

ChemMedChem

Supporting Information

Scaffold Hopping from Amodiaquine to Novel Nurr1 Agonist Chemotypes via Microscale Analogue Libraries

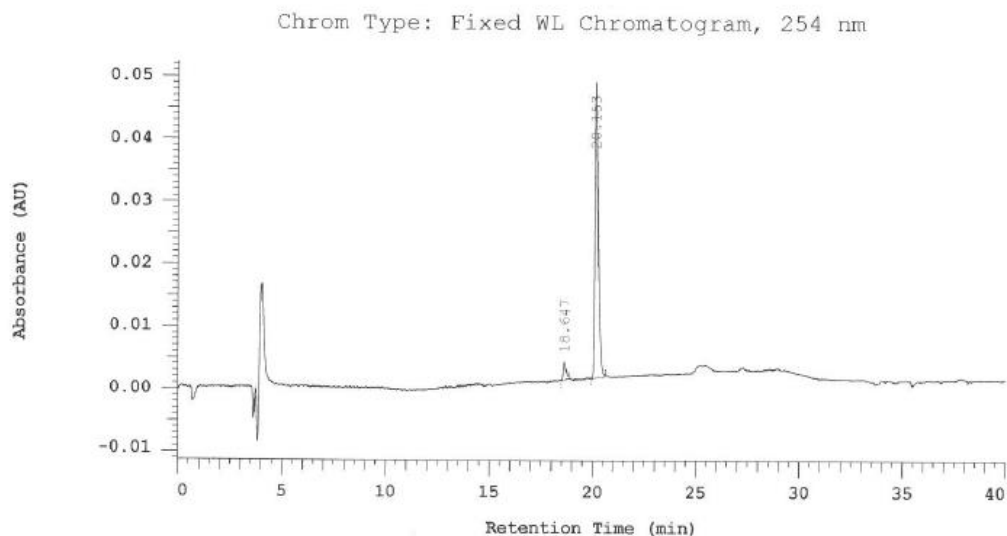
Sabine Willems[†], Marcel Müller[†], Julia Ohrndorf, Jan Heering, Ewgenij Proschak, and Daniel Merk*

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HPLC purity data for compounds 3j, 4, 4e and 5

7-Chloro-N-((5-(4-chlorophenyl)furan-2-yl)methyl)quinolin-4-amine (3j)



Pump 1: 5160

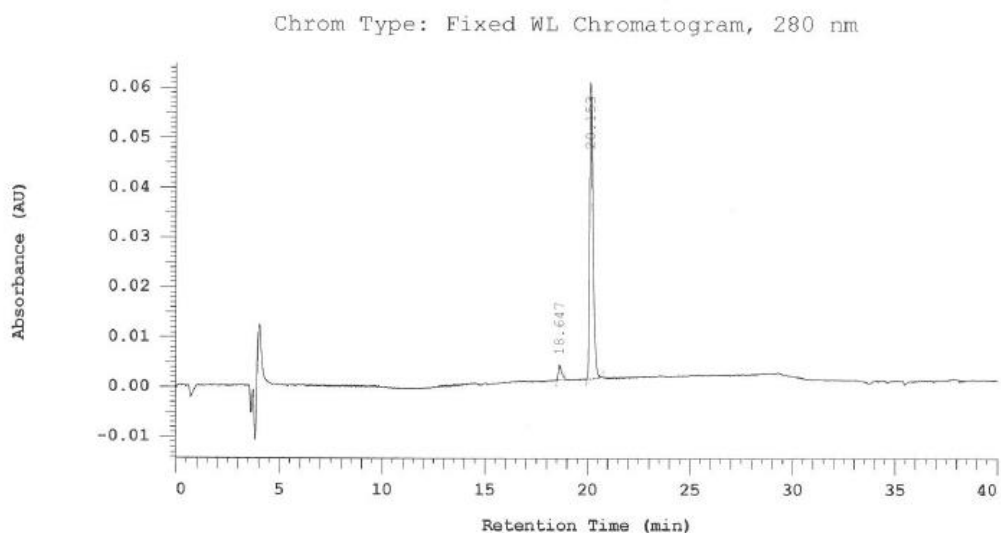
Pump 1 Solvent A: MeOH

Pump 1 Solvent B: Wasser

Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	18.647	12643	4.945	1379
2	20.153	243032	95.055	23752
		255675	100.000	25131



Pump 1: 5160

Pump 1 Solvent A: MeOH

Pump 1 Solvent B: Wasser

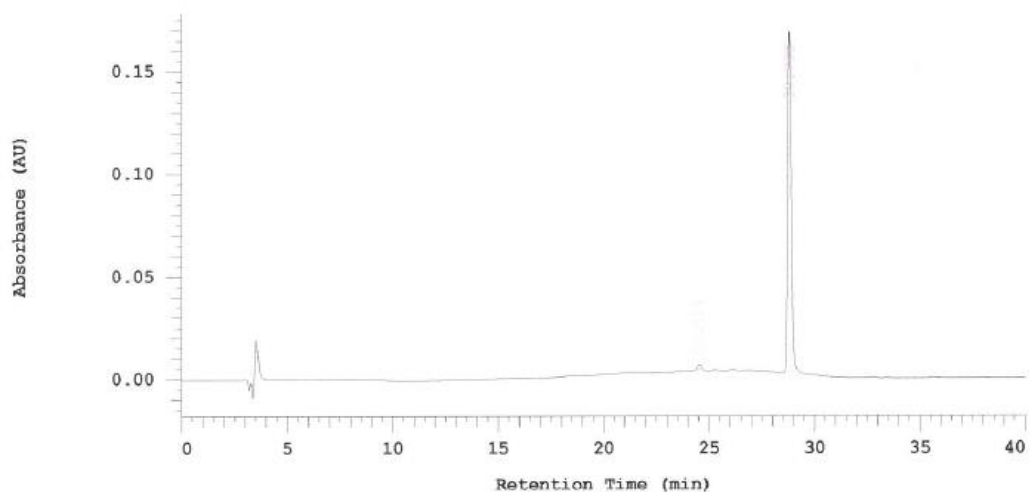
Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	18.647	13882	4.362	1478
2	20.153	304355	95.638	29713
		318237	100.000	31191

5-(4-Chlorophenyl)-*N*-(7-chloroquinolin-4-yl)furan-2-carboxamide (**4**)

Chrom Type: Fixed WL Chromatogram, 254 nm



Pump 1: 5160

Pump 1 Solvent A: MeOH

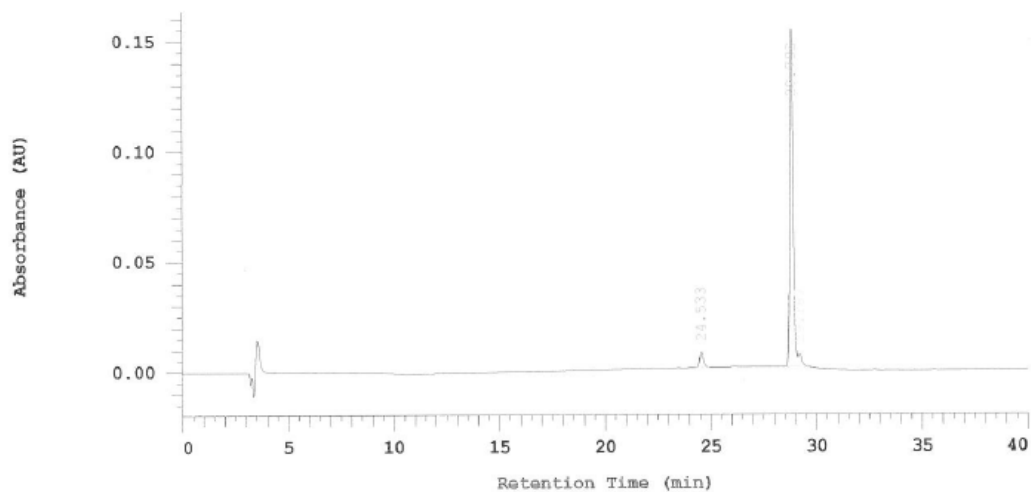
Pump 1 Solvent B: Wasser

Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	24.513	13976	1.507	1245
2	28.793	913589	98.493	83052
		927565	100.000	84297

Chrom Type: Fixed WL Chromatogram, 280 nm



Pump 1: 5160

Pump 1 Solvent A: MeOH

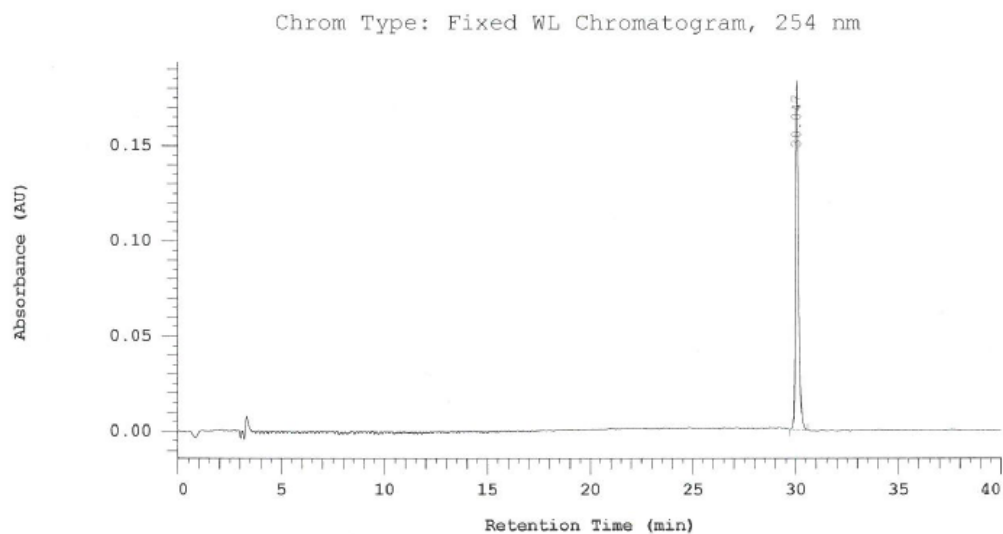
Pump 1 Solvent B: Wasser

Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	24.533	40059	4.366	3489
2	28.793	844876	92.082	76556
3	29.187	32587	3.552	2908
		917522	100.000	82953

7-Chloro-2,3-dihydro-4*H*-benzo[*b*][1,4]oxazin-4-yl)(5-(4-chlorophenyl)furan-2-yl)methanone
(4e)



Pump 1: 5160

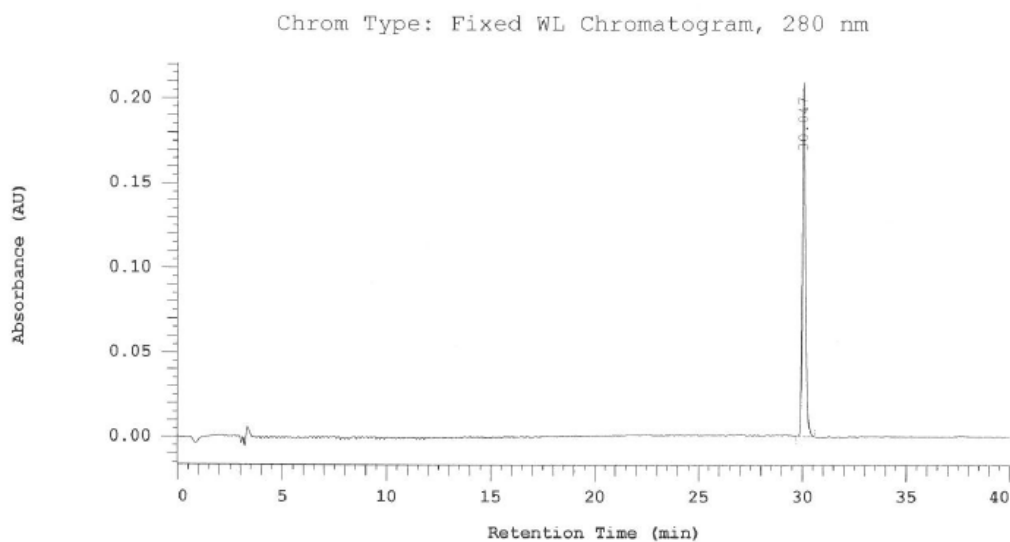
Pump 1 Solvent A: MeOH

Pump 1 Solvent C: MeOH

Pump 1 Solvent B: Wasser

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	30.047	934597	100.000	91514
		934597	100.000	91514



Pump 1: 5160

Pump 1 Solvent A: MeOH

Pump 1 Solvent C: MeOH

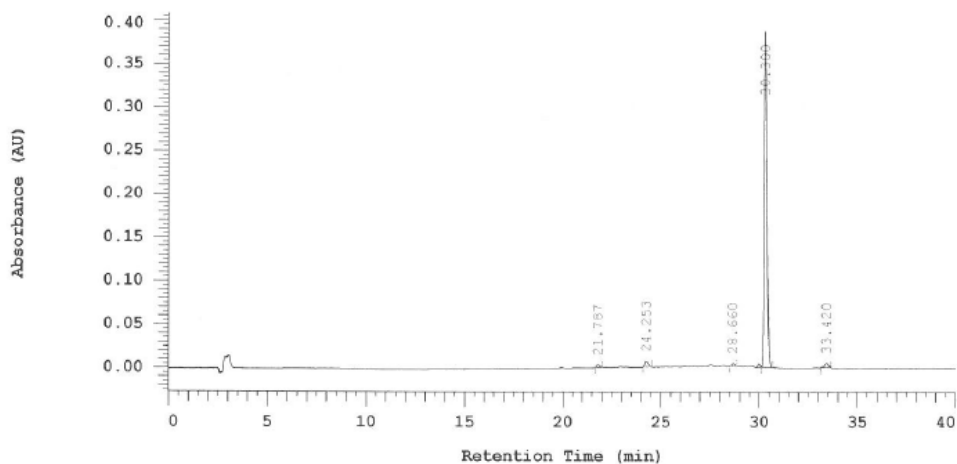
Pump 1 Solvent B: Wasser

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	30.047	1067396	100.000	104562
		1067396	100.000	104562

7-Chloro-4-((5-(4-chlorophenyl)furan-2-yl)methyl)-3,4-dihydro-2H-benzo[*b*][1,4]oxazine (5)

Chrom Type: Fixed WL Chromatogram, 254 nm



Pump 1: 5160

Pump 1 Solvent A: MeOH

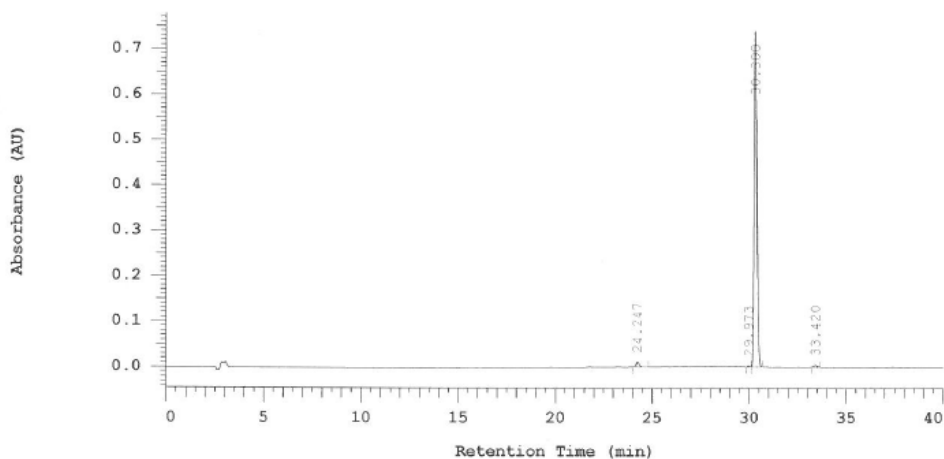
Pump 1 Solvent B: Wasser

Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	21.787	15942	0.840	1557
2	24.253	34534	1.819	3334
3	28.660	13810	0.727	1572
4	30.300	1804880	95.054	193618
5	33.420	29621	1.560	2351
		1898787	100.000	202432

Chrom Type: Fixed WL Chromatogram, 280 nm



Pump 1: 5160

Pump 1 Solvent A: MeOH

Pump 1 Solvent B: Wasser

Pump 1 Solvent C: MeOH

Pump 1 Solvent D: MeOH

No.	RT	Area	Area %	Height
1	24.247	57046	1.618	5140
2	29.973	10635	0.302	1351
3	30.300	3436319	97.444	368971
4	33.420	22459	0.637	1902
		3526459	100.000	377364