

# European Journal of Organic Chemistry

Supporting Information

## **RNA Hydrolysis by Heterocyclic Amidines and Guanidines: Parameters Affecting Reactivity**

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## Supporting Information

### Table of contents:

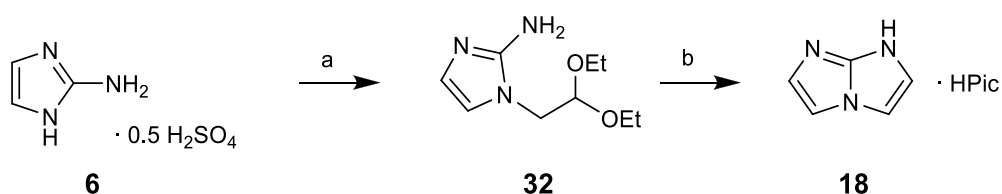
General.....	S2
1 <i>H</i> -Imidazo[1,2- <i>a</i> ]imidazole <b>18</b> .....	S2
9 <i>H</i> -Imidazo[1,2- <i>a</i> ]benzimidazole <b>19</b> .....	S4
5 <i>H</i> -Benzimidazo[1,2- <i>a</i> ]benzimidazole <b>20</b> .....	S5
3,9-Dimethoxy-benzimidazo[1,2- <i>a</i> ]benzimidazole <b>21</b> .....	S6
Methyl benzimidazo[1,2- <i>a</i> ]benzimidazole-3-carboxylate <b>22</b> .....	S8
2-Amino-6-methyl-1 <i>H</i> -perimidine hydrobromide <b>28</b> .....	S10
Methyl 2-amino-1 <i>H</i> -perimidine-6-carboxylate hydrobromide <b>29</b> .....	S12
Methyl 2-(2-amino-1 <i>H</i> -perimidin-7-yl)acetate hydrobromide <b>30</b> .....	S13
Methyl 3-(2-amino-1 <i>H</i> -perimidin-6-yl)propanoate hydrobromide <b>31</b> .....	S15
Cleavage and aggregation studies.....	S17
Estimation of p <i>K</i> <sub>a</sub> values.....	S19
References.....	S19
Additional computational details.....	S20
Energies of compounds and their tautomers.....	S22
xyz-Structures of compounds and their tautomers.....	S23
NMR spectra.....	S84

## General

2-Aminobenzimidazole derivative **11**,<sup>[1]</sup> bislactam **23**,<sup>[2]</sup> as well as 2-aminoperimidine derivatives **25**,<sup>[3]</sup> **26**,<sup>[3]</sup> and **27**<sup>[4]</sup> 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. <sup>1</sup>H and <sup>13</sup>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*<sub>5</sub> ( $\delta_{\text{H}} = 2.50$ ,  $\delta_{\text{C}} = 39.43$ ) or CHCl<sub>3</sub> ( $\delta_{\text{H}} = 7.26$ ,  $\delta_{\text{C}} = 77.00$ ) 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 (Perceptive 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*]imidazole **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**



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**<sup>[5]</sup>

To a suspension of 2-aminoimidazole hemisulfate **6**<sup>[6]</sup> (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 %). <sup>1</sup>H-NMR (250 MHz, CDCl<sub>3</sub>): δ = 6.61 (d, 1H, *J* = 1.4 Hz, *H*-C5), 6.51 (d, 1H, *J* = 1.4 Hz, *H*-C4), 4.59 (t, 1H, *J* = 5.3 Hz, acetal-*H*), 4.30 (br s, 2H, NH<sub>2</sub>), 3.84 (d, 2H, *J* = 5.3 Hz, H<sub>2</sub>C-N1), 3.80 - 3.68 (m, 2H, H<sub>2</sub>C-O), 3.56 - 3.44 (m, 2H, H<sub>2</sub>C-O), 1.20 (t, 6H, *J* = 7.0 Hz, CH<sub>3</sub>). <sup>13</sup>C-NMR (62.9 MHz, CDCl<sub>3</sub>): δ = 149.0, 124.3, 116.0, 102.6, 64.0, 48.5, 15.3. IR (KBr):  $\tilde{\nu}$  = 3399 (s), 3146 (m), 2977 (m), 1655 (m), 1560 (s), 1497 (m), 1381 (m), 1129 (m), 1064 (s), 702 (w).

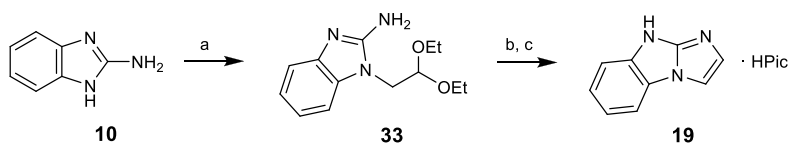
#### Picrate and hydrochloride of 1*H*-imidazo[1,2-*a*]imidazole **18** <sup>[5,7]</sup>

**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<sub>2</sub>O, 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, <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>): δ = 13.11 (br s, 2H, NH), 8.58 (s, 2H, picrate), 7.64 (dd, 2H, *J* = 2.8 Hz, *J* = 0.7 Hz, *H*-C3, *H*-C5), 7.51 (dd, 2H, *J* = 2.8 Hz, *J* = 0.7 Hz, *H*-C2 and *H*-C6). <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>): δ = 160.8, 141.9, 139.2, 125.2, 120.5, 108.8. Elemental analysis for C<sub>13</sub>H<sub>8</sub>N<sub>6</sub>O<sub>7</sub> (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<sup>-</sup>-form).

Alternatively, the crude product was directly purified by HPLC, yielding the TFA salt of **18** as a slightly yellow solid. *R*<sub>f</sub> = 0.22 (DCM/MeOH 9:1). Mp.: decomposition at 280 °C. <sup>1</sup>H-NMR (250 MHz, DMSO-*d*<sub>6</sub>): δ = 13.25 (br. s, 2H, NH), 7.64 (d, 2H, *J* = 2.0 Hz, *H*-C3, *H*-C5), 7.51 (d, 2H, *J* = 2.0 Hz, *H*-C2 und *H*-C6). <sup>13</sup>C-NMR (62.9 MHz, DMSO-*d*<sub>6</sub>): δ = 120.4, 108.6. IR (KBr):  $\tilde{\nu}$  = 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<sup>+</sup>): *m/z* (%) = 107.5 (100) [M+H]<sup>+</sup>, 214.7 (5) [2M+H]<sup>+</sup>, calcd for C<sub>5</sub>H<sub>5</sub>N<sub>3</sub>: 107.05. HRMS (MALDI) *m/z* = 108.05549 [M+H]<sup>+</sup>, calcd for C<sub>5</sub>H<sub>5</sub>N<sub>3</sub>+H<sup>+</sup>: 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*<sub>R</sub> = 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<sup>-</sup>-form). Elemental analysis for C<sub>5</sub>H<sub>5</sub>N<sub>3</sub> · 1.5 HCl · 0.3 H<sub>2</sub>O (167.21): calcd: C, 35.92; H, 4.28; N, 25.13; found: C, 35.55; H, 4.37; N, 25.30.

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

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

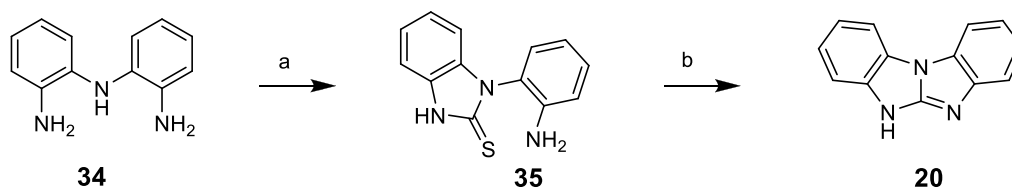
**1-(2,2-Diethoxyethyl)-1H-benzo[*d*]imidazol-2-amine 33** <sup>[7]</sup>

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. <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>): 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, NH<sub>2</sub>), 4.73 (t, 1H, *J* = 5.3 Hz, CH), 4.05 (d, 2H, *J* = 5.3 Hz, CH<sub>2</sub>N), 3.63 (dq, 2H, *J* = 9.5 Hz, *J* = 7.1 Hz, OCH<sub>2</sub>), 3.40 (dq, 2H, *J* = 9.5 Hz, *J* = 7.1 Hz, OCH<sub>2</sub>), 1.01 (t, 6H, *J* = 7.0 Hz, CH<sub>3</sub>). <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>): 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<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub> (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 9H-imidazo[1,2-*a*]benzimidazole 19** <sup>[7]</sup>

**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<sub>2</sub>O, 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<sub>f</sub> = 0.60 (DCM/MeOH 9:1). Mp: decomposition at 234.6 °C. <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>): 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). <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>): 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<sub>15</sub>H<sub>10</sub>N<sub>6</sub>O<sub>7</sub> (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<sup>-</sup>-form).

**5*H*-Benzimidazo[1,2-*a*]benzimidazole 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** <sup>[see also 8]</sup>

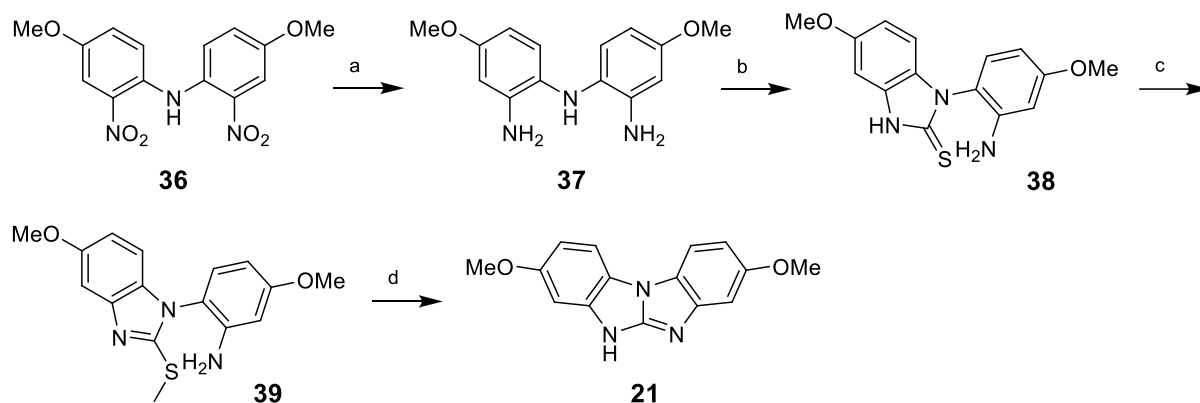
To a solution of bis-(2-aminophenyl)amine **34** (300 mg, 1.51 mmol), which was prepared as described in literature,<sup>[9]</sup> and imidazole (34 mg, 0.5 mmol) in 10 mL of dry MeCN, a solution of 1,1'-thiocarbonyl diimidazole (282 mg, 1.51 mmol) in 10 mL of dry MeCN was added dropwise at 0 °C. After 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.  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 12.90$  (br s, 1H, NH), 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<sub>2</sub>).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta = 168.8, 145.0, 133.4, 131.5, 129.7, 129.2, 122.9, 122.1, 119.6, 116.3, 116.2, 109.54, 109.50$ . IR (neat):  $\tilde{\nu} = 3361$  (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<sub>13</sub>H<sub>11</sub>N<sub>3</sub>S (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** <sup>[see also 10]</sup>

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.  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 12.04$  (br s, 1H, NH), 8.11 - 8.08 (m, 2H, Aryl-H), 7.52 - 7.48 (m, 2H, Aryl-H), 7.33 - 7.20 (m, 4H, Aryl-H).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta = 153.2, 141.0, 126.0, 122.7, 119.7, 114.4, 110.6$ . IR (neat):  $\tilde{\nu} = 2981$  (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<sup>+</sup>):

$m/z$  (%) = 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<sub>2</sub>, Pd/C (10%), MeOH, 60 °C, 16 h, 96 %; b: TCDI, imidazole, MeCN, rt, 16 h, 57 %; c: MeI, AcOH, MeNO<sub>2</sub>, 101 °C, 3 h, rt, overnight, 94 %; d: DMF, 153 °C, 3 days, 12 %.

#### Bis(4-methoxy-2-aminophenyl)amine 37 <sup>[11]</sup>

Bis(4-methoxy-2-nitrophenyl)amine **36** <sup>[11]</sup> (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 %). <sup>1</sup>H-NMR: (250 MHz, DMSO-*d*<sub>6</sub>): 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, NH), 4.67 (s, 4H, NH<sub>2</sub>) 3.61 (s, 6H, OCH<sub>3</sub>).

#### 1-(2-Amino-4-methoxyphenyl)-5-methoxy-1H-benzo[*d*]imidazole-2(3H)-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<sub>4</sub>. 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. <sup>1</sup>H-NMR (250 MHz, DMSO-*d*<sub>6</sub>): δ = 12.74 (s, 1H, NH), 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<sub>2</sub>), 3.76 (s, 3H, OCH<sub>3</sub>), 3.74 (s, 3H, OCH<sub>3</sub>). <sup>13</sup>C-NMR (125.8 MHz, DMSO-*d*<sub>6</sub>): 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):  $\tilde{\nu}$  = 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<sup>+</sup>): m/z (%) = 302.1 [M+H]<sup>+</sup>, calcd for C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>S: 301.09. HRMS (MALDI) m/z = 302.09577 [M+H]<sup>+</sup>, calcd for C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>S+H<sup>+</sup>: 302.09577.

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

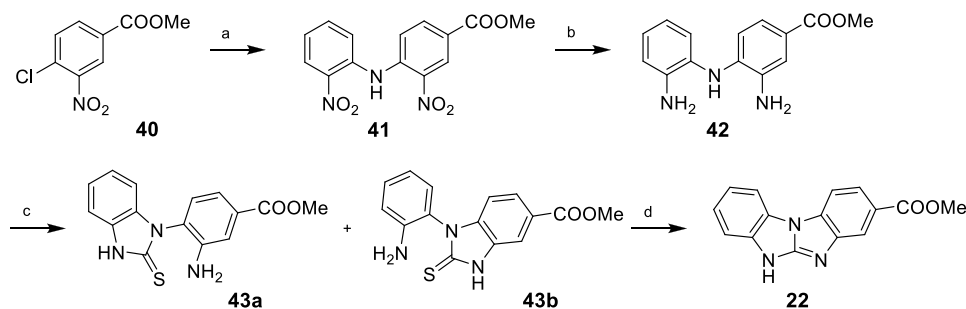
To a solution of thiourea **38** (307 mg, 1.01 mmol) in 20 ml nitromethane, glacial acetic acid (0.23 mL, 4.04 mmol) and MeI (126  $\mu$ L, 2.02 mmol) were added. The reaction mixture was refluxed for 3 h and then stirred at rt overnight. After evaporation of the solvent, the residue was dissolved in 50 mL DCM. The organic phase was washed with 50 mL of a saturated solution of NaHCO<sub>3</sub> and brine, dried over MgSO<sub>4</sub> and evaporated to dryness. Column chromatography (cyclohexane/EtOAc 2:1) yielded 300 mg of the product as a colorless solid (94 %). Mp: 187 °C. <sup>1</sup>H-NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  = 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, NH<sub>2</sub>), 3.77 (s, 3H, OCH<sub>3</sub>), 3.74 (s, 3H, OCH<sub>3</sub>), 2.63 (s, 3H, SCH<sub>3</sub>). <sup>13</sup>C-NMR (125.8 MHz, DMSO-d<sub>6</sub>):  $\delta$  = 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):  $\tilde{\nu}$  = 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<sup>+</sup>): m/z (%) = 316.2 (100) [M+H]<sup>+</sup>, calcd for C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S: 315.1. HRMS (MALDI) m/z = 316.11191 [M+H]<sup>+</sup>, calcd for C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S+H<sup>+</sup>: 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. <sup>1</sup>H-NMR (250 MHz, DMSO-d<sub>6</sub>):  $\delta$  = 11.93 (s, 1H, NH), 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, OCH<sub>3</sub>). IR (neat):  $\tilde{\nu}$  = 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<sup>+</sup>): m/z (%) = 267.8 (100) [M+H]<sup>+</sup>, calcd for C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub>: 267.1. HRMS (MALDI) m/z = 268.10849 [M+H]<sup>+</sup>, calcd for C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub>+H<sup>+</sup>: 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.  $^1H$ -NMR (250 MHz, DMSO- $d_6$ ):  $\delta$  = 10.77 (br s, 1H, NH), 8.68 (d, 1H,  $J$  = 2.2 Hz, *H*-C2), 8.21 (dd, 1H,  $J$  = 8.5 Hz,  $J$  = 1.5 Hz, *H*-C3'), 8.07 (dd, 1H,  $J$  = 8.8 Hz,  $J$  = 2.1 Hz, *H*-C6), 7.83 - 7.72 (m, 2H, *H*-C5', *H*-C6'), 7.49 (d, 1H,  $J$  = 9.0 Hz, *H*-C5), 7.45 - 7.39 (m, 1H, *H*-C4'), 3.87 (s, 3H, OCH<sub>3</sub>).  $^{13}C$ -NMR (62.9 MHz, DMSO- $d_6$ ):  $\delta$  = 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):  $\tilde{\nu}$  = 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.  $^1H$ -NMR (250 MHz, DMSO- $d_6$ ):  $\delta$  = 7.30 (d, 1H,  $J$  = 2.0 Hz, *H*-C2), 7.10 (dd, 1H,  $J$  = 8.2 Hz,  $J$  = 2.0 Hz, *H*-C6), 6.94 - 6.88 (m, 2H, Aryl-*H*), 6.76 (dd, 1H,  $J$  = 8.6 Hz,  $J$  = 1.7 Hz, Aryl-*H*), 6.64 (br s, 1H, NH), 6.60 - 6.54 (m, 1H, Aryl-*H*), 6.31 (d, 1H,  $J$  = 8.2 Hz, *H*-C5), 4.95 (br s, 2H,  $NH_2$ ), 4.73 (br s, 2H,  $NH_2$ ), 3.73 (s, 3H, OCH<sub>3</sub>).  $^{13}C$ -NMR (62.9 MHz, DMSO- $d_6$ ):  $\delta$  = 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):  $\tilde{\nu}$  = 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.

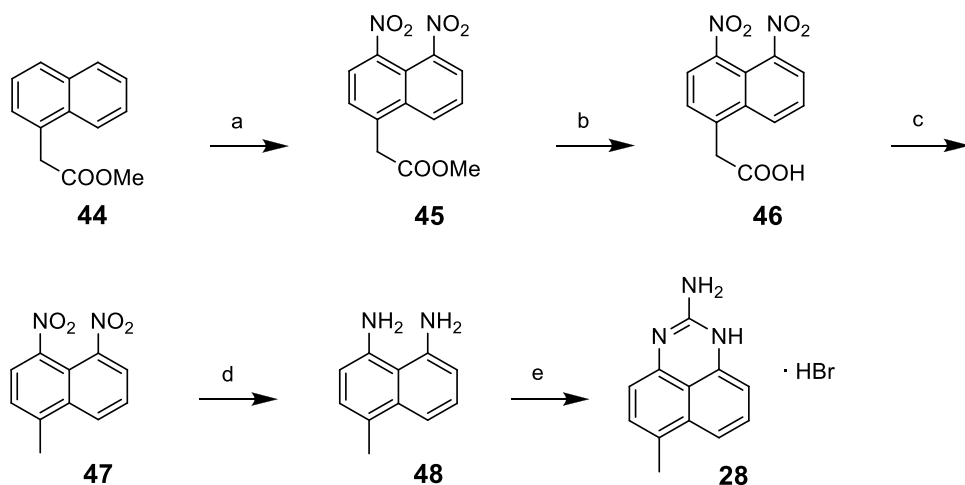
**Mixture of methyl 3-amino-4-(1,2-dihydro-2-thioxobenzo[d]imidazol-3-yl)benzoate 43a and methyl 1-(2-aminophenyl)-2,3-dihydro-2-thioxo-1H-benzo[d]imidazole-5-carboxylate 43b**

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):  $\tilde{\nu}$  = 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<sup>-</sup>):  $m/z$  (%) = 297.9 (100) [M-H]<sup>-</sup>, 148.6 (15) [M-2H]<sup>2-</sup>, 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. <sup>1</sup>H-NMR (250 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  = 12.26 (br s, 1H, NH), 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, OCH<sub>3</sub>). <sup>13</sup>C-NMR (125.8 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  = 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):  $\tilde{\nu}$  = 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<sup>+</sup>):  $m/z$  (%) = 265.9 (100) [M+H]<sup>+</sup>, 531.5 (6) [2M+H]<sup>+</sup>, calcd for  $C_{15}H_{11}N_3O_2$ : 265.09. HRMS (MALDI)  $m/z$  = 266.09323 [M+H]<sup>+</sup>, 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:  $\text{HNO}_3/\text{H}_2\text{SO}_4$ , 0 °C, 10 min, 42%; b: 6 N HCl, 100 °C, 2 h 15 min, 89 %; c:  $\text{NEt}_3$ , acetone, rt, 3 h, 97 %; d:  $\text{Et}_3\text{SiH}$ , Pd/C (10 %), MeOH, rt, 18 min, 93 %; e: 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** <sup>[13]</sup> (3.0 g, 15 mmol) in 6.6 mL conc.  $\text{H}_2\text{SO}_4$  the mixture of 2.2 mL conc.  $\text{HNO}_3$  and 2 mL conc.  $\text{H}_2\text{SO}_4$  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  $\text{Na}_2\text{CO}_3$  four times followed by washing with 15 mL of a 1:1 mixture of *n*-hexane and  $\text{Et}_2\text{O}$ . 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.  $^1\text{H-NMR}$  (250 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 8.55$  (dd, 1H,  $J = 8.5$  Hz,  $J = 1.0$  Hz, *H*-C7 or C5), 8.51 - 8.44 (m, 2H, *H*-C2, *H*-C5 or C7), 7.95 (dd, 1H,  $J = 8.6$  Hz,  $J = 7.7$  Hz, *H*-C6), 7.88 (d, 1H,  $J = 8.0$  Hz, *H*-C3), 4.47 (s, 2H,  $\text{CH}_2$ ), 3.65 (s, 3H,  $\text{OCH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 170.4, 145.1, 144.0, 139.0, 133.4, 131.2, 129.1, 127.1, 127.0, 126.8, 115.5, 52.1, 38.0$ . IR (neat):  $\tilde{\nu} = 3113$  (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  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_6$  (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.  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 12.81$  (br s, 1H, COOH), 8.55 (dd, 1H,  $J = 8.5$  Hz,  $J = 1.1$  Hz, *H-C7* or *C5*), 8.50 - 8.43 (m, 2 H, *H-C2*, *H-C5* or *C7*), 7.95 (dd, 1H,  $J = 8.5$  Hz,  $J = 7.9$  Hz, *H-C6*), 7.87 (d, 1 H,  $J = 7.9$  Hz, *H-C3*), 4.36 (s, 2 H,  $\text{CH}_2$ ).  $^{13}\text{C-NMR}$  (125.8 MHz, DMSO- $d_6$ ):  $\delta = 171.6, 145.1, 143.9, 140.0, 133.5, 131.3, 129.0, 127.1, 127.0, 126.9, 115.6, 38.6$ . IR (neat):  $\tilde{\nu} = (2861$  (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) [ $\text{M-NO}_2$ ], calcd for  $\text{C}_{12}\text{H}_8\text{N}_2\text{O}_6$ : 276.04.

#### 4-Methyl-1,8-dinitronaphthalene **47** <sup>[14]</sup>

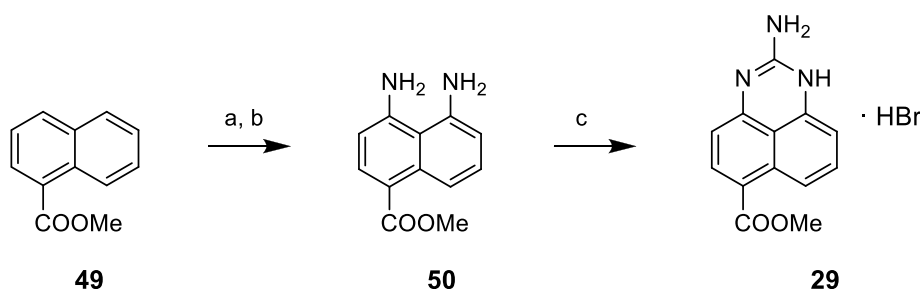
Carboxylic acid **46** (200 mg, 0.72 mmol) was dissolved in 7 mL acetone and  $\text{NEt}_3$  was added (0.10 mL, 0.72 mmol). The reaction mixture was stirred at rt for 3 h. After evaporation of the solvent, column chromatography (*n*-hexane/EtOAc 3:1) yielded in 162 mg of the title compound as a colorless solid (97 %).  $R_f = 0.19$  (*n*-hexane/EtOAc 3:1). Mp: 143 – 144 °C; Lit: 143 °C.<sup>[14]</sup>  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 8.63$  (dd, 1H,  $J = 8.5$  Hz,  $J = 1.1$  Hz, *H-C5* or *C7*), 8.48 (dd, 1H,  $J = 7.8$  Hz,  $J = 1.1$  Hz, *H-C7* or *C5*), 8.39 (d, 1H,  $J = 7.8$  Hz, *H-C2*), 7.94 (dd, 1H,  $J = 8.5$  Hz,  $J = 7.7$  Hz, *H-C6*), 7.77 (dd, 1H,  $J = 7.9$  Hz,  $J = 1.0$  Hz, *H-C3*), 2.85 (d, 3H,  $J = 0.5$  Hz,  $\text{CH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta = 145.1, 143.1, 142.9, 133.4, 131.1, 127.3, 126.9, 126.8, 126.8, 115.4, 19.8$ . IR (neat):  $\tilde{\nu} = 2970$  (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  $\text{C}_{11}\text{H}_8\text{N}_2\text{O}_4$  (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** <sup>[14]</sup>

To the suspension of dinitro compound **47** (277 mg, 1.19 mmol) and Pd/C (28 mg) in 10 mL of dry MeOH,  $\text{Et}_3\text{SiH}$  (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.<sup>[14]</sup>  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 7.12$  (m, 1H, *H-C6*), 7.02 (dd, 1H,  $J = 8.3$  Hz,  $J = 1.3$  Hz, *H-C5* or *C7*), 6.93 (d, 1H,  $J = 7.4$  Hz, *H-C2* or *C3*), 6.59 (dd, 1H,  $J = 7.3$  Hz,  $J = 1.3$  Hz, *H-C7* or *C5*), 6.51 (d, 1H,  $J = 7.5$  Hz, *H-C3* or *C2*), 5.60 (br s, 2H,  $\text{NH}_2$ ), 5.19 (br s, 2H,  $\text{NH}_2$ ), 2.36 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta = 146.7, 144.2, 135.1, 126.6, 126.0, 122.1, 116.0, 112.8, 110.1, 109.7, 19.3$ . IR (neat):  $\tilde{\nu} = 3351$  (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:  $\text{C}_{11}\text{H}_{12}\text{N}_2$  (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-1H-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.  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta = 11.29$  (br s, 2H, NH), 7.81 (br s, 2H,  $\text{NH}_2$ ), 7.45 - 7.34 (m, 2H, H-C8, H-C7), 7.22 (dd, 1H,  $J = 7.6$  Hz,  $J = 0.9$  Hz, H-C5), 6.85 (dd, 1H,  $J = 6.7$  Hz,  $J = 1.5$  Hz, H-C9), 6.24 (d, 1H,  $J = 7.6$  Hz, H-C4), 2.41 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta = 149.6, 133.0, 132.5, 130.7, 128.0, 128.0, 126.7, 117.3, 115.0, 106.7, 106.2, 18.1$ . IR (neat):  $\tilde{\nu} = 3275$  (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  $\text{C}_{12}\text{H}_{11}\text{N}_3 \cdot \text{HBr}$  (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-1H-perimidine-6-carboxylate hydrobromide 29**

a:  $\text{HNO}_3/\text{H}_2\text{SO}_4$ , 0 °C, 10 min; b:  $\text{Et}_3\text{SiH}$ , 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**

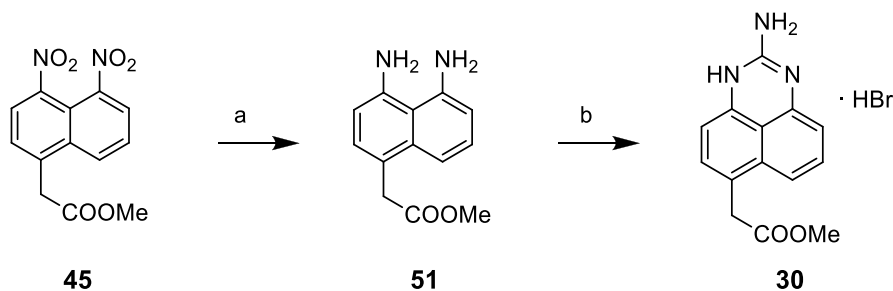
To a solution of methyl 1-naphthoic acid **49** <sup>[15]</sup> (3.70 g, 19.9 mmol) in 8.8 mL conc.  $\text{H}_2\text{SO}_4$  the mixture of 2.9 mL conc.  $\text{HNO}_3$  and 2.7 mL conc.  $\text{H}_2\text{SO}_4$  was added at 0 °C. The dark, viscous mixture was stirred at 0 °C for 10 min before it was poured on ice resulting in precipitation of an off-white solid. The precipitate was filtered off and washed with 10 mL of 2 M  $\text{Na}_2\text{CO}_3$  five times followed by washing with 40 mL of a 1:1 mixture of *n*-hexane and  $\text{Et}_2\text{O}$ . 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),  $\text{Et}_3\text{SiH}$  (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.  $^1\text{H-NMR}$  (250 MHz,  $\text{CDCl}_3$ ):  $\delta = 8.60$  (dd, 1H,  $J = 8.7$  Hz,  $J = 0.9$  Hz, *H-C8*), 8.02 (d, 1H,  $J = 8.1$  Hz, *H-C2*), 7.32 (dd, 1H,  $J = 8.7$  Hz,  $J = 7.4$  Hz, *H-C7*), 6.70 (dd, 1H,  $J = 7.3$  Hz,  $J = 0.8$  Hz, *H-C6*); 6.50 (d, 1H,  $J = 8.1$  Hz, *H-C3*), 5.42 (br s, 2H,  $\text{NH}_2$ ), 4.21 (br s, 2H,  $\text{NH}_2$ ), 3.90 (s, 3H,  $\text{OCH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz,  $\text{CDCl}_3$ ):  $\delta = 168.1, 150.4, 143.9, 135.7, 132.8, 128.0, 118.6, 116.3, 115.8, 113.6, 108.5, 51.5$ . IR (KBr):  $\tilde{\nu} = 3407$  (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  $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2$  (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.  $^1\text{H-NMR}$  (250 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 11.76$  (br s, 2H,  $\text{NH}$ ), 8.41 (dd, 1H,  $J = 8.8$  Hz,  $J = 0.8$  Hz, *H-C7*), 8.13 (d, 1H,  $J = 8.1$  Hz, *H-C5*), 8.07 (br s, 2H,  $\text{NH}_2$ ), 7.56 (dd, 1H,  $J = 8.8$  Hz,  $J = 7.6$  Hz, *H-C8*), 6.97 (dd, 1H,  $J = 7.6$  Hz,  $J = 0.8$  Hz, *H-C9*), 6.89 (d, 1H,  $J = 8.1$  Hz, *H-C4*), 3.87 (s, 3H,  $\text{OCH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 166.0, 149.4, 137.8, 133.8, 133.1, 132.0, 130.1, 118.6, 117.9, 115.3, 107.5, 105.8, 51.7$ . IR (neat):  $\tilde{\nu} = 3114$  (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<sup>+</sup>):  $m/z$  (%) = 242.6 (100)  $[\text{M}+\text{H}]^+$ , calcd for  $\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}_2$ : 241.09. Elemental analysis for  $\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}_2 \cdot \text{HBr}$  (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



a:  $\text{Et}_3\text{SiH}$ , Pd/C (10%), MeOH, rt, 15 min, 91 %; b: BrCN, DCM (abs.), 40 °C, 6.5 h, rt, 16 h, 76 %.

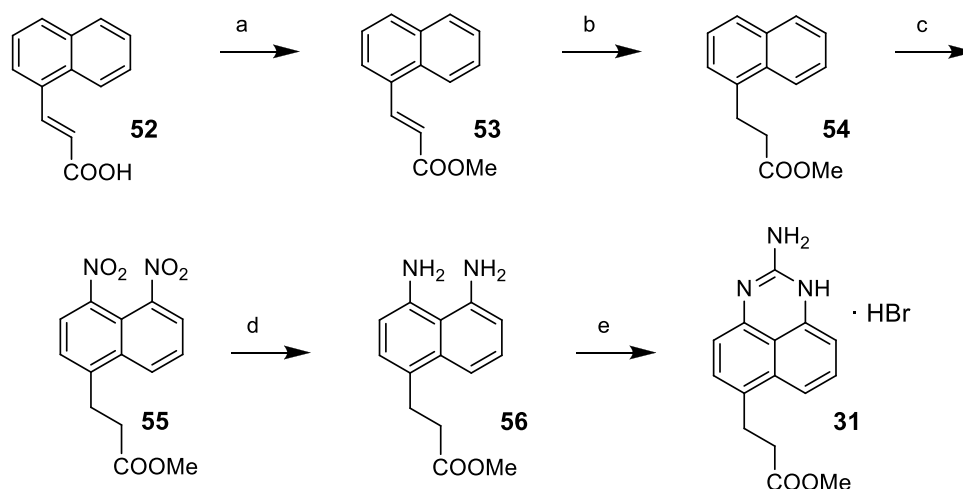
**Methyl 2-(1,8-diaminonaphthalen-4-yl)acetate 51**

To the suspension of dinitro compound **45** (352 mg, 1.21 mmol) and Pd/C (40 mg) in 5 mL of dry MeOH, Et<sub>3</sub>SiH (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<sub>f</sub>* = 0.33 (*n*-hexane/EtOAc 1:1). Mp: 107 – 109 °C. <sup>1</sup>H-NMR (250 MHz, DMSO-d<sub>6</sub>): δ = 7.11 (dd, 1H, *J* = 8.4 Hz, *J* = 7.5 Hz, *H*-C6), 7.00 (d, 1H, *J* = 7.8 Hz, *H*-C3), 6.94 (dd, 1H, *J* = 8.5 Hz, *J* = 1.1 Hz, *H*-C5), 6.61 (dd, 1H, *J* = 7.5 Hz, *J* = 1.1 Hz, *H*-C7), 6.53 (d, 1H, *J* = 7.5 Hz, *H*-C2), 5.56 (br s, 2H, NH<sub>2</sub>), 5.43 (br s, 2H, NH<sub>2</sub>), 3.80 (s, 2H, CH<sub>2</sub>), 3.56 (s, 3H, OCH<sub>3</sub>). <sup>13</sup>C-NMR (62.9 MHz, DMSO-d<sub>6</sub>): 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):  $\tilde{\nu}$  = 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<sub>13</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> (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<sub>f</sub>* = 0.26 (DCM/MeOH 9:1 + 1 % AcOH). Mp: 215 – 217 °C. <sup>1</sup>H-NMR (250 MHz, DMSO-d<sub>6</sub>): δ = 11.36 (br s, 2H, NH), 7.86 (br s, 2H, NH<sub>2</sub>), 7.40 (dd, 1H, *J* = 8.5 Hz, *J* = 7.3 Hz, *H*-C8), 7.32 - 7.28 (m, 2H, *H*-C5, *H*-C7), 6.86 (dd, 1H, *J* = 7.3 Hz, *J* = 0.9 Hz, *H*-C9), 6.79 (d, 1H, *J* = 7.6 Hz, *H*-C4), 3.93 (s, 2H, CH<sub>2</sub>), 3.59 (s, 3H, OCH<sub>3</sub>). <sup>13</sup>C-NMR (62.9 MHz, DMSO-d<sub>6</sub>): 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):  $\tilde{\nu}$  = 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<sub>14</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub> · 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:  $\text{SOCl}_2$ , MeOH (abs.), 0 °C - RT, 20 h, 97 %; b: 5 bar  $\text{H}_2$ , Pd/C (10%), EtOAc (abs.), 4 h, 97 %; c:  $\text{HNO}_3/\text{H}_2\text{SO}_4$ , -5 °C, 5 min, 36 %; d: 4 bar  $\text{H}_2$ , 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,  $\text{SOCl}_2$  (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  $\text{NaHCO}_3$ . The combined organic phases were dried over  $\text{Na}_2\text{SO}_4$  and evaporated to dryness, yielding 1.04 g of an orange oil (97 %).  $R_f = 0.23$  (*n*-hexane/EtOAc 19:1).  $^1\text{H-NMR}$  (250 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 8.46$  (d, 1H,  $J = 15.8$  Hz, =CH-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, =CH-COOMe), 3.78 (s, 3H,  $\text{OCH}_3$ ).  $^{13}\text{C-NMR}$  (62.9 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 166.3, 140.6, 133.2, 130.6, 130.5, 128.6, 127.1, 126.2, 125.5, 125.3, 122.8, 120.3, 51.4$ . IR (neat):  $\tilde{\nu} = 2949$  (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  $\text{C}_{14}\text{H}_{12}\text{O}_2 \cdot 0.1 \text{H}_2\text{O}$  (214.05): calcd: C, 78.56; H, 5.74; found: C, 78.62; H, 5.70.

#### Methyl 3-(naphthalen-1-yl)propanoate **54** <sup>[16]</sup>

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).  $^1\text{H-NMR}$  (250 MHz,  $\text{DMSO-d}_6$ ):  $\delta = 8.08 - 8.04$  (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, OCH<sub>3</sub>), 3.33 (t, 2H, *J* = 7.3 Hz, CH<sub>2</sub>-Aryl, overlaps with H<sub>2</sub>O signal), 2.73 (t, 2H, *J* = 7.3 Hz, CH<sub>2</sub>-COOMe). <sup>13</sup>C-NMR (62.9 MHz, DMSO-d<sub>6</sub>): 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):  $\tilde{\nu}$  = 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<sub>14</sub>H<sub>14</sub>O<sub>2</sub> (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<sub>2</sub>SO<sub>4</sub> the mixture of 1.9 mL conc. HNO<sub>3</sub> and 1.6 mL conc. H<sub>2</sub>SO<sub>4</sub> 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<sub>2</sub>CO<sub>3</sub> and 100 mL EtOAc were added and the insoluble 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<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. The residue was combined with the insoluble 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<sub>f</sub> = 0.34 (*n*-hexane/EtOAc 1:1). Mp: 187 – 189 °C. <sup>1</sup>H-NMR (250 MHz, DMSO-d<sub>6</sub>): δ = 8.71 (dd, 1H, *J* = 8.7 Hz, *J* = 1.1 Hz, *H*-C7), 8.49 (dd, 1H, *J* = 7.6 Hz, *J* = 1.1 Hz, *H*-C5), 8.42 (d, 1H, *J* = 7.9 Hz, *H*-C2), 7.95 (dd, 1H, *J* = 8.7 Hz, *J* = 7.6 Hz, *H*-C6), 7.79 (d, 1H, *J* = 7.9 Hz, *H*-C3), 3.60 (s, 3H, OCH<sub>3</sub>), 3.51 (t, 2H, *J* = 7.5 Hz, CH<sub>2</sub>-Aryl), 2.82 (t, 2H, *J* = 7.5 Hz, CH<sub>2</sub>-COOMe). <sup>13</sup>C-NMR (62.9 MHz, DMSO-d<sub>6</sub>): 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):  $\tilde{\nu}$  = 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<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub> (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<sub>f</sub> = 0.10 (*n*-hexane/EtOAc). <sup>1</sup>H-NMR (250 MHz, DMSO-d<sub>6</sub>): δ = 7.16 - 7.04 (m, 2H, *H*-C6, *H*-C5), 6.93 (d, 1H, *J* = 7.6 Hz, *H*-C3), 6.59 (dd, 1H, *J* = 7.0 Hz, *J* = 1.6 Hz, *H*-C7), 6.51 (d, 1H, *J* = 7.6 Hz, *H*-C2), 5.58 (br s, 2H, NH<sub>2</sub>), 5.30 (br s, 2H, NH<sub>2</sub>), 3.58 (s, 3H, OCH<sub>3</sub>), 3.04 (t, 2H, *J* = 7.5 Hz, CH<sub>2</sub>-Aryl), 2.62 - 2.52 (m, 2H, CH<sub>2</sub>-COOMe, overlaps with DMSO). <sup>13</sup>C-NMR (62.9 MHz, DMSO-d<sub>6</sub>): 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):  $\tilde{\nu}$  = 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-1H-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.  $^1\text{H-NMR}$  (250 MHz, DMSO- $d_6$ ):  $\delta$  = 11.33 (br s, 2H, NH), 7.83 (br s, 2H, NH<sub>2</sub>), 7.43 - 7.41 (m, 2H, H-C7, H-C8), 7.22 (d, 1H,  $J$  = 7.8 Hz, H-C5), 6.85 (m, 1H, H-C9), 6.76 (d, 1H,  $J$  = 7.6 Hz, H-C4), 3.58 (s, 3H, OCH<sub>3</sub>), 3.09 (t, 2H,  $J$  = 7.3 Hz, CH<sub>2</sub>-Aryl), 2.63 (t, 2H,  $J$  = 7.3 Hz, CH<sub>2</sub>-COOMe).  $^{13}\text{C-NMR}$  (62.9 MHz, DMSO- $d_6$ ):  $\delta$  = 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):  $\tilde{\nu}$  = 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<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub> · 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<sub>2</sub>O and

desalted on a NAP-10 column. The pooled fractions were lyophilized to dryness, and the pellet was dissolved in DEPC-treated H<sub>2</sub>O 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<sub>2</sub>O) 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<sub>2</sub>O-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<sub>20</sub>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<sub>a</sub> 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<sub>2</sub>O 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<sub>a</sub> values.

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## Additional computational details

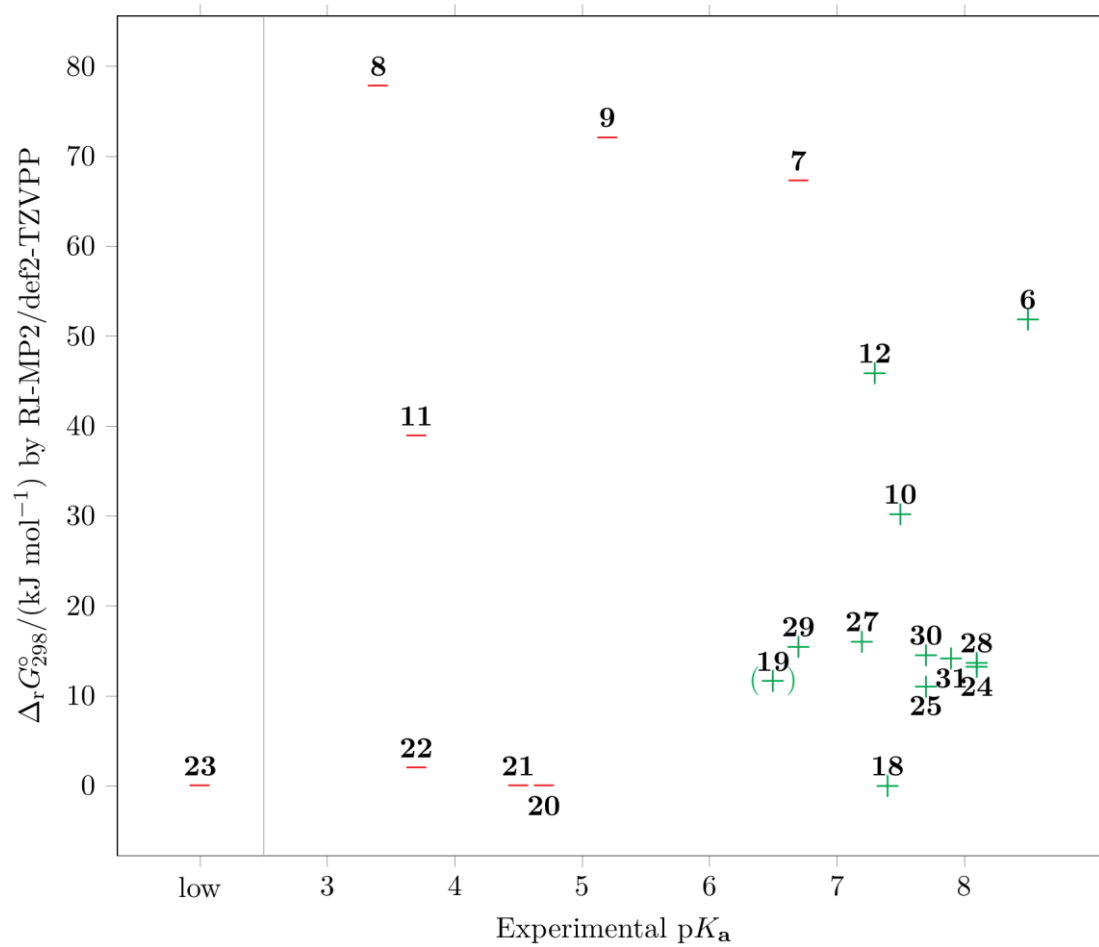
### Choice of tautomers

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<sup>-1</sup> 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 were considered in the calculations. For compounds **7** and **12** AM1 favors the disallowed (*Z*)-isomer (by 4.0 and 6.7 kJ mol<sup>-1</sup>) 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 ( $\leq 1.0$  kJ mol<sup>-1</sup> 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<sup>-1</sup> 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<sup>-1</sup> 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  $\Delta_r G_{298}^\circ$  is small (the average of the absolute differences is 0.08 kJ mol<sup>-1</sup> and for all structures the effect is  $< 0.7$  kJ mol<sup>-1</sup>).



**Figure S1.** Variant of Figure 12 with  $\Delta_r G_{298}^\circ$  from RI-MP2 instead of  $\Delta_r H_{298}^\circ$  from AM1.

## Energies of compounds and their tautomers

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

**Table S1.** Calculated heat of formation  $\Delta_f H_{298}^\circ$  and Gibbs free energies  $\Delta G_{298}^\circ$  for the various compounds by different methods.

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

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

Compound	$\Delta_r H_{298}^\circ / (\text{kJ mol}^{-1})$	$\Delta_r G_{298}^\circ / (\text{kJ mol}^{-1})$				<i>E</i> RI-CCSD(T)/cc-pVTZ + Thermal of RI-MP2
	AM1	RI-B3LYP/ def2-TZVPP	B3LYP/ def2-TZVPP	RI-MP2/ def2-TZVPP		
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 <sup>[a]</sup>	0.0	0.0	0.0	0.0	0.0	
19	17.2	9.3	9.3	11.6	-	
20 <sup>[a]</sup>	0.0	0.0	0.0	0.0	0.0	
21 <sup>[a]</sup>	0.0	0.0	0.0	0.0	0.0	
22	2.8	1.4	1.4	2.0	-	
23 <sup>[a]</sup>	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

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### 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

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**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

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**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

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### 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<sub>h</sub>

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<sub>h</sub>

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

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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

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**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

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**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

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**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
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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

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**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

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**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

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**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<sub>h</sub>

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<sub>h</sub>

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

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**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

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**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<sub>h</sub>

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

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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

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**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

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**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

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**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

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**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

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**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<sub>h</sub>

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<sub>h</sub>

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

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**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<sub>h</sub>

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<sub>h</sub>

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

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**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

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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

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**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

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### 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

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**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

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**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
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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<sub>h</sub>

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<sub>h</sub>

C	-0.2586427	-2.1533802	0.0733910
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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

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**Compound 30**

32

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

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**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

35

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

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**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

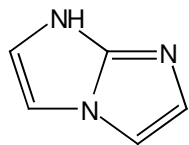
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RI-B3LYP electronic energy -895.20113707343 E\_h  
C -0.9727203 -2.0752662 -0.0000335  
C 0.3305035 -1.5435169 -0.0000273  
C 0.5902715 -0.1911761 -0.0000070  
C -0.5236284 0.7091452 0.0000129  
C -1.8429797 0.1753589 0.0000078  
C -2.0555977 -1.2273982 -0.0000173  
C -0.3856653 2.1207801 0.0000380  
C -1.4934202 2.9345069 0.0000588  
C -2.7944542 2.4070952 0.0000542  
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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  
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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  
H 7.4434927 -1.3239393 0.0004202  
H 6.9980511 0.1631414 0.8863909  
H 6.9981473 0.1626034 -0.8864987  
35  
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  
C -2.9666236 1.0386685 -0.0001066  
N -4.2327879 0.4585859 -0.0003066  
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
H	6.9980681	0.1629195	0.8858298
H	6.9976820	0.1627199	-0.8871933

35

RI-MP2 electronic energy -893.646538884530 E\_h

C	-1.2234901	-2.0959936	-0.0004589
C	0.0817854	-1.5718957	-0.0005365
C	0.3370103	-0.2118659	-0.0004481
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
H	7.1598431	-1.2935383	0.0015203
H	6.6648690	0.1764777	0.8850152
H	6.6654240	0.1753245	-0.8842015



HPic

**18**

13.11

8.58

7.64

7.64

7.63

7.63

7.52

7.51

7.51

7.50

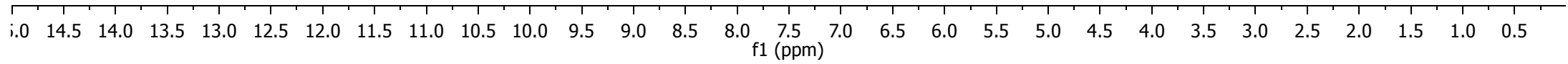
2.50 DMSO-d6

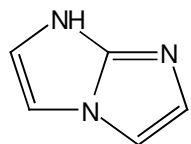
1.81

2.00

2.00

2.01





HPic

**18**

— 160.81

— 141.88

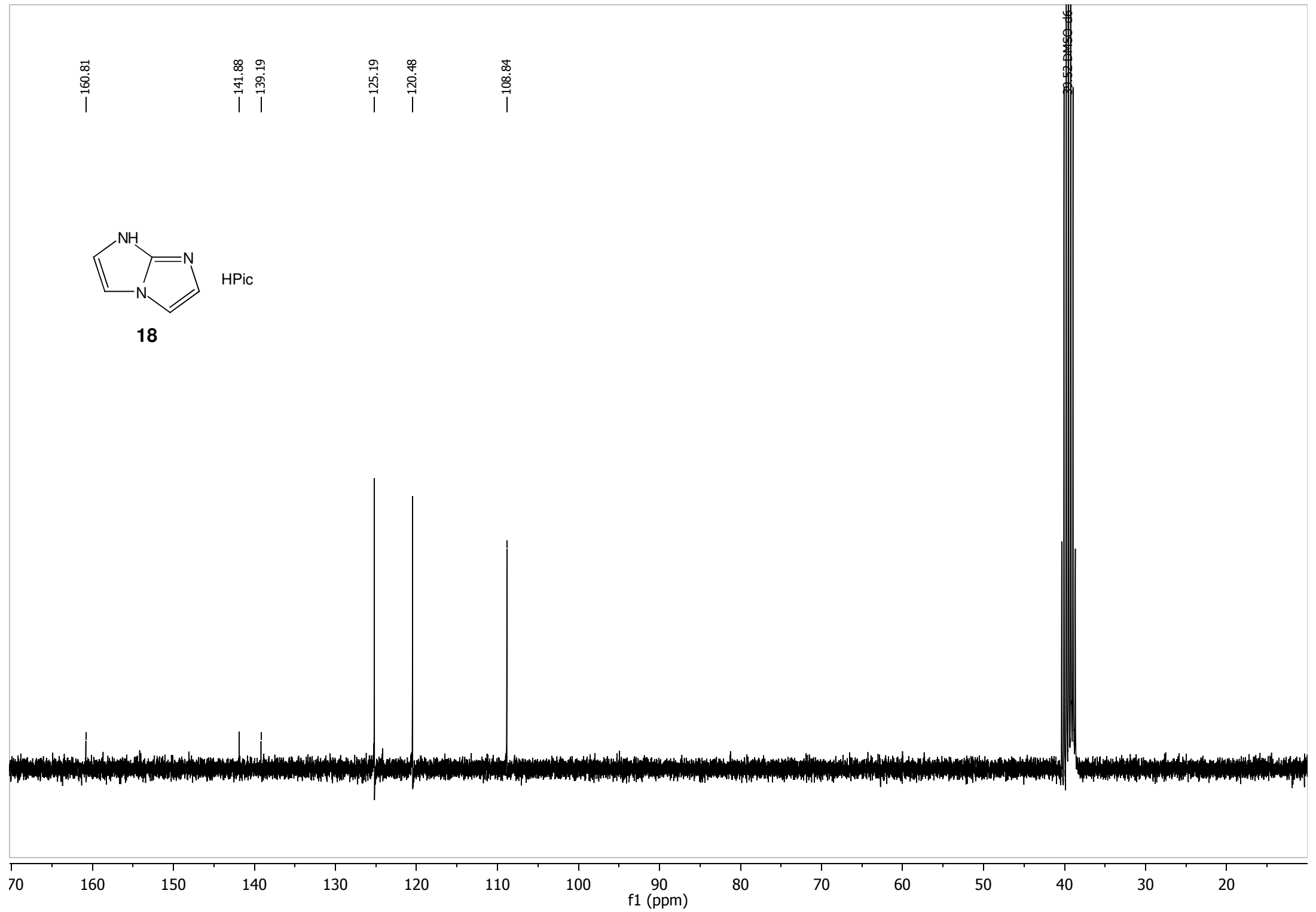
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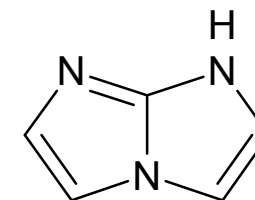
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39.52, 39.50, 39.48, 39.46

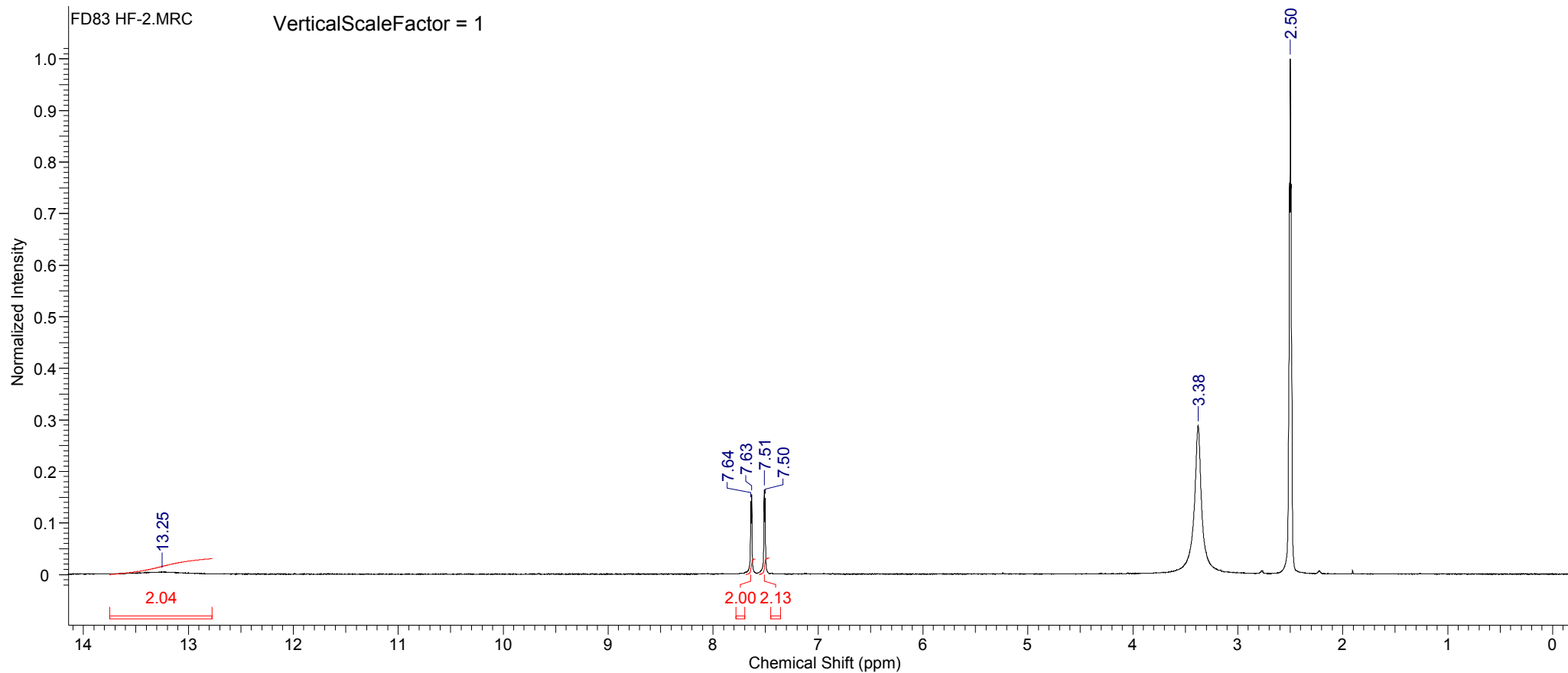


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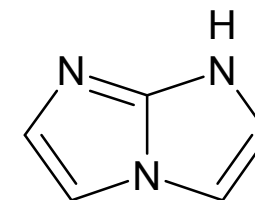
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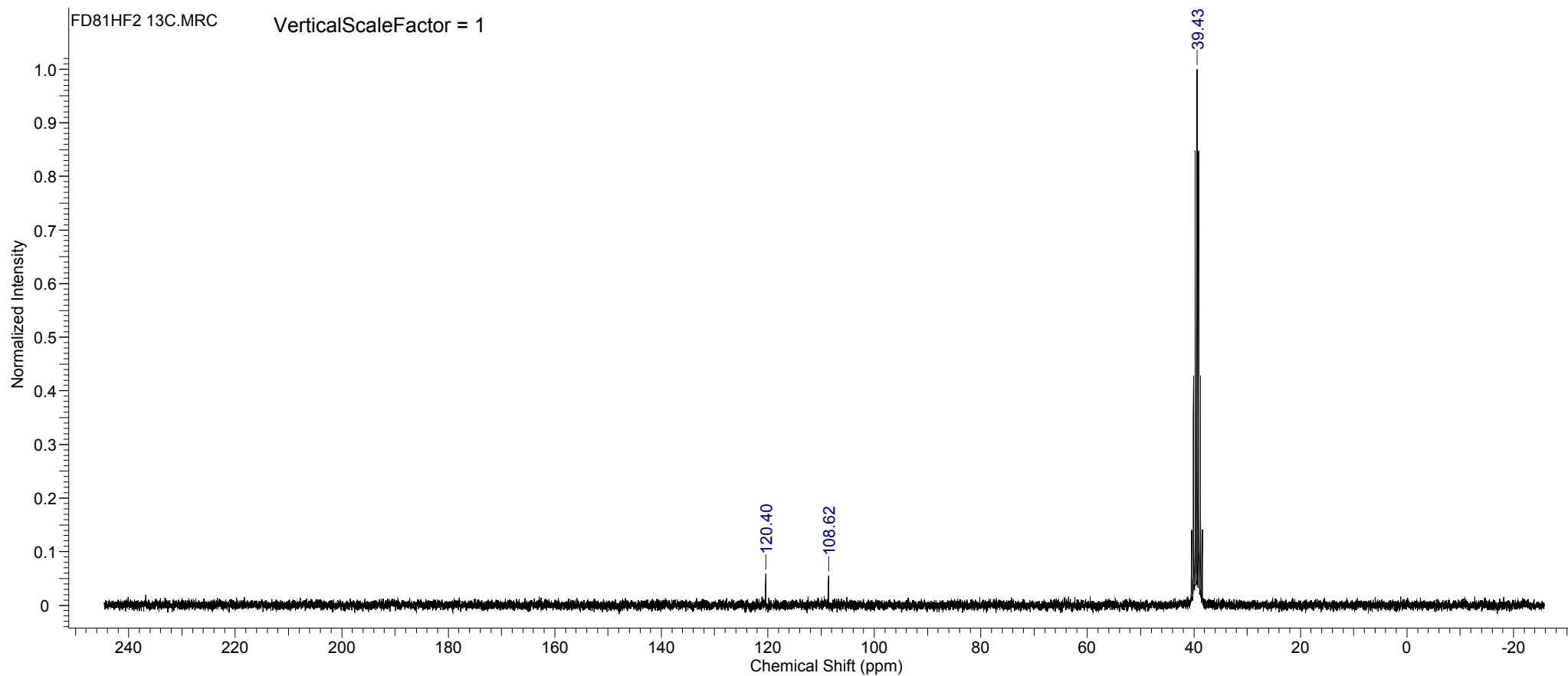
This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

## Compound 18

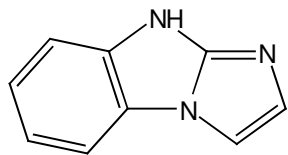
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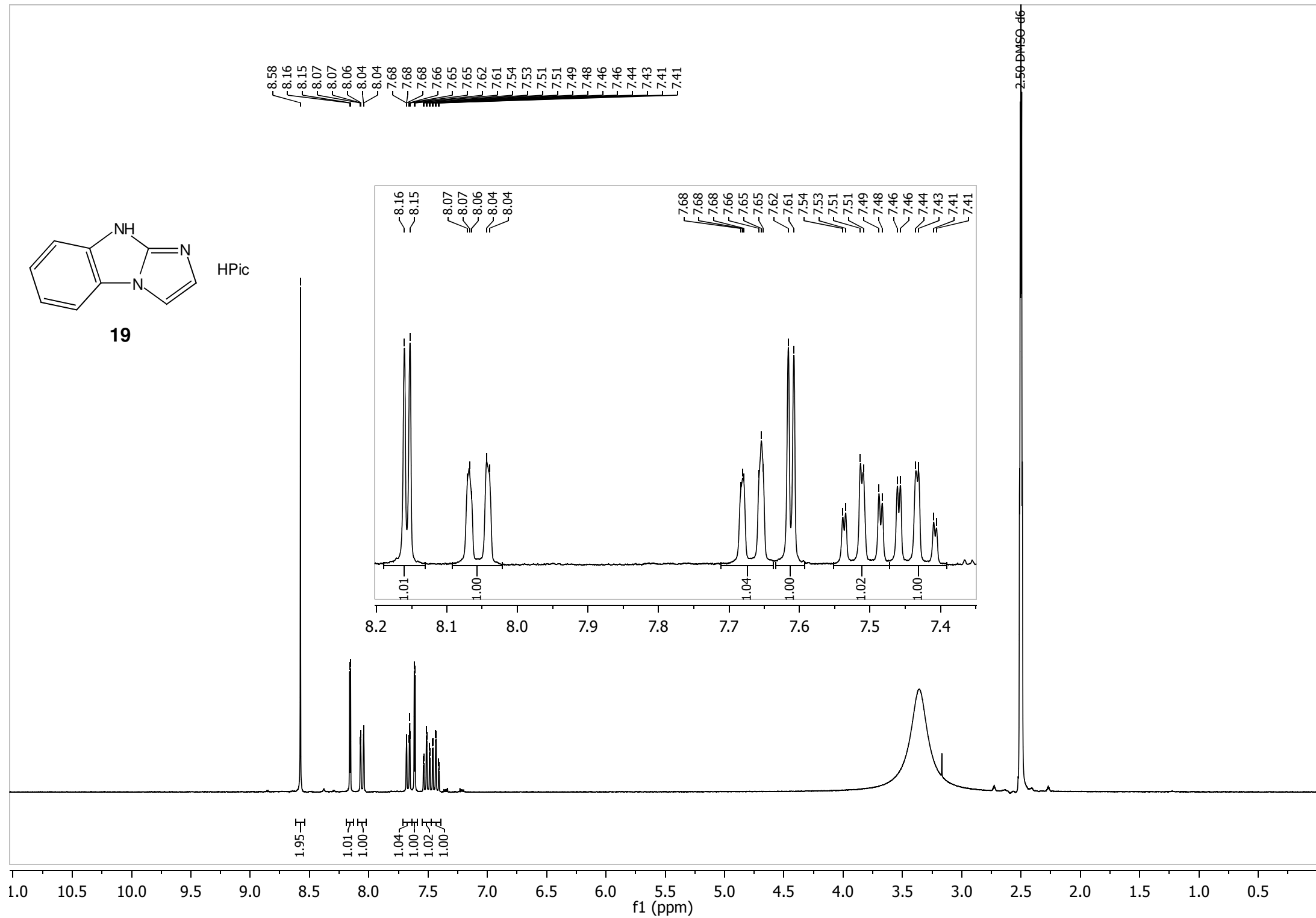


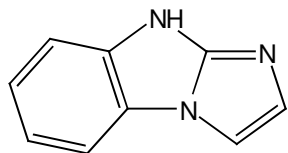




HPic

19





HPic

**19**

142.50  
141.85

134.49

125.61  
125.18  
123.99  
122.50  
120.19

113.61  
112.76  
109.12

39.52, 39.50, 39.48

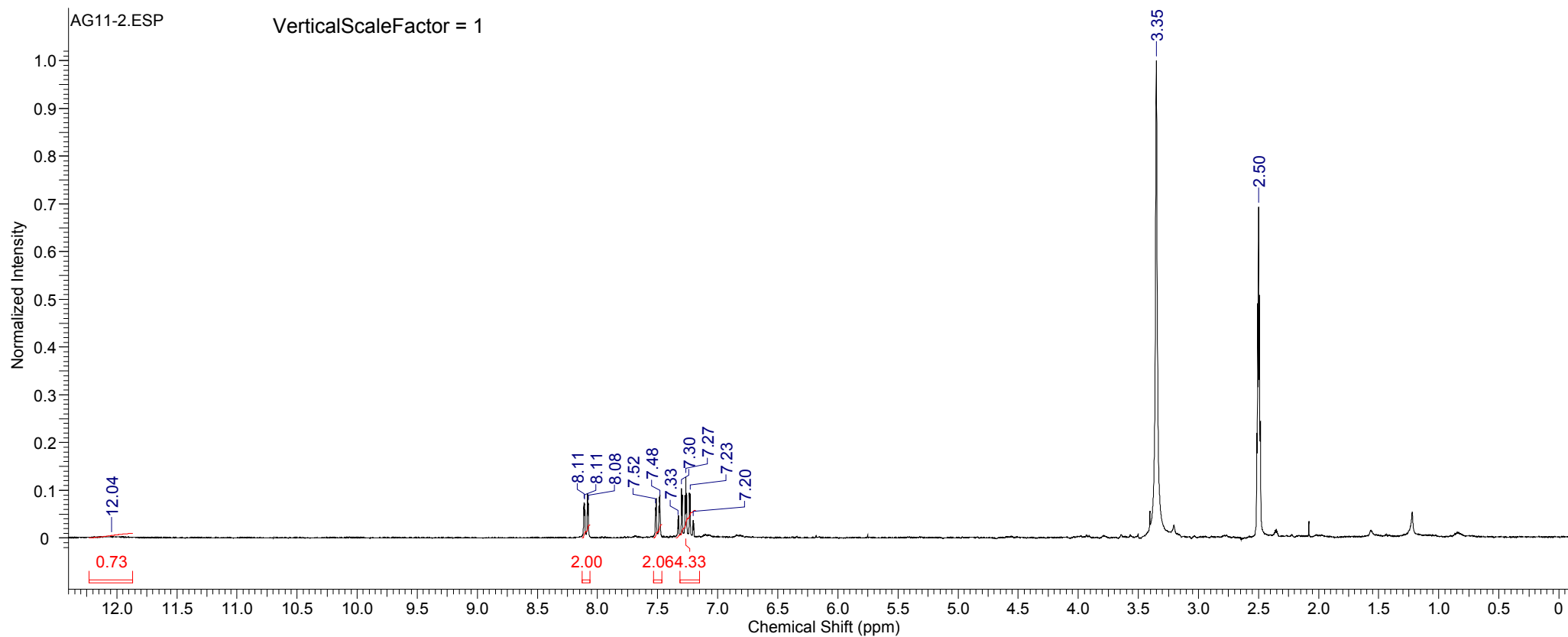
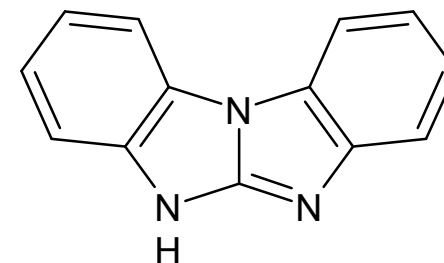
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15

f1 (ppm)

## Compound 20

AG11-2

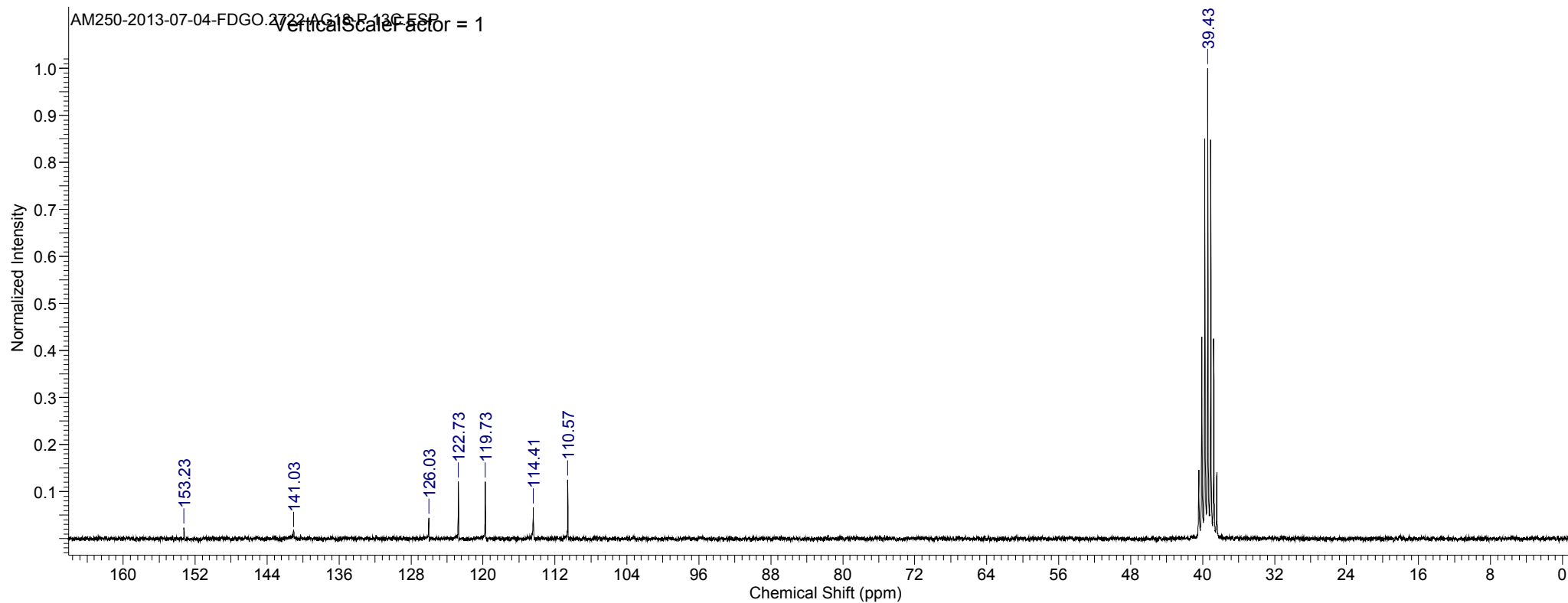
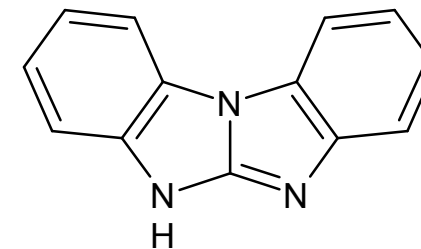
<b>Acquisition Time (sec)</b>	3.9998	<b>Comment</b>	AG11-2	<b>Date</b>	13 May 2013 17:38:40	<b>Date Stamp</b>	13 May 2013 17:38:40
<b>File Name</b>	C:\USERS\RIKE\DESKTOP\ALEX\NMR\AG11-2\1\FID	<b>Frequency (MHz)</b>	250.13	<b>Nucleus</b>	1H	<b>Number of Transients</b>	32
<b>Origin</b>	spect	<b>Original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



## Compound 20

AG18-P

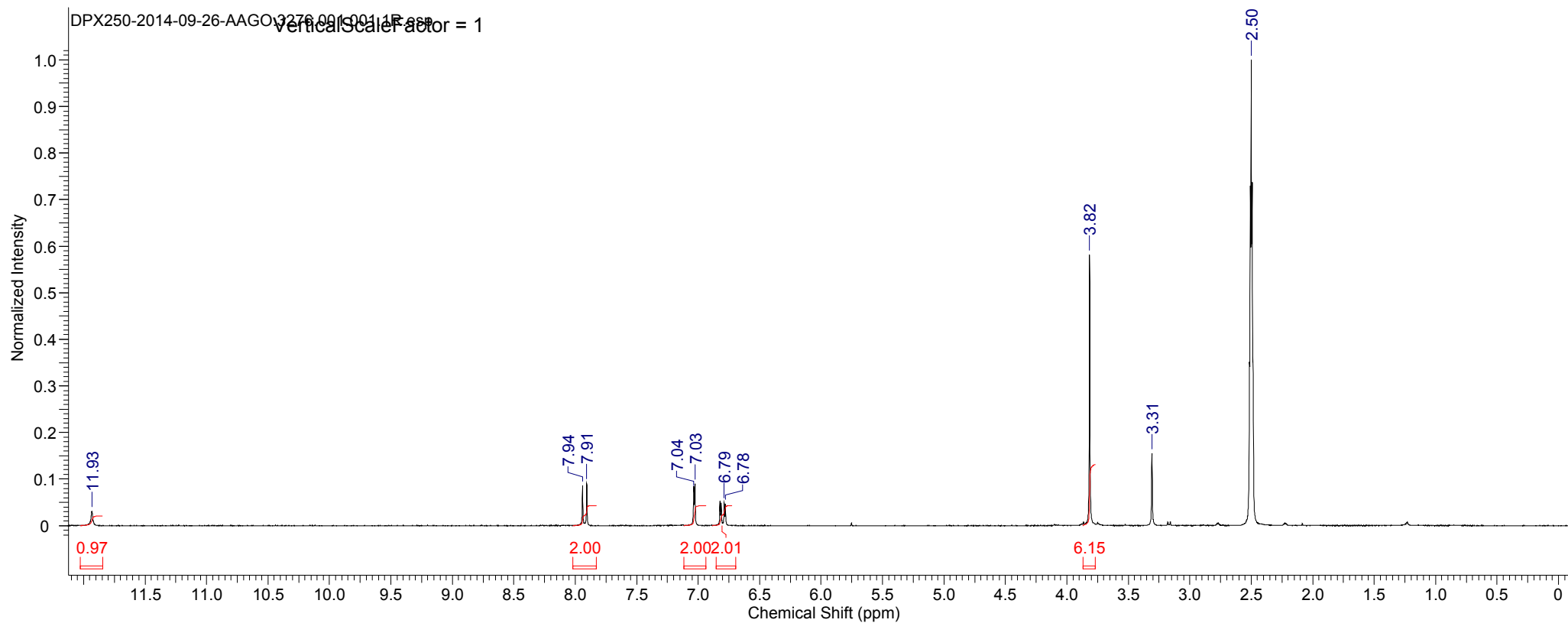
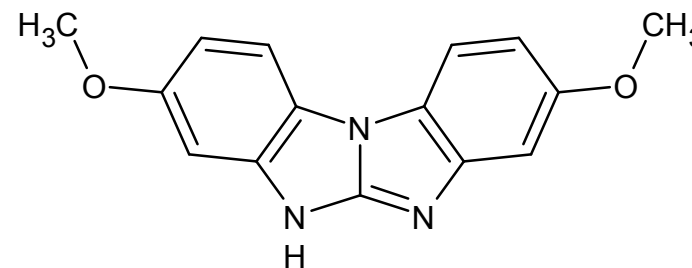
<b>Acquisition Time (sec)</b>	1.0420	<b>Comment</b>	AG18-P	<b>Date</b>	05 Jul 2013 01:55:44
<b>Date Stamp</b>	05 Jul 2013 01:55:44				
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\NMR AK-PRAKTIS\NMR AG01 - 18\AG18\AM250-2013-07-04-FDGO.2722 AG18-P 13C\1\PDATA\1\1R				
<b>Frequency (MHz)</b>	62.90	<b>Nucleus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



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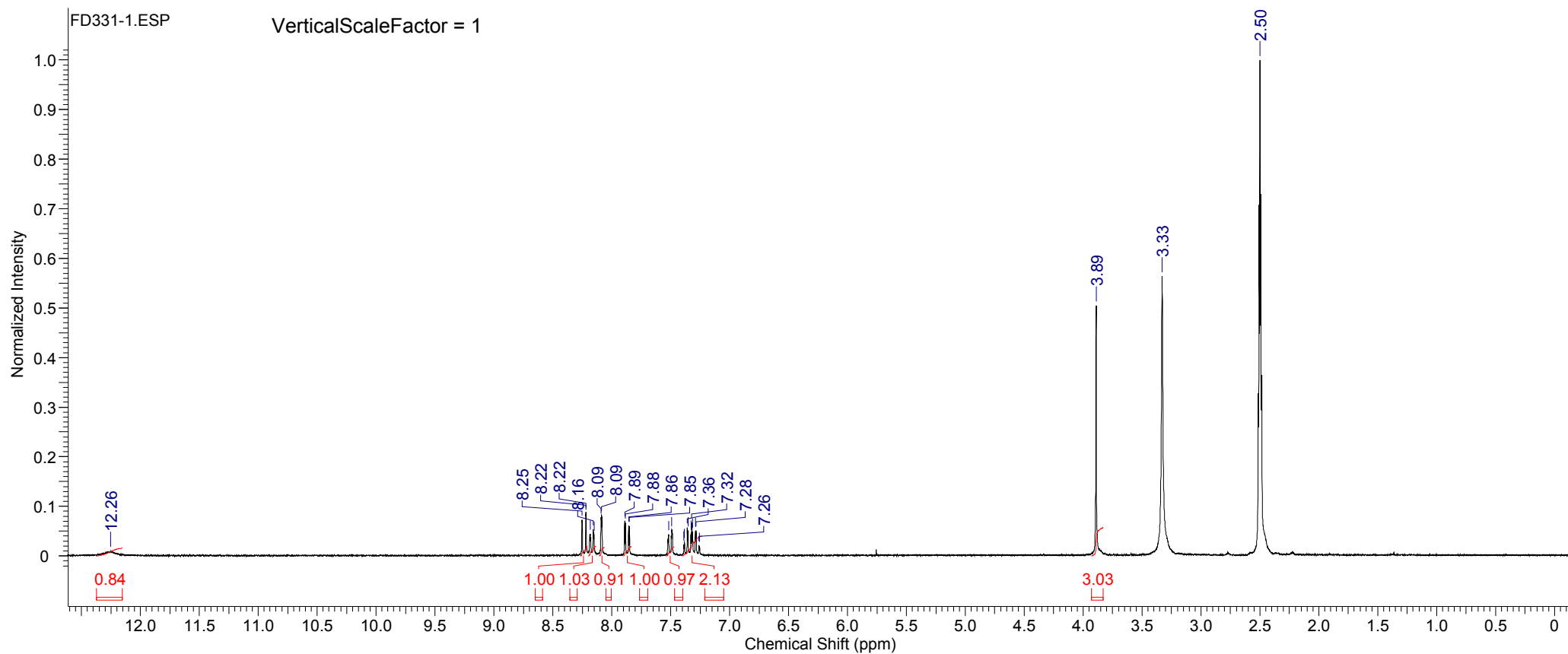
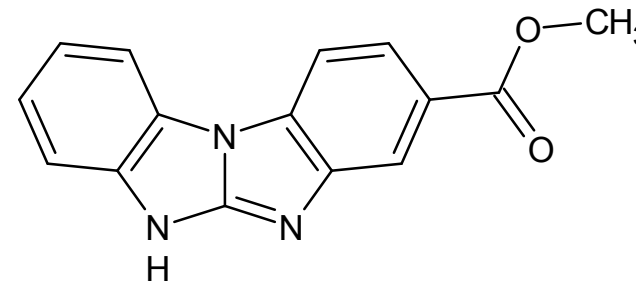
## Compound 21

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\APISPEKTREN 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		



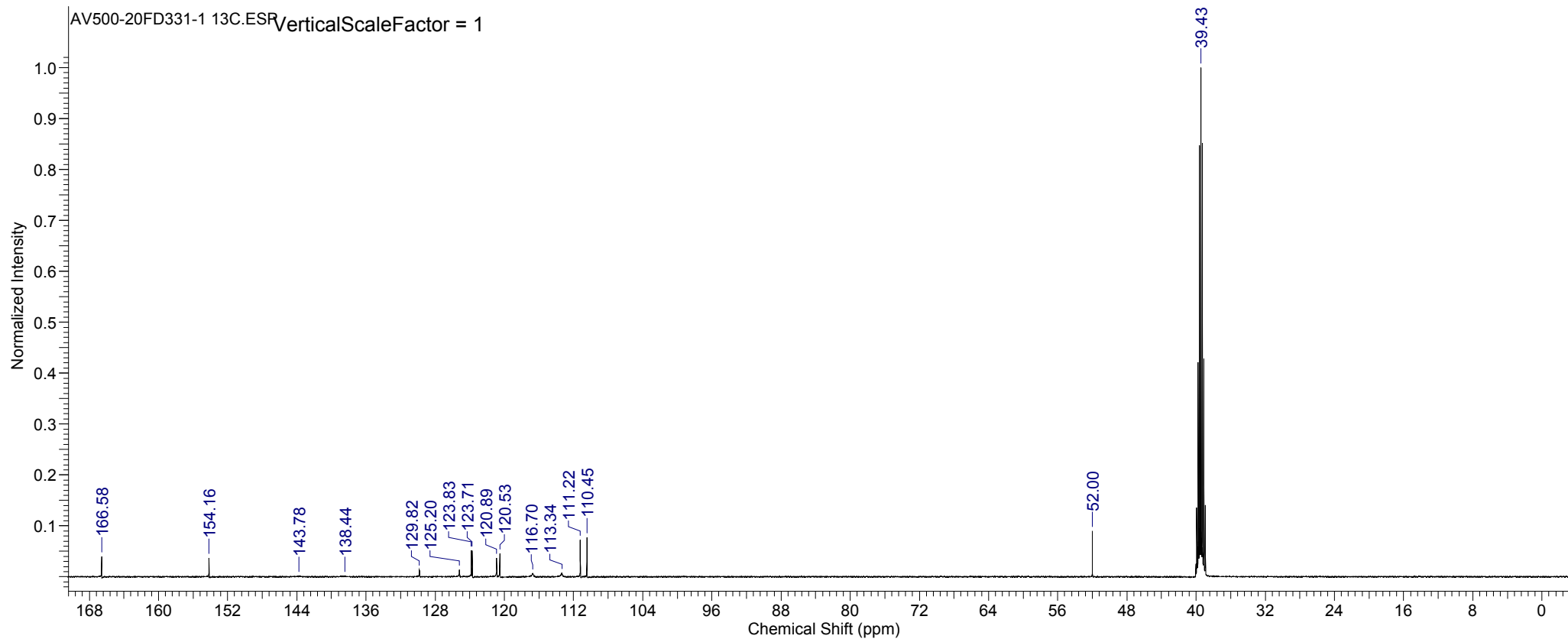
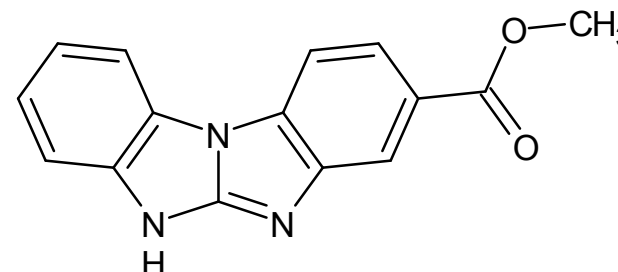
## Compound 22

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



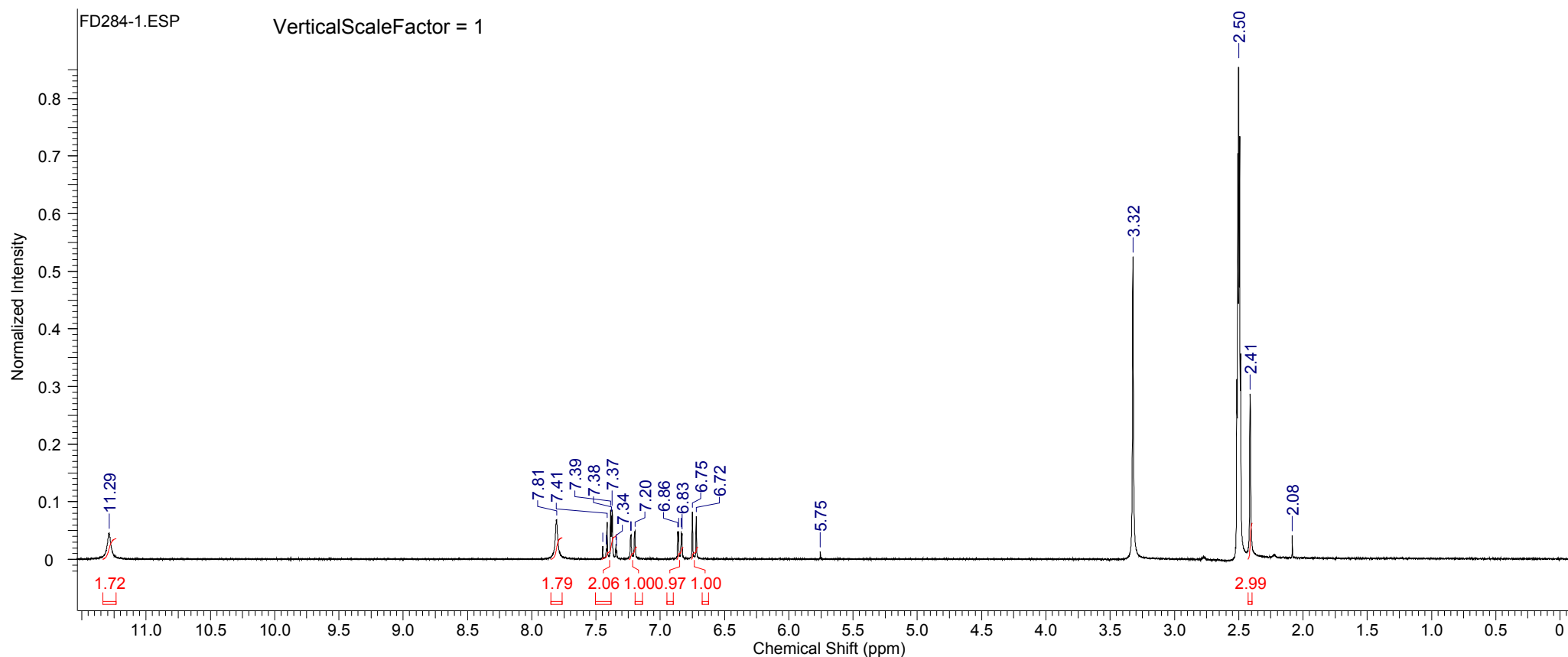
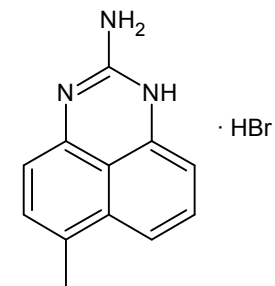
## Compound 22

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
Original Points Count	32678	Owner	service	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	31249.52	Temperature (degree C)	25.002
				Origin	spect
				Pulse Sequence	zggp30
				Spectrum Offset (Hz)	12431.8789



## 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
Receiver Gain	812.70	SW(cyclical) (Hz)	4990.02	Solvent	DMSO-d6	Spectrum Offset (Hz)	1747.4247
Sweep Width (Hz)	4989.87	Temperature (degree C)	27.000	Spectrum Type	STANDARD		

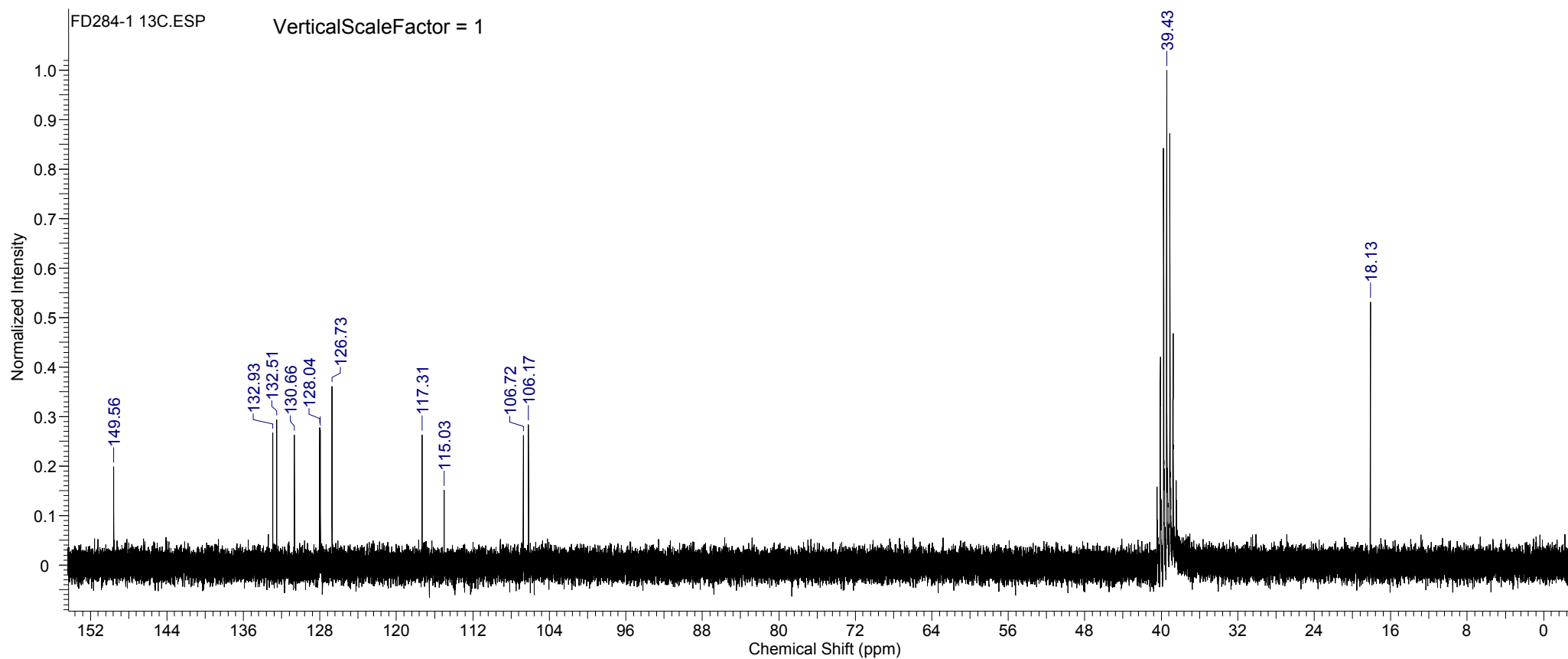
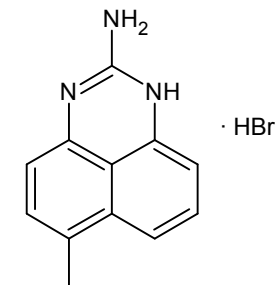




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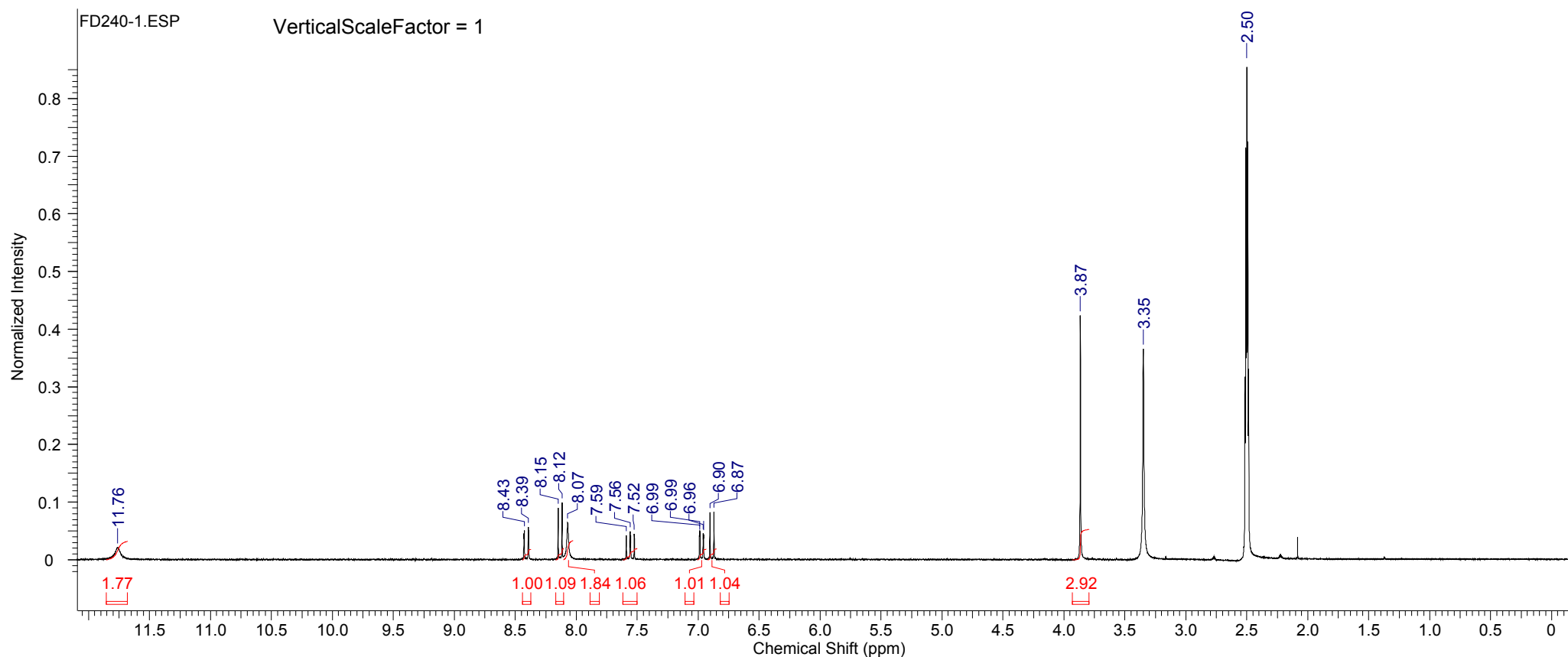
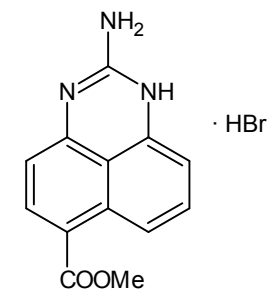
## Compound 28

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



## Compound 29

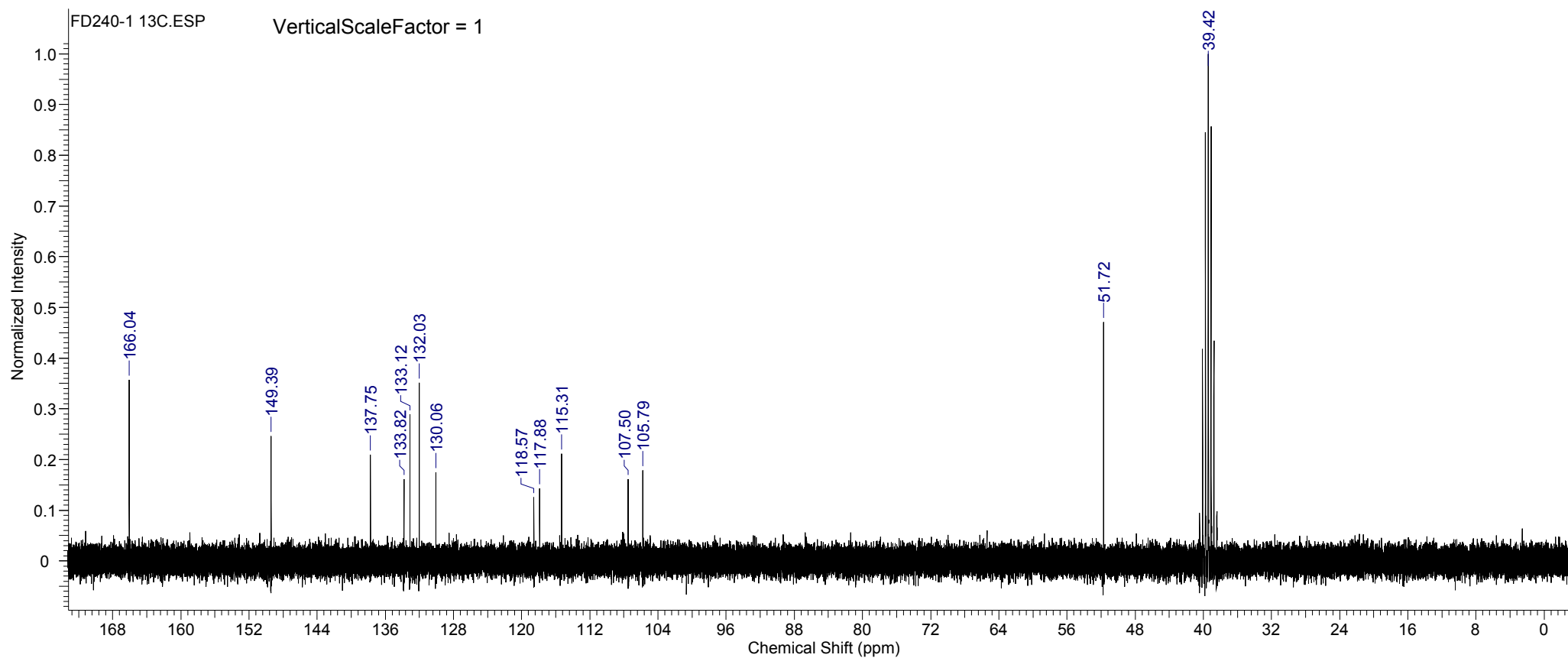
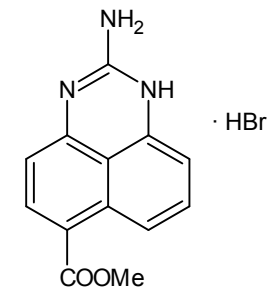
Acquisition Time (sec)	6.1563	Comment	FD240-1	Date	21 Mar 2012 12:58:56	Date Stamp	21 Mar 2012 12:58:56
File Name	C:\USERS\RIKE\DATEN\RIKE\NMR\FD240-1\1\FID	Frequency (MHz)	250.13	Nucleus	1H	Number of Transients	24
Origin	spect	Original Points Count	30720	Owner	service	Points Count	32768
Receiver Gain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



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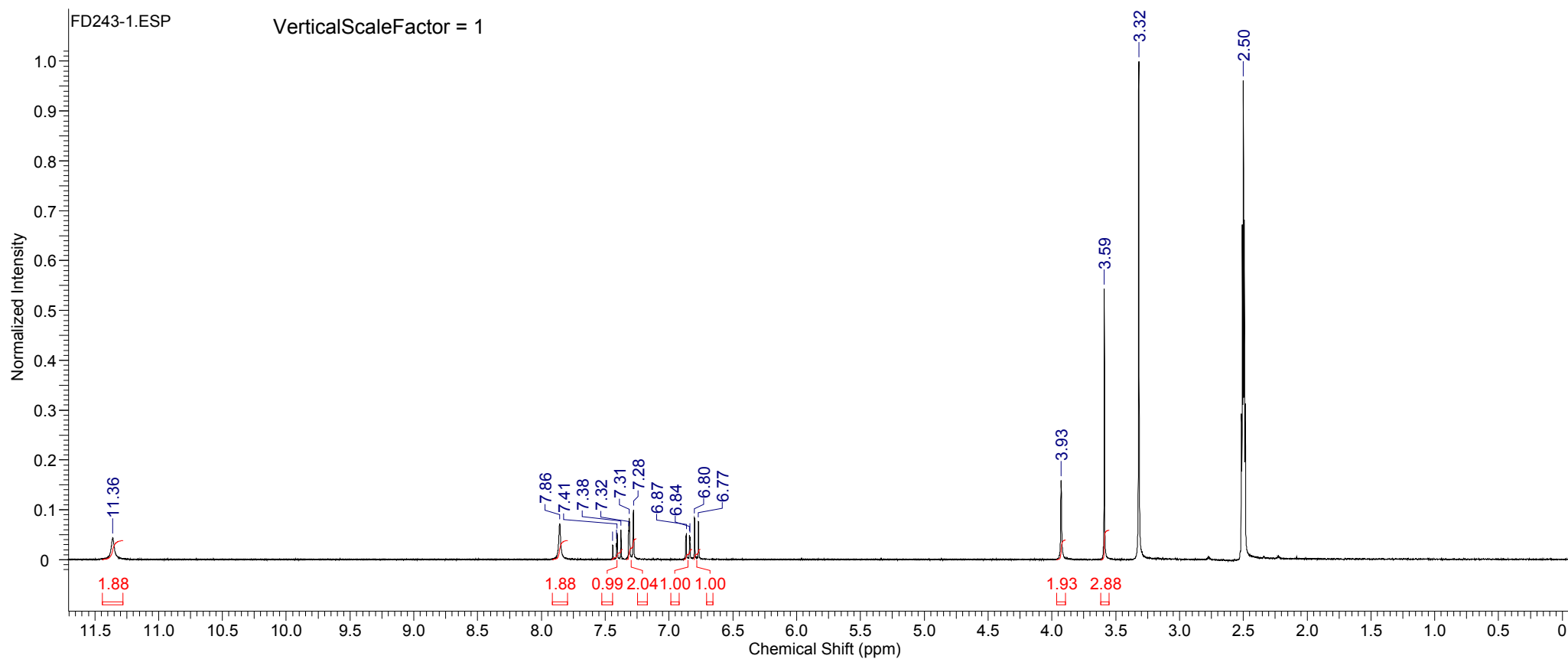
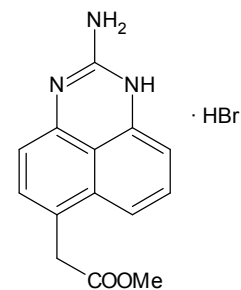
## Compound 29

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
Points Count	131072	Pulse Sequence	zpggvar	Receiver Gain	7298.20	SW(cyclical) (Hz)	15723.27
Spectrum Offset (Hz)	6566.0649	Spectrum Type	STANDARD	Sweep Width (Hz)	15723.15	Temperature (degree C)	27.000
						Owner	service
						Solvent	DMSO-d6



## Compound 30

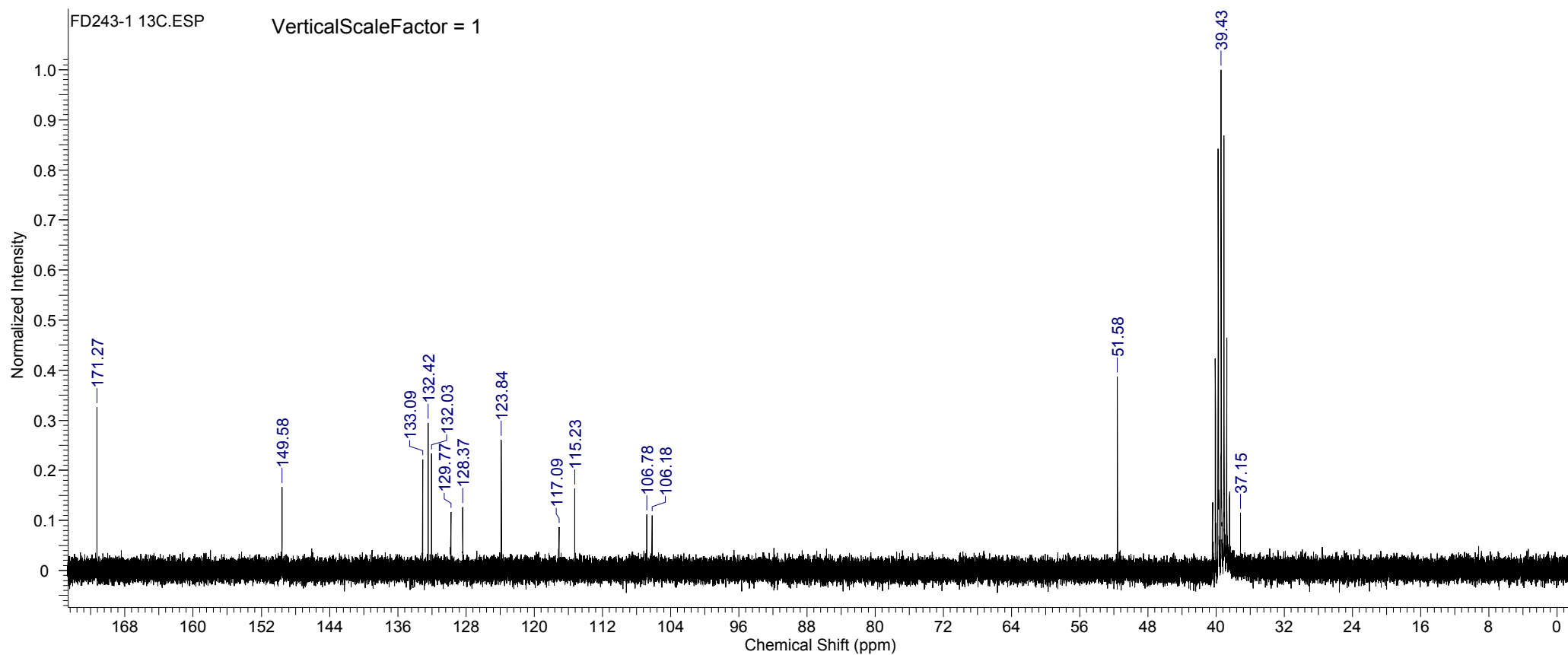
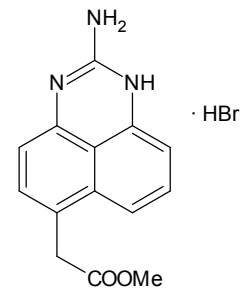
<b>Acquisition Time (sec)</b>	6.1563	<b>Comment</b>	FD243-1	<b>Date</b>	28 Mar 2012 15:56:16	<b>Date Stamp</b>	28 Mar 2012 15:56:16
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\FD243-1\1\FID	<b>Frequency (MHz)</b>	250.13	<b>Nucleus</b>	1H	<b>Number of Transients</b>	16
<b>Origin</b>	spect	<b>Original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



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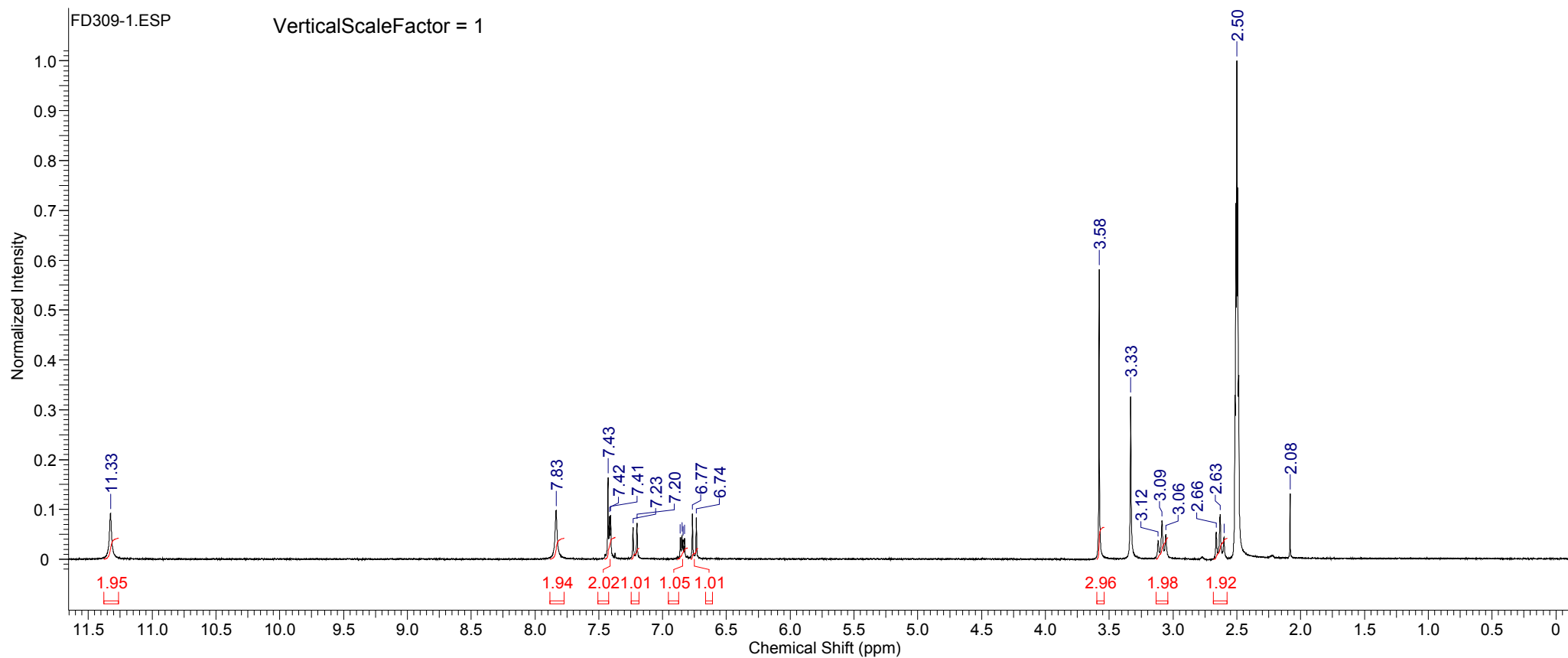
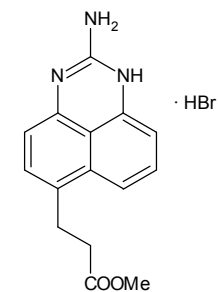
## Compound 30

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
Points Count	131072	Pulse Sequence	zpggvar	Receiver Gain	11585.20	SW(cyclical) (Hz)	15723.27
Spectrum Offset (Hz)	6564.2656	Spectrum Type	STANDARD	Sweep Width (Hz)	15723.15	Temperature (degree C)	27.000
						Owner	service
						Solvent	DMSO-d6



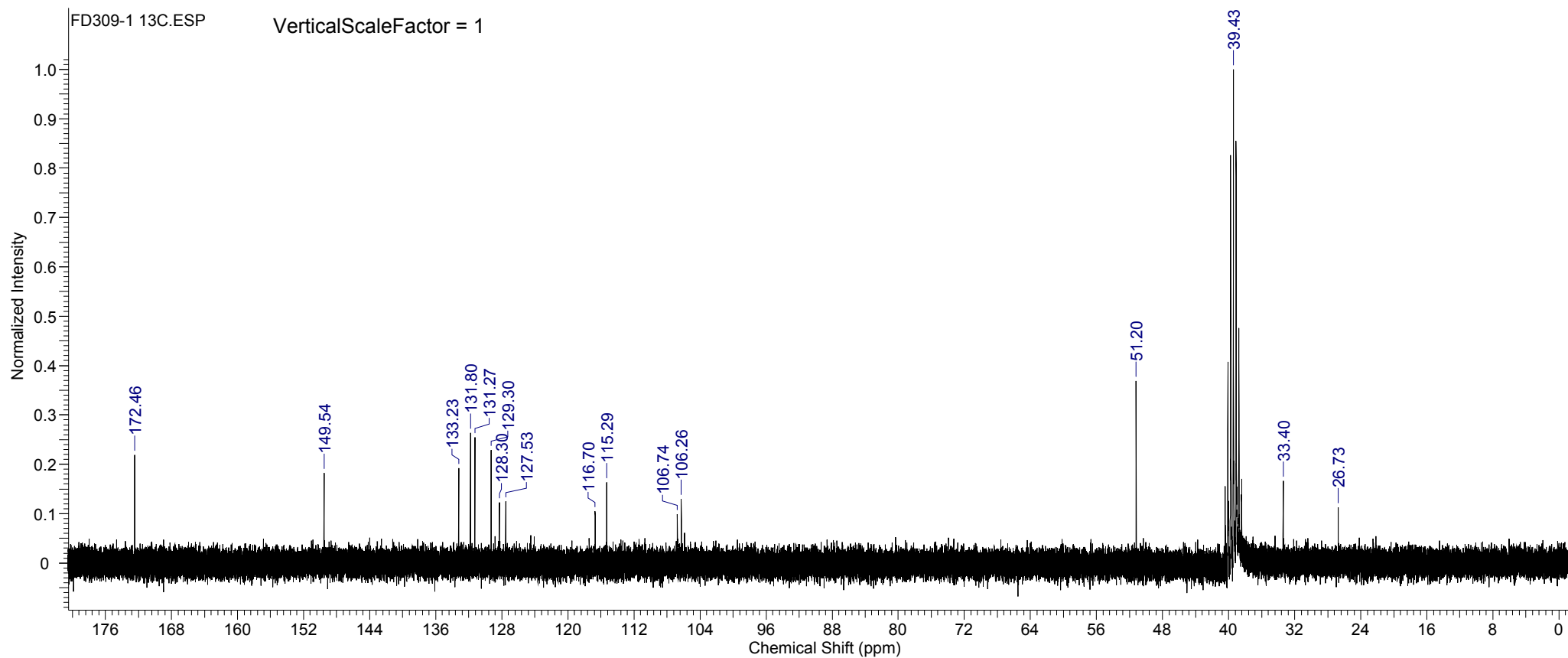
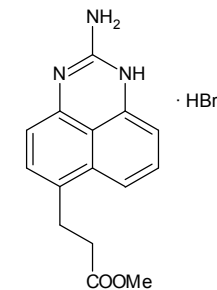
## Compound 31

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



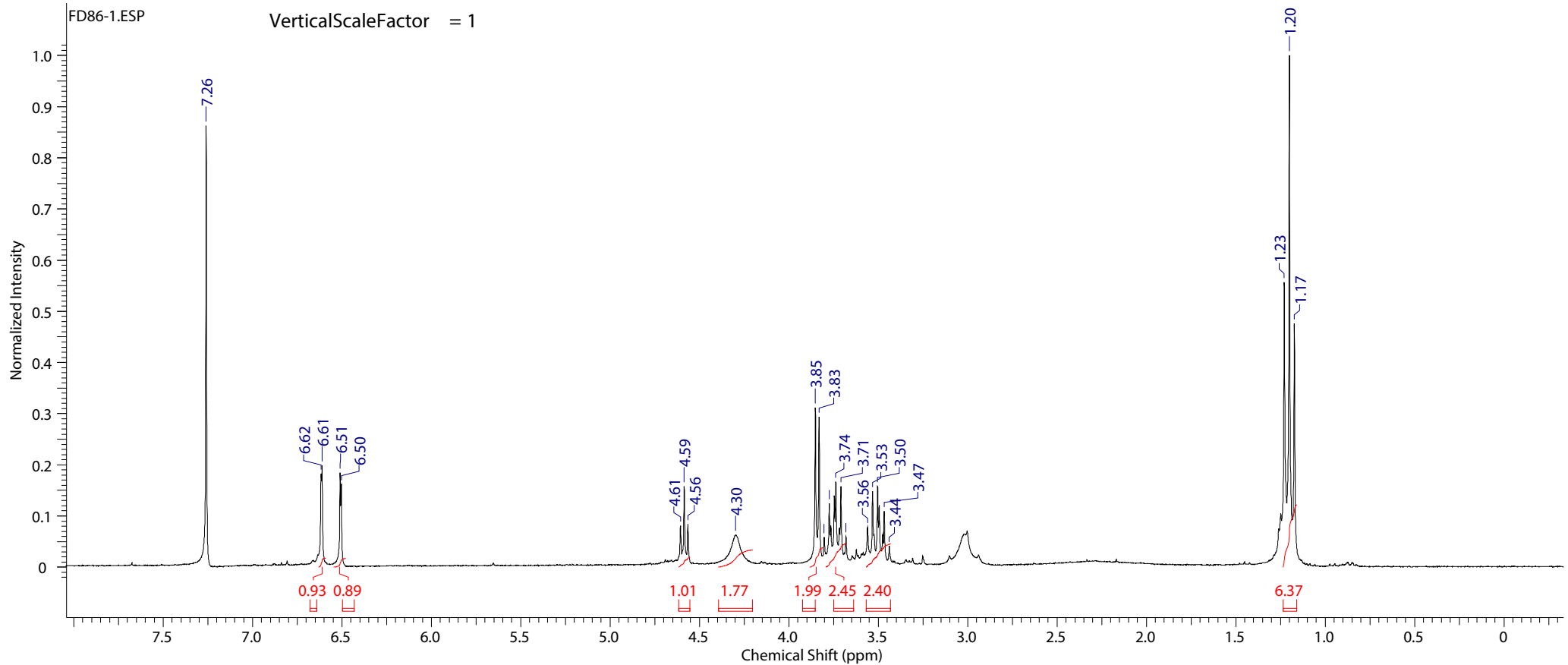
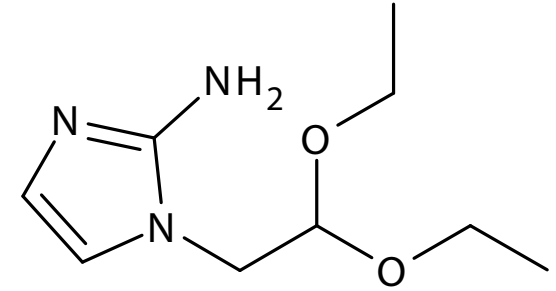
## Compound 31

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



## Compound 32

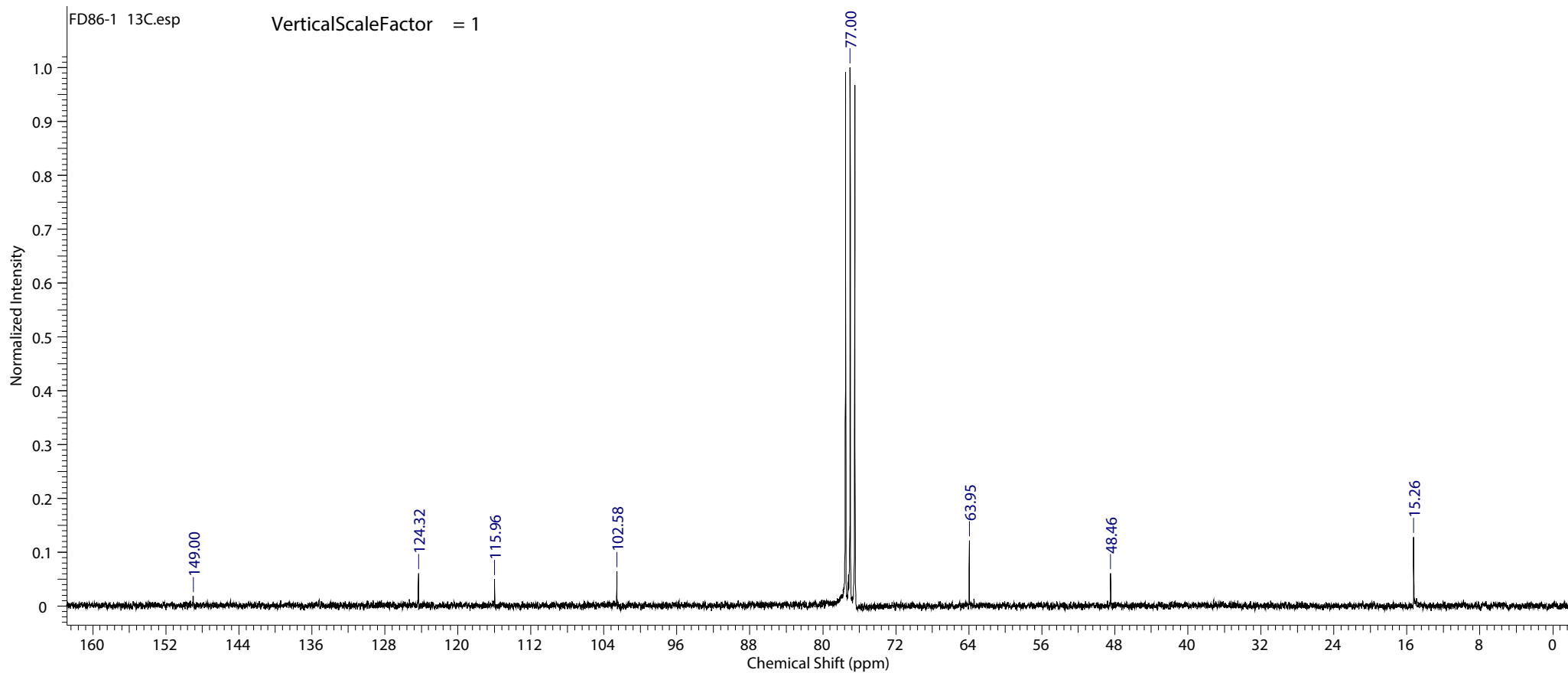
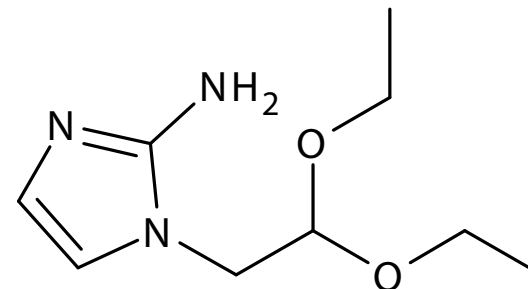
Acquisition Time (sec)	3.1261	Date	15 Feb 2012 09:55:18				
File Name	C:\USERS\RIKE\DATEN	RIKE\NMR\NMR	FD54 - 97\FD86\FD86-1.MRC	Frequency (MHz)	250.13	Nucleus	1H
Origin	Bruker	Original Points Count	32768	Points Count	65536	Pulse Sequence	ZG30
Spectrum Type	STANDARD	Sweep Width (Hz)	10482.18		Spectrum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





## Compound 32

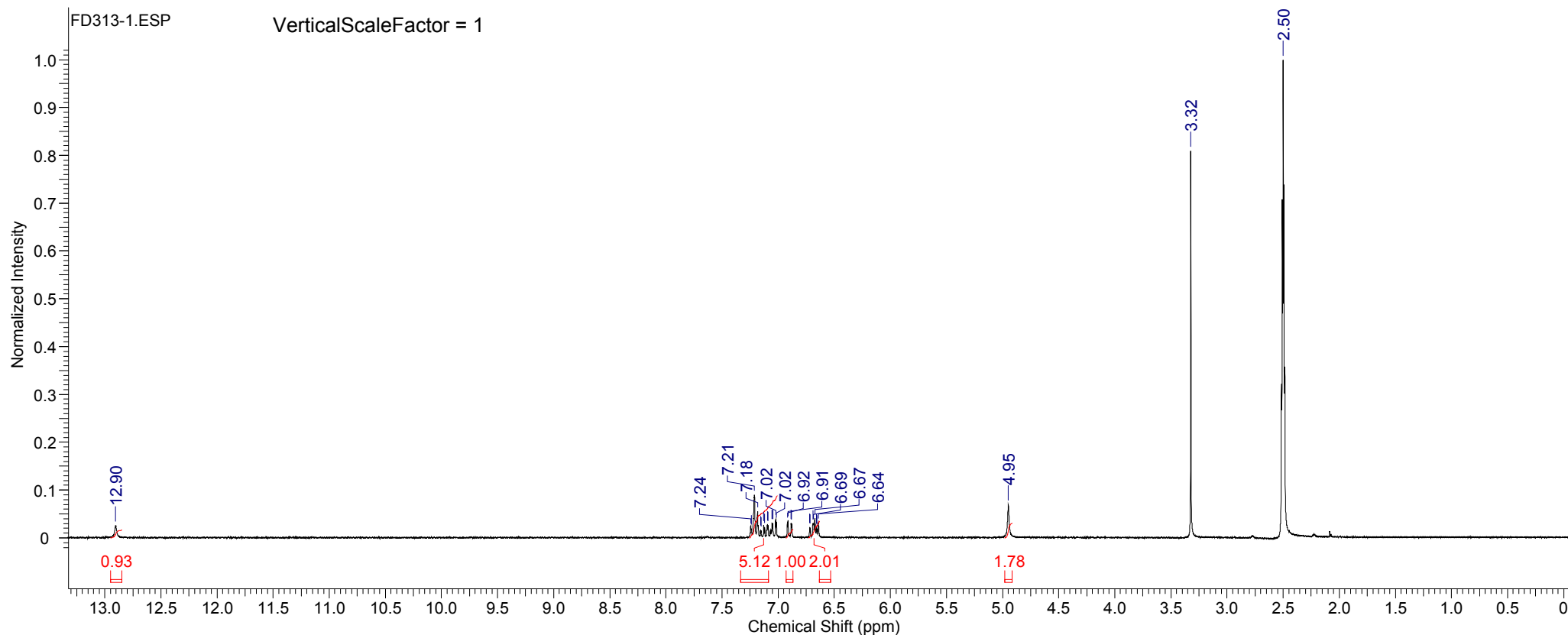
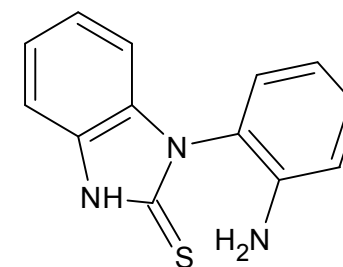
Acquisition Time (sec)	1.3849	Date	15 Feb 2012 09:55:18			Frequency (MHz)	62.90		
File Name	C:\USERS\RIKE\DATEN	RIKE\NMR\NMR	FD54 - 97\FD86\FD86-1	13C.MRC	Original Points Count	23552	Points Count	65536	
Nucleus	13C	Origin	Bruker	Spectrum Offset (Hz)	6918.8745	Spectrum Type	STANDARD	Sweep Width (Hz)	17006.80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



## Compound 35

FD313-1

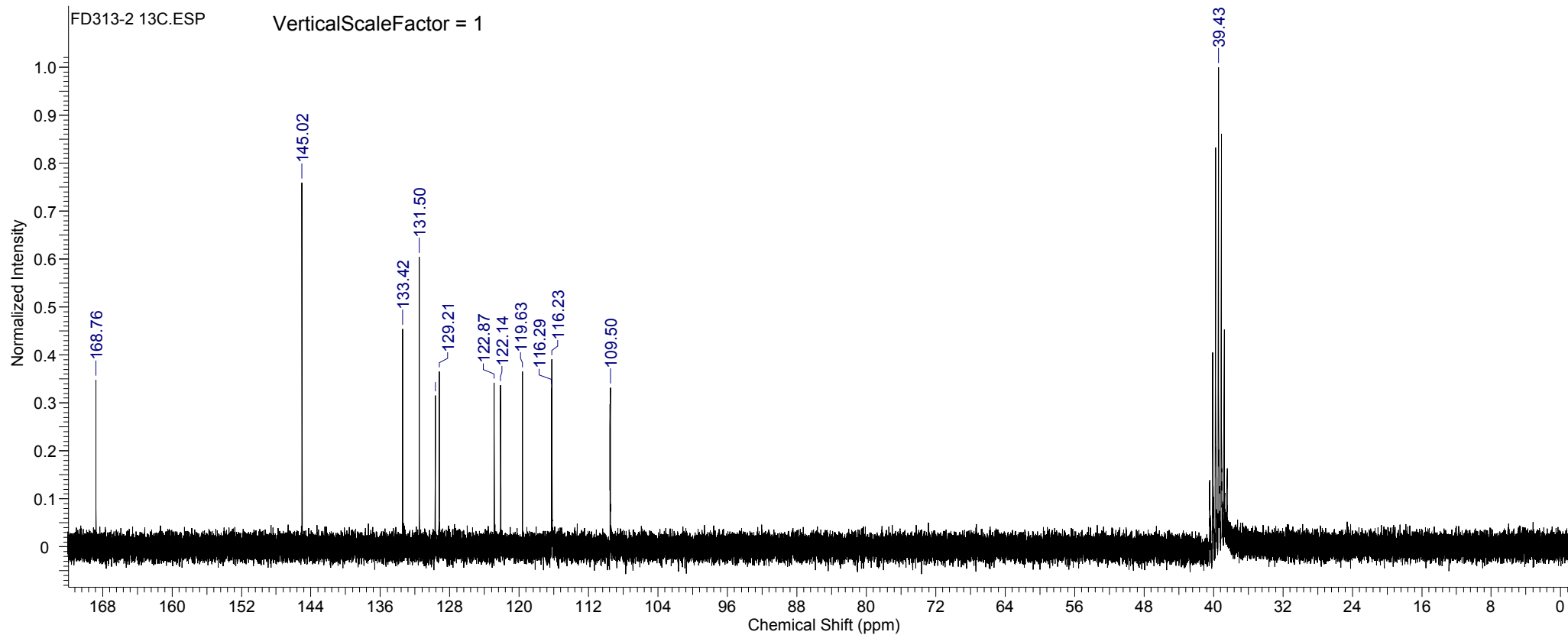
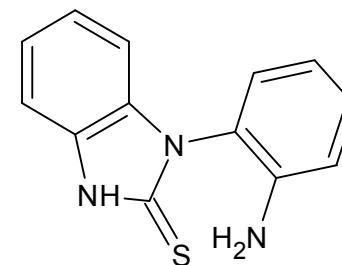
<b>Acquisition Time (sec)</b>	4.5146	<b>Comment</b>	FD313-1	<b>Date</b>	20 Mar 2013 12:48:16	<b>Date Stamp</b>	20 Mar 2013 12:48:16
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\FD313-1\1\FID	<b>Frequency (MHz)</b>	250.13	<b>Nucleus</b>	1H	<b>Number of Transients</b>	24
<b>Origin</b>	spect	<b>Original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



# Compound 35

FD313-2

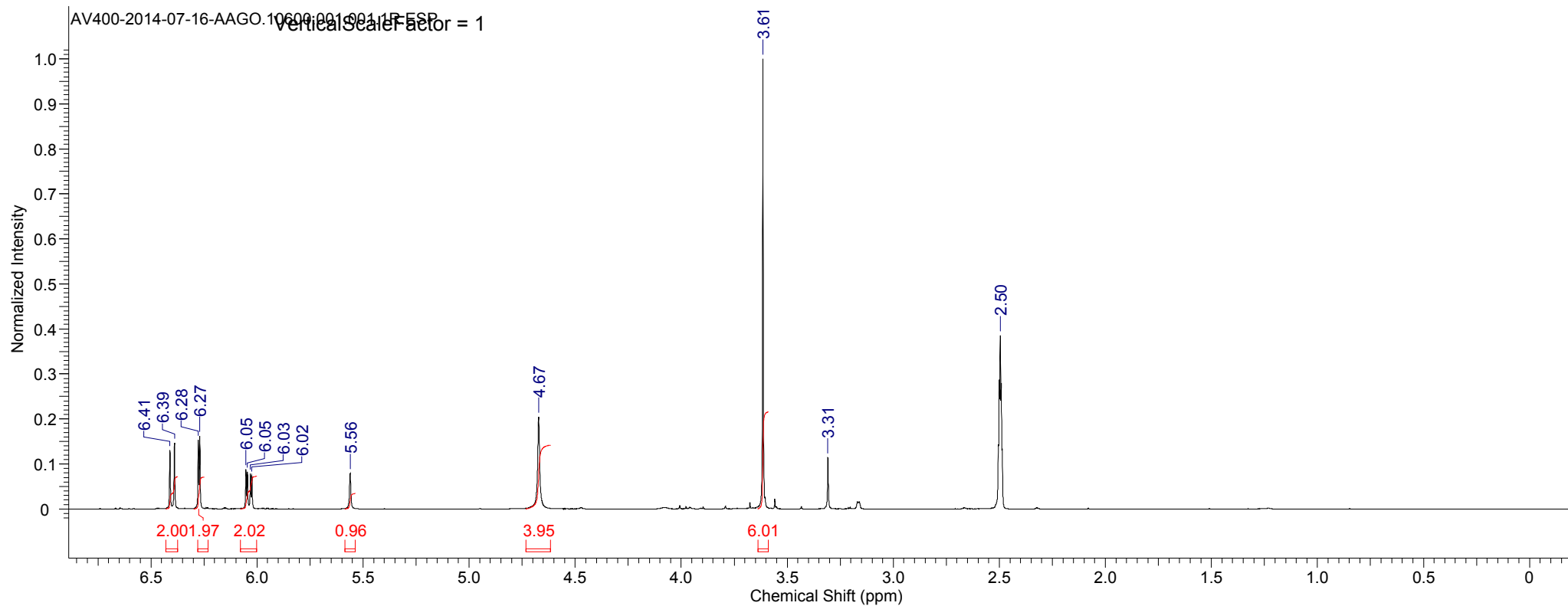
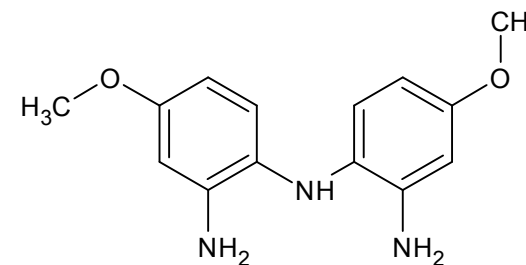
<b>Acquisition Time (sec)</b>	4.8845	<b>Comment</b>	FD313-2	<b>Date</b>	25 Mar 2013 21:16:00				
<b>Date Stamp</b>	25 Mar 2013 21:16:00		<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKENMR\FD313-2 13C\1\FID					
<b>Frequency (MHz)</b>	62.90	<b>Nucleus</b>	13C	<b>Number of Transients</b>	1400	<b>Origin</b>	spect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



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## Compound 37

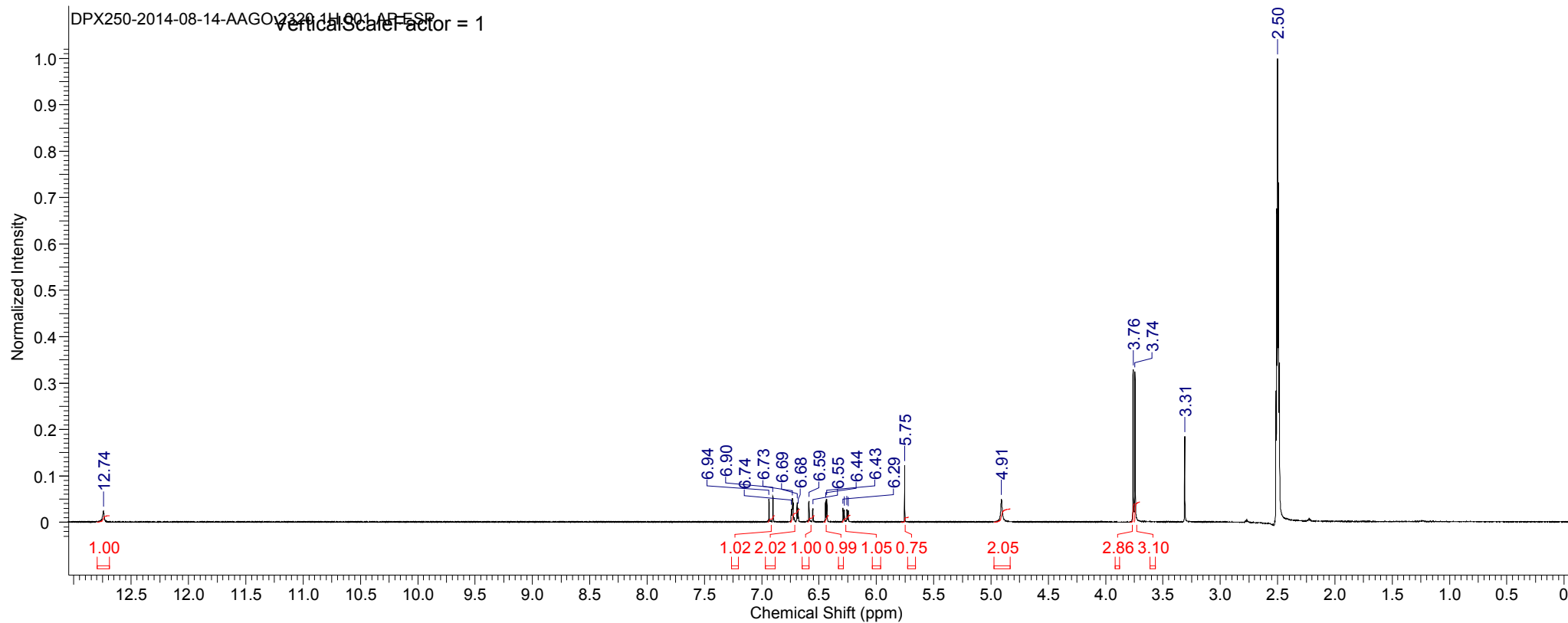
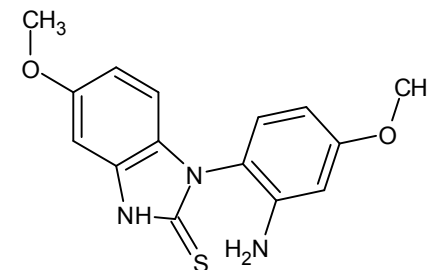
<b>Acquisition Time (sec)</b>	4.0894						
<b>Comment</b>	Goethe-Universität Frankfurt NMR Service Abteilung Spektrometer AV400 HH003200 Probenkopf BBI Z-Grad Z862701 0065 Arbeitskreis AK Goebel AA5						
<b>Date</b>	16 Jul 2014 15:11:28	<b>Date Stamp</b>	16 Jul 2014 15:11:28				
<b>File Name</b>	C:\USERS\PLAM\DESKTOP\ABDULLAH\AV400-2014-07-16-AAGO.10600\1\PDATA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



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## Compound 38

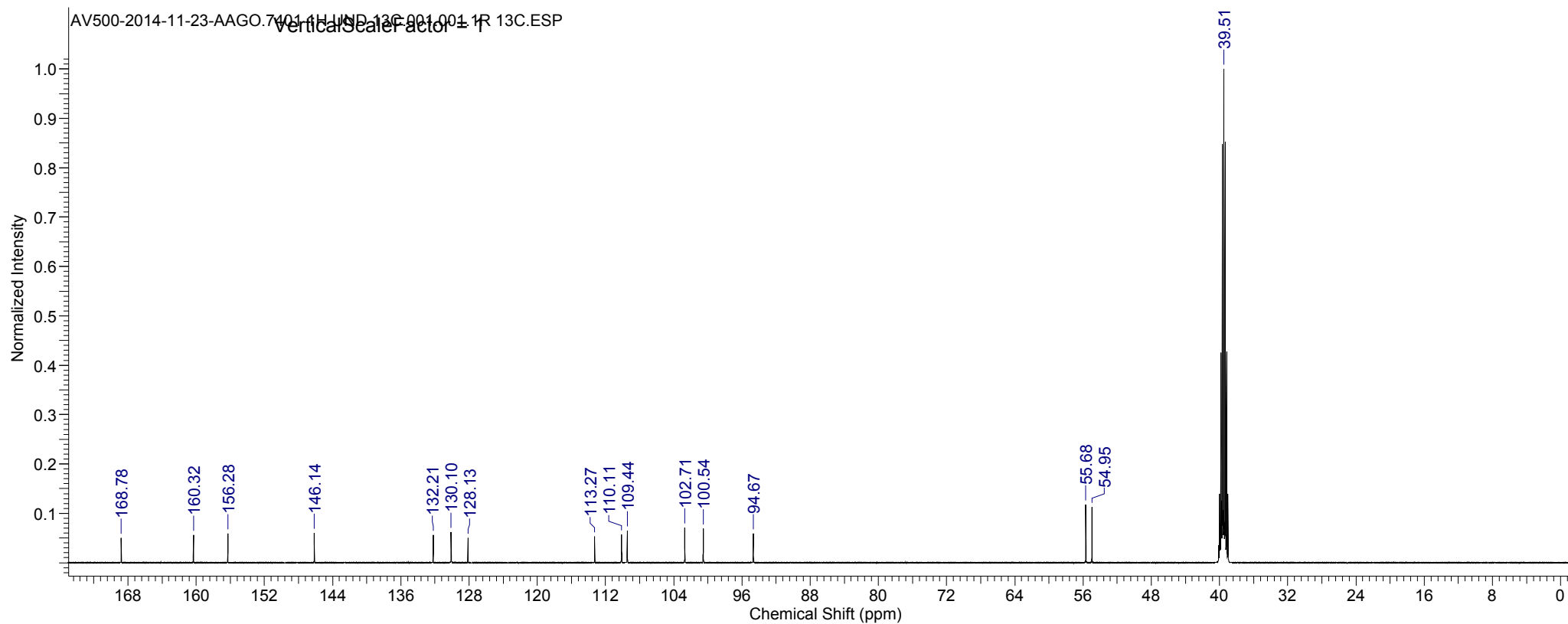
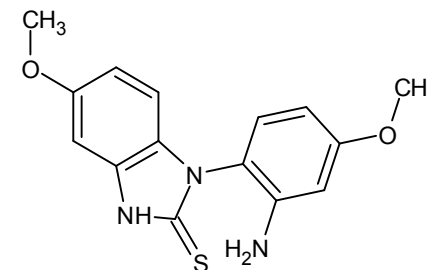
Acquisition Time (sec)	3.9998	Comment	AA6-SI	Date	14 Aug 2014 19:14:40		
Date Stamp	14 Aug 2014 19:14:40						
File Name	C:\USERS\RIKE\DATEN\RIKE\WRT\APISPEKTREN\ABDULLAH\THIOHARNSTOFF\NMR\DPX250-2014-08-14-AAGO.2320 1H\1\FID						
Frequency (MHz)	250.13	Nucleus	1H	Number of Transients	64	Origin	spect
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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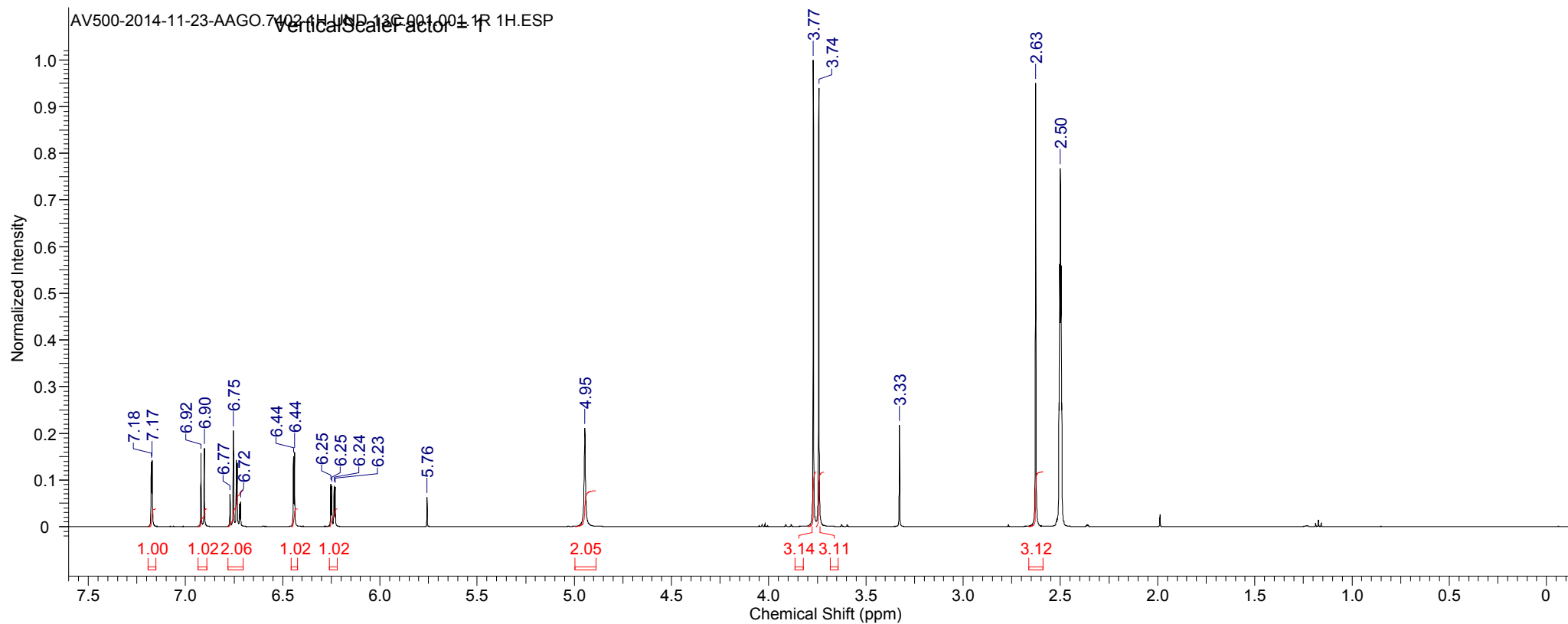
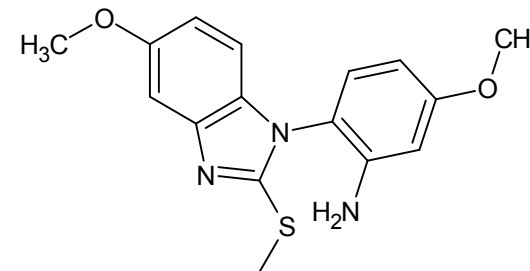
## Compound 38

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\APISPEKTREN\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	zpgg30
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		



## Compound 39

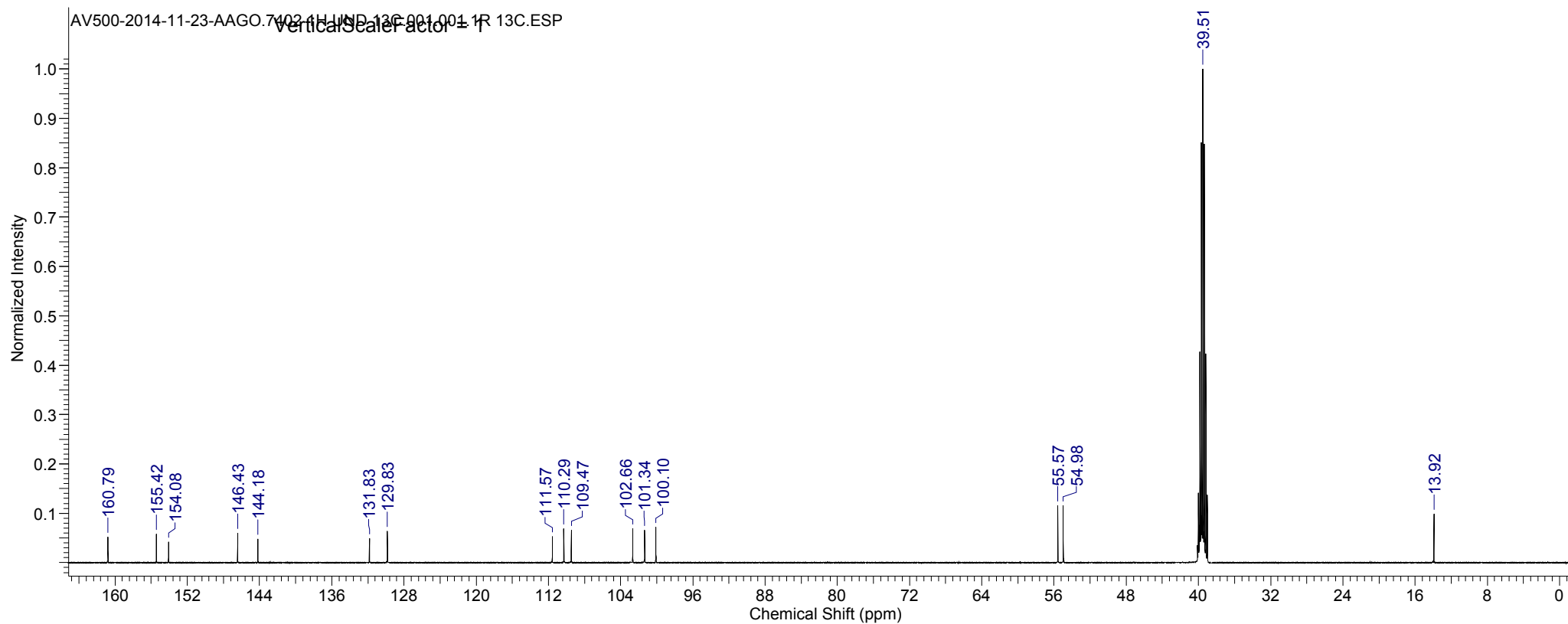
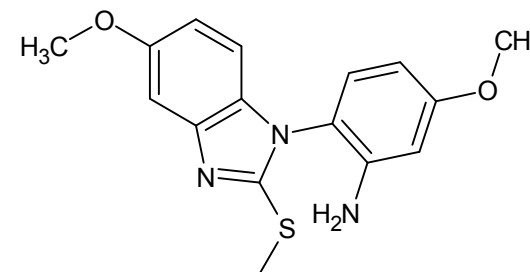
<b>Acquisition Time (sec)</b>	3.9999	<b>Comment</b>	AA6SMe	<b>Date</b>	24 Nov 2014 00:02:24
<b>Date Stamp</b>	24 Nov 2014 00:02:24				
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\WRT\APISPEKTREN\ABDULLAH\METHYLTHIOHARNSTOFF\NMR\AV500-2014-11-23-AAGO.7402 1H UND 13C\1\PDATA\1\1R				
<b>Frequency (MHz)</b>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



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## Compound 39

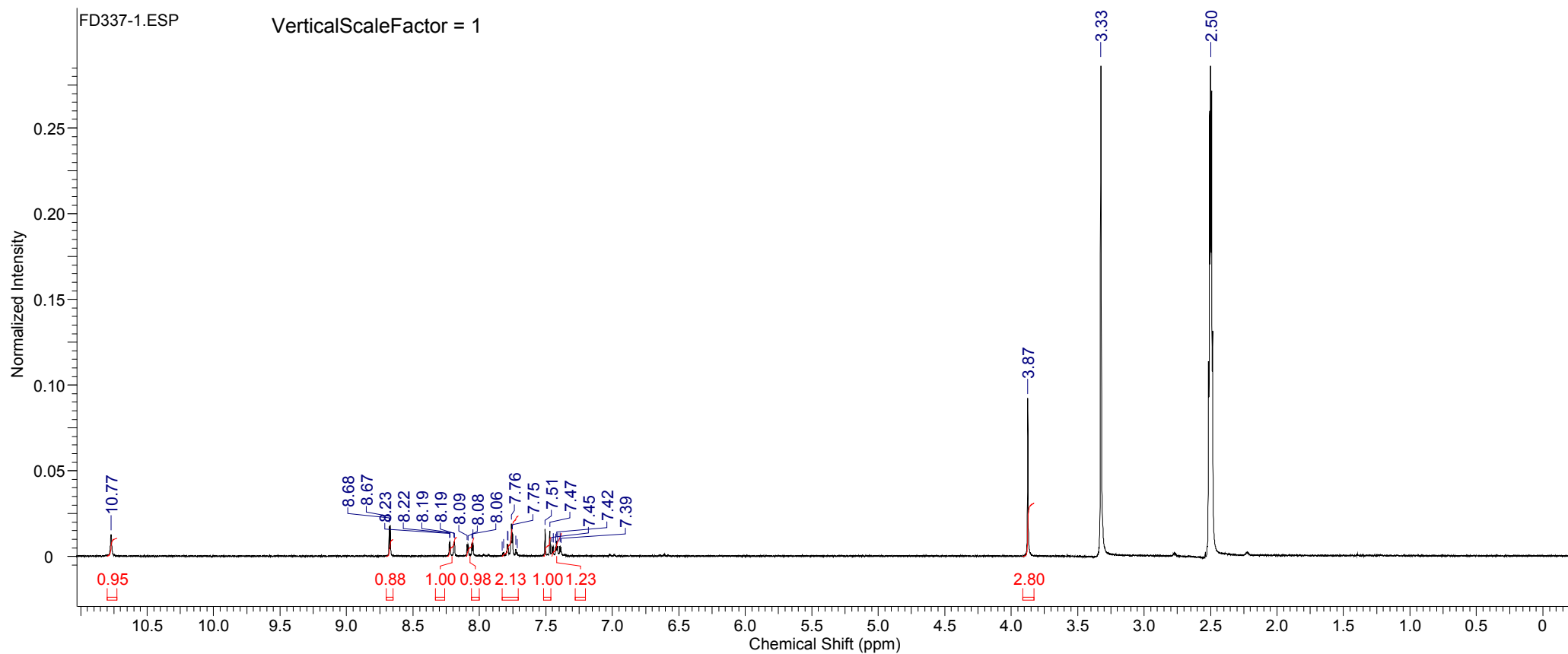
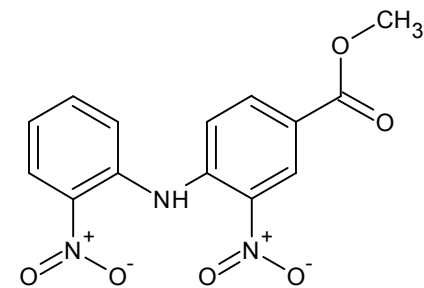
Acquisition Time (sec)	1.0457	Comment	AA6SMe	Date	24 Nov 2014 00:57:52		
Date Stamp	24 Nov 2014 00:57:52						
File Name	C:\USERS\RIKE\DATEN\RIKE\WRT\APISPEKTREN\ABDULLAH\METHYLTHIOHARNSTOFF\NMR\AV500-2014-11-23-AAGO.7402 1H UND 13C\2\PDATA\1\1R						
Frequency (MHz)	125.77	Nucleus	13C	Number of Transients	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		





## Compound 41

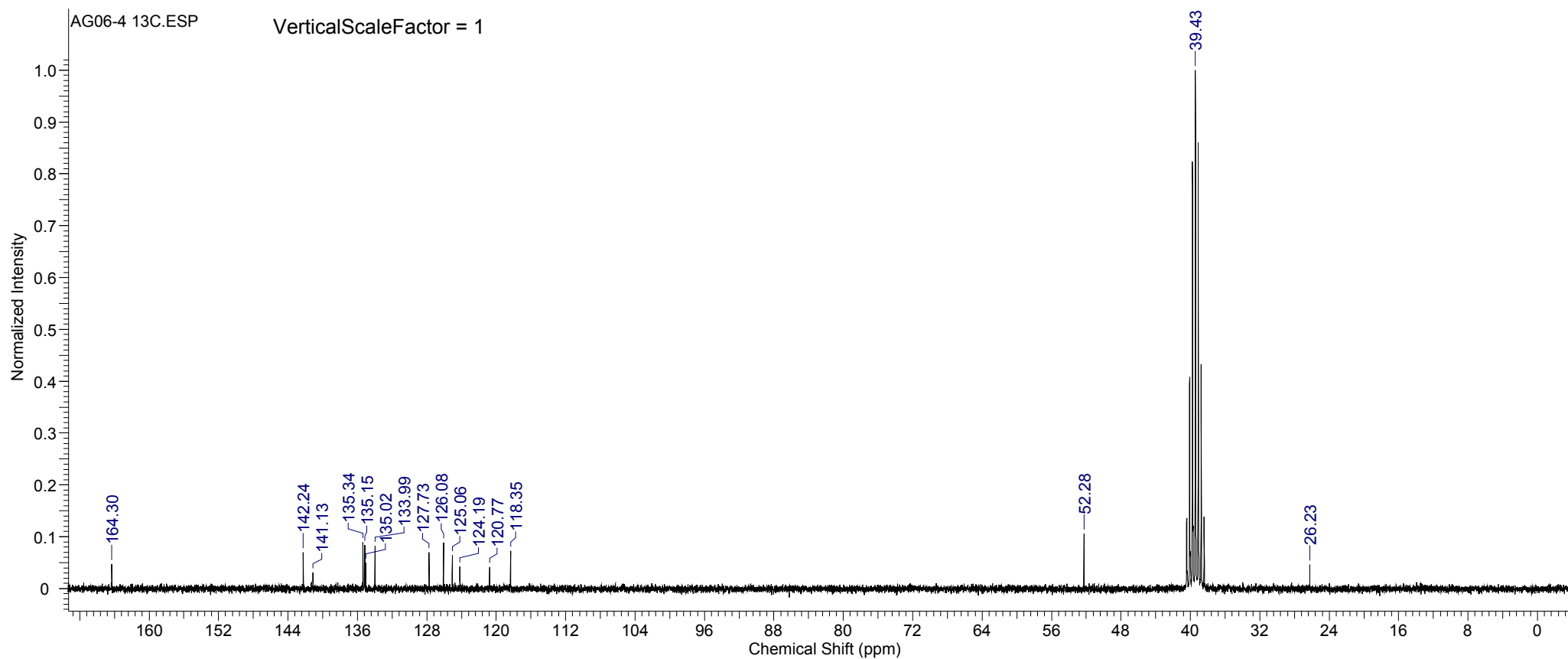
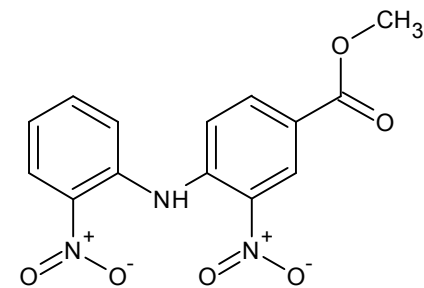
<b>Acquisition Time (sec)</b>	3.9999	<b>Comment</b>	FD337-1	<b>Date</b>	09 Sep 2013 11:42:24	<b>Date Stamp</b>	09 Sep 2013 11:42:24
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\FD337-1\1\FID	<b>Frequency (MHz)</b>	250.13	<b>Nucleus</b>	1H	<b>Number of Transients</b>	32
<b>Origin</b>	spect	<b>Original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



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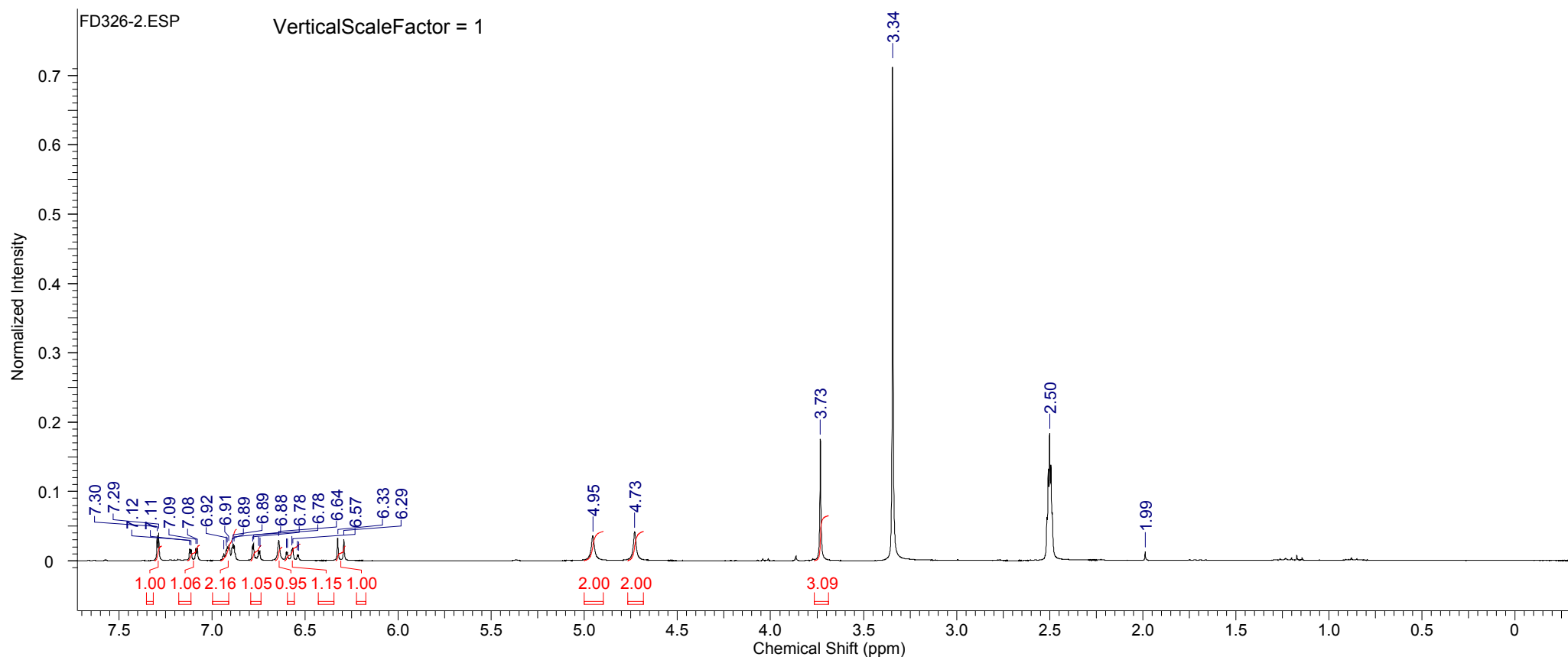
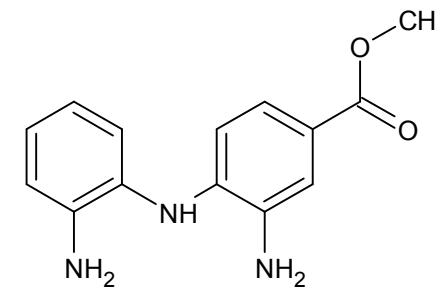
## Compound 41

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 13C1\FID				
Frequency (MHz)	62.90	Nucleus	13C	Number of Transients	4096	Origin	spect	Original Points Count	16384
Owner	service	Points Count	16384	Pulse Sequence	zpgpg30	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



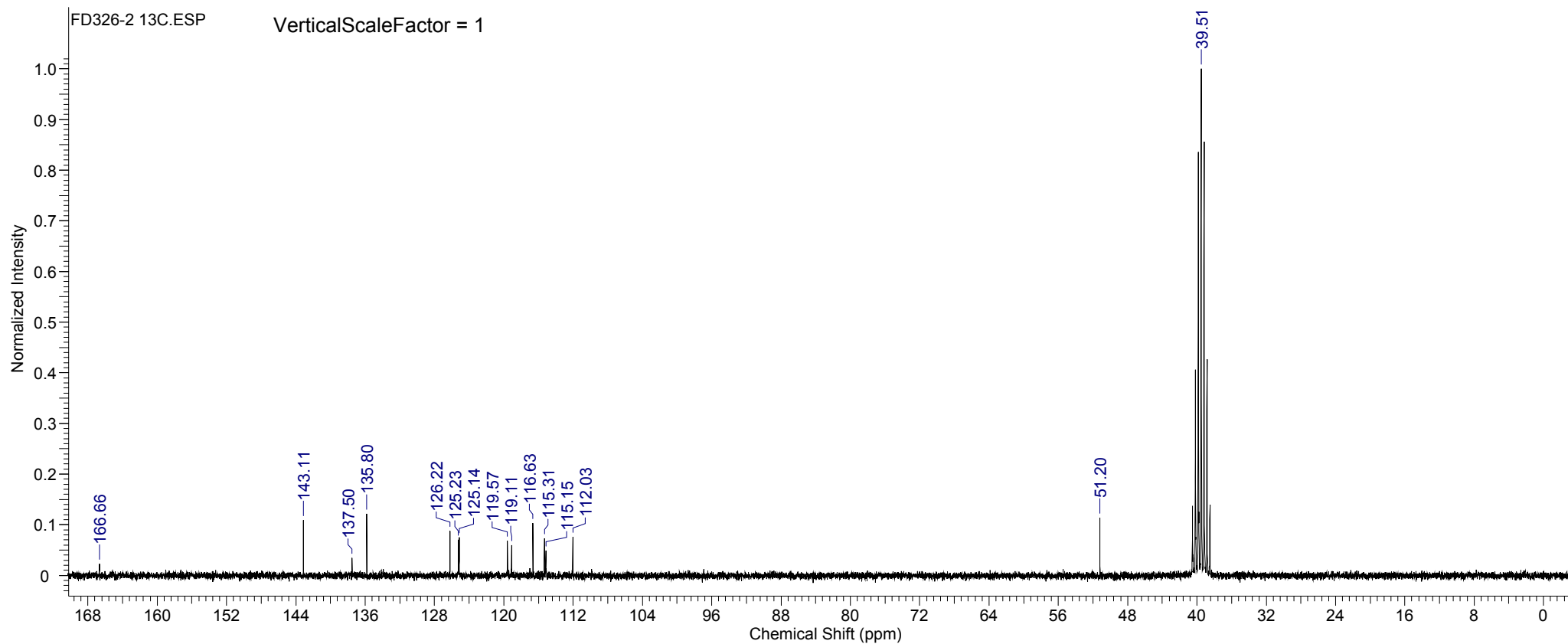
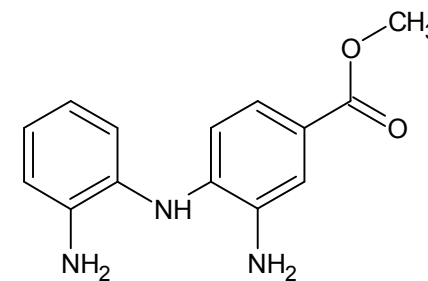
## Compound 42

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



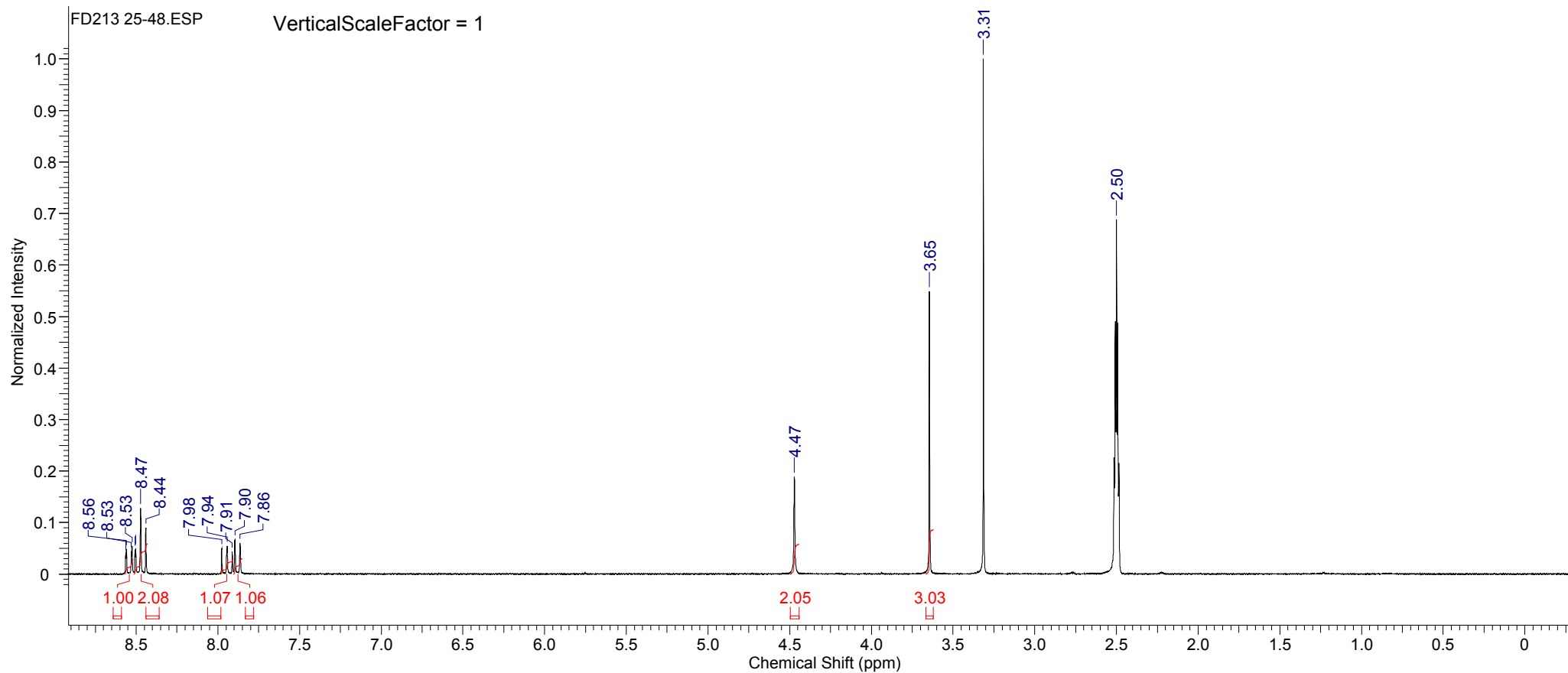
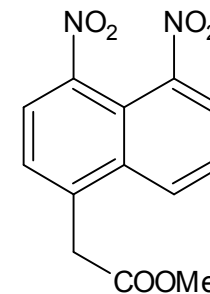
## Compound 42

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\FID			Frequency (MHz)	62.90	Nucleus	13C
Number of Transients	4096	Origin	spect	Original Points Count	16384	Owner	service
Pulse Sequence	zgpg30	Receiver Gain	11585.20	SW(cyclical) (Hz)	15723.27	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	15722.31	Temperature (degree C)	27.000	Spectrum Offset (Hz)	6258.9033



## Compound 45

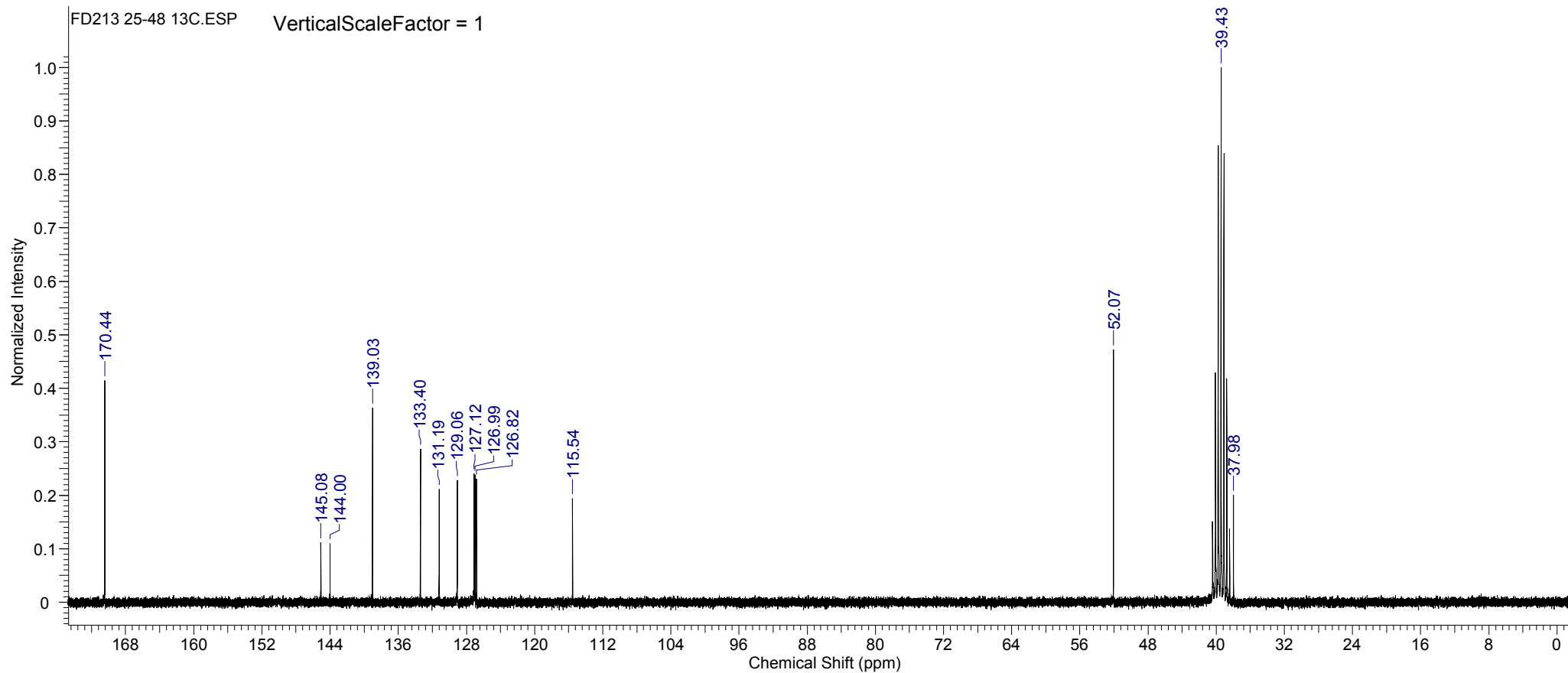
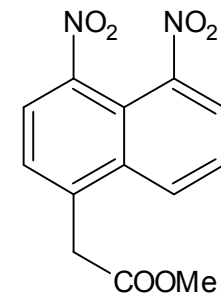
Acquisition Time (sec)	5.3809	Date	15 Feb 2012 11:27:22				
File Name	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD213\FD213 25-48\FD213 25-48.MRC			Frequency (MHz)	250.13		
Nucleus	1H	Origin	Bruker	Original Points Count	29696	Points Count	65536
Pulse Sequence	ZG30	Spectrum Offset (Hz)	1747.4260	Spectrum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



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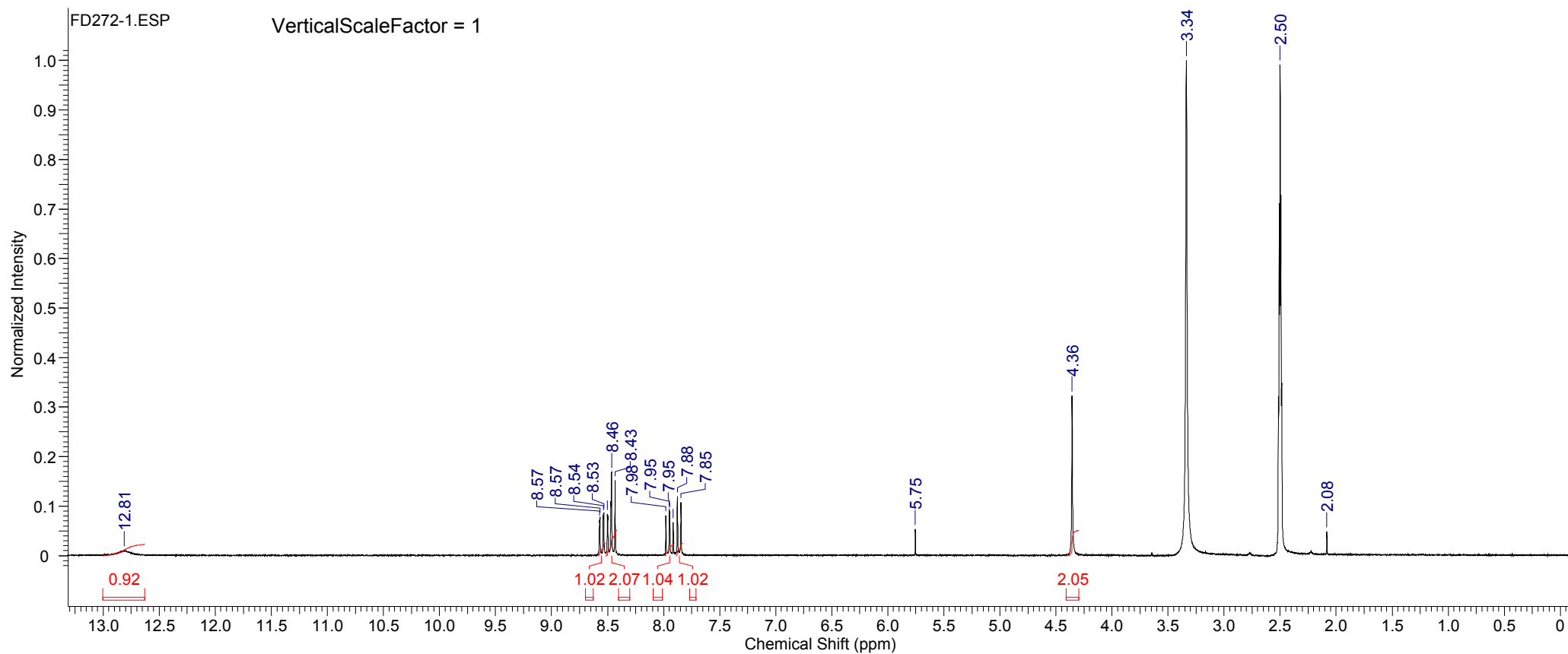
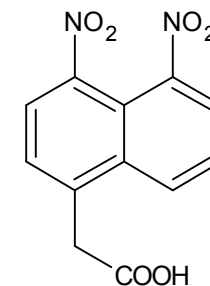
## Compound 45

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



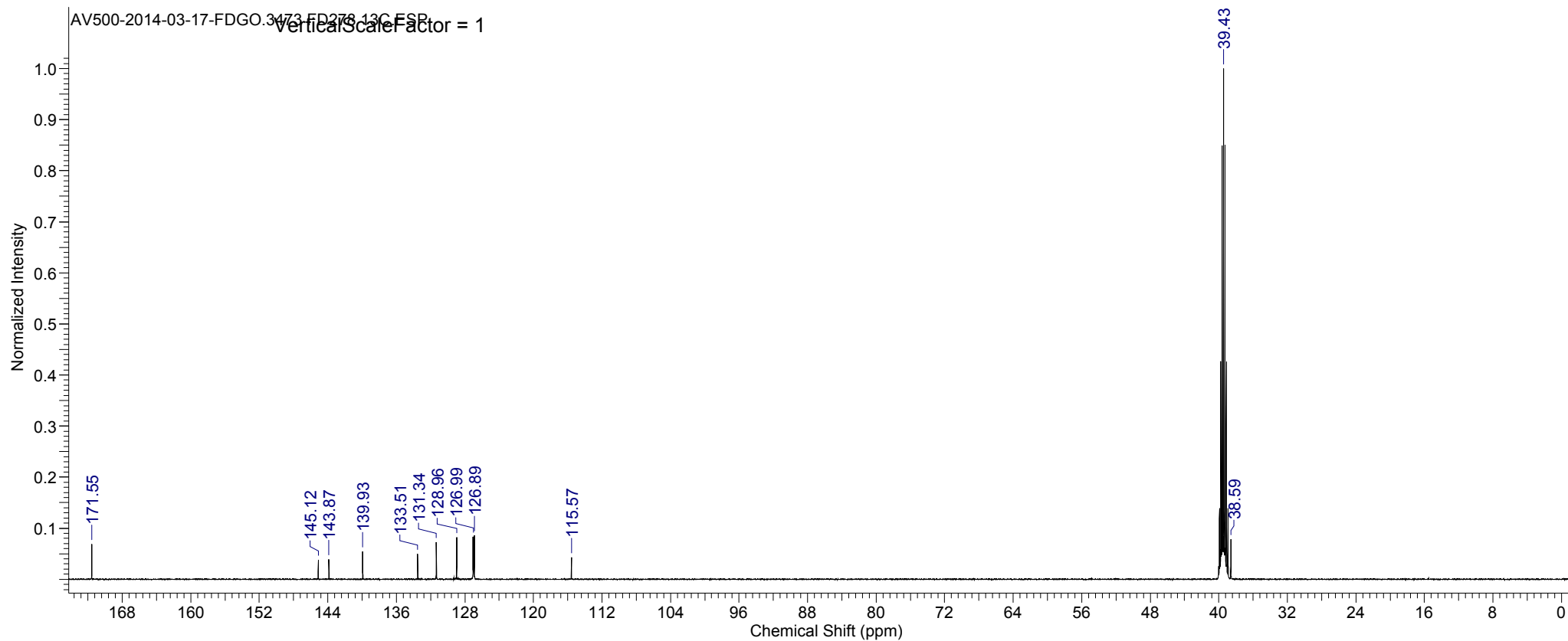
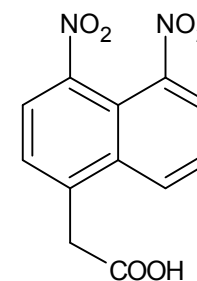
## Compound 46

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
Receiver Gain	645.10	SW(cyclical) (Hz)	4761.90	Solvent	DMSO-d6	Spectrum Offset (Hz)	1754.1121
Sweep Width (Hz)	4761.76	Temperature (degree C)	27.000	Spectrum Type	STANDARD		



## Compound 46

<b>Acquisition Time (sec)</b>	1.0457	<b>Comment</b>	FD278	<b>Date</b>	17 Mar 2014 13:22:24
<b>Date Stamp</b>	17 Mar 2014 13:22:24	<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKENMR\AV500-2014-03-17-FDGO.3473 FD278 13C\1\PDATA\1\1R		
<b>Frequency (MHz)</b>	125.77	<b>Nucleus</b>	13C	<b>Number of Transients</b>	1926
<b>Original Points Count</b>	32678	<b>Owner</b>	service	<b>Points Count</b>	65536
<b>Receiver Gain</b>	2050.00	<b>SW(cyclical) (Hz)</b>	31250.00	<b>Solvent</b>	DMSO-d6
<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	31249.52	<b>Temperature (degree C)</b>	25.001
				<b>Origin</b>	spect
				<b>Pulse Sequence</b>	zpgg30
				<b>Spectrum Offset (Hz)</b>	12431.8789

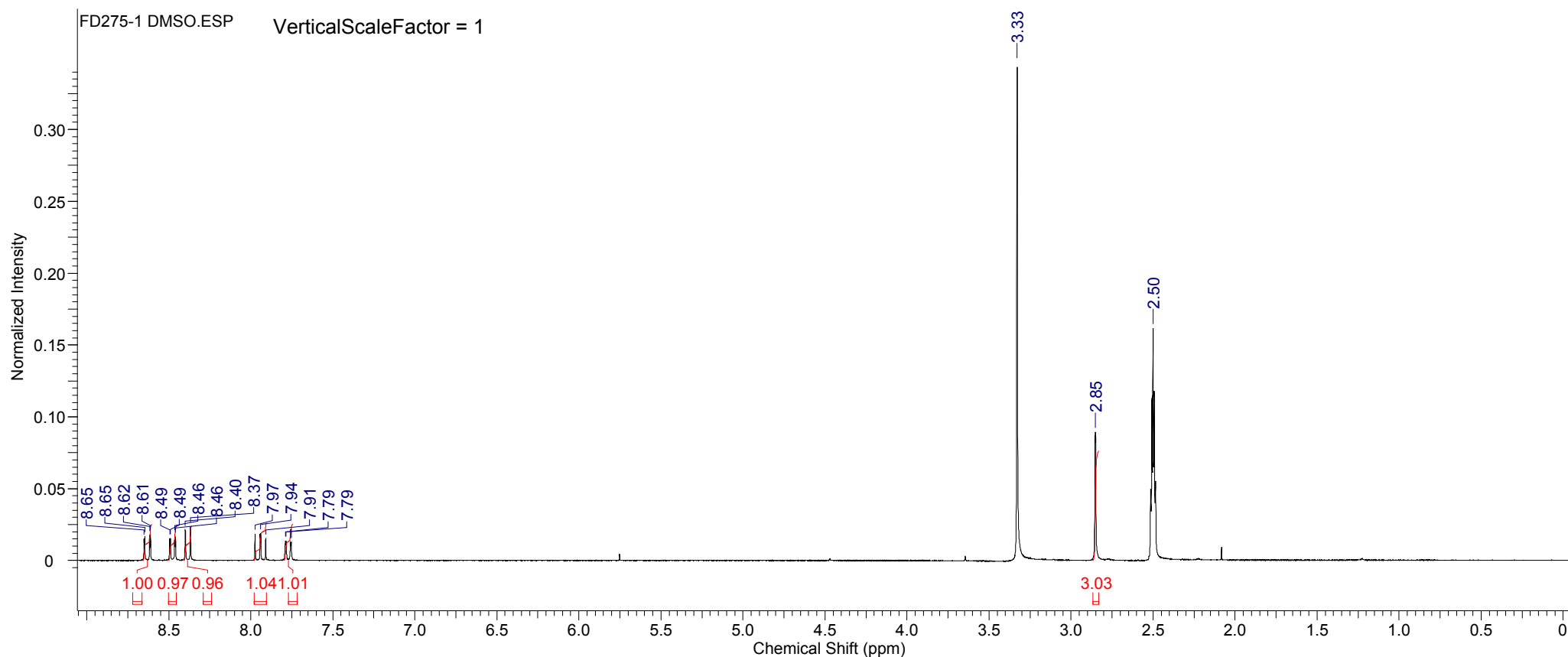
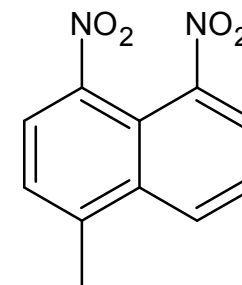




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## Compound 47

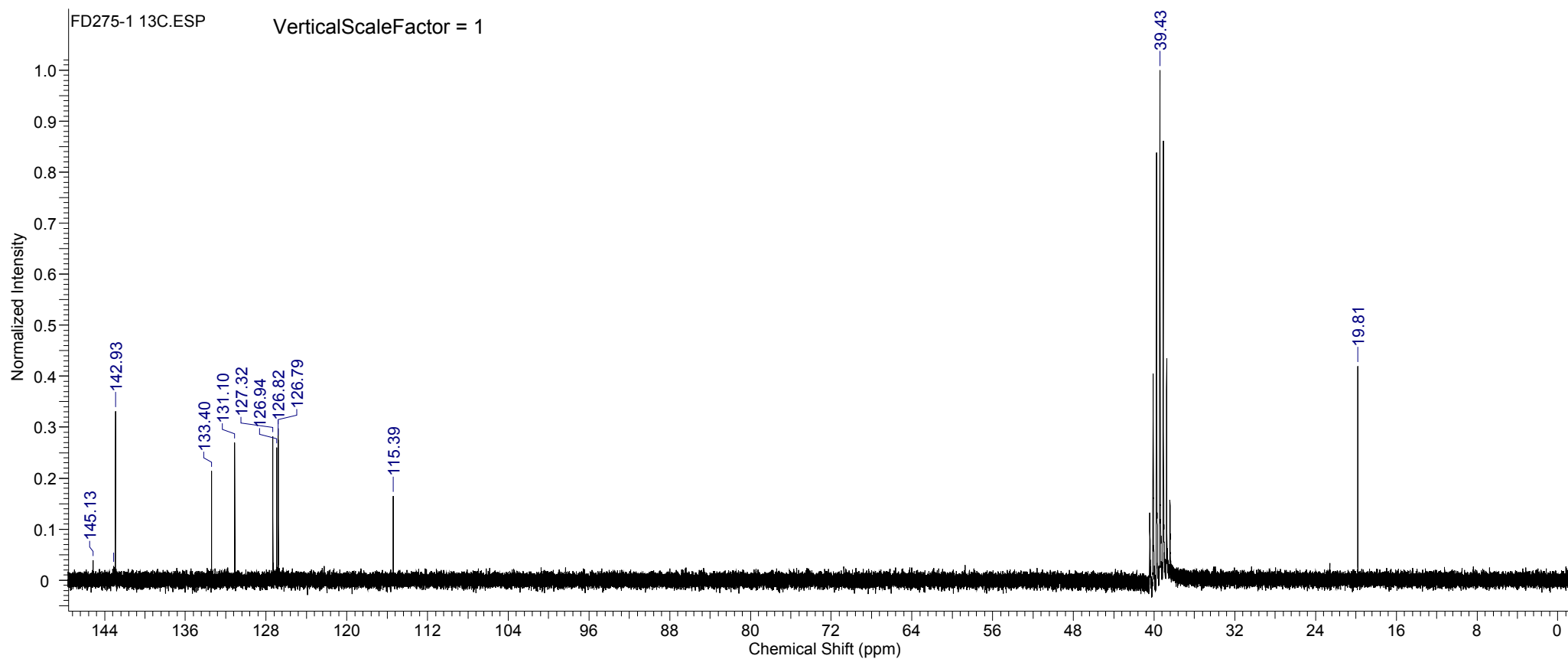
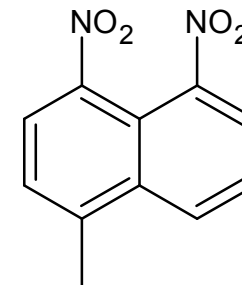
Acquisition Time (sec)	4.5158	Comment	FD275-1	Date	11 Sep 2012 10:32:00	Date Stamp	11 Sep 2012 10:32:00
File Name	C:\USERS\RIKE\DATEN\RIKE\NMR\FD275-1\1\FID	Frequency (MHz)	250.13	Nucleus	1H	Number of Transients	32
Origin	spect	Original Points Count	21504	Owner	service	Points Count	32768
Receiver Gain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



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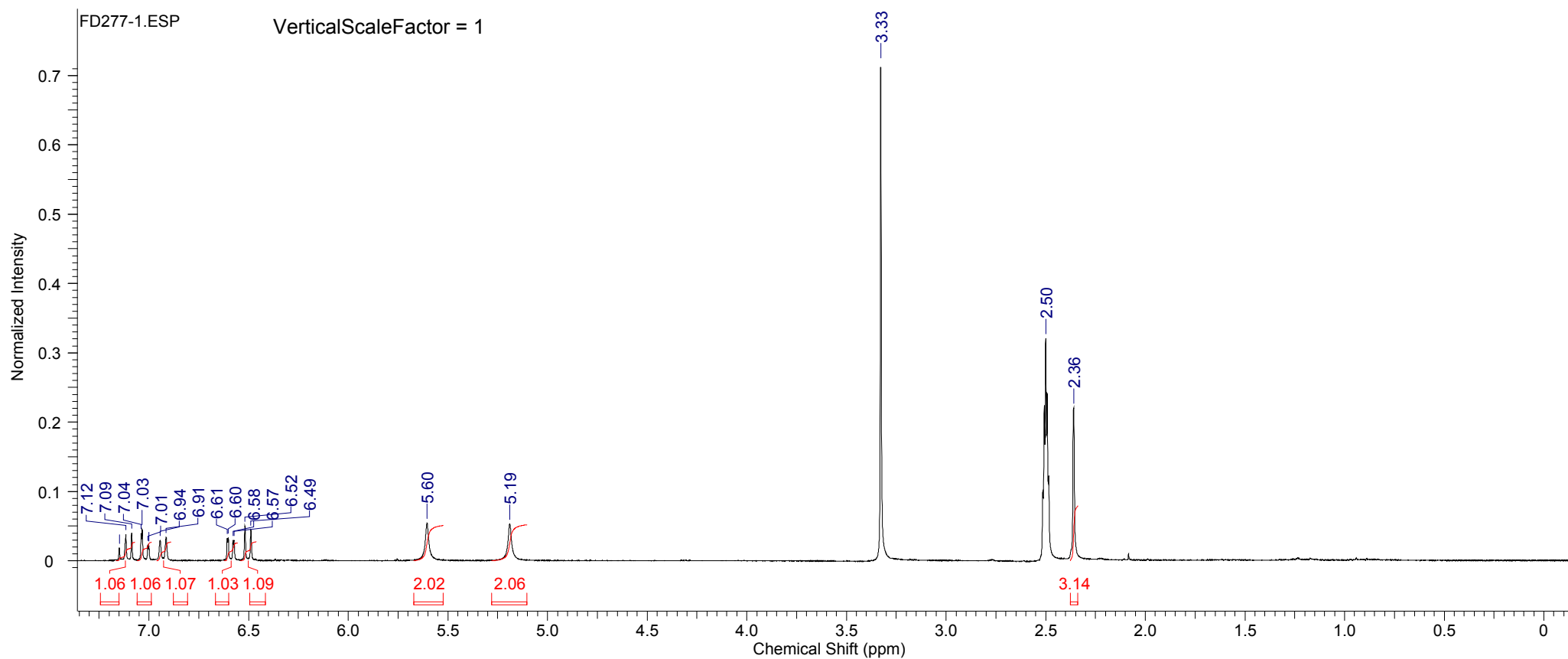
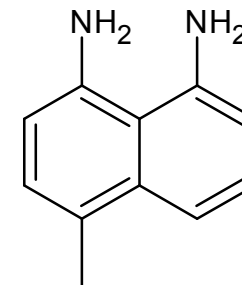
## Compound 47

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
Points Count	131072	Pulse Sequence	zgig30	Receiver Gain	13004.00	SW(cyclical) (Hz)	15060.24
Spectrum Offset (Hz)	6816.8232	Spectrum Type	STANDARD	Sweep Width (Hz)	15060.13	Temperature (degree C)	27.000
						Owner	service
						Solvent	DMSO-d6



## Compound 48

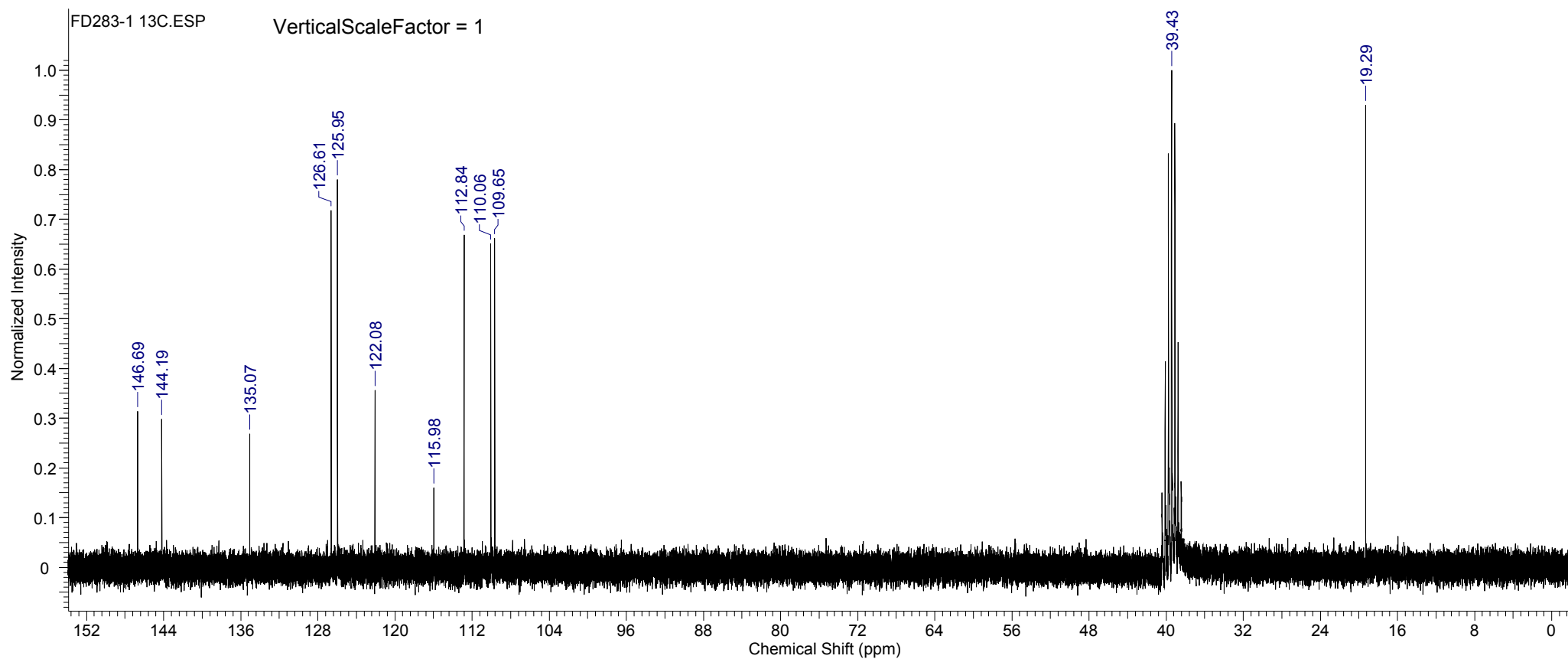
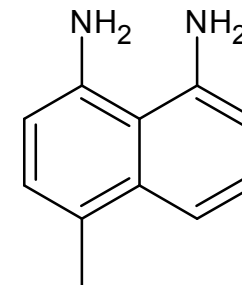
<b>Acquisition Time (sec)</b>	4.8384	<b>Comment</b>	FD277-1	<b>Date</b>	14 Sep 2012 11:48:48	<b>Date Stamp</b>	14 Sep 2012 11:48:48
<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\FD277-1\1\FID	<b>Frequency (MHz)</b>	250.13	<b>Nucleus</b>	1H	<b>Number of Transients</b>	32
<b>Origin</b>	spect	<b>Original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



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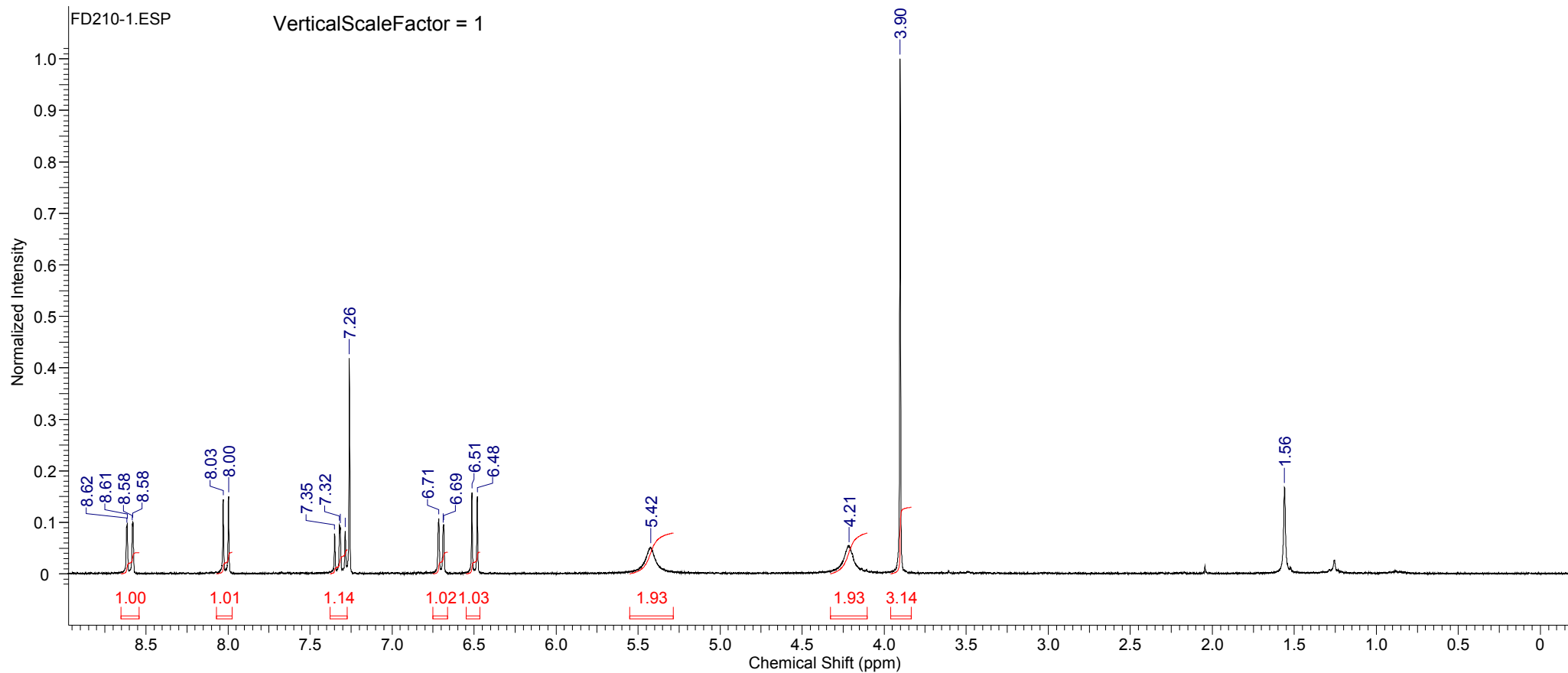
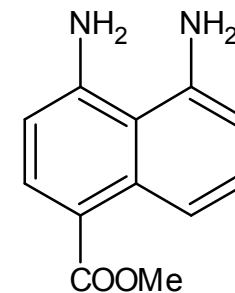
## Compound 48

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



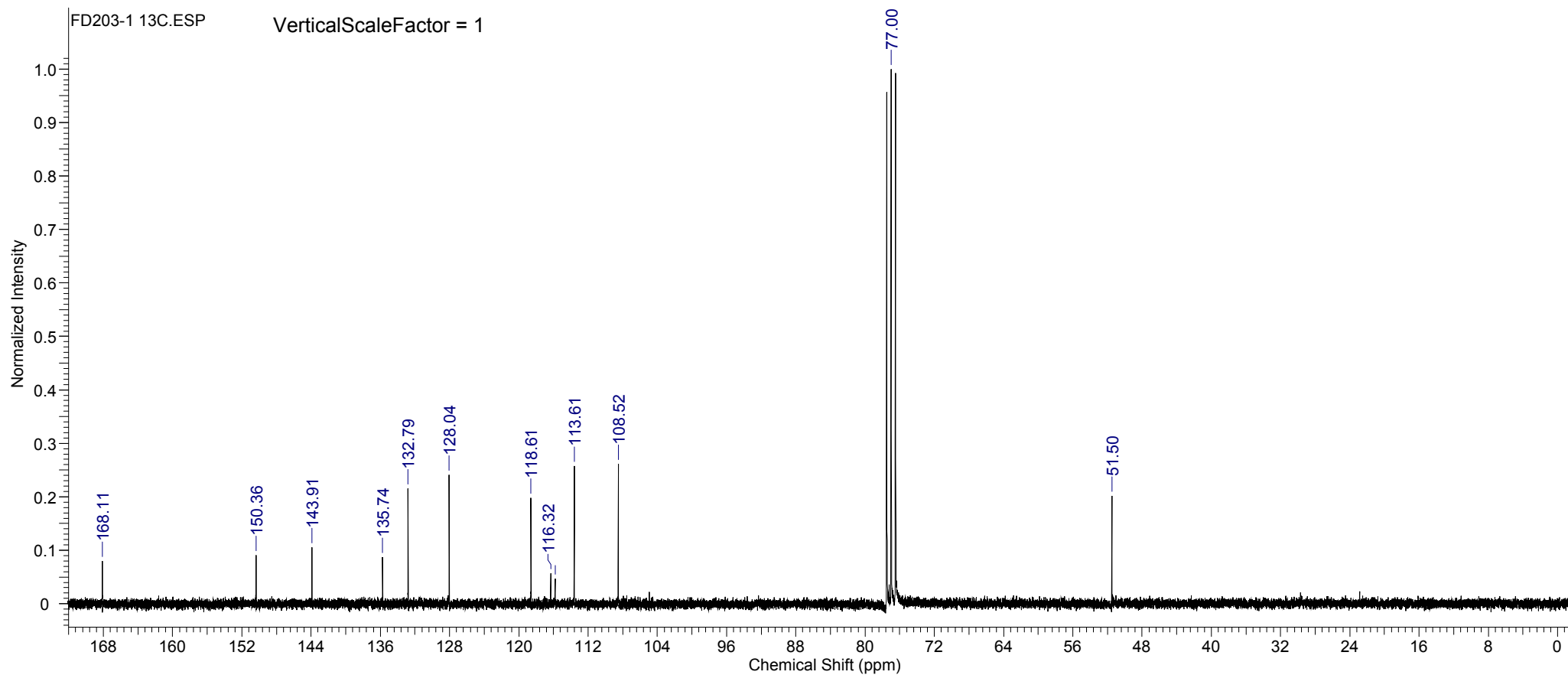
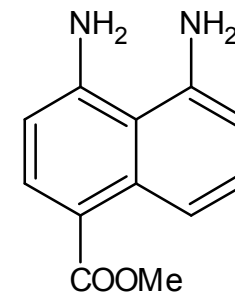
## Compound 50

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



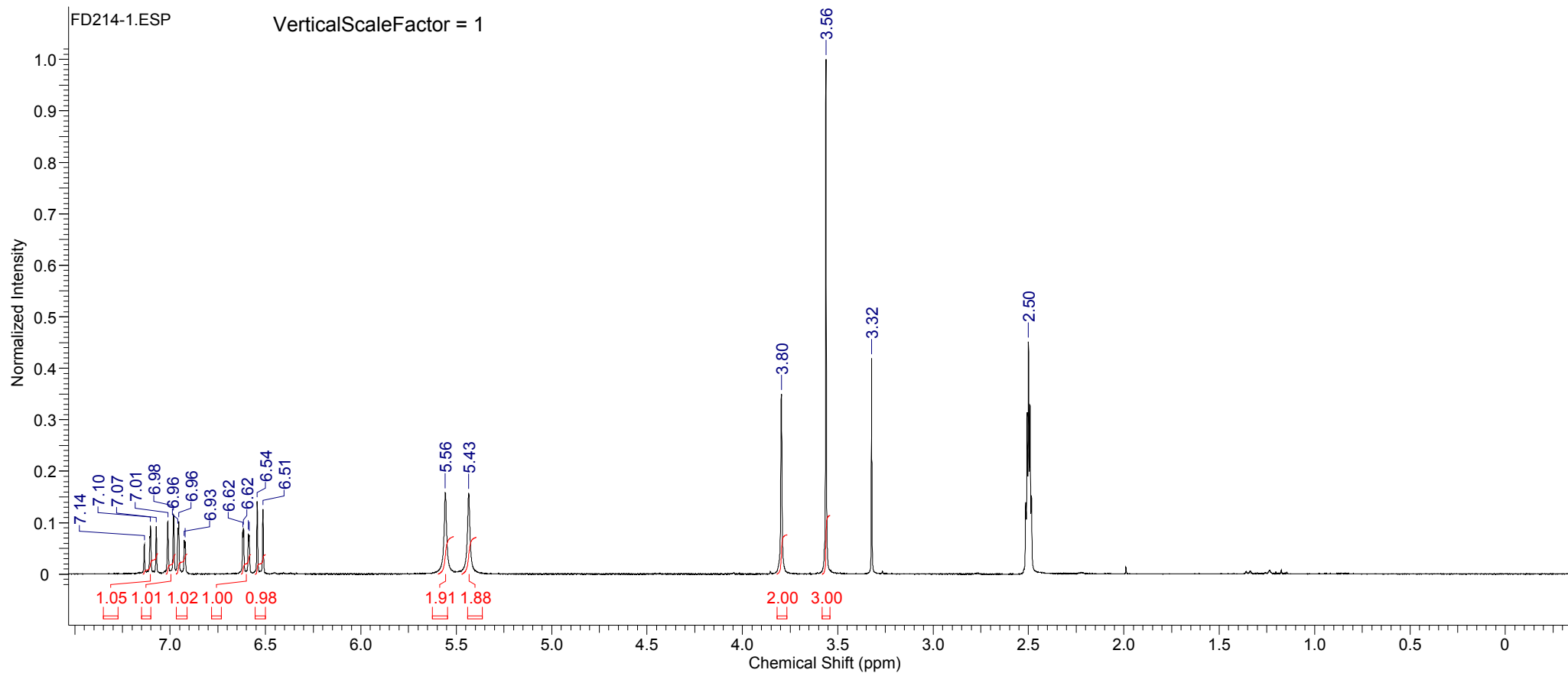
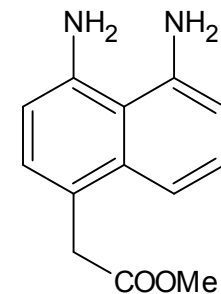
## Compound 50

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



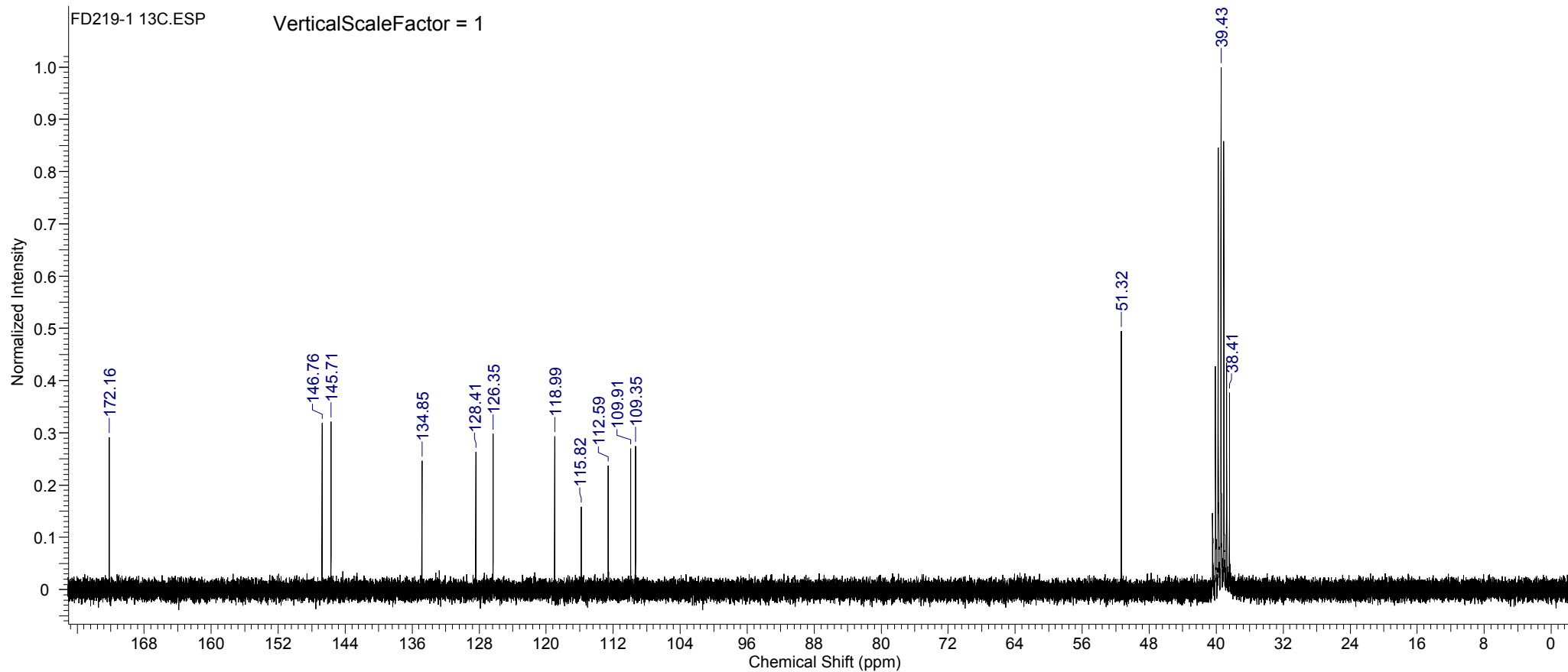
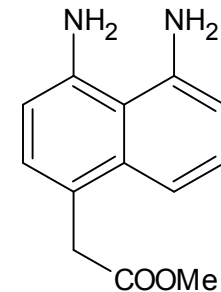
## Compound 51

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



## Compound 51

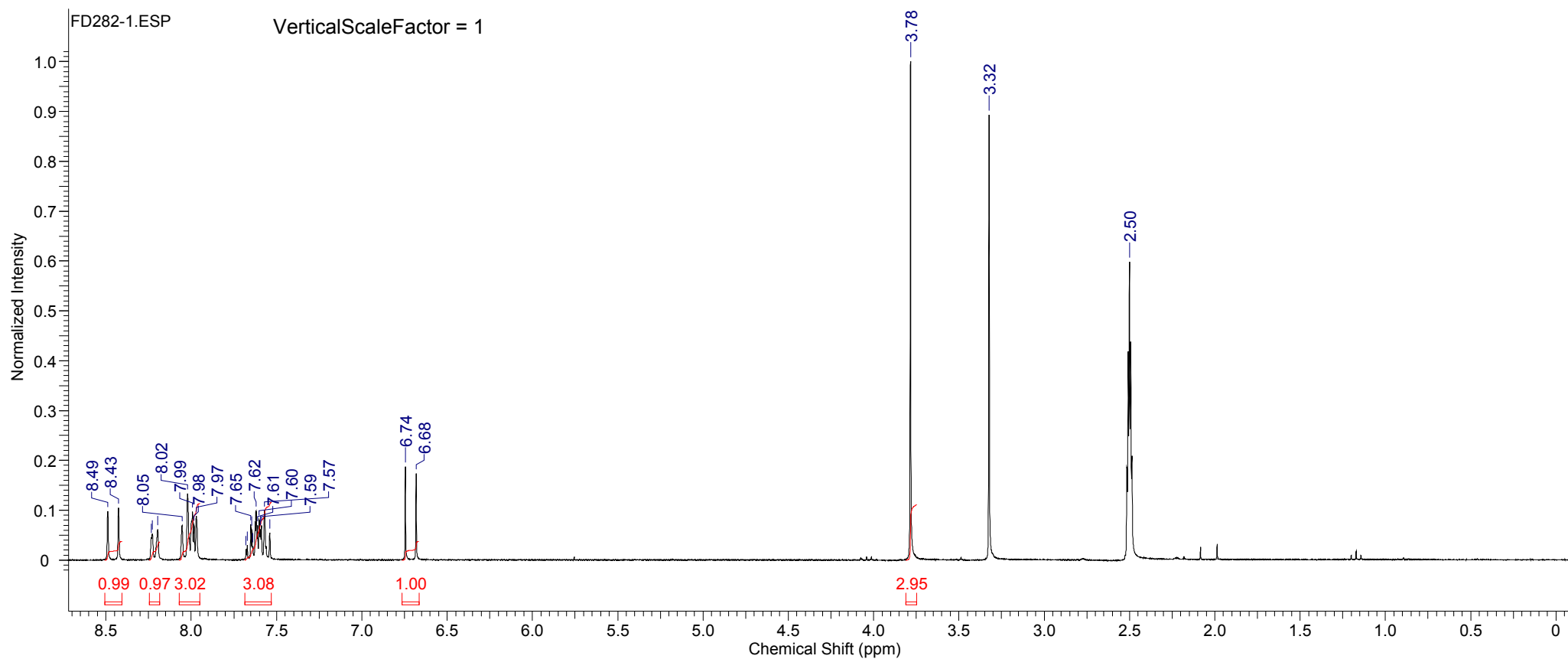
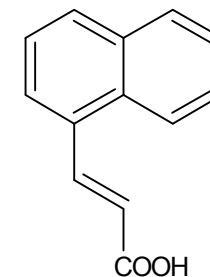
<b>Acquisition Time (sec)</b>	3.2358	<b>Date</b>	15 Feb 2012 11:27:56		
<b>File Name</b>	C:\USERS\RIKE\DATEN RIKE\NMR\NMR FD201 -247\FD219\FD219-1 13C.MRC			<b>Frequency (MHz)</b>	62.90
<b>Nucleus</b>	13C	<b>Origin</b>	Bruker	<b>Original Points Count</b>	51200
<b>Pulse Sequence</b>	ZGPGVAR	<b>Spectrum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





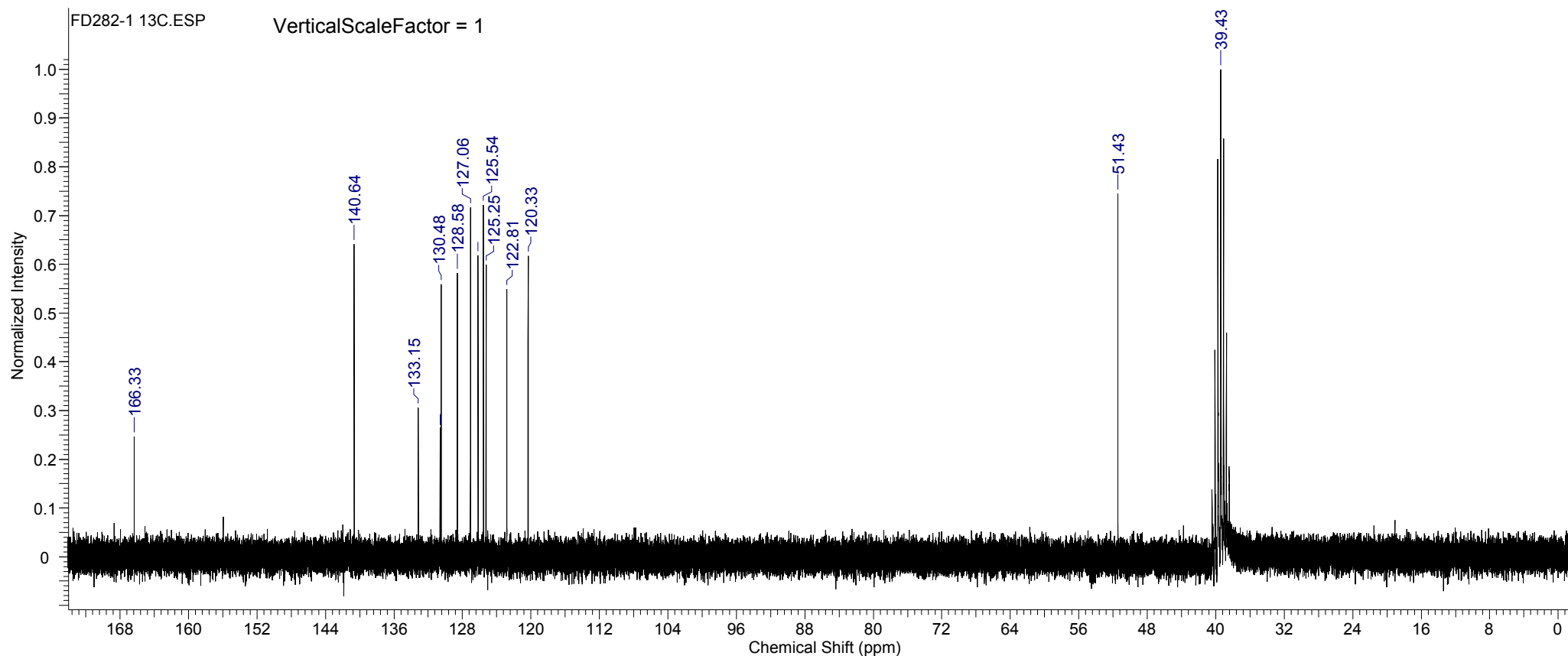
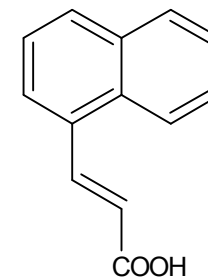
## Compound 53

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



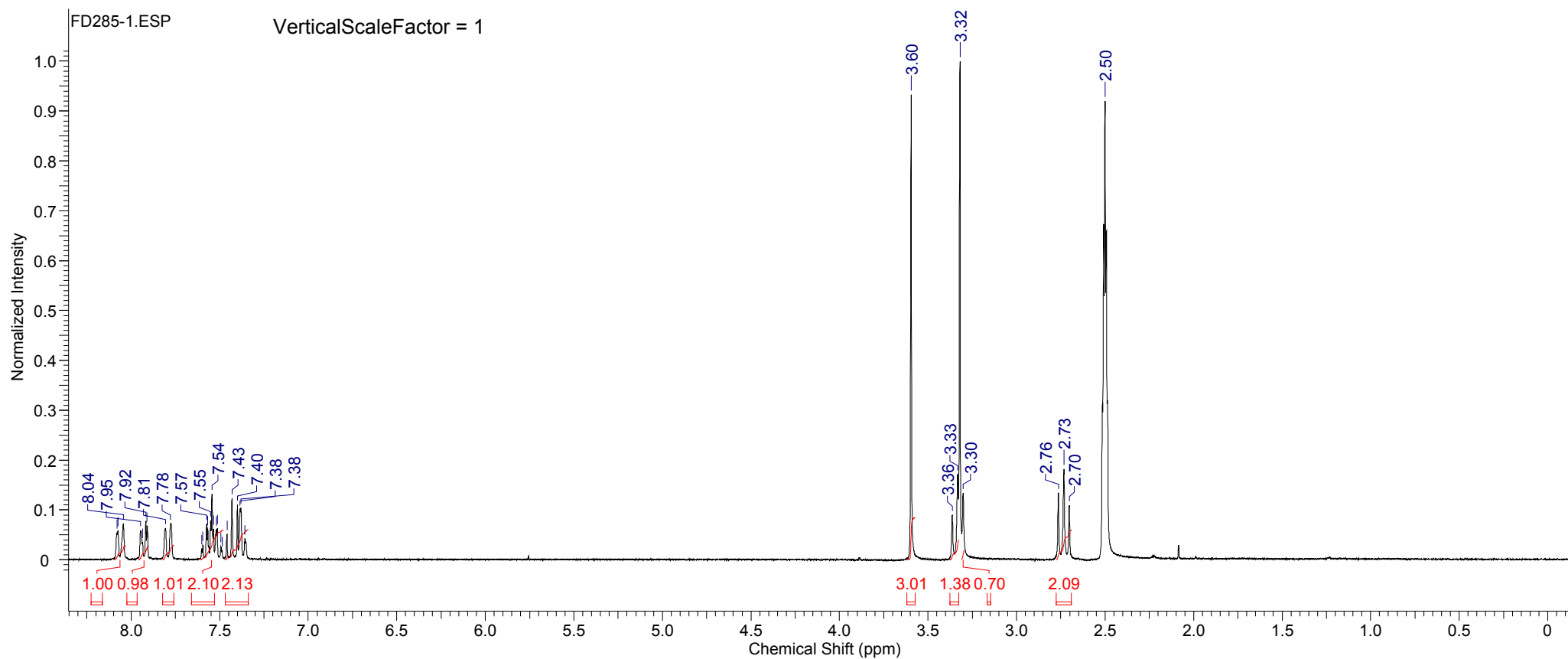
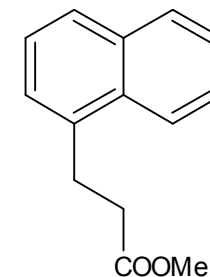
## Compound 53

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



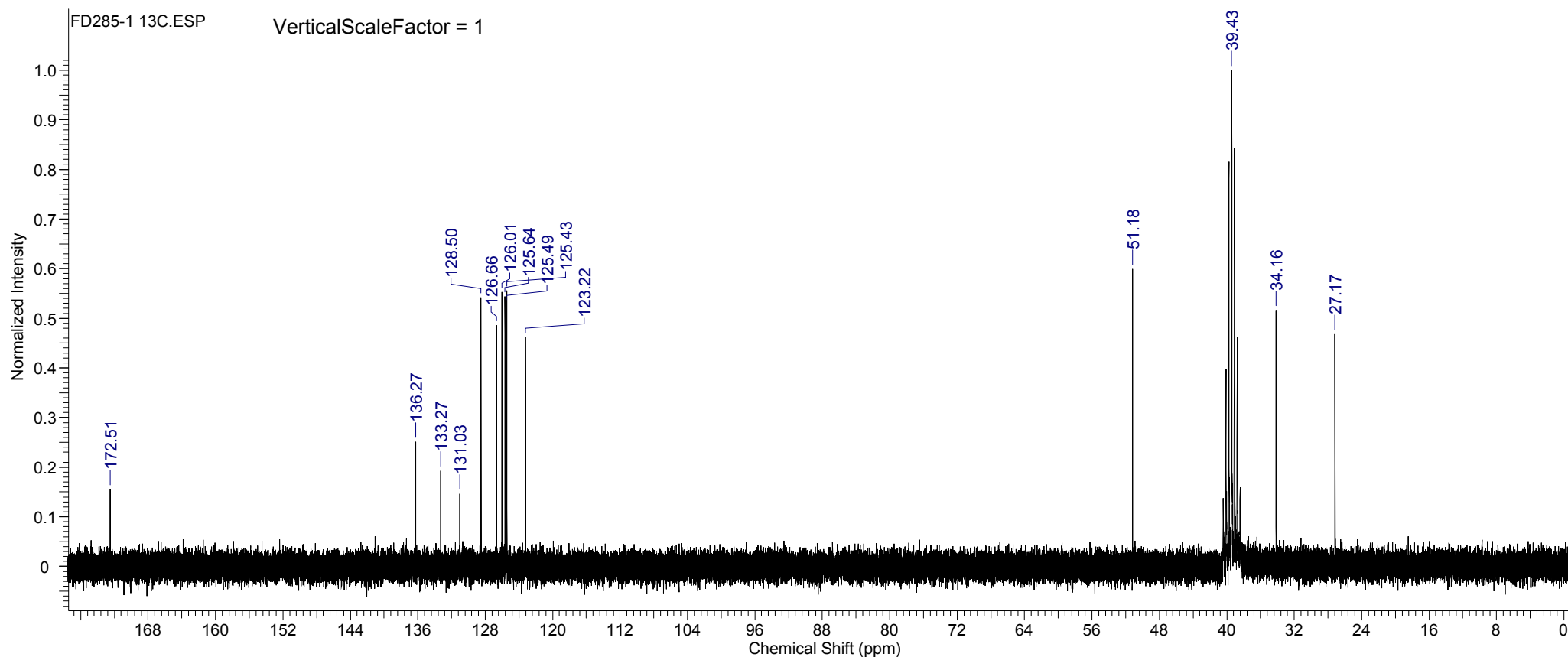
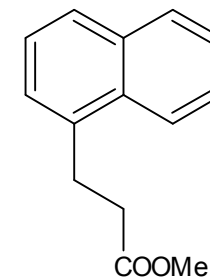
## Compound 54

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
Receiver Gain	645.10	SW(cyclical) (Hz)	4990.02	Solvent	DMSO-d6	Spectrum Offset (Hz)	1747.7292
Sweep Width (Hz)	4989.87	Temperature (degree C)	27.000	Spectrum Type	STANDARD		



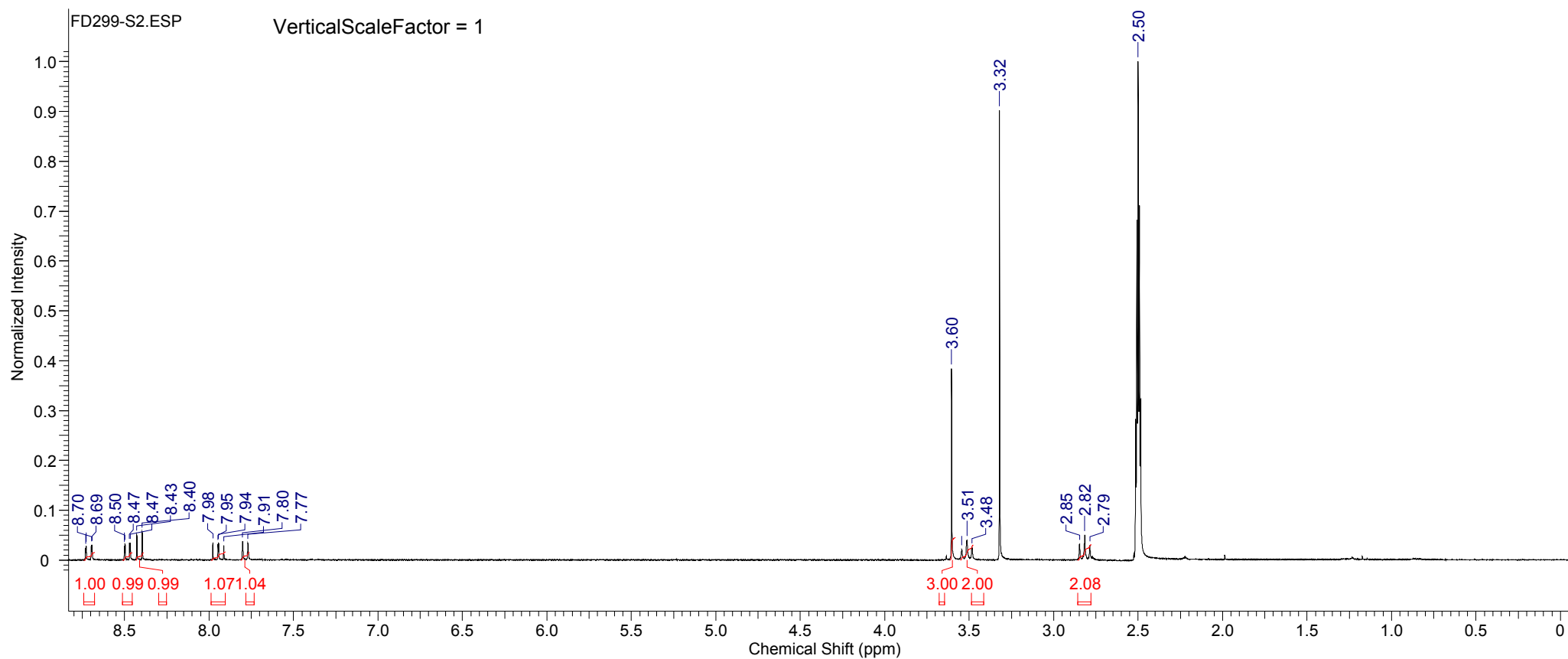
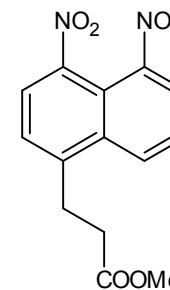
## Compound 54

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



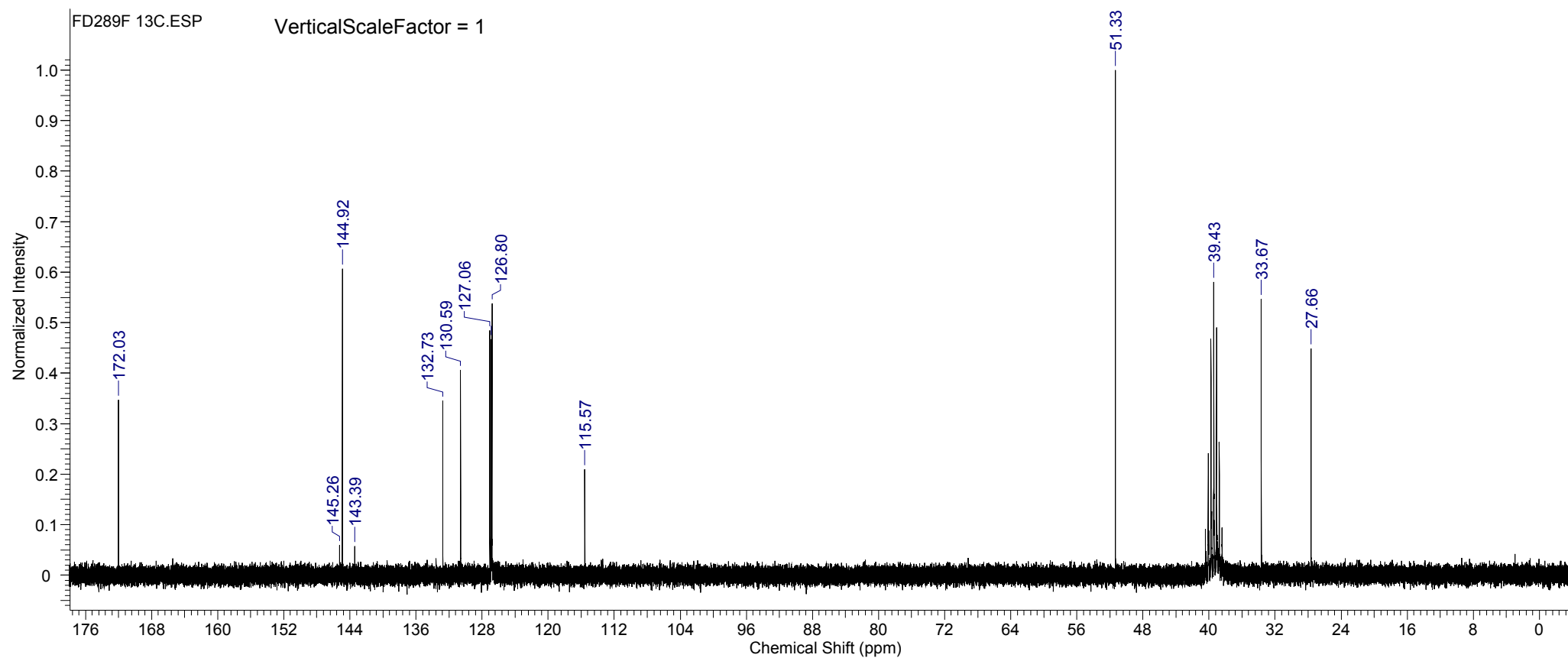
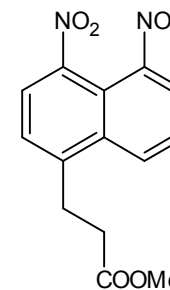
## Compound 55

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



## Compound 55

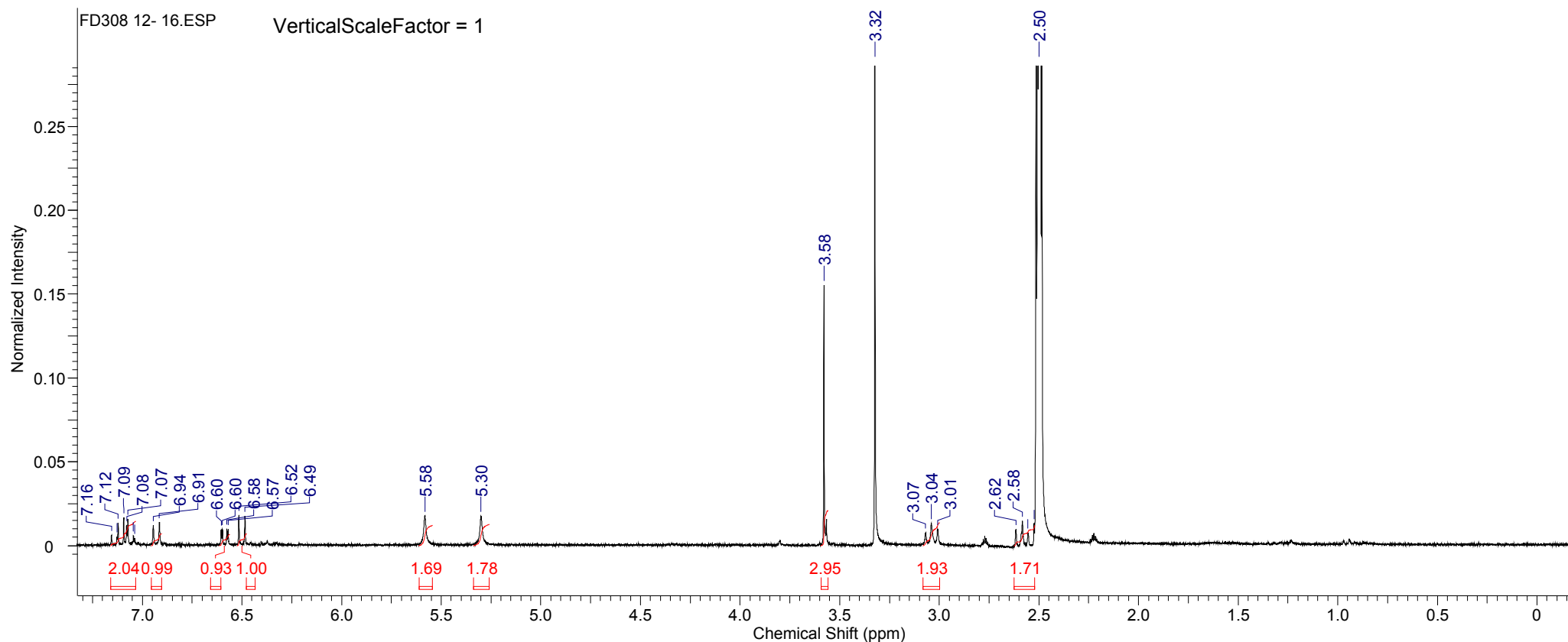
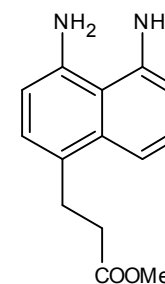
<b>Acquisition Time (sec)</b>	4.5588	<b>Comment</b>	FD289F	<b>Date</b>	04 Nov 2012 05:56:32		
<b>Date Stamp</b>	04 Nov 2012 05:56:32			<b>File Name</b>	C:\USERS\RIKE\DATEN\RIKE\NMR\FD289F_13C\1\FID	<b>Frequency (MHz)</b>	62.90
<b>Nucleus</b>	13C	<b>Number of Transients</b>	1520	<b>Origin</b>	spect	<b>Original Points Count</b>	71680
<b>Points Count</b>	131072	<b>Pulse Sequence</b>	zqig	<b>Receiver Gain</b>	13004.00	<b>SW(cyclical) (Hz)</b>	15723.27
<b>Spectrum Offset (Hz)</b>	6564.7456	<b>Spectrum Type</b>	STANDARD	<b>Sweep Width (Hz)</b>	15723.15	<b>Temperature (degree C)</b>	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
Pulse Sequence	zg30	Receiver Gain	724.10	SW(cyclical) (Hz)	4990.02	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	4989.87	Temperature (degree C)	27.000	Points Count	32768
						Spectrum Offset (Hz)	1747.4247



## 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
Receiver Gain	13004.00	SW(cyclical) (Hz)	15723.27	Solvent	DMSO-d6	Spectrum Offset (Hz)	6567.8647
Sweep Width (Hz)	15723.15	Temperature (degree C)	27.000	Spectrum Type	STANDARD		

