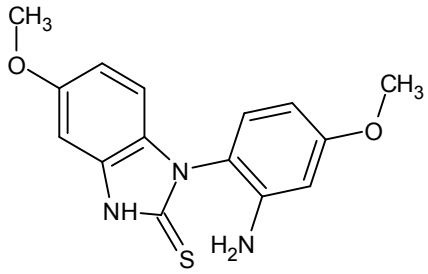
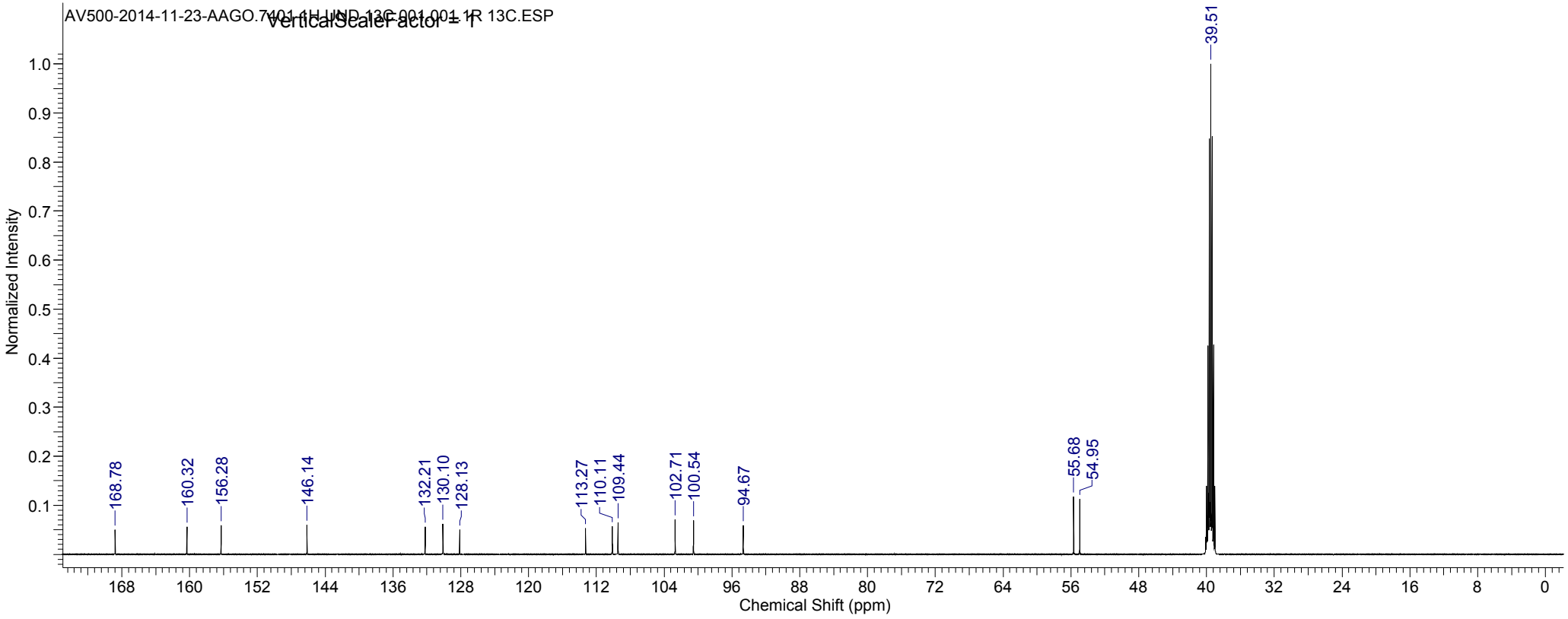
Compound 38

Acquisition Time (sec)	1.0457	***Comment***	AA6S	***Date***	23 Nov 2014 23:47:28		
Date Stamp	23 Nov 2014 23:47:28						
File Name	C:\USERS\RIKE\DATEN RIKE\WRT\AP\SPEKTREN ABDULLAH\THIOHARNSTOFF\NMR\AV500-2014-11-23-AAGO.7401 1H UND 13C\1\PDATA\1\1R						
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	2048	***Origin***	spect
Original Points Count	32678	***Owner***	service	***Points Count***	65536	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	12440.5098
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.52	***Temperature (degree C)***	25.200		

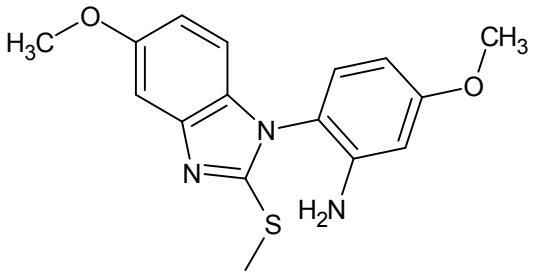


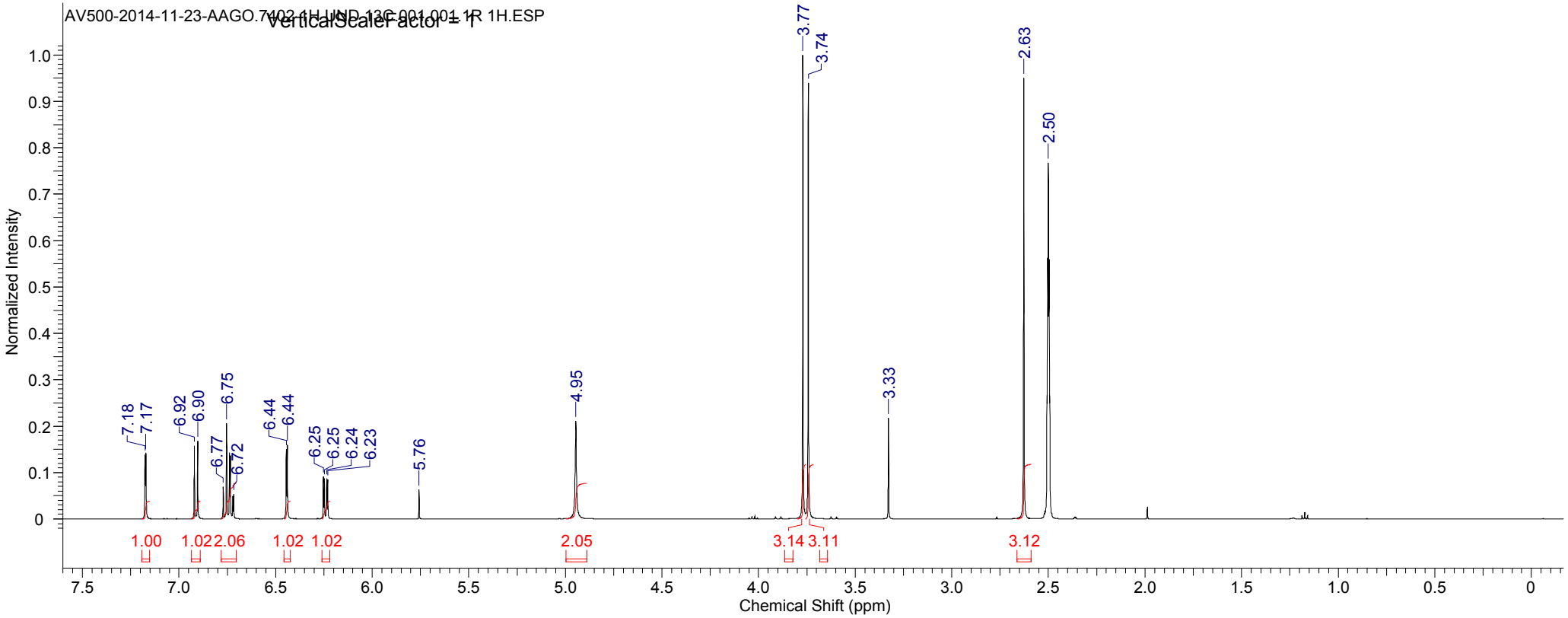


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 39

Acquisition Time (sec)	3.9999	***Comment***	AA6SMe	***Date***	24 Nov 2014 00:02:24		
Date Stamp	24 Nov 2014 00:02:24						
File Name	C:\USERS\RIKE\DATEN RIKE\WRT\AP\SPEKTREN ABDULLAH\METHYLTHIOHARNSTOFF\NMR\AV500-2014-11-23-AAGO.7402 1H UND 13C\1\PDATA\1\1R						
Frequency (MHz)	500.18	***Nucleus***	1H	***Number of Transients***	32	***Origin***	spect
Original Points Count	39999	***Owner***	service	***Points Count***	131072	***Pulse Sequence***	zg30_ns
Receiver Gain	45.20	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2996.7039
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.92	***Temperature (degree C)***	25.199		

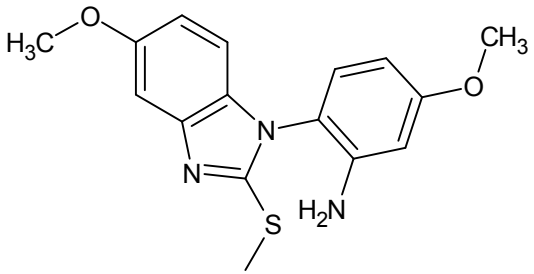


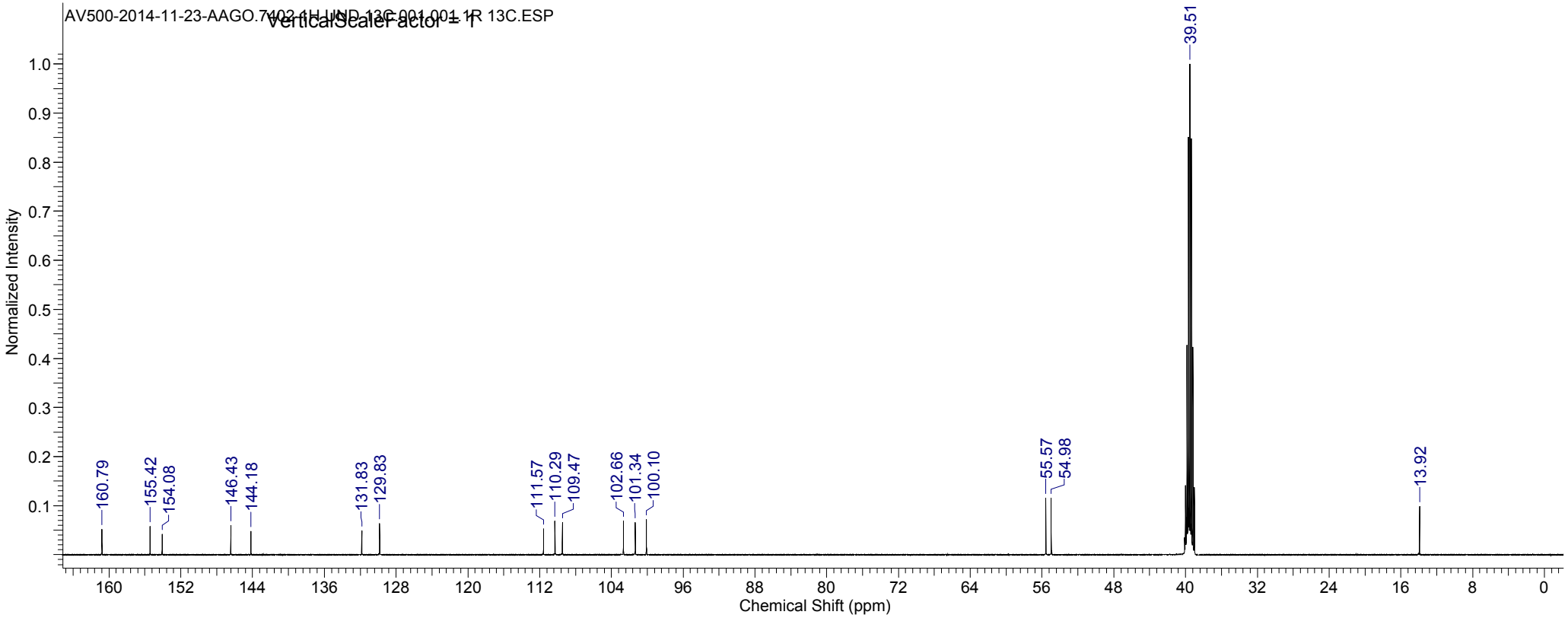


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 39

Acquisition Time (sec)	1.0457	***Comment***	AA6SMe	***Date***	24 Nov 2014 00:57:52		
Date Stamp	24 Nov 2014 00:57:52						
File Name	C:\USERS\RIKE\DATEN RIKE\WRT\AP\SPEKTREN ABDULLAH\METHYLTHIOHARNSTOFF\NMR\AV500-2014-11-23-AAGO.7402 1H UND 13C\2\PDATA\1\1R						
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	2048	***Origin***	spect
Original Points Count	32678	***Owner***	service	***Points Count***	65536	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	12440.0332
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.52	***Temperature (degree C)***	25.202		

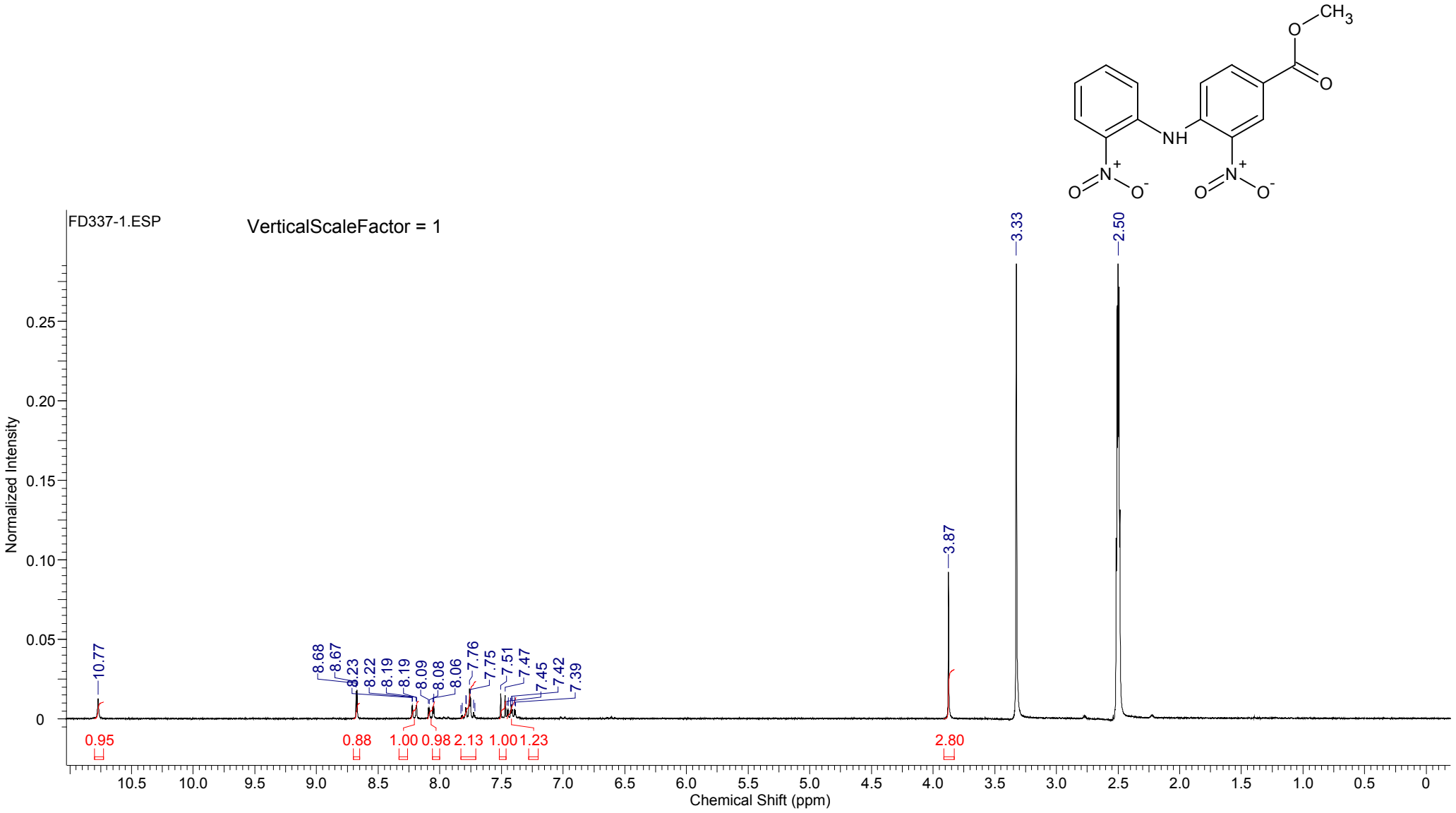




This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 41

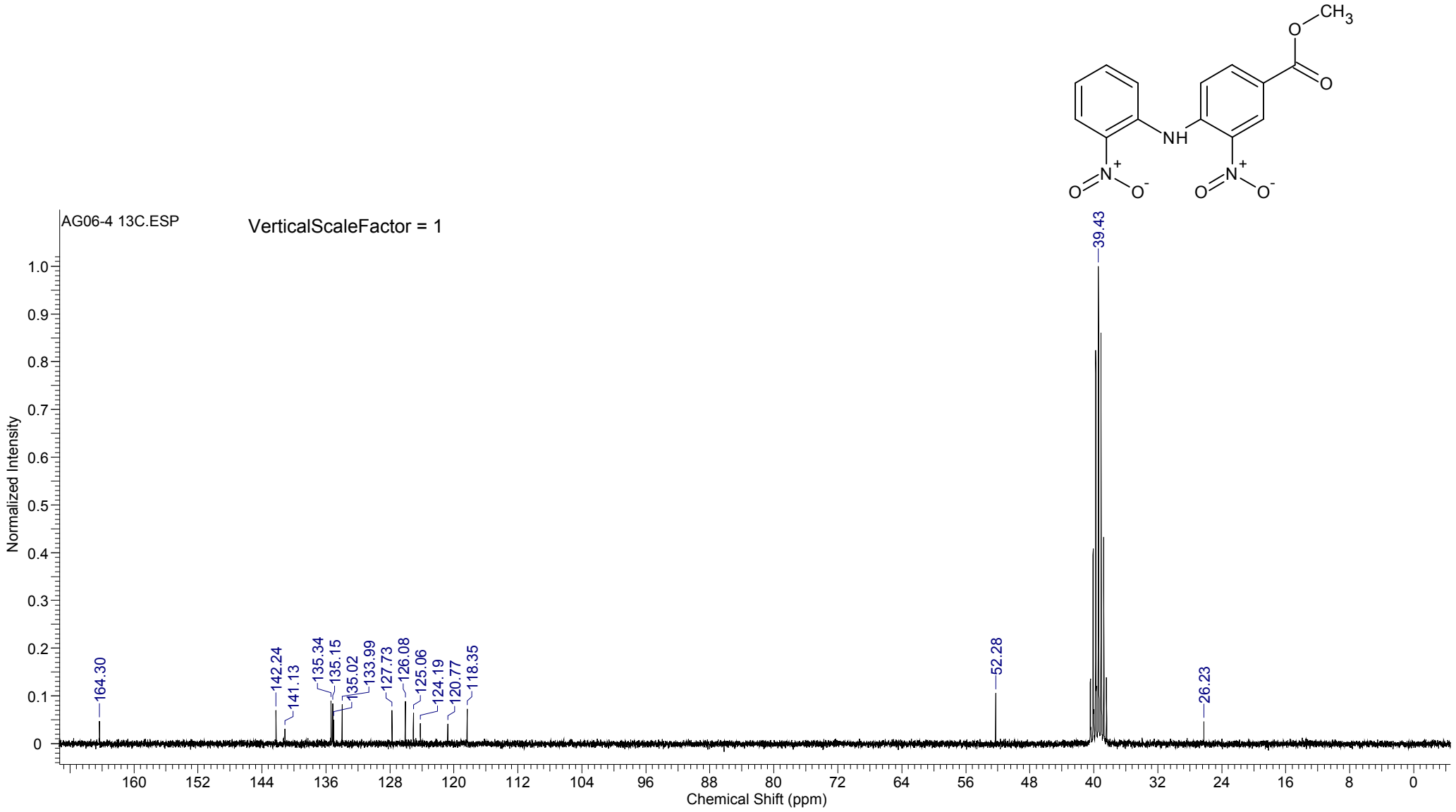
Acquisition Time (sec)	3.9999	***Comment***	FD337-1	***Date***	09 Sep 2013 11:42:24			***Date Stamp***	09 Sep 2013 11:42:24
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD337-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	17985	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30_ns
Receiver Gain	645.10	***SW(cyclical) (Hz)***	4496.40	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1247.2716	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.27	***Temperature (degree C)***	27.000						



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 41

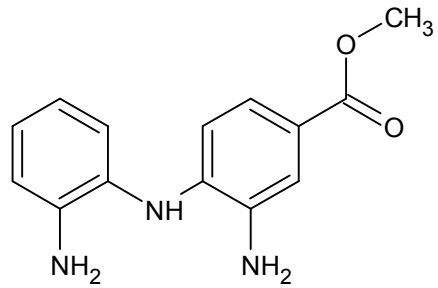
Acquisition Time (sec)	1.0420	***Comment***	AG06-4	***Date***	21 Jun 2013 06:07:28				
Date Stamp	21 Jun 2013 06:07:28			***File Name***	C:\USERS\RIKE\DESKTOP\ALEX\NMR\AG06\AG06-4 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	4096	***Origin***	spect	***Original Points Count***	16384
Owner	service	***Points Count***	16384	***Pulse Sequence***	zgpg30	***Receiver Gain***	11585.20	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6253.8716	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15722.31	***Temperature (degree C)***	27.000

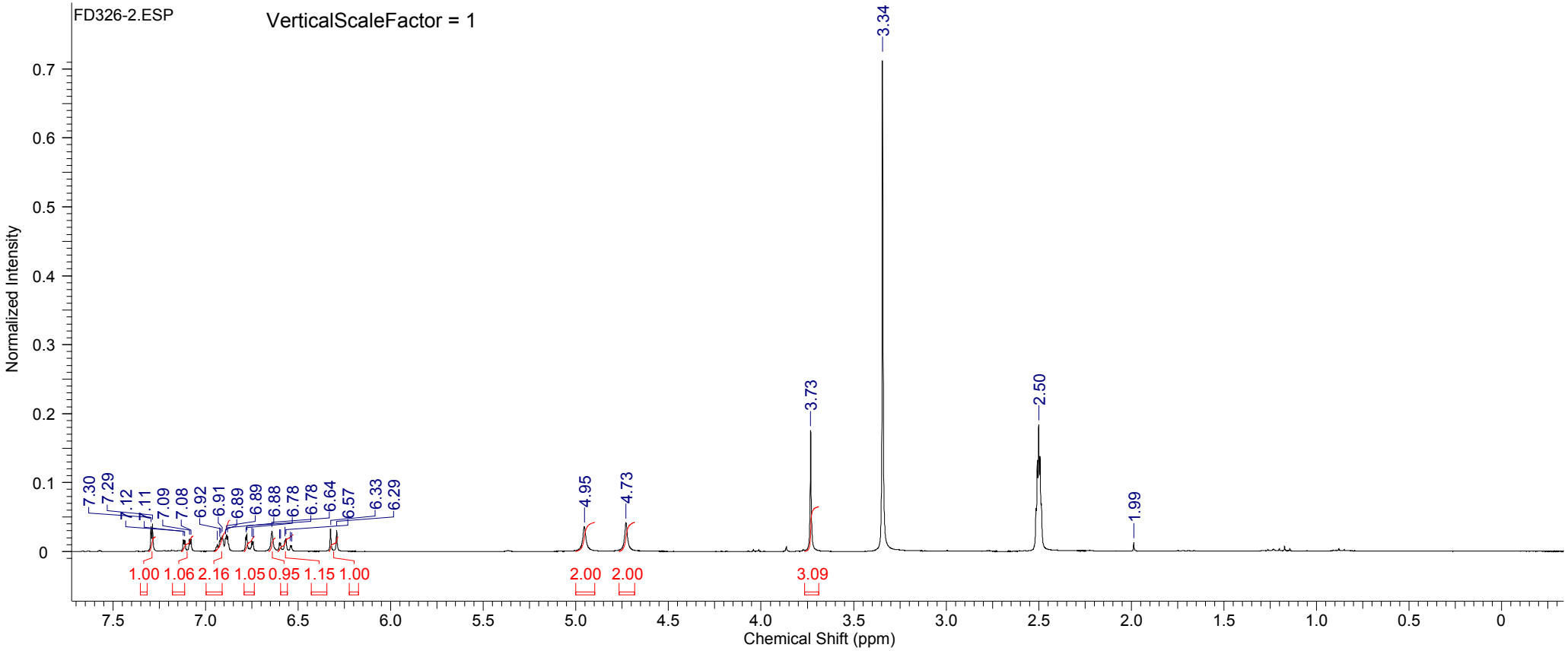


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 42

Acquisition Time (sec)	3.9998	***Comment***	FD326-2	***Date***	01 Jul 2013 10:49:04			***Date Stamp***	01 Jul 2013 10:49:04
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD326-2\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	128
Origin	spect	***Original Points Count***	19959	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30_new
Receiver Gain	406.40	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1504.5327	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						

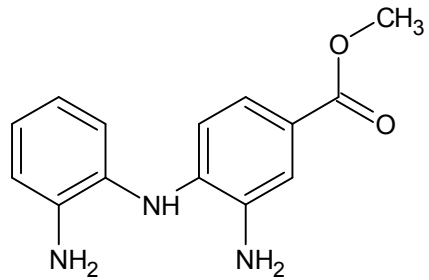


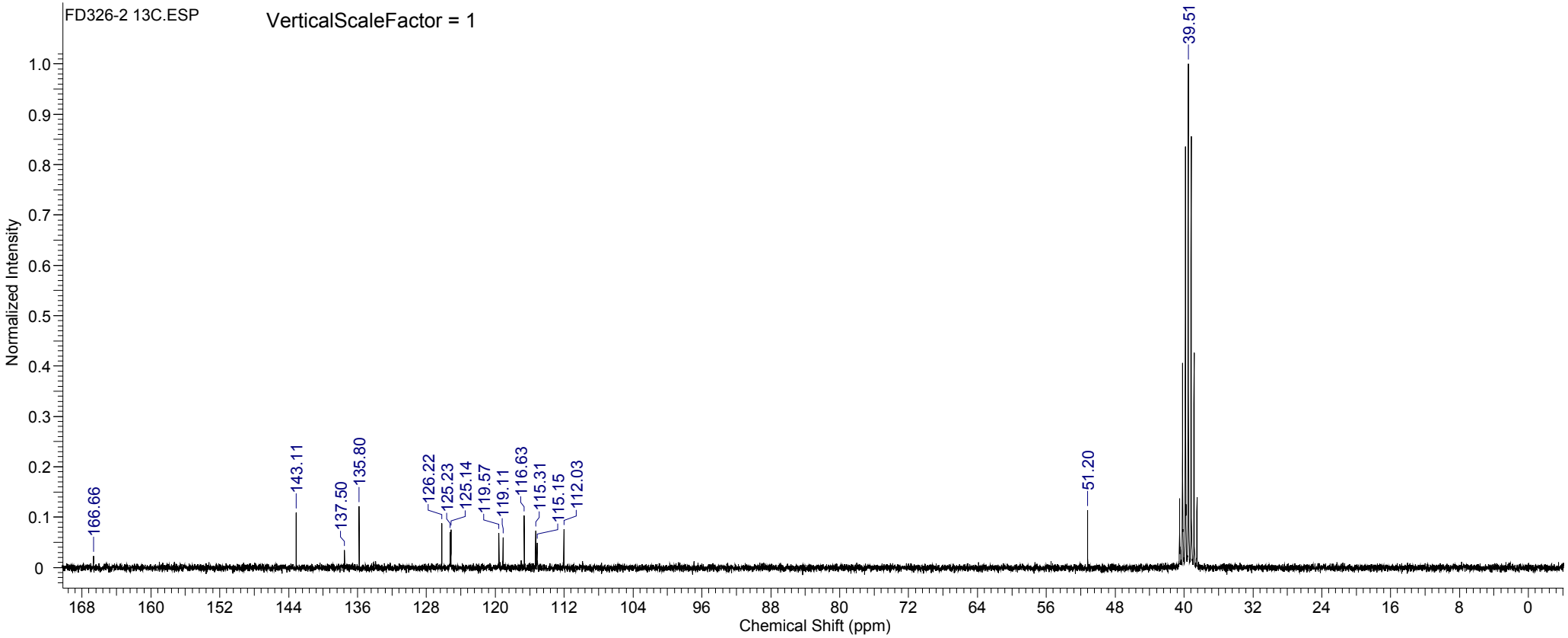


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 42

Acquisition Time (sec)	1.0420	***Comment***	FD326-2	***Date***	02 Jul 2013 02:21:20			***Date Stamp***	02 Jul 2013 02:21:20
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD326-2 13C\2\FID					***Frequency (MHz)***	62.90	***Nucleus***	13C
Number of Transients	4096	***Origin***	spect	***Original Points Count***	16384	***Owner***	service	***Points Count***	16384
Pulse Sequence	zgpg30	***Receiver Gain***	11585.20	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6258.9033
Spectrum Type	STANDARD	***Sweep Width (Hz)***	15722.31	***Temperature (degree C)***	27.000				

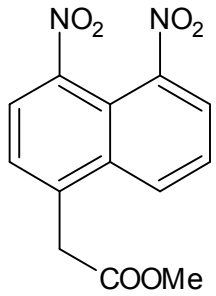


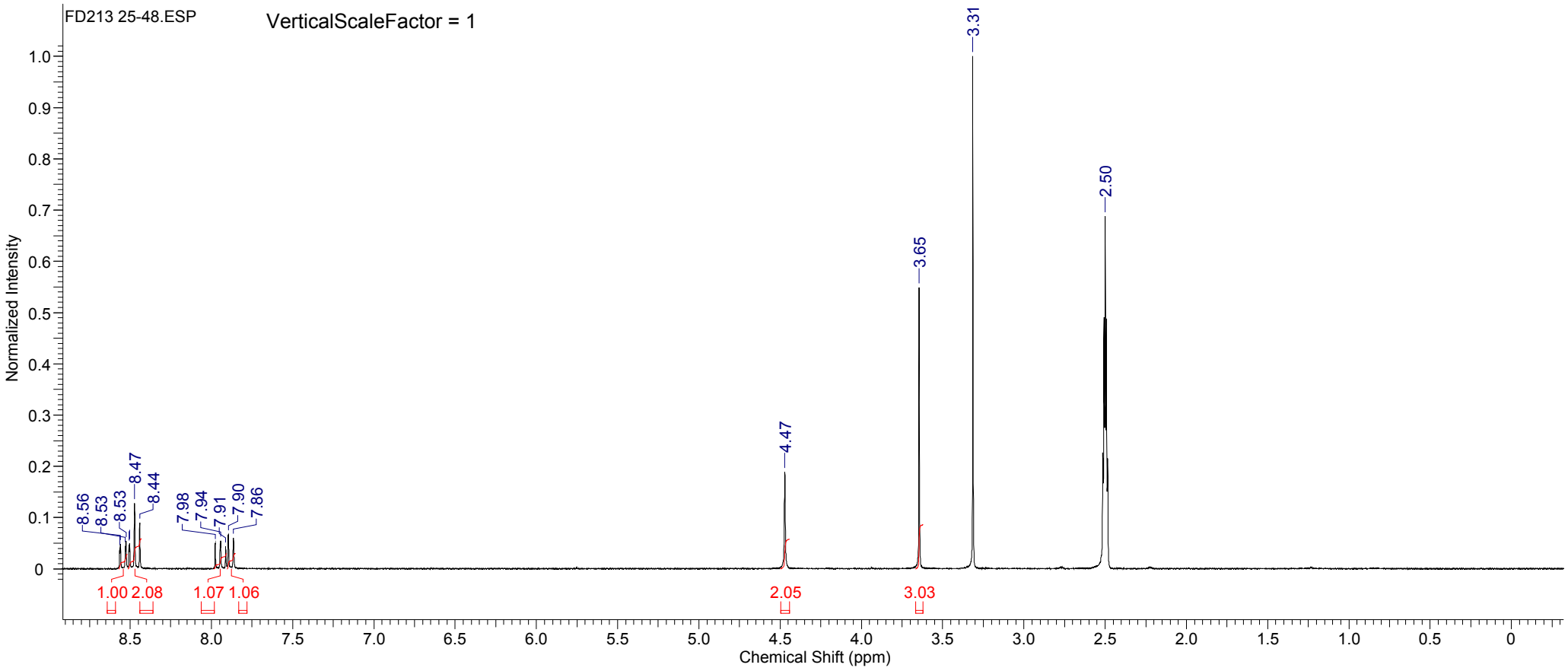


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 45

Acquisition Time (sec)	5.3809	***Date***	15 Feb 2012 11:27:22				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD213\FD213 25-48\FD213 25-48.MRC					***Frequency (MHz)***	250.13
Nucleus	1H	***Origin***	Bruker	***Original Points Count***	29696	***Points Count***	65536
Pulse Sequence	ZG30	***Spectrum Offset (Hz)***	1747.4260	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	5518.76

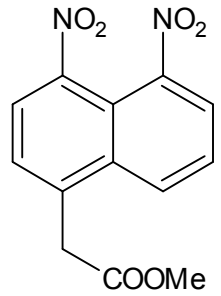


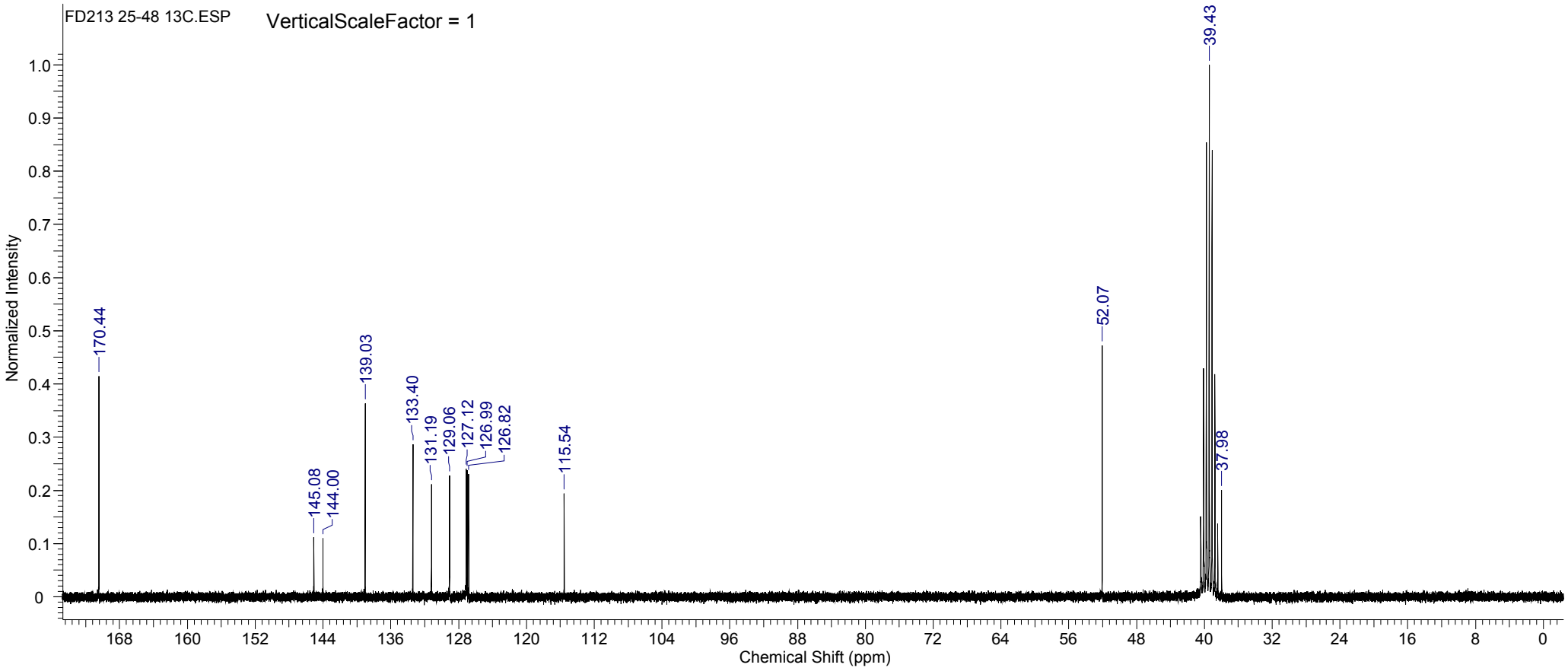


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 45

Acquisition Time (sec)	4.1681	***Date***	15 Feb 2012 11:27:28				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD213\FD213 25-48 13C\FD213 25-48 13C.MRC					***Frequency (MHz)***	62.90
Nucleus	13C	***Origin***	Bruker	***Original Points Count***	65536	***Points Count***	131072
Pulse Sequence	ZGPG30	***Spectrum Offset (Hz)***	6541.5146	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.27

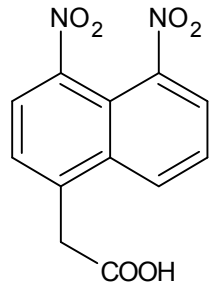


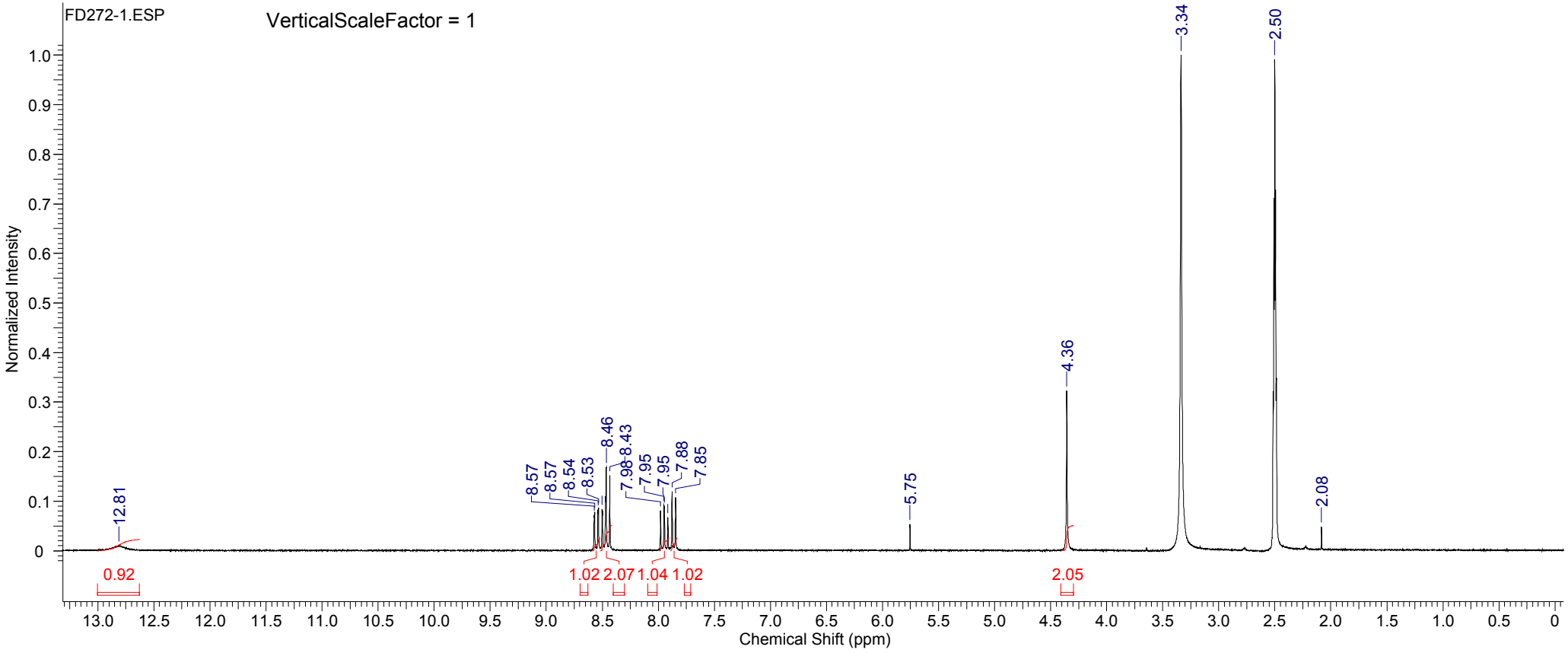


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 46

Acquisition Time (sec)	4.0858	***Comment***	FD272-1	***Date***	04 Sep 2012 15:13:36			***Date Stamp***	04 Sep 2012 15:13:36
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD272-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	19456	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	645.10	***SW(cyclical) (Hz)***	4761.90	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1754.1121	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4761.76	***Temperature (degree C)***	27.000						





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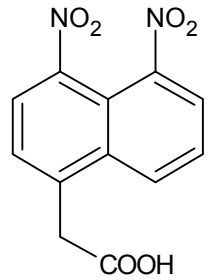
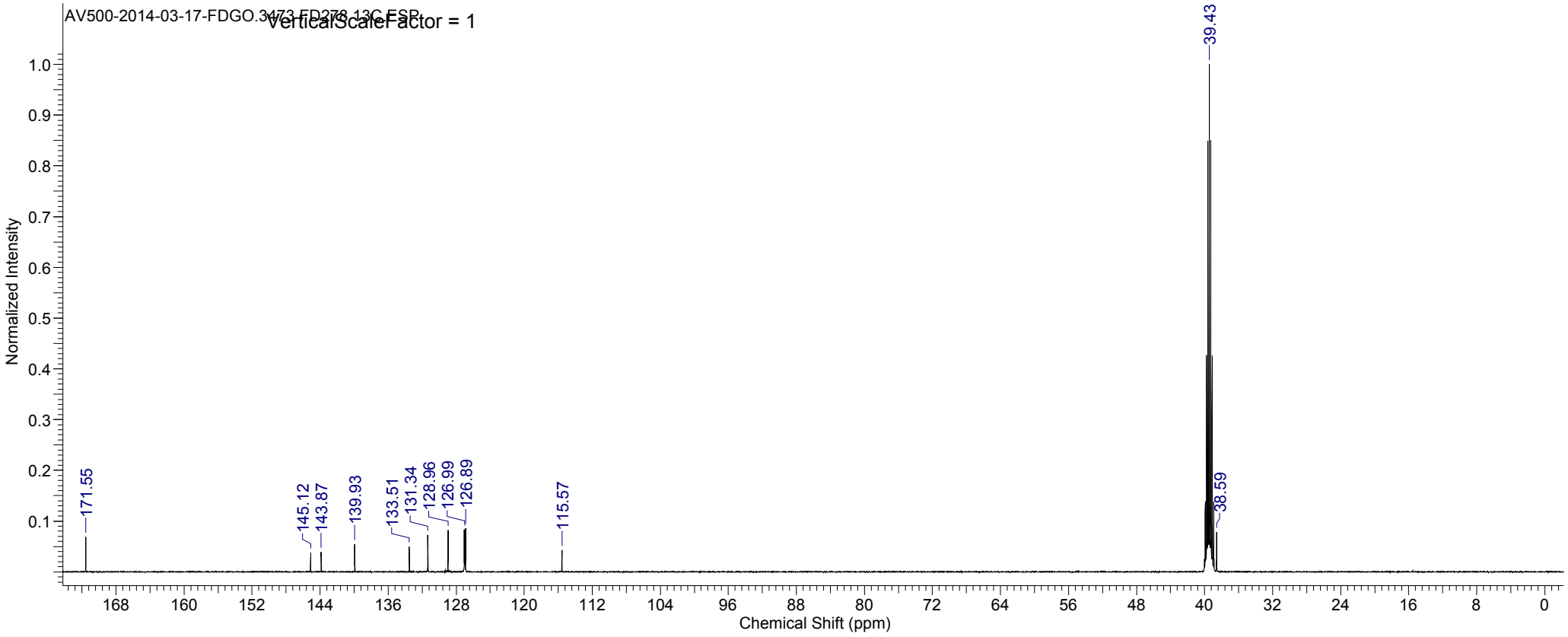
Compound 46

Acquisition Time (sec)	1.0457	***Comment***	FD278	***Date***	17 Mar 2014 13:22:24		
Date Stamp	17 Mar 2014 13:22:24			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\AV500-2014-03-17-FDGO.3473 FD278 13C\1\PDATA\1\1R		
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	1926	***Origin***	spect
Original Points Count	32678	***Owner***	service	***Points Count***	65536	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	12431.8789
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.52	***Temperature (degree C)***	25.001		





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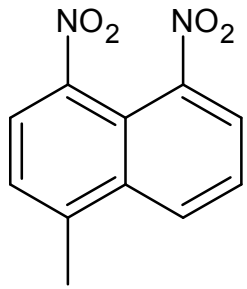
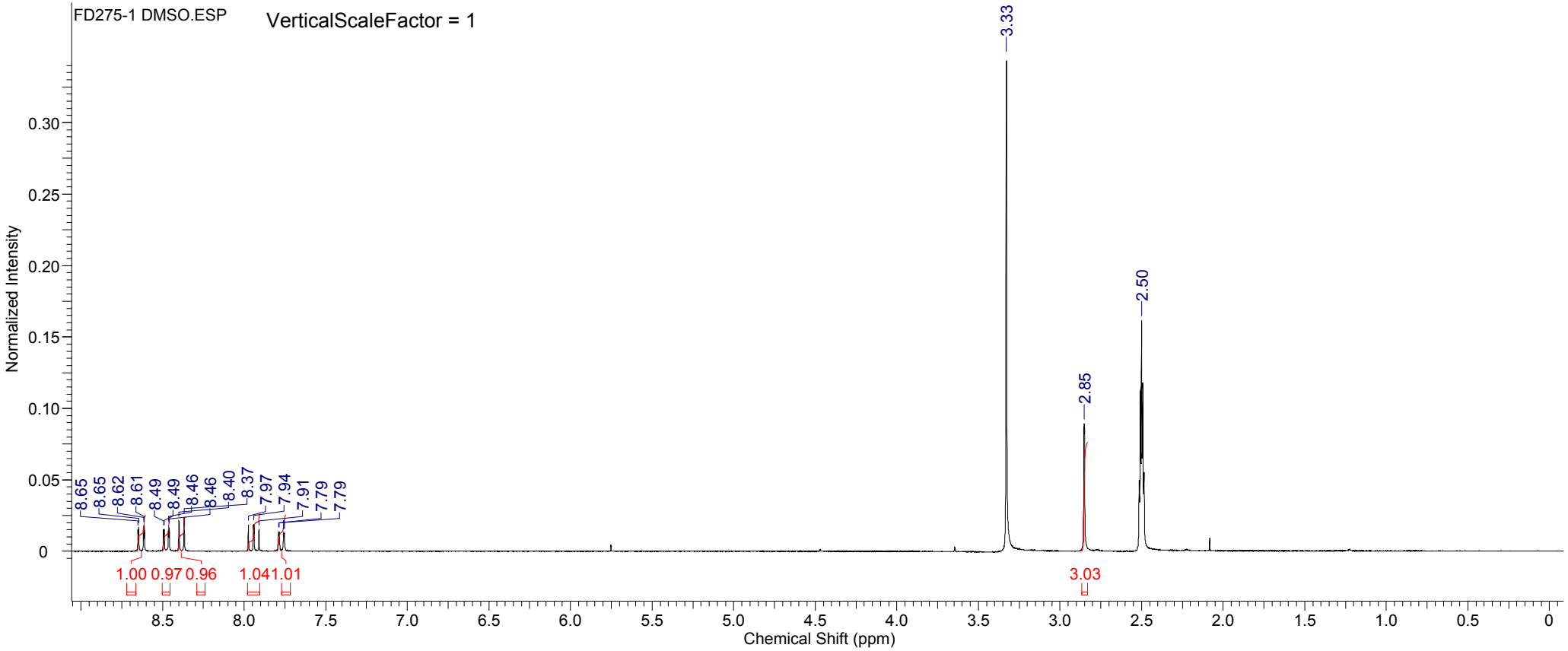
Compound 47

Acquisition Time (sec)	4.5158	***Comment***	FD275-1	***Date***	11 Sep 2012 10:32:00			***Date Stamp***	11 Sep 2012 10:32:00
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD275-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	21504	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4761.90	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4272	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4761.76	***Temperature (degree C)***	27.000						

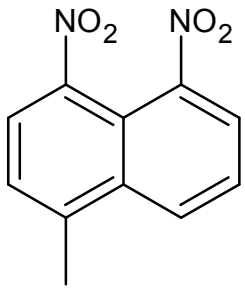


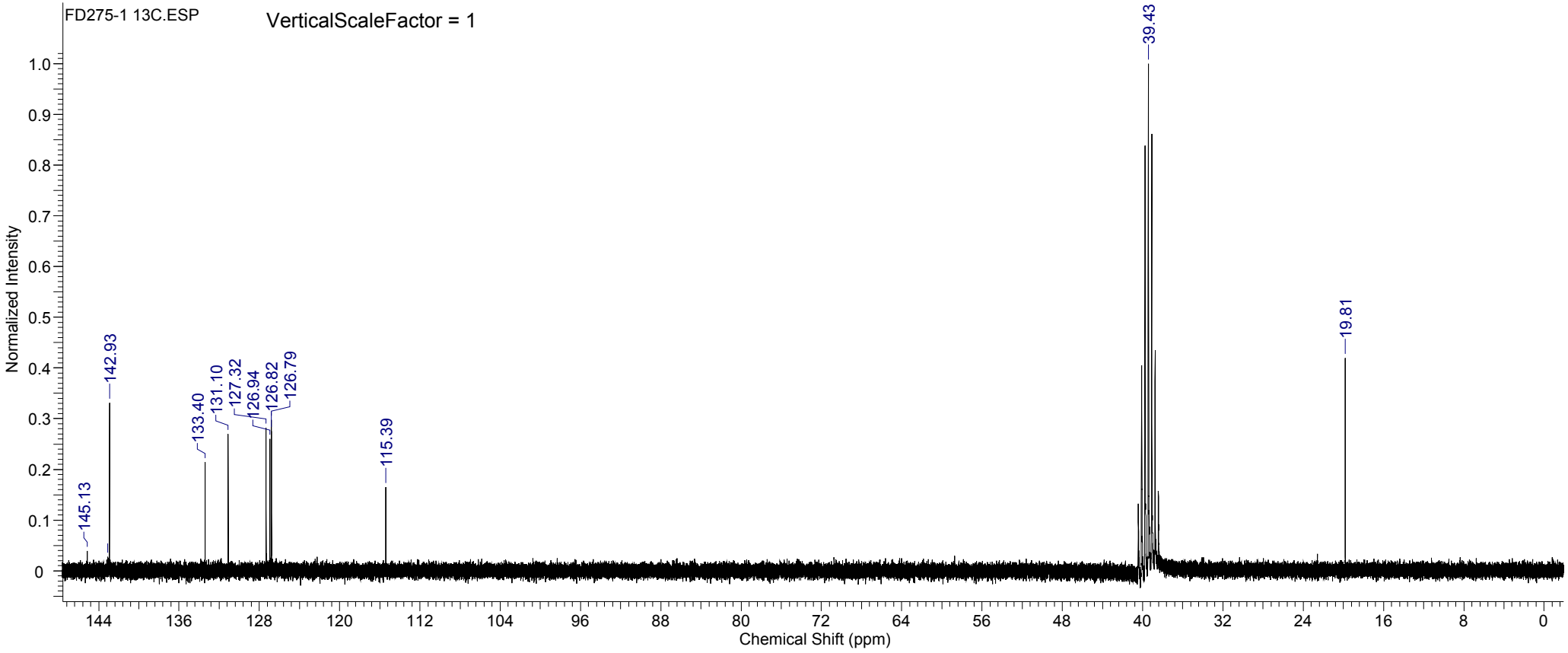


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 47

Acquisition Time (sec)	4.8955	***Comment***	FD275-1	***Date***	14 Sep 2012 21:22:40				
Date Stamp	14 Sep 2012 21:22:40			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD275-1 13C\1\FID			***Frequency (MHz)***	62.90
Nucleus	13C	***Number of Transients***	1600	***Origin***	spect	***Original Points Count***	73728	***Owner***	service
Points Count	131072	***Pulse Sequence***	zgig30	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15060.24	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	6816.8232	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15060.13	***Temperature (degree C)***	27.000		

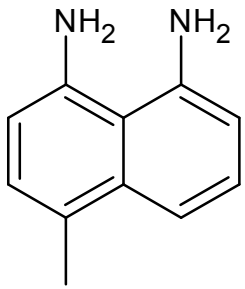


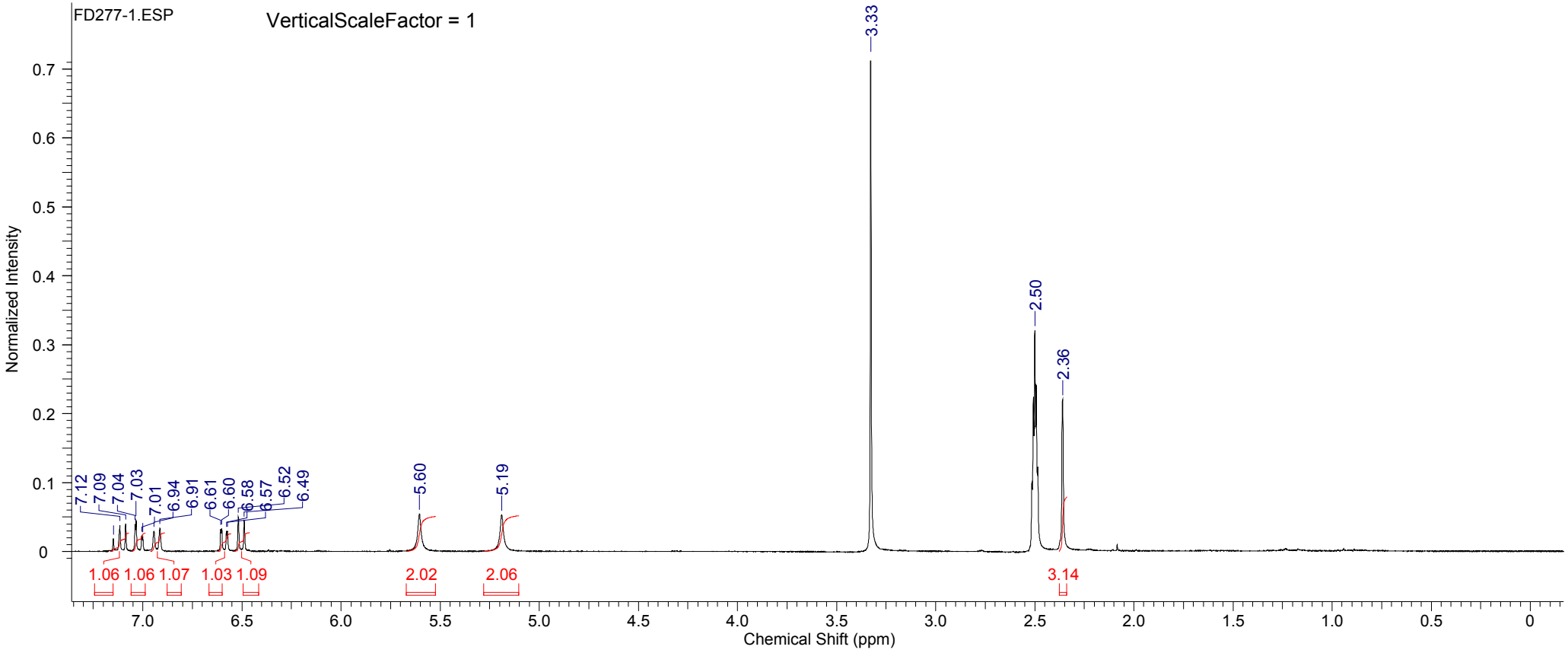


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 48

Acquisition Time (sec)	4.8384	***Comment***	FD277-1	***Date***	14 Sep 2012 11:48:48			***Date Stamp***	14 Sep 2012 11:48:48
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD277-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	23040	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4761.90	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4272	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4761.76	***Temperature (degree C)***	27.000						

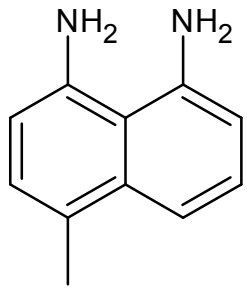


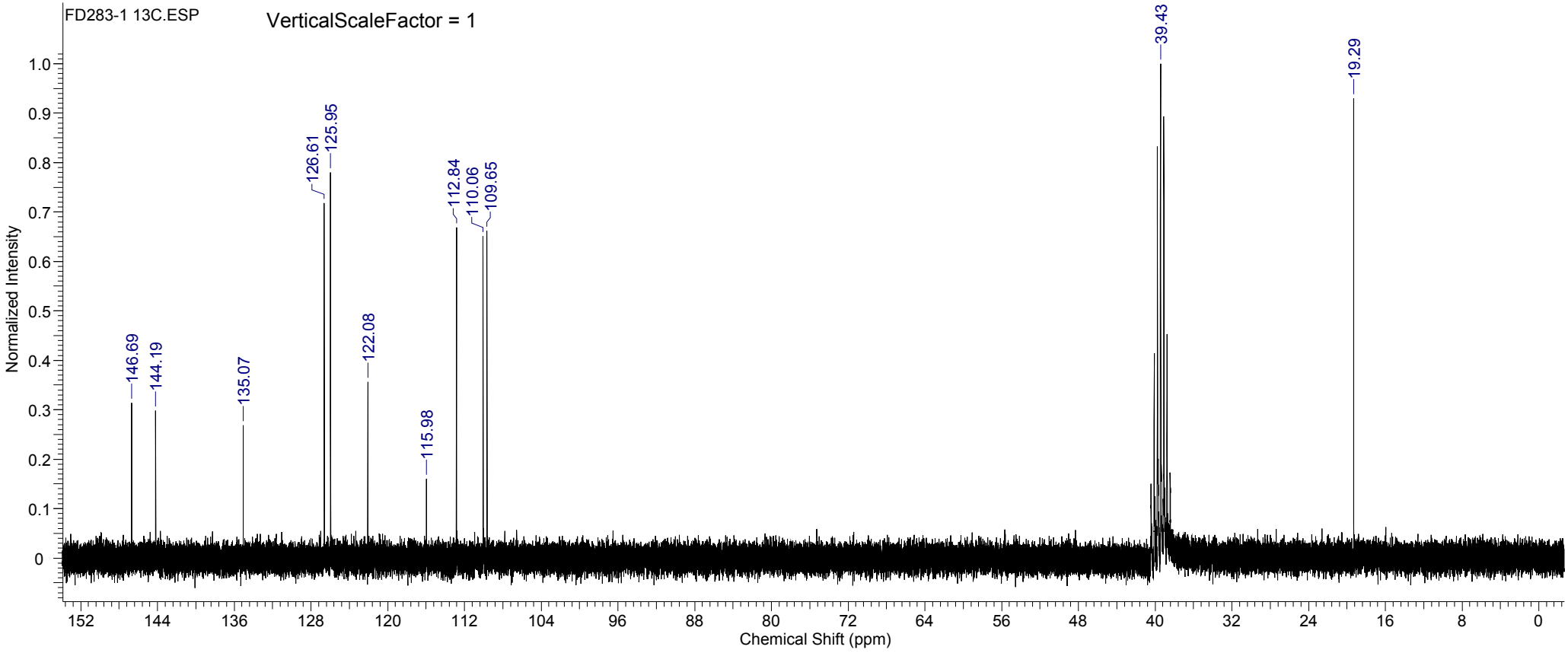


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 48

Acquisition Time (sec)	4.5588	***Comment***	FD283-1	***Date***	30 Sep 2012 16:53:52				
Date Stamp	30 Sep 2012 16:53:52			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD283-1 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1520	***Origin***	spect	***Original Points Count***	71680
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6564.3857	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000

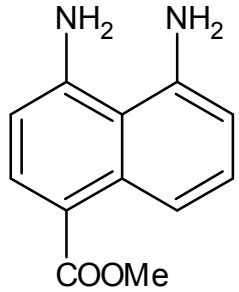


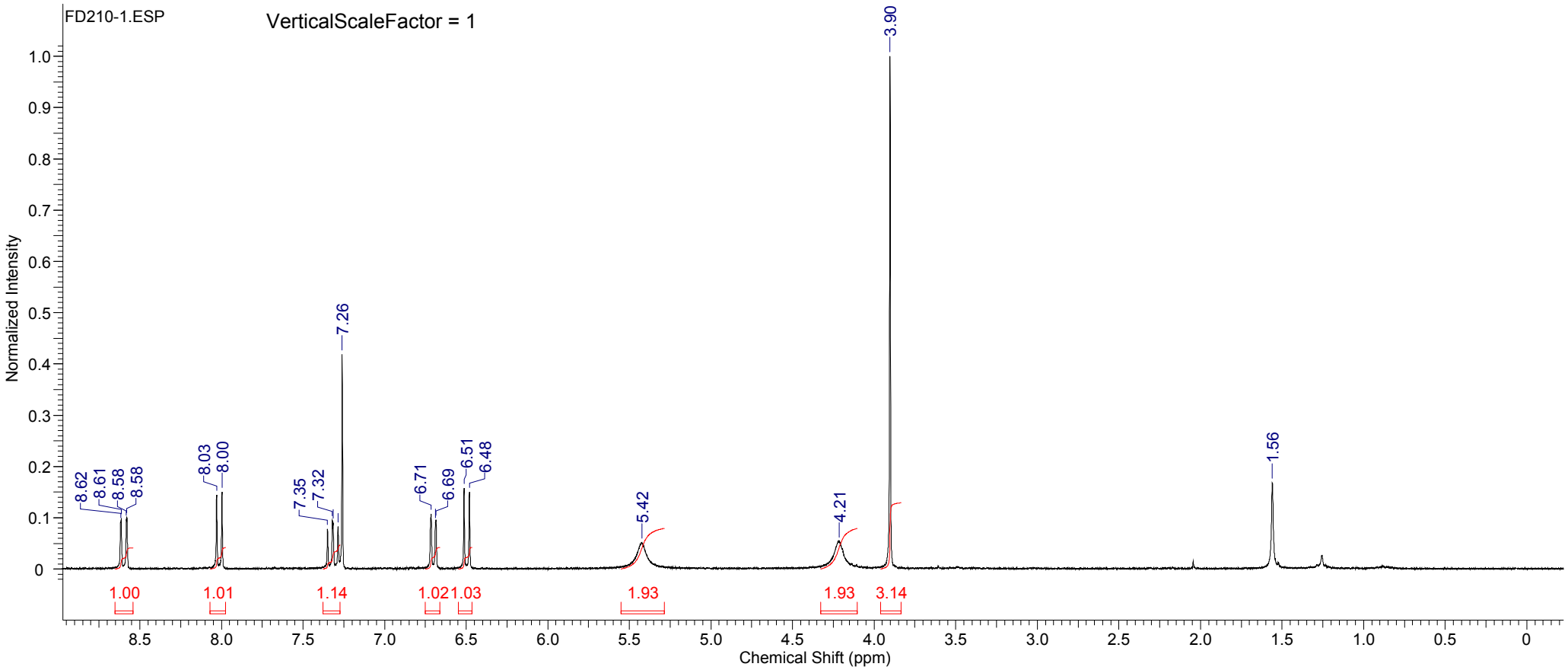


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 50

Acquisition Time (sec)	4.4532	***Date***	15 Feb 2012 11:26:14				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD210\FD210-1\FD210-1.MRC					***Frequency (MHz)***	250.13
Nucleus	1H	***Origin***	Bruker	***Original Points Count***	24576	***Points Count***	65536
Pulse Sequence	ZG30	***Spectrum Offset (Hz)***	1738.2355	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	5518.76





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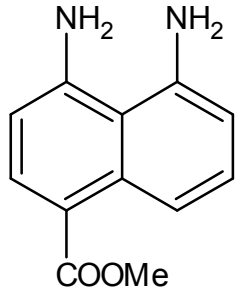
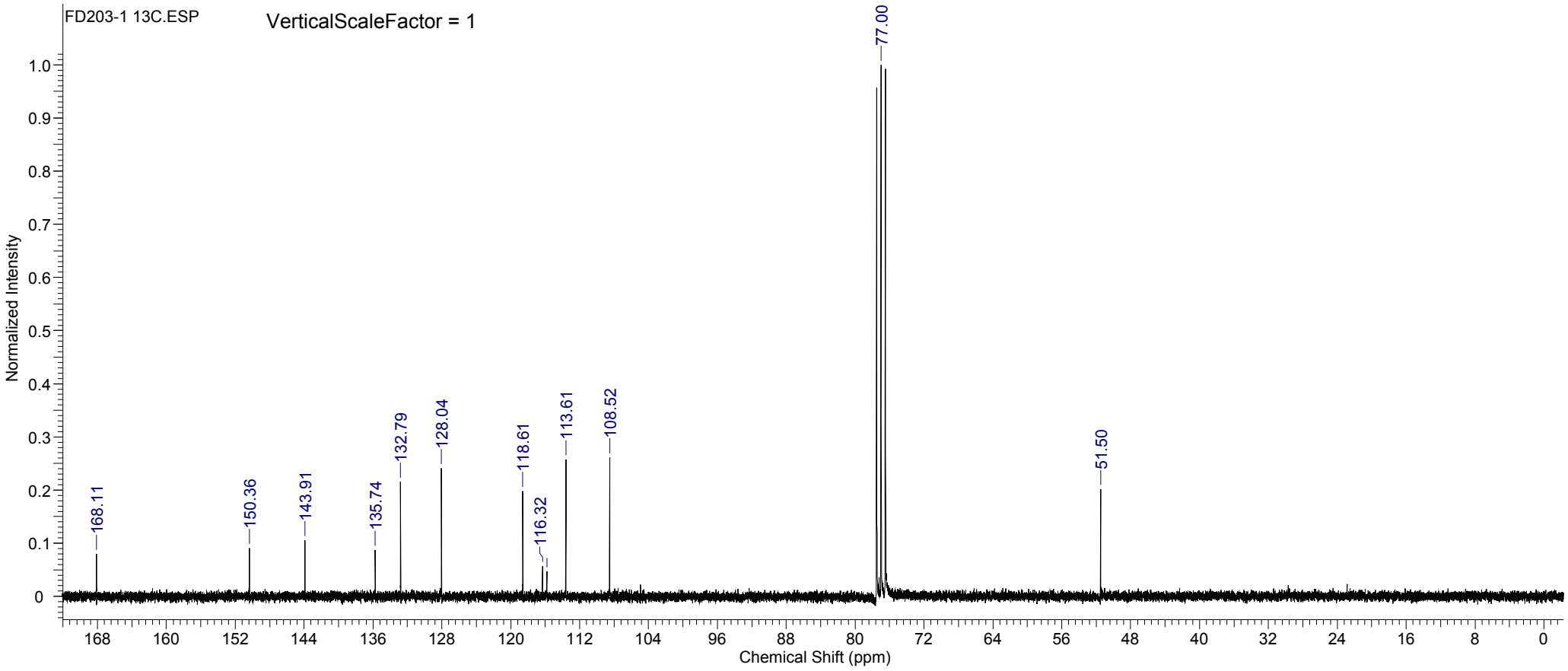
Compound 50

Acquisition Time (sec)	1.6933	***Date***	15 Feb 2012 11:25:20				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD203\FD203-1 13C\FD203-1 13C.MRC					***Frequency (MHz)***	62.90
Nucleus	13C	***Origin***	Bruker	***Original Points Count***	26624	***Points Count***	65536
Pulse Sequence	ZGIG30	***Spectrum Offset (Hz)***	6601.9658	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.27





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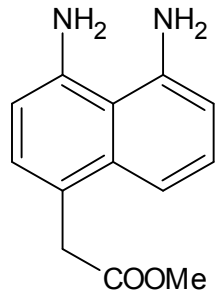
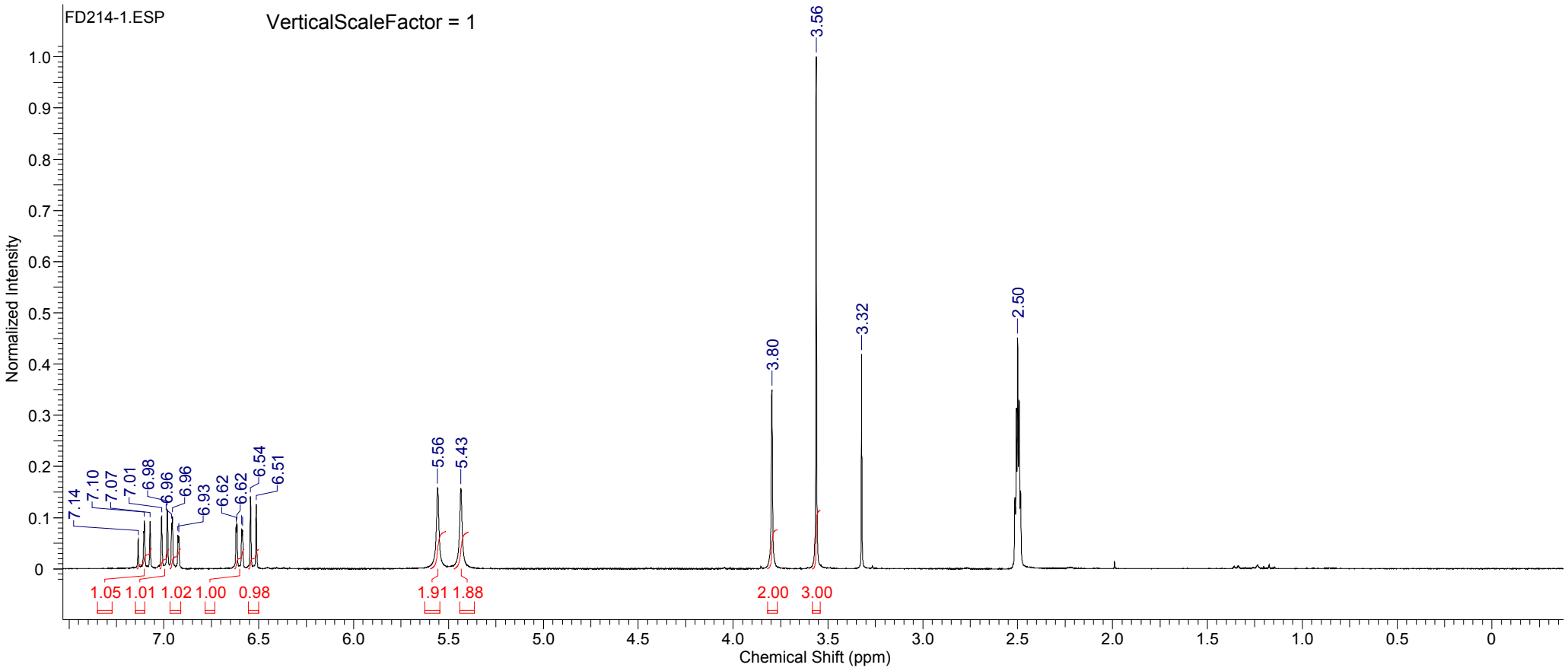
Compound 51

Acquisition Time (sec)	5.3809	***Date***	15 Feb 2012 11:27:40				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD214\FD214-1\FD214-1.MRC					***Frequency (MHz)***	250.13
Nucleus	1H	***Origin***	Bruker	***Original Points Count***	29696	***Points Count***	65536
Pulse Sequence	ZG30	***Spectrum Offset (Hz)***	1747.4584	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	5518.76

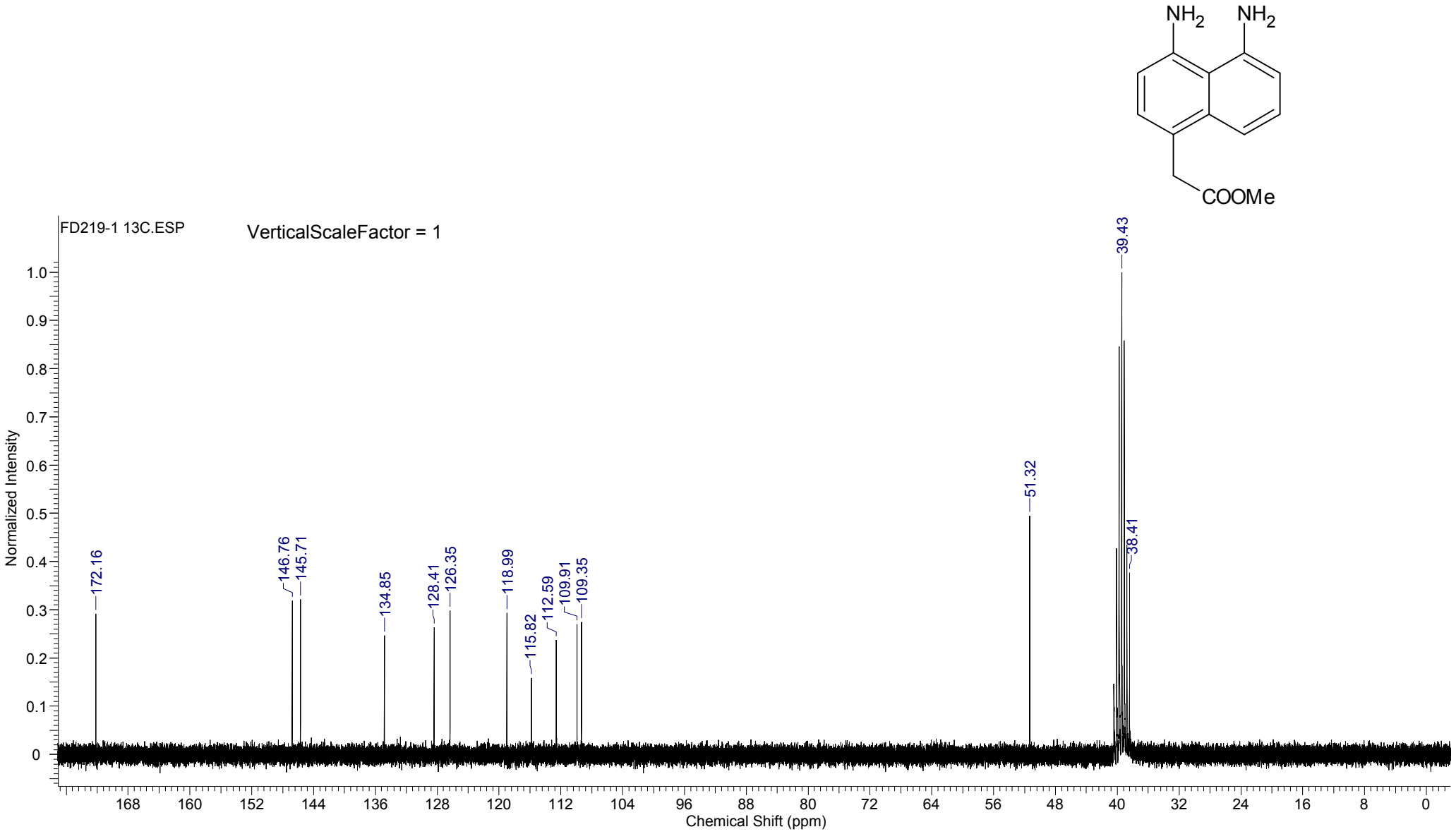




This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 51

Acquisition Time (sec)	3.2358	***Date***	15 Feb 2012 11:27:56				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD219\FD219-1 13C.MRC					***Frequency (MHz)***	62.90
Nucleus	13C	***Origin***	Bruker	***Original Points Count***	51200	***Points Count***	131072
Pulse Sequence	ZGPGVAR	***Spectrum Offset (Hz)***	6564.8369	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15822.79



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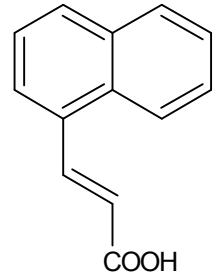
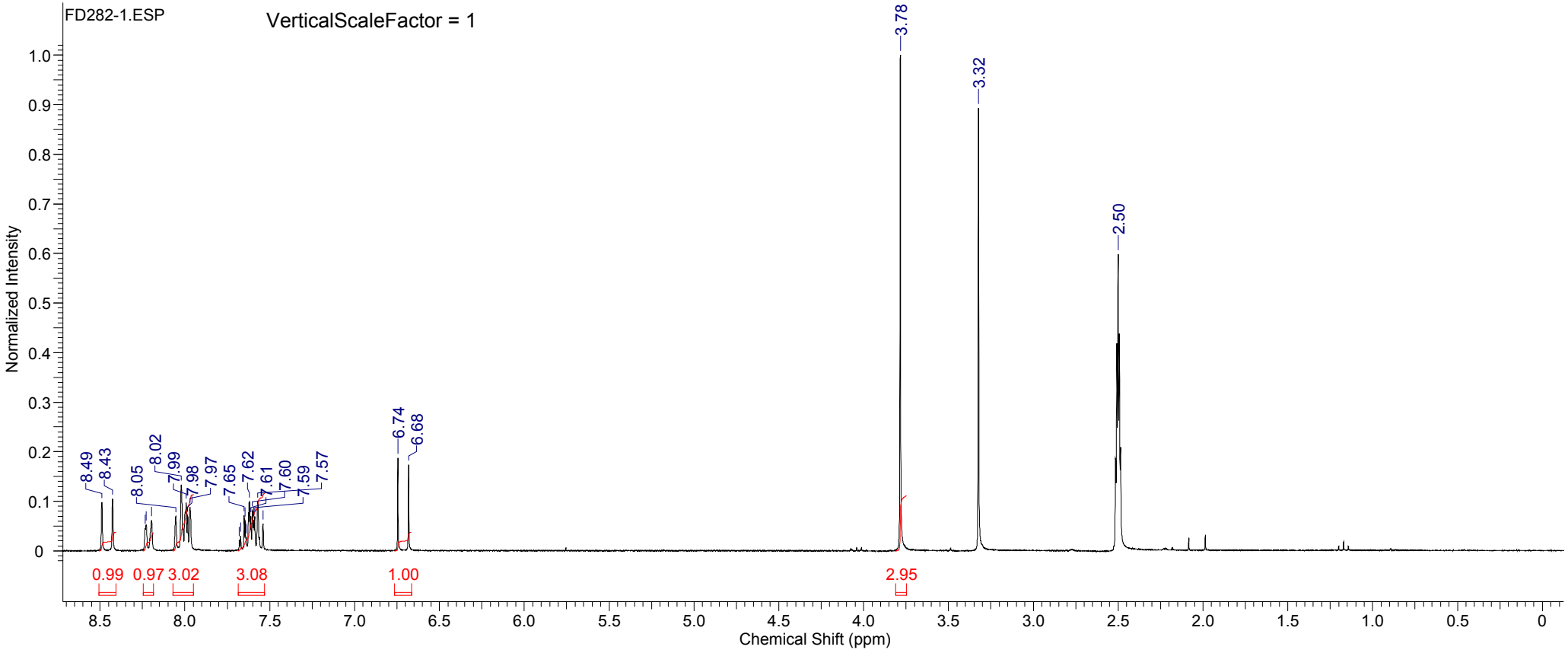
Compound 53

Acquisition Time (sec)	4.9545	***Comment***	FD282-1	***Date***	27 Sep 2012 07:26:24			***Date Stamp***	27 Sep 2012 07:26:24
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD282-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	24576	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4960.32	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.5575	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4960.17	***Temperature (degree C)***	27.000						

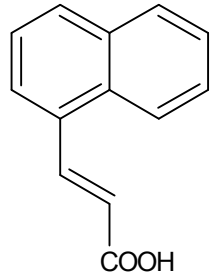


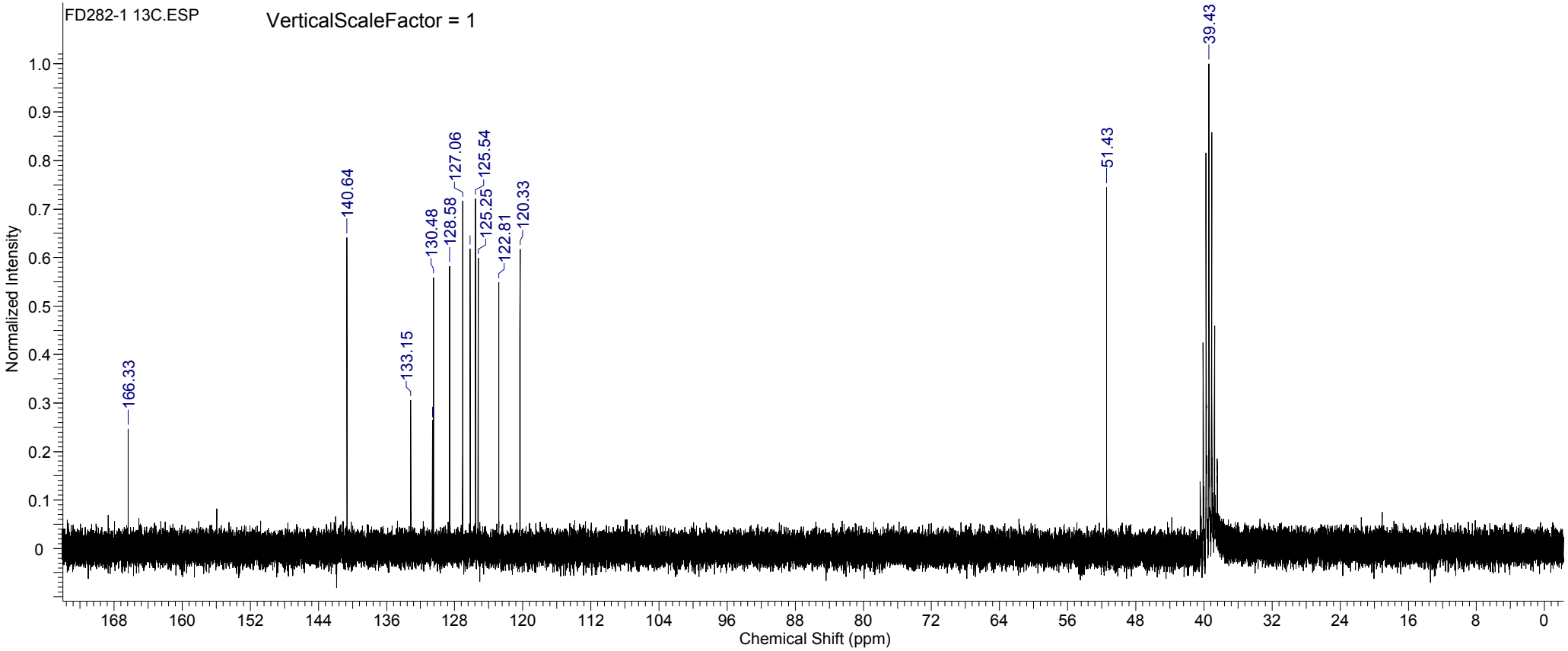


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Compound 53

Acquisition Time (sec)	4.5588	***Comment***	FD282-1	***Date***	29 Sep 2012 02:53:20				
Date Stamp	29 Sep 2012 02:53:20			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD282-1 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1520	***Origin***	spect	***Original Points Count***	71680
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6564.3857	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000





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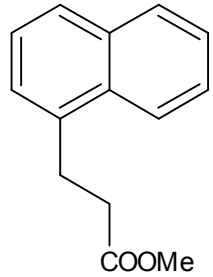
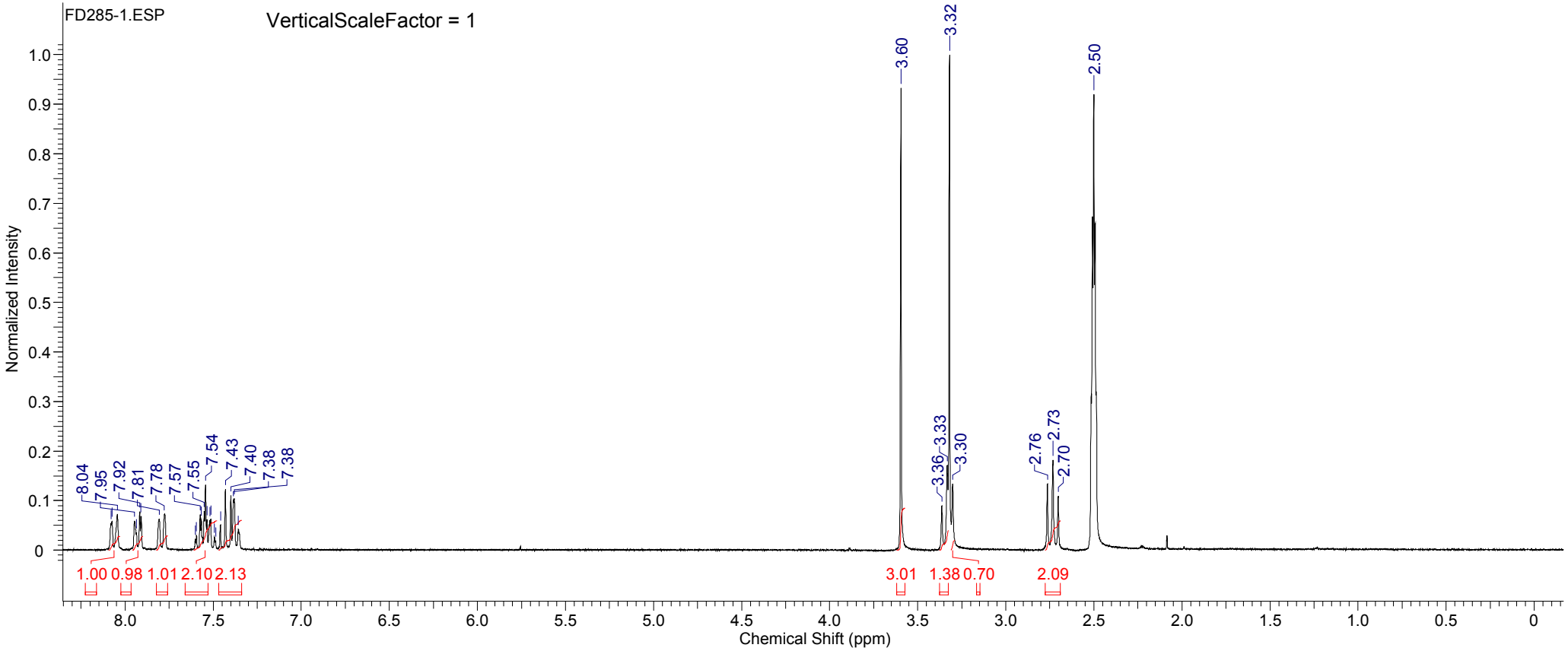
Compound 54

Acquisition Time (sec)	5.1302	***Comment***	FD285-1	***Date***	02 Oct 2012 12:52:48			***Date Stamp***	02 Oct 2012 12:52:48
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD285-1\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	25600	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	645.10	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.7292	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						





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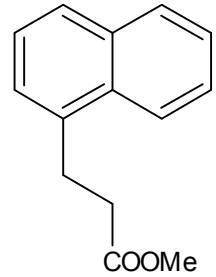
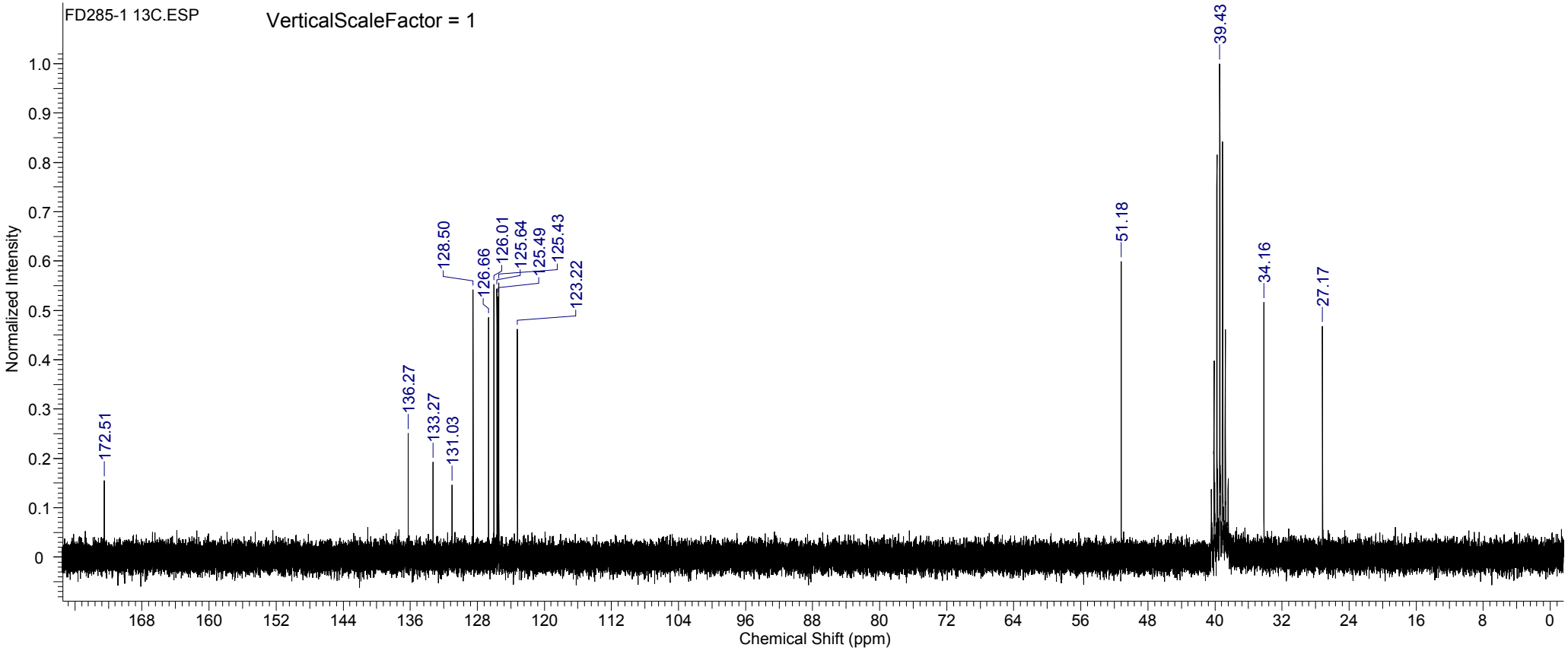
Compound 54

Acquisition Time (sec)	4.5588	***Comment***	FD285-1	***Date***	03 Oct 2012 05:22:40				
Date Stamp	03 Oct 2012 05:22:40			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD285-1 13C\1\FID				
Frequency (MHz)	62.90	***Nucleus***	13C	***Number of Transients***	1520	***Origin***	spect	***Original Points Count***	71680
Owner	service	***Points Count***	131072	***Pulse Sequence***	zgig	***Receiver Gain***	10321.30	***SW(cyclical) (Hz)***	15723.27
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	6564.3857	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000





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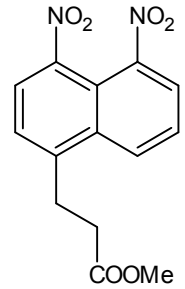
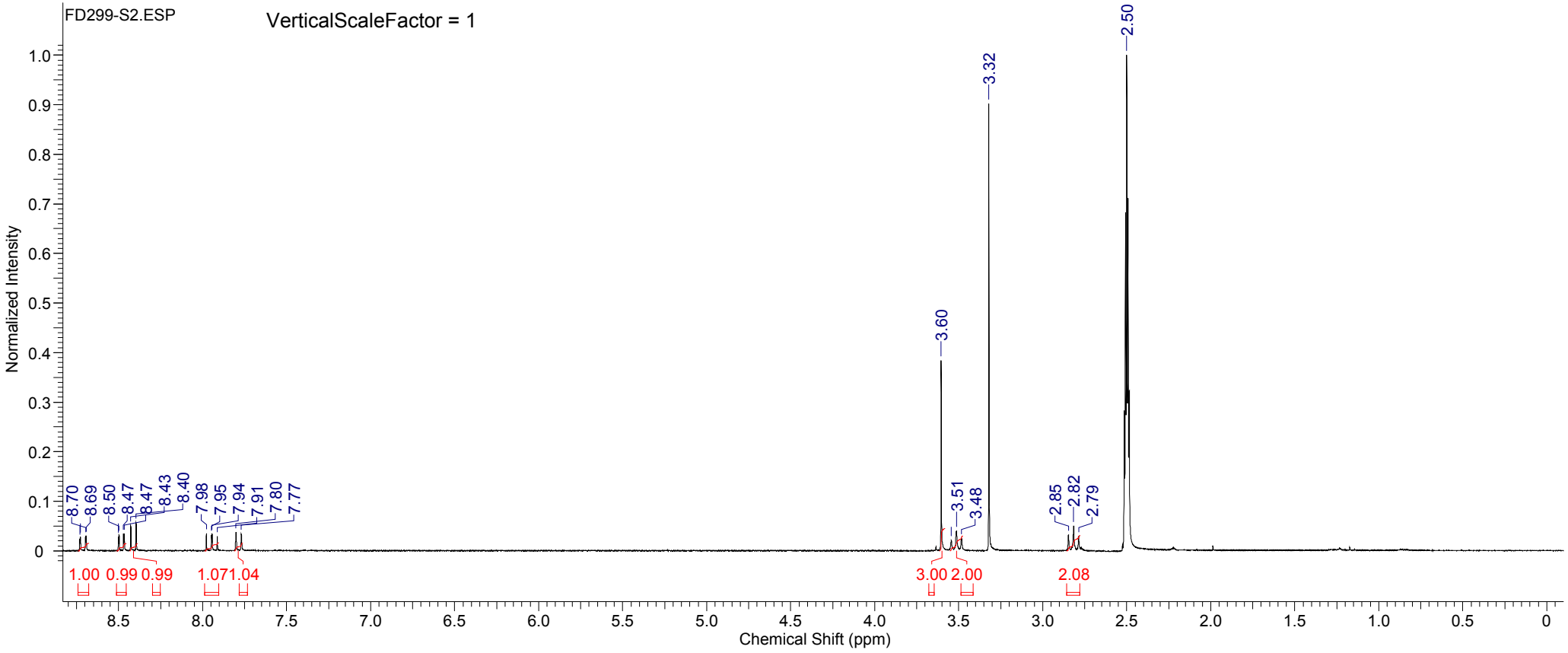
Compound 55

Acquisition Time (sec)	4.5146	***Comment***	FD299-S2	***Date***	11 Jan 2013 15:02:40			***Date Stamp***	11 Jan 2013 15:02:40
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD299-S2\1\FID			***Frequency (MHz)***	250.13	***Nucleus***	1H	***Number of Transients***	24
Origin	spect	***Original Points Count***	22528	***Owner***	service	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	574.70	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4247	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4989.87	***Temperature (degree C)***	27.000						





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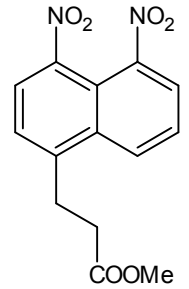
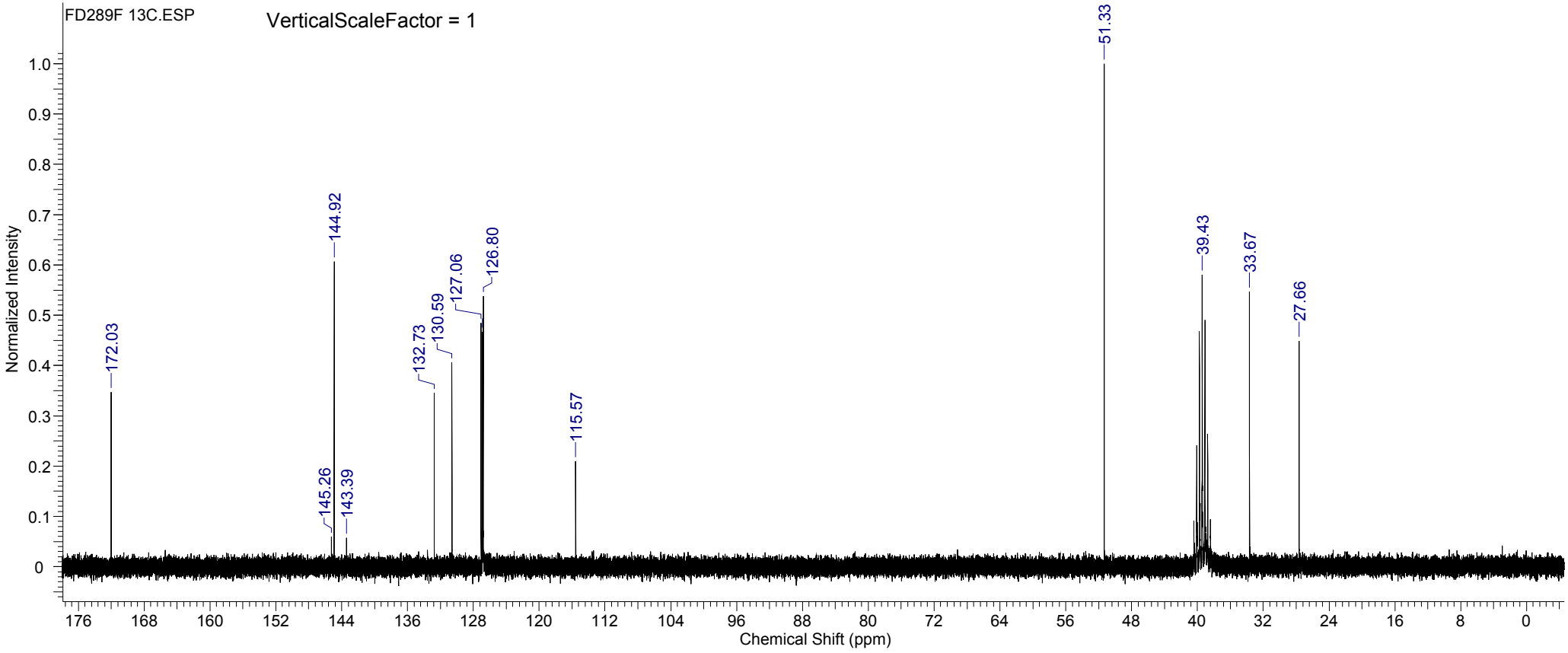
Compound 55

Acquisition Time (sec)	4.5588	***Comment***	FD289F	***Date***	04 Nov 2012 05:56:32				
Date Stamp	04 Nov 2012 05:56:32			***File Name***	C:\USERS\RIKE\DATEN RIKE\NMR\FD289F 13C\1\FID			***Frequency (MHz)***	62.90
Nucleus	13C	***Number of Transients***	1520	***Origin***	spect	***Original Points Count***	71680	***Owner***	service
Points Count	131072	***Pulse Sequence***	zgig	***Receiver Gain***	13004.00	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	6564.7456	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	15723.15	***Temperature (degree C)***	27.000		





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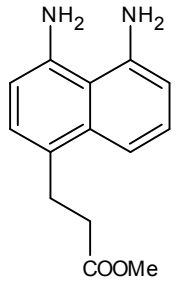
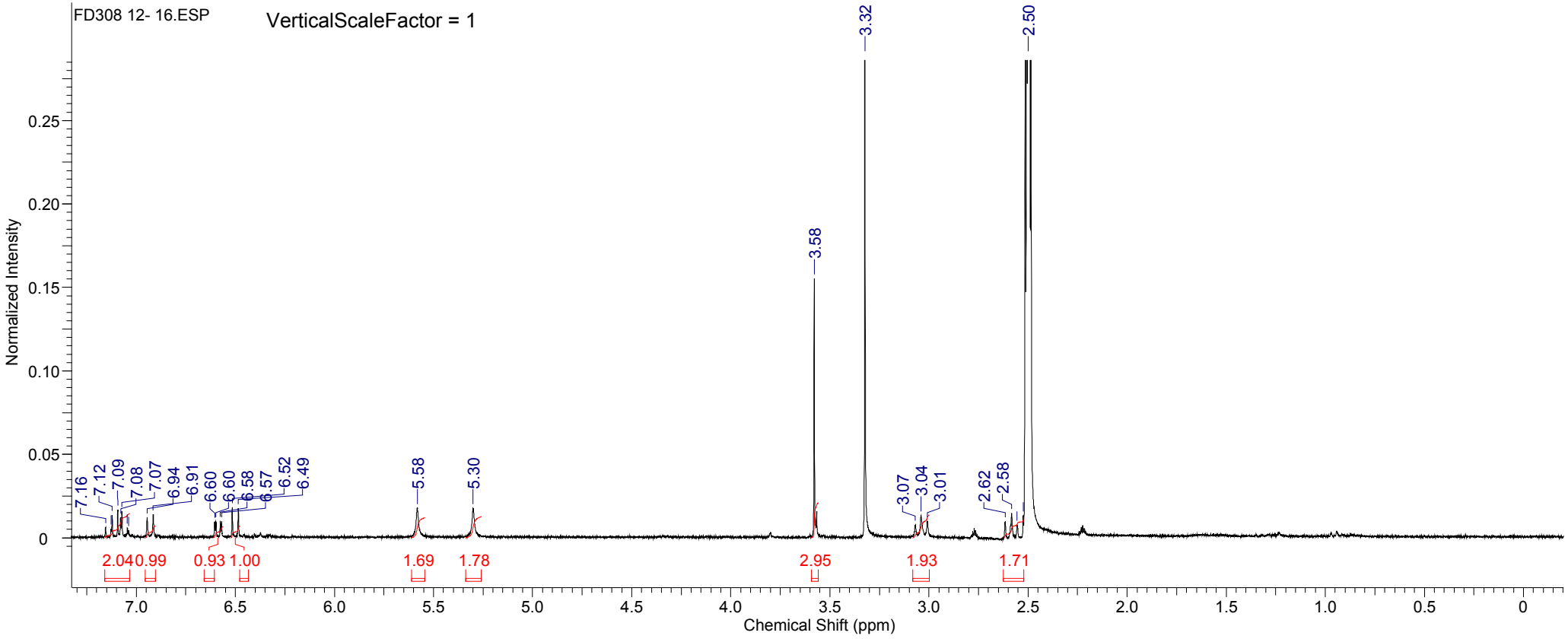
Compound 56

Acquisition Time (sec)	4.5146	***Comment***	FD308 12-16	***Date***	26 Feb 2013 15:24:00			***Date Stamp***	26 Feb 2013 15:24:00
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD308 12- 16\1\FID					***Frequency (MHz)***	250.13	***Nucleus***	1H
Number of Transients	24	***Origin***	spect	***Original Points Count***	22528	***Owner***	service	***Points Count***	32768
Pulse Sequence	zg30	***Receiver Gain***	724.10	***SW(cyclical) (Hz)***	4990.02	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1747.4247
Spectrum Type	STANDARD	***Sweep Width (Hz)***	4989.87	***Temperature (degree C)***	27.000				





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Compound 56

Acquisition Time (sec)	4.8845	***Comment***	FD316-1	***Date***	18 Apr 2013 05:37:36			***Date Stamp***	18 Apr 2013 05:37:36
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\FD316 13C\1\FID			***Frequency (MHz)***	62.90	***Nucleus***	13C	***Number of Transients***	1400
Origin	spect	***Original Points Count***	76800	***Owner***	service	***Points Count***	131072	***Pulse Sequence***	zgig
Receiver Gain	13004.00	***SW(cyclical) (Hz)***	15723.27	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6567.8647	***Spectrum Type***	STANDARD
Sweep Width (Hz)	15723.15	***Temperature (degree C)***	27.000