SUPPORTING INFORMATION

Structure Based Design, Synthesis, Pharmacophore Modeling, Virtual Screening, and Molecular Docking Studies for Identification of Novel Cyclophilin D Inhibitors

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Chemistry

General

All reagents were commercially available and used without further purification. Melting points were determined in open capillary tubes on a Laboratory Devices Mel-Temp apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded in d_6-DMSO on a Bruker DRX-500 spectrometer operating at 500 MHz, and 125 MHz, respectively and calibrated to the solvent peak. Abbreviations used for the split patterns of proton NMR signals are: singlet (s), doublet (d), triplet (t), quartet (q), quintet (qui), multiplet (m) and broad signal (br). High-resolution mass spectrometry (HRMS) was recorded on a LCT Premier Spectrometer. Single crystal structural analyses were performed using monochromated CuKα radiation with a Bruker Proteum diffractometer.

Ethyl 3-(4-fluorophenyl)-5-(4-hydroxyphenyl)-7-methyl-5H-thiazolo [3, 2-a] pyrimidine-6-carboxylate (6e)

Color less solid, R_f 0.28; (hexane: ethyl acetate, 1:1 v/v). Yield: 78%; m.p.: 186-189 ºC; ^{1}H NMR (DMSO-d_6) δ 1.20 (t, 3H), 2.41 (*s*, 3H), 4.00-4.15 (m, 2H), 5.31 (s, 1H), 6.42 (s, 1H), 7.08-7.01 (m, 3H), 7.19-7.11 (m, 2H), 7.36-7.30 (m, 2H), 7.84 (d, 1H), 9.56 (s, 1H); ^{13}C NMR (DMSO-d_6) δ 13.8, 19.2, 60.7, 62.3, 101.1, 109.4, 115.5, 119.1, 126.8, 127.4, 128.8, 129.3, 130.1, 131.5, 133.6, 137.9, 140.2, 158.2, 160.1, 163.5, 168.4. HRMS cald for $C_{22}H_{19}FN_2O_3S$ (M+H) 411.1179; found 411.1127 (TOF MS ES^+).

Ethyl 3-(3,4-dichlorophenyl)-5-(4-hydroxyphenyl)-7-methyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6f)

Color less solid, R_f 0.33; (hexane: ethyl acetate, 1:1 v/v). Yield: 81%; m.p.: 236-238 ºC; ^{1}H NMR (DMSO-d_6) δ 1.10 (t, 3H), 2.40 (*s*, 3H), 4.10-3.92 (m, 2H), 5.32 (s, 1H), 6.53-6.42 (m, 3H), 6.95-6.81 (m, 1H), 7.40-7.36 (m, 2H), 7.90-7.87 (m, 1H), 8.61 (s, 1H), 9.52 (s, 1H); ^{13}C NMR (DMSO-d_6) δ 14.01, 30.67, 55.14, 59.23, 101.10, 114.2, 115.08, 125.68, 126.01, 127.3, 127.9, 128.14, 129.45, 130.89, 131.48, 134.05, 134.90, 136.39, 140.85, 144.48, 156.65, 156.85, 164.87, 165.15. HRMS cald for $C_{22}H_{18}C_{l2}N_2O_3S$ (M+H) 461.0492; found 461.0493 (TOF MS ES^+).

Methyl 5-(4-hydroxy-3-(methoxycarbonyl) phenyl)-3-(4-hydroxyphenyl)-7-methyl-5H-thiazolo [3, 2-a] pyrimidine-6-carboxylate (6j)

Color less solid, R_f 0.28; (hexane: ethyl acetate, 1:1 v/v). Yield: 67%; m.p.: 253-254 ºC; ^{1}H NMR (DMSO-d_6) δ 2.48 (s, 3H), 3.60 (s, 3H), 3.84 (s, 3H), 6.27 (d, 1H), 6.70 (s, 1H), 6.91-6.83 (m, 3H), 7.13-7.09 (m, 3H), 7.30 (s, 1H), 10.12 (s, 1H), 10.52 (s, 1H). ^{13}C NMR (DMSO-d_6) δ 13.72, 18.17, 52.50, 58.13, 60.44, 102.1, 109.9, 112.5, 115.5, 117.6, 118.1, 129.3, 130.1, 133.7, 140.3, 159.8, 160.2, 164.5, 168.2. HRMS cald for $C_{23}H_{20}N_2O_6S$ (M+H) 479.1641; found 479.1646 (TOF MS ES$^+$).

Methyl 3,5-bis(4-hydroxyphenyl)-7-methyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6l)

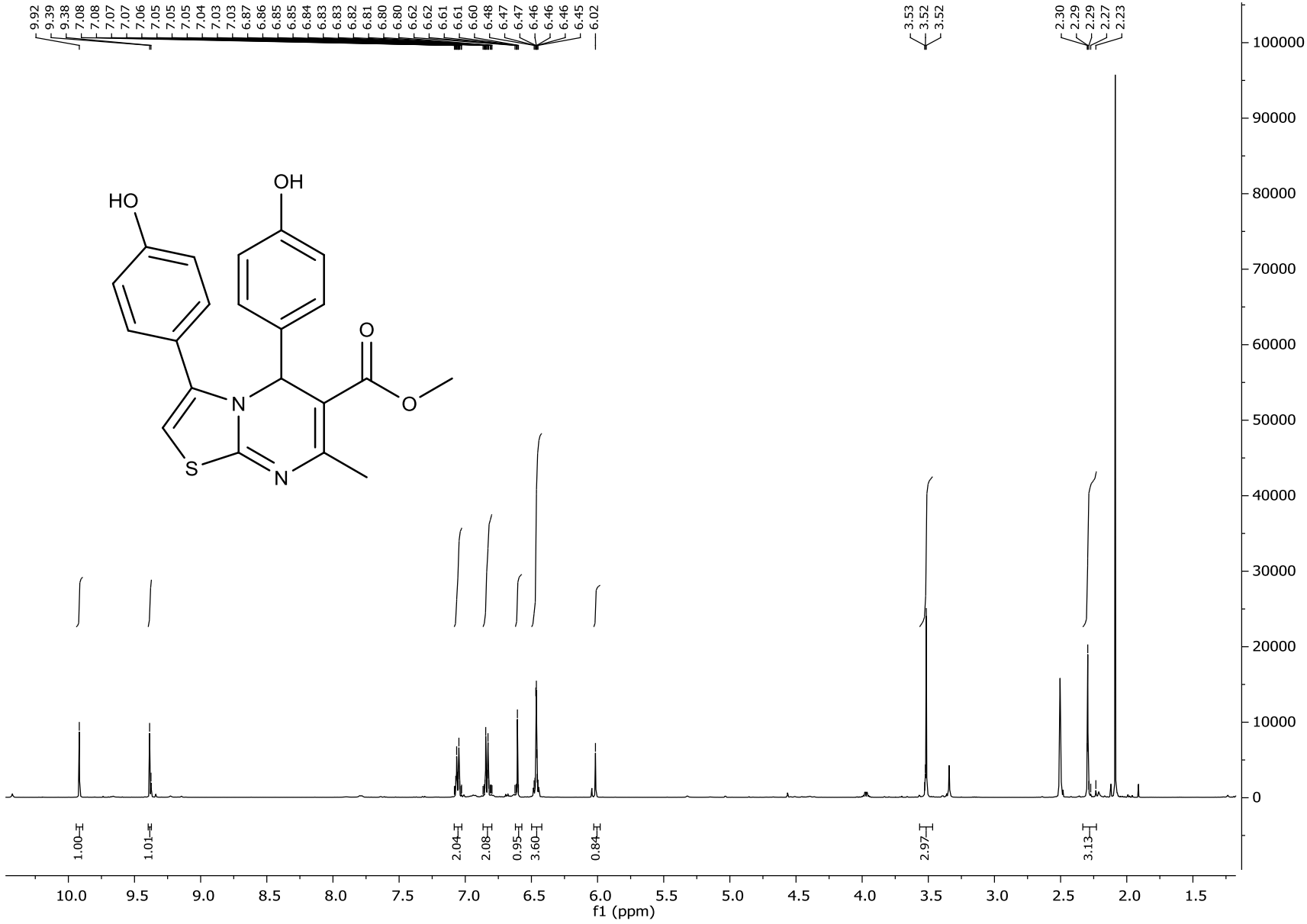
Color less solid, R_f 0.38; (hexane: ethyl acetate, 1:1 v/v). Yield: 86%; m.p.: 285-287 ºC; ^{1}H NMR (DMSO-d_6) δ 2.30 (s, 3H), 3.52 (s, 3H), 6.03 (d, 1H), 6.49-6.45 (m, 4H), 6.60 (s, 1H), 6.85-6.83 (m, 2H), 7.08-7.05 (m, 2H), 9.37 (s, 1H), 9.90 (s, 1H). ^{13}C NMR (DMSO-d_6) δ 23.2, 50.7, 56.2, 59.0, 100.4, 102.3, 114.8, 115.0, 115.3, 120.0, 127.1, 130.1, 130.8, 132.8, 139.2, 155.0, 157.0, 158.4, 162.2, 165.8, 166.3. HRMS cald for $C_{21}H_{18}N_2O_4S$ (M+H) 395.1066; found 395.1057 (TOF MS ES$^+$).

Ethyl 3-(4-fluorophenyl)-5-(4-hydroxy-3-(methoxycarbonyl) phenyl)-7-methyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6k)

Color less solid, R_f 0.40; (hexane: ethyl acetate, 1:1 v/v). Yield: 74%; m.p.: 224-226 ºC; ^{1}H NMR (DMSO-d_6) δ 1.12 (t, 3H), 2.39 (s, 3H), 3.56 (s, 3H), 4.08-3.94 (m, 2H), 5.28 (s, 1H), 6.51-6.44 (m, 3H), 7.01-6.95 (m, 1H), 7.33-7.26 (m, 2H), 7.86-7.81 (m, 1H), 8.62 (s, 1H), 10.52 (s, 1H); ^{13}C NMR (DMSO-d_6) δ 13.4, 29.8, 54.1, 58.4, 101.6, 115.4, 116.0, 124.5, 125.4, 126.5, 128.0, 129.2, 130.2, 131.7, 131.9, 135.0, 136.3, 136.8, 140.8, 143.5, 155.5, 156.8, 165.0, 166.1. HRMS cald for $C_{24}H_{21}FN_2O_5S$ (M+H) 468.1077; found 468.1071 (TOF MS ES$^+$).

2-(3-Cyano-4-isobutoxyphenyl)-4-methyl-N-(4-sulfamoylphenyl) thiazole-5-carboxamide (9)

Yield 92%, m p. 297-299 °C. R_f 0.62; (methylene dichloride: methanol, 9:1 v/v). ^{1}H NMR (DMSO-d_6) *δ:* 1.03 (d, 6H, *J* = 13.6 Hz), 2.12-2.08 (m, 1H), 2.65 (s, 3H), 4.02 (d, 2H, *J* = 12.4 Hz), 7.31 (s, 2H), 7.44-7.40 (m, 1H), 8.87-8.81 (m, 4H), 8.25-8.21(m, 1H), 8.31 (s, 1H), 10.59 (s, 1H); ^{13}C NMR (DMSO-d_6) 164.4, 161.9, 160.0, 156.2, 141.4, 139.5, 132.9, 131.3, 126.5, 125.8, 125.2, 119.8, 115.3, 113.9, 101.5, 75.0, 27.5, 18.6, 17.1; HRMS cald for $C_{22}H_{22}N_4O_4S_2$ $(M+H)^+$ 471.1130; found 471.1098 (TOF MS ES^+).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O
O
N
S
N
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90000
80000
70000
60000
50000
40000
30000
20000
10000
0
1.00 1.01 2.04 2.08 0.95 3.60 0.84 2.97 3.13
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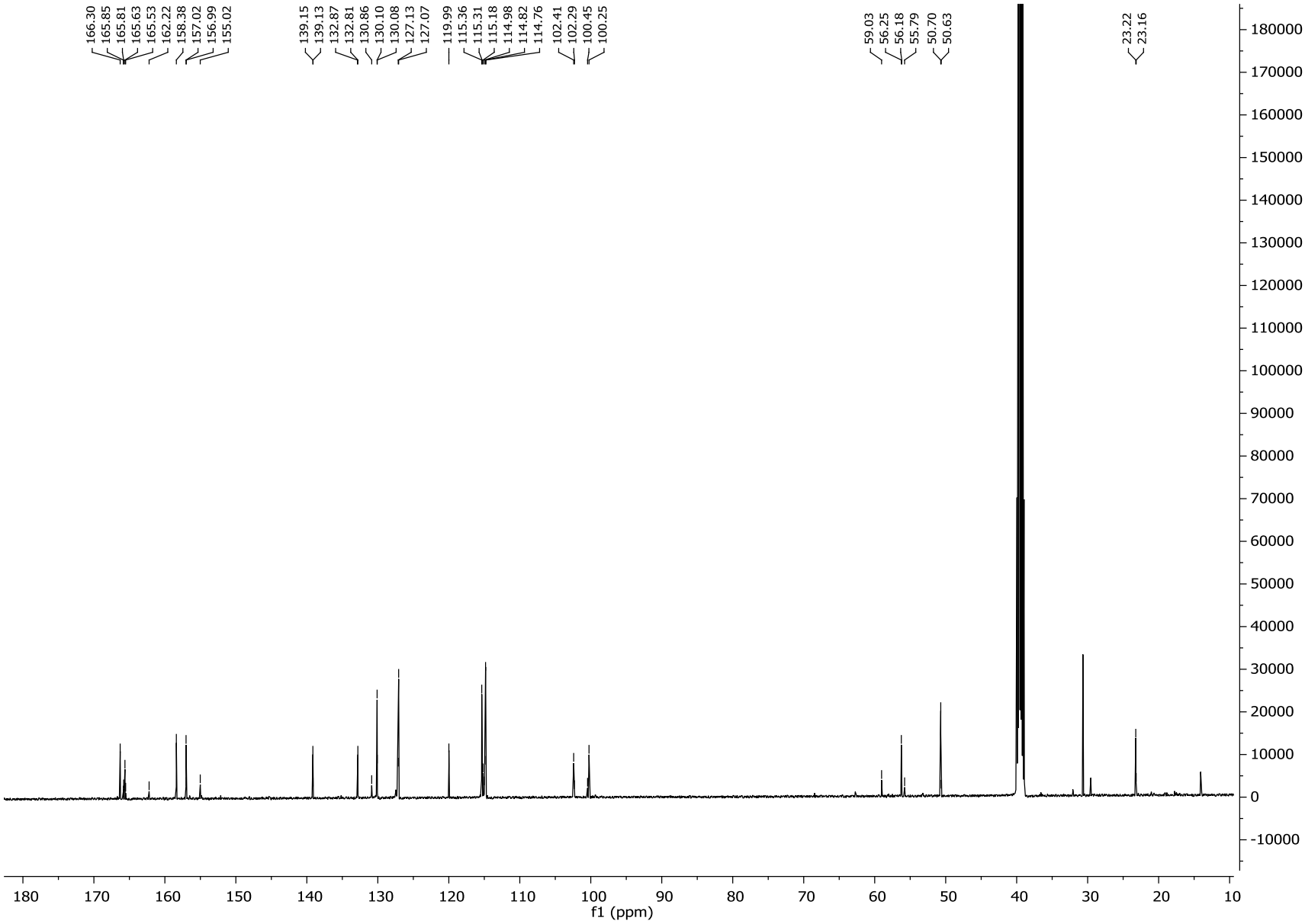
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56.18
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50.70
50.63
23.22
23.16
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160000
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130000
120000
110000
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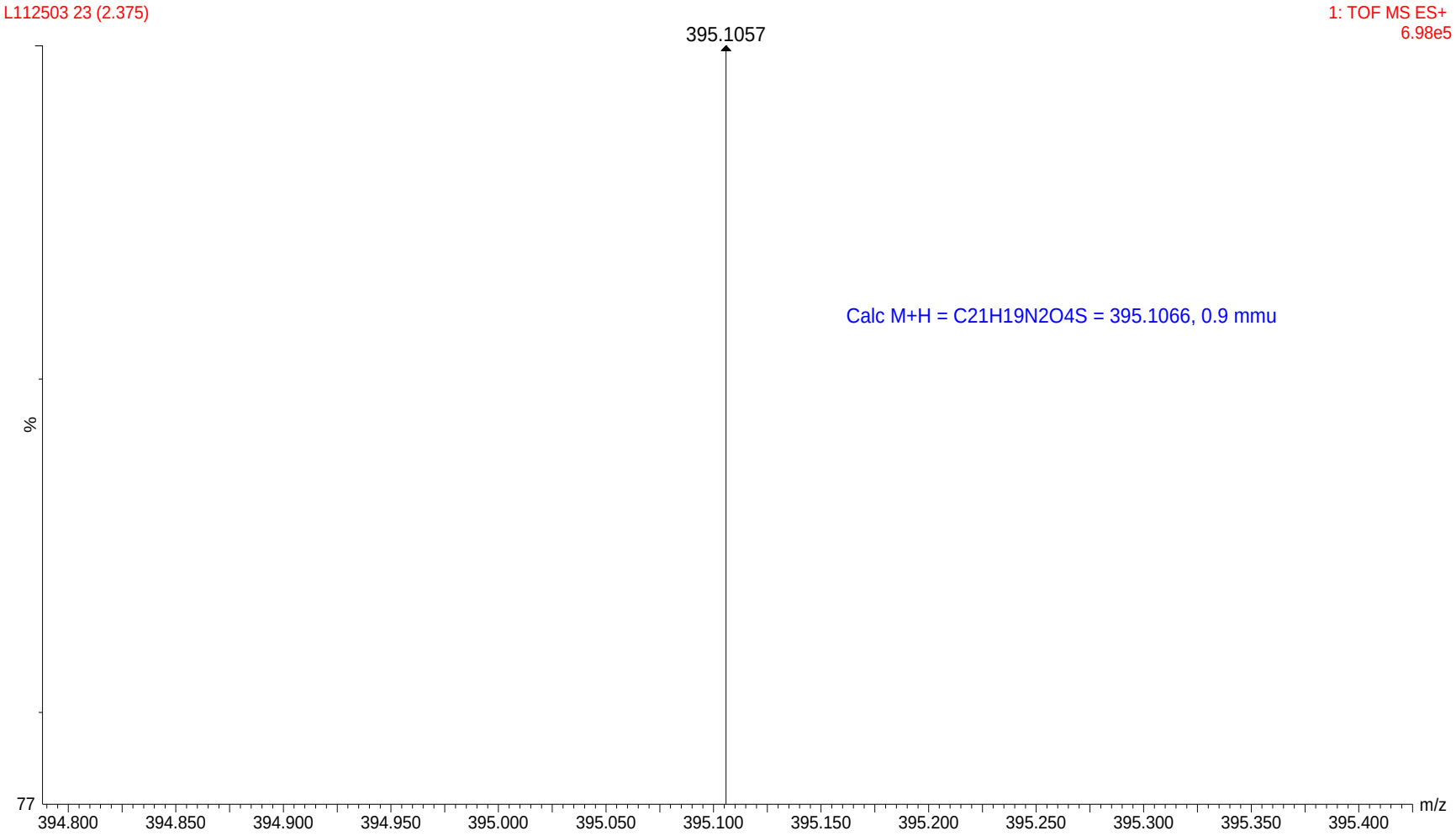
f1 (ppm)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%
77
394.800
394.850
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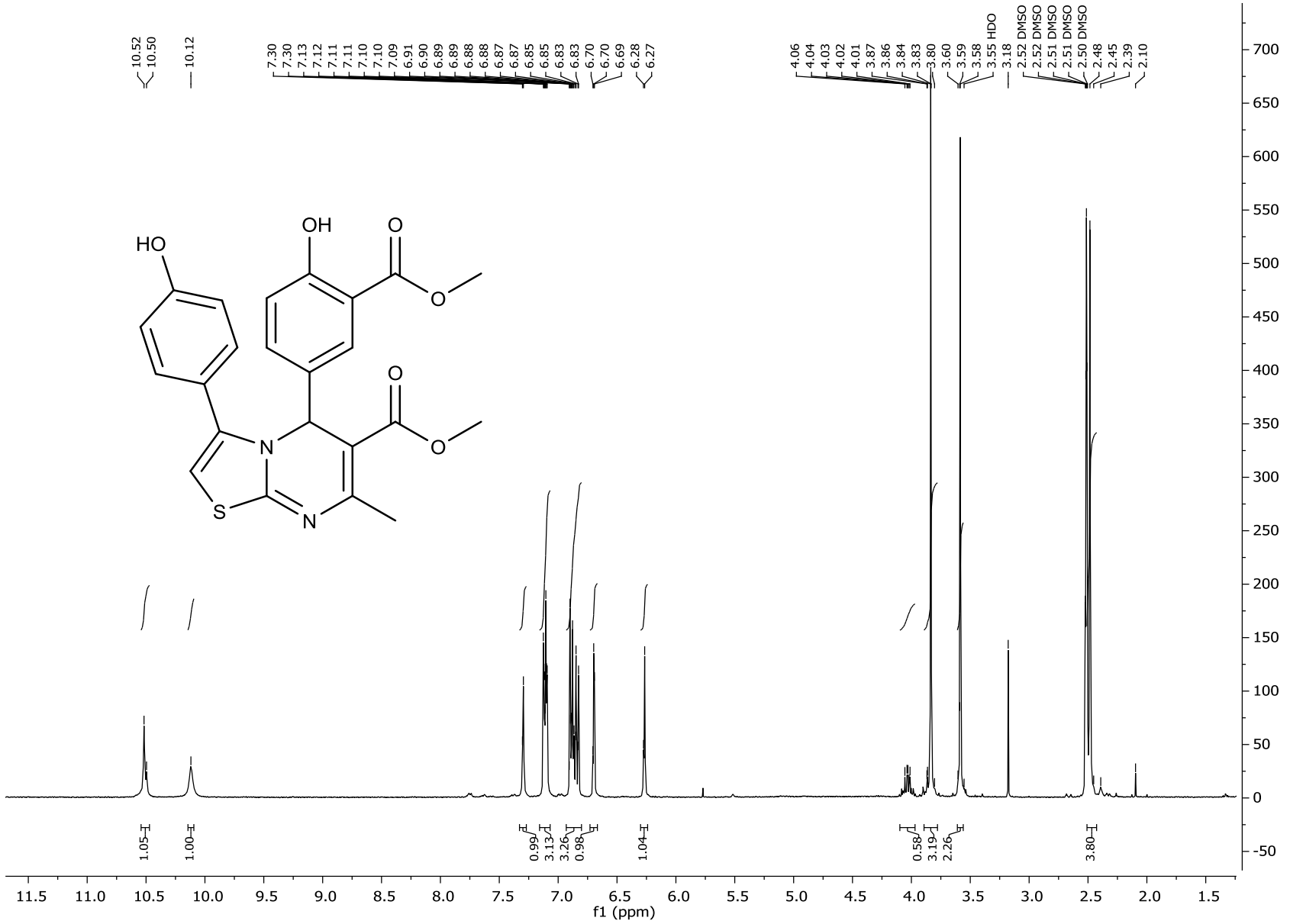
395.300
395.350
395.400
m/z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4.01
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3.83
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2.51 DMSO
2.51 DMSO
2.50 DMSO
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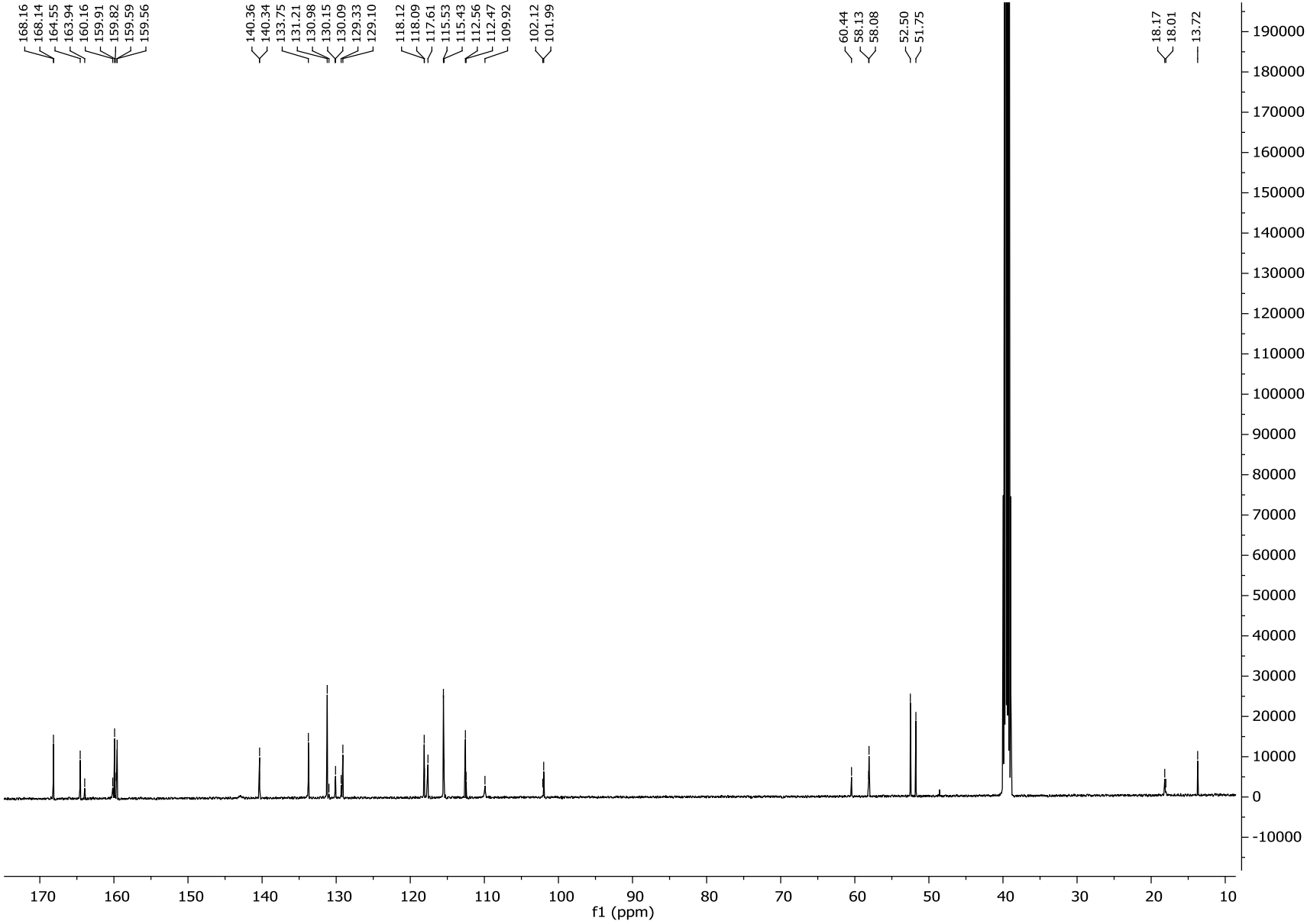
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117.61
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115.43
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112.47
109.92
102.12
101.99
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18.17
18.01
13.72
f1 (ppm)


L112501 7 (0.723)
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%
0
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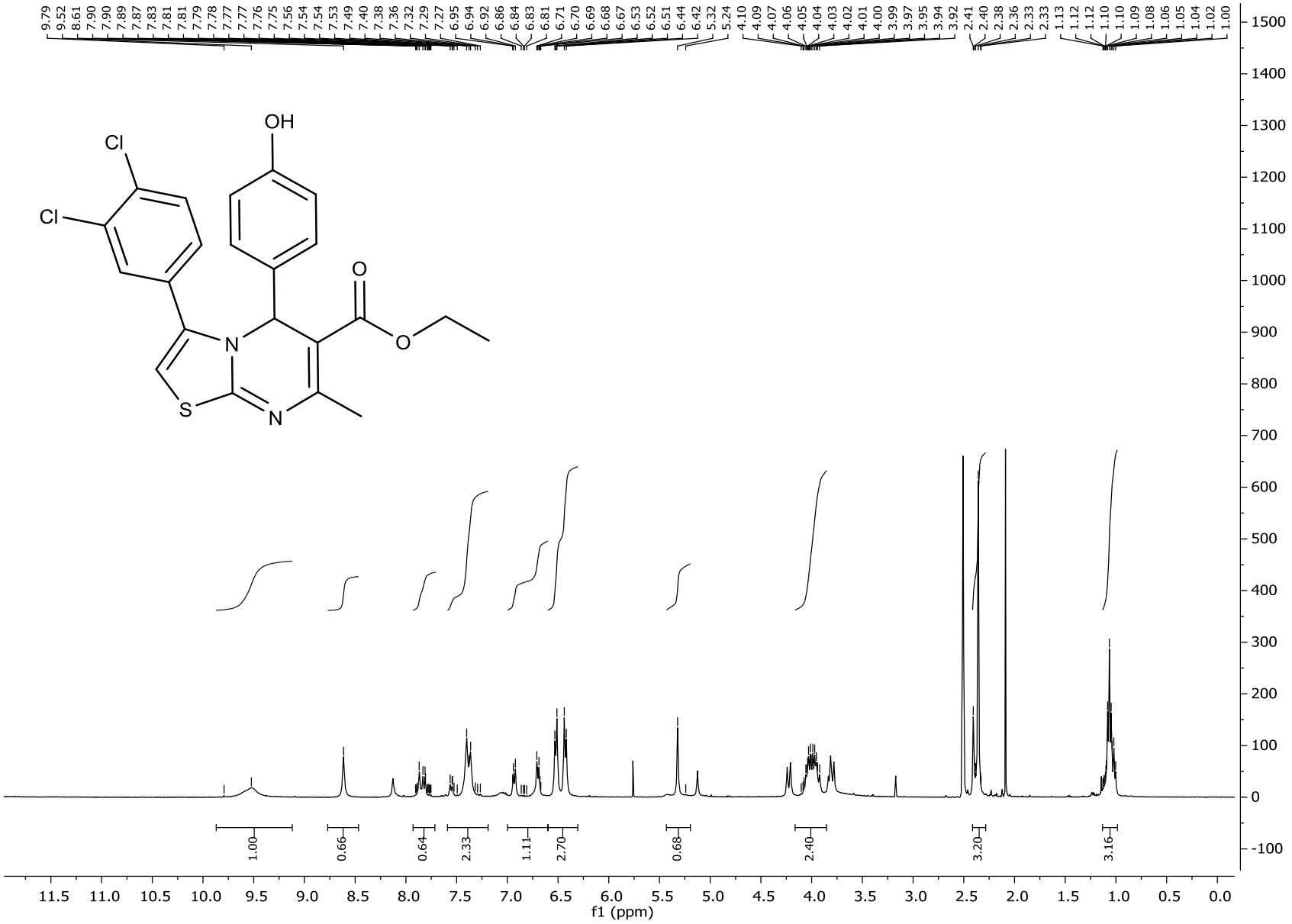
m/z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OH
Cl
Cl
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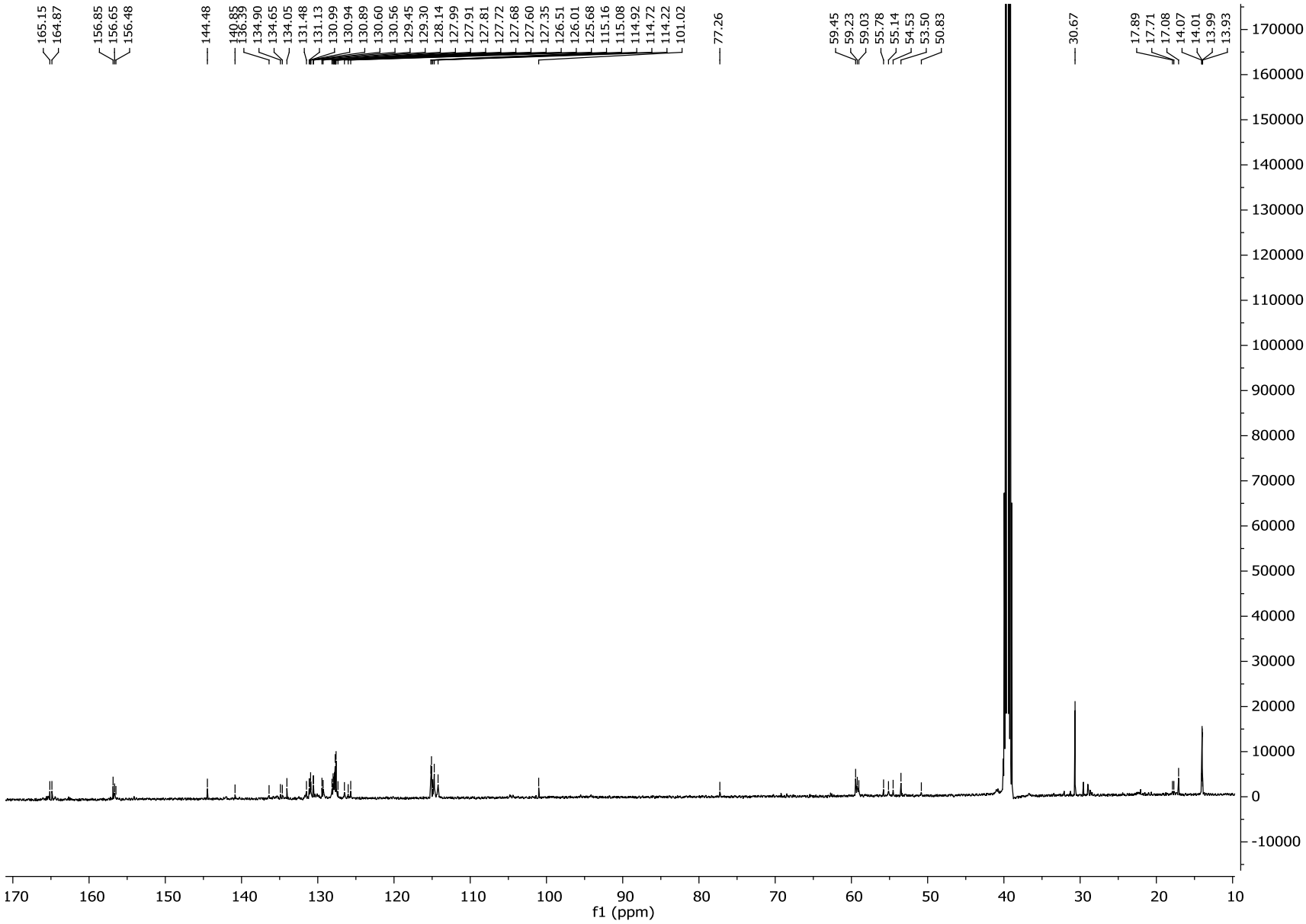
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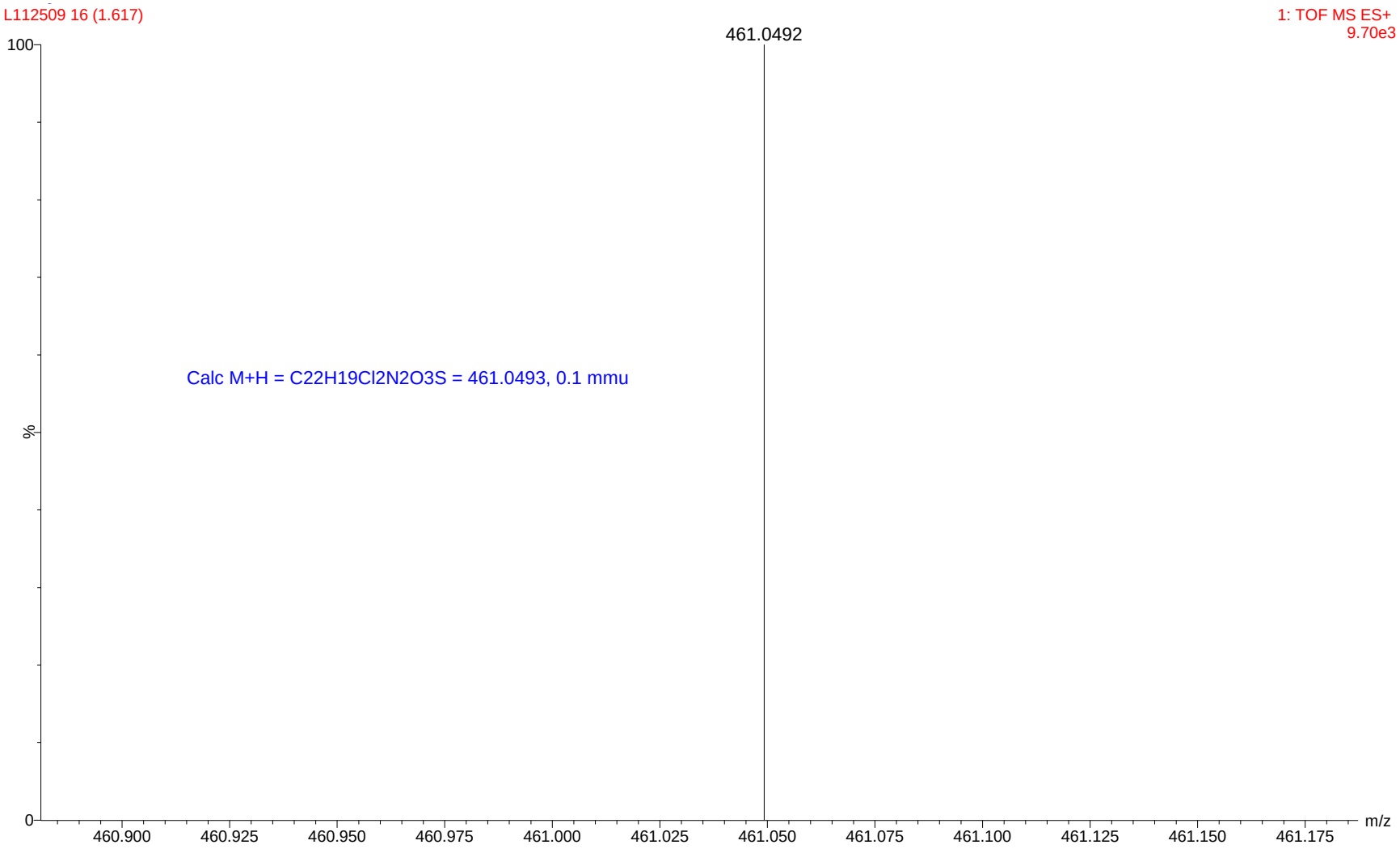
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%
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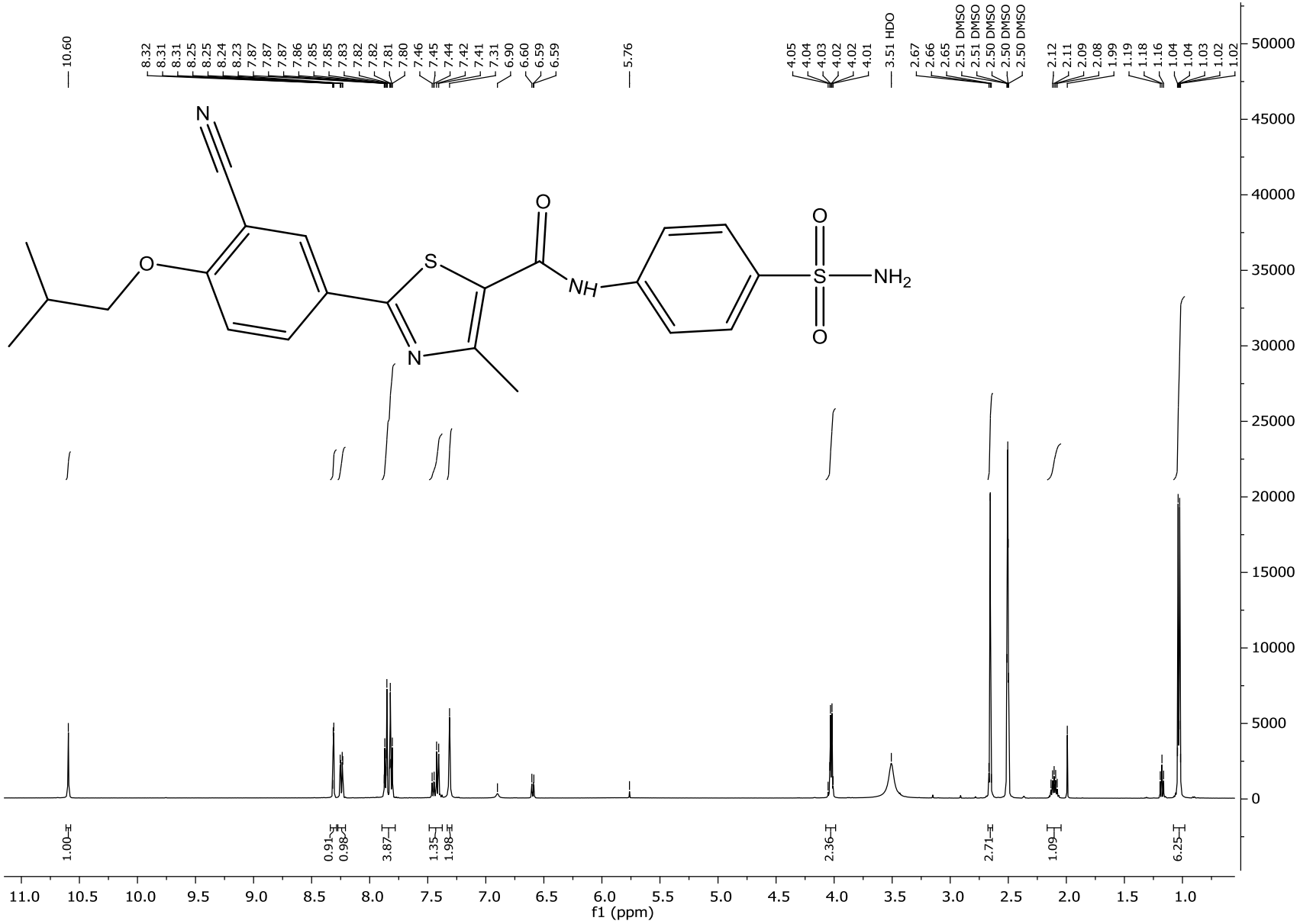
m/z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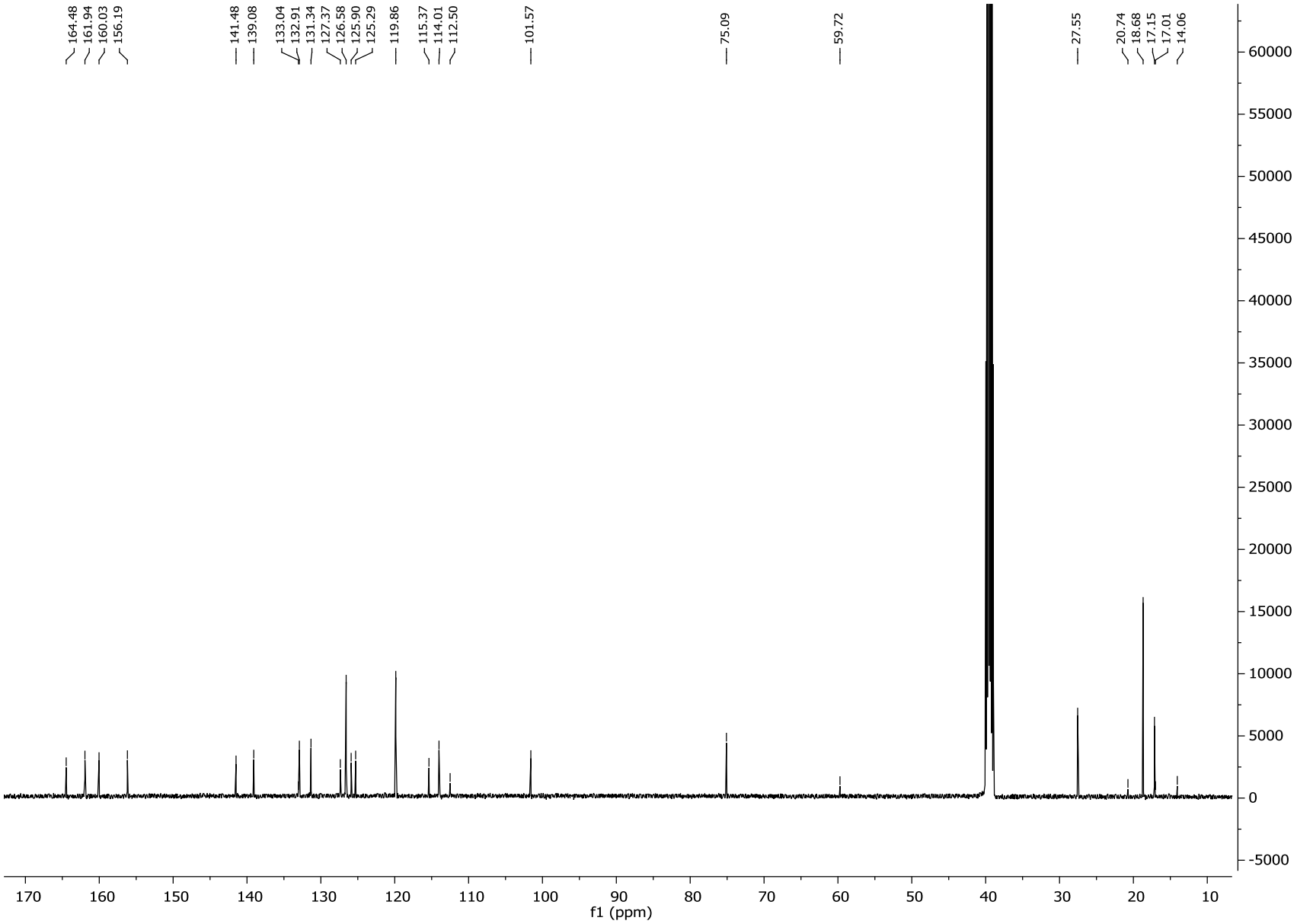
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17.15
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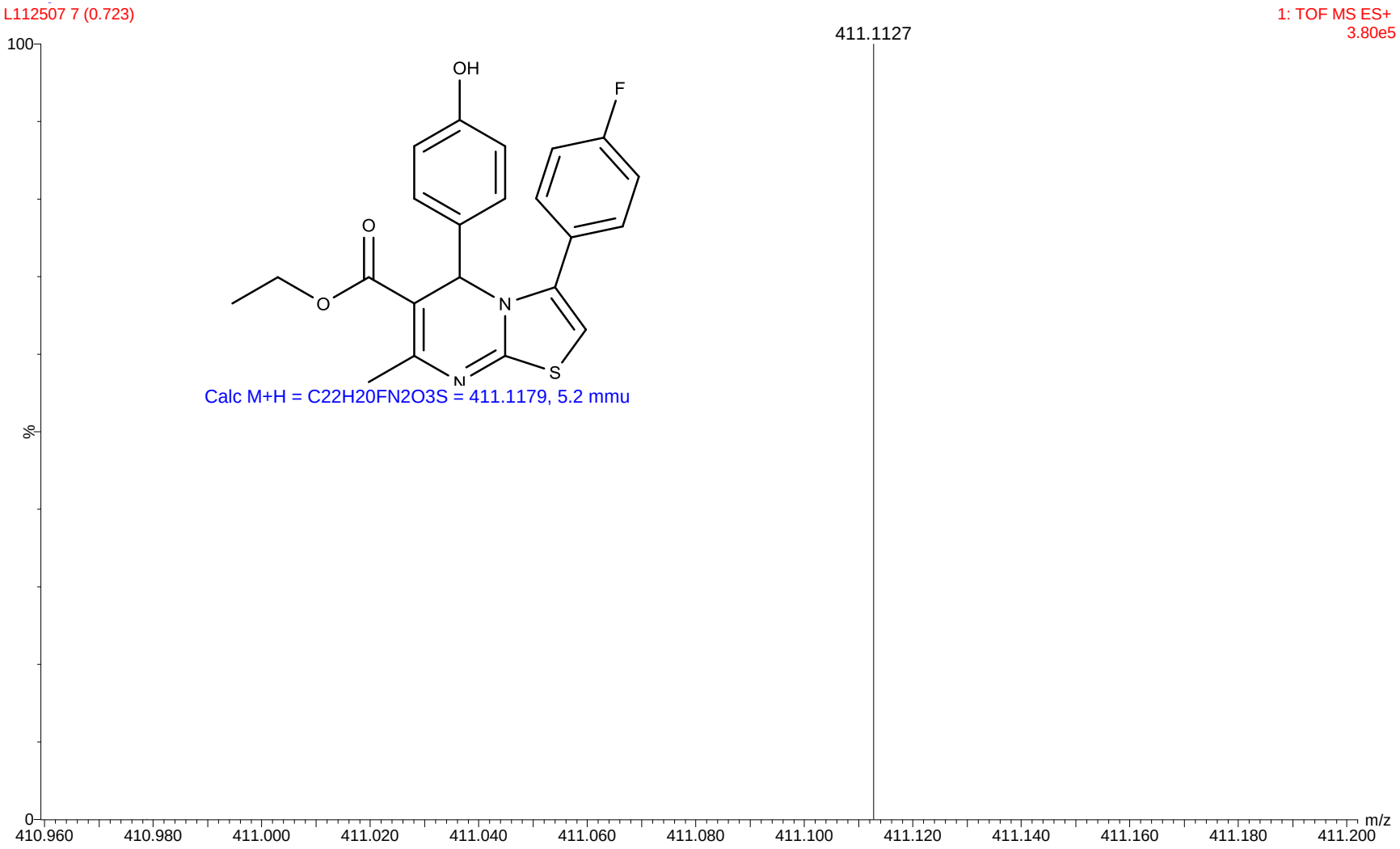
f1 (ppm)


L112507 7 (0.723)
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411.1127
100
%
0
OH
F
O
O
N
N
S
Calc M+H = C22H20FN2O3S = 411.1179, 5.2 mmu
410.960
410.980
411.000
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411.060
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411.120
411.140
411.160
411.180
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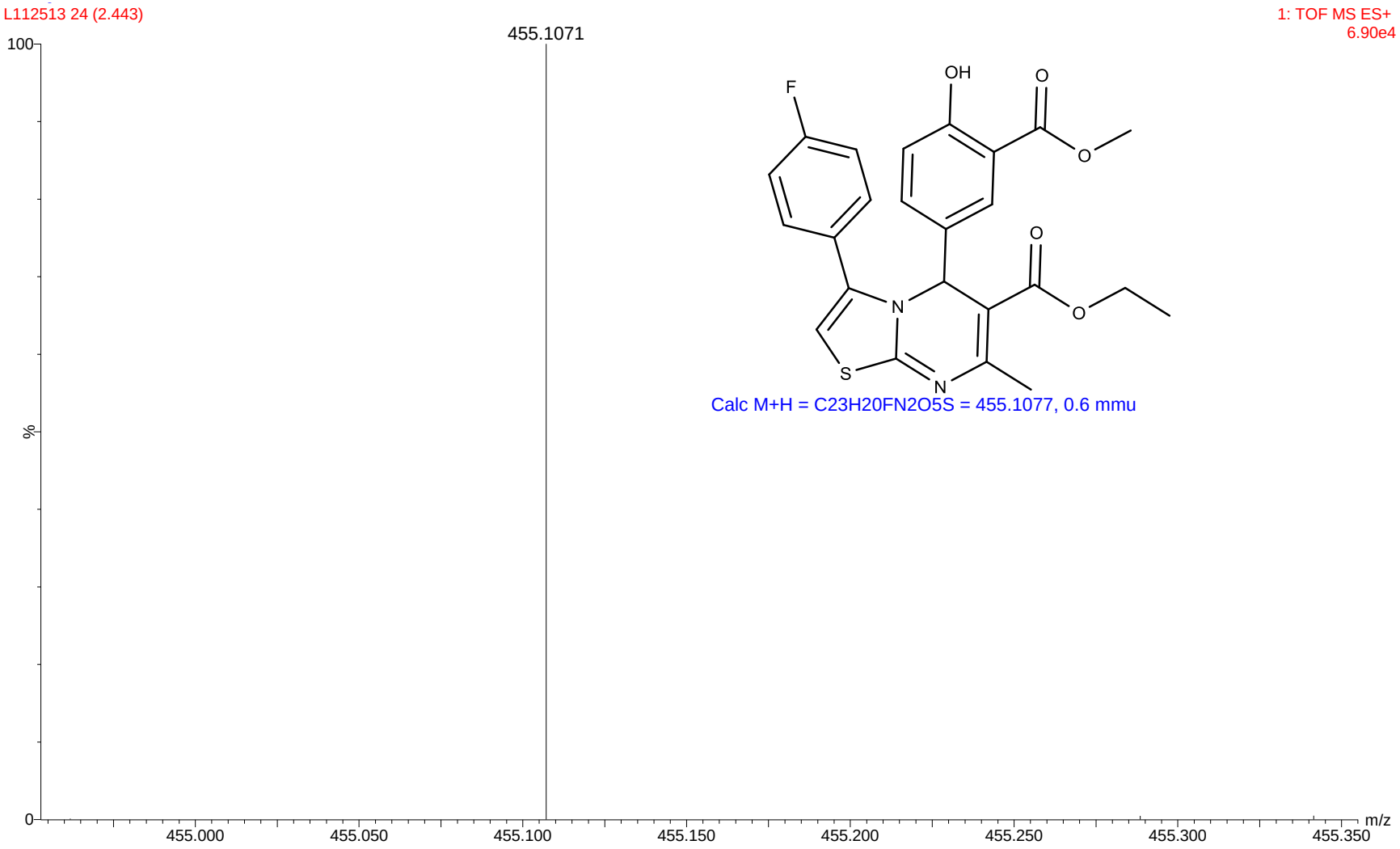
m/z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100
%
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455.000
455.050
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455.200
455.250
455.300
455.350
m/z
F
OH
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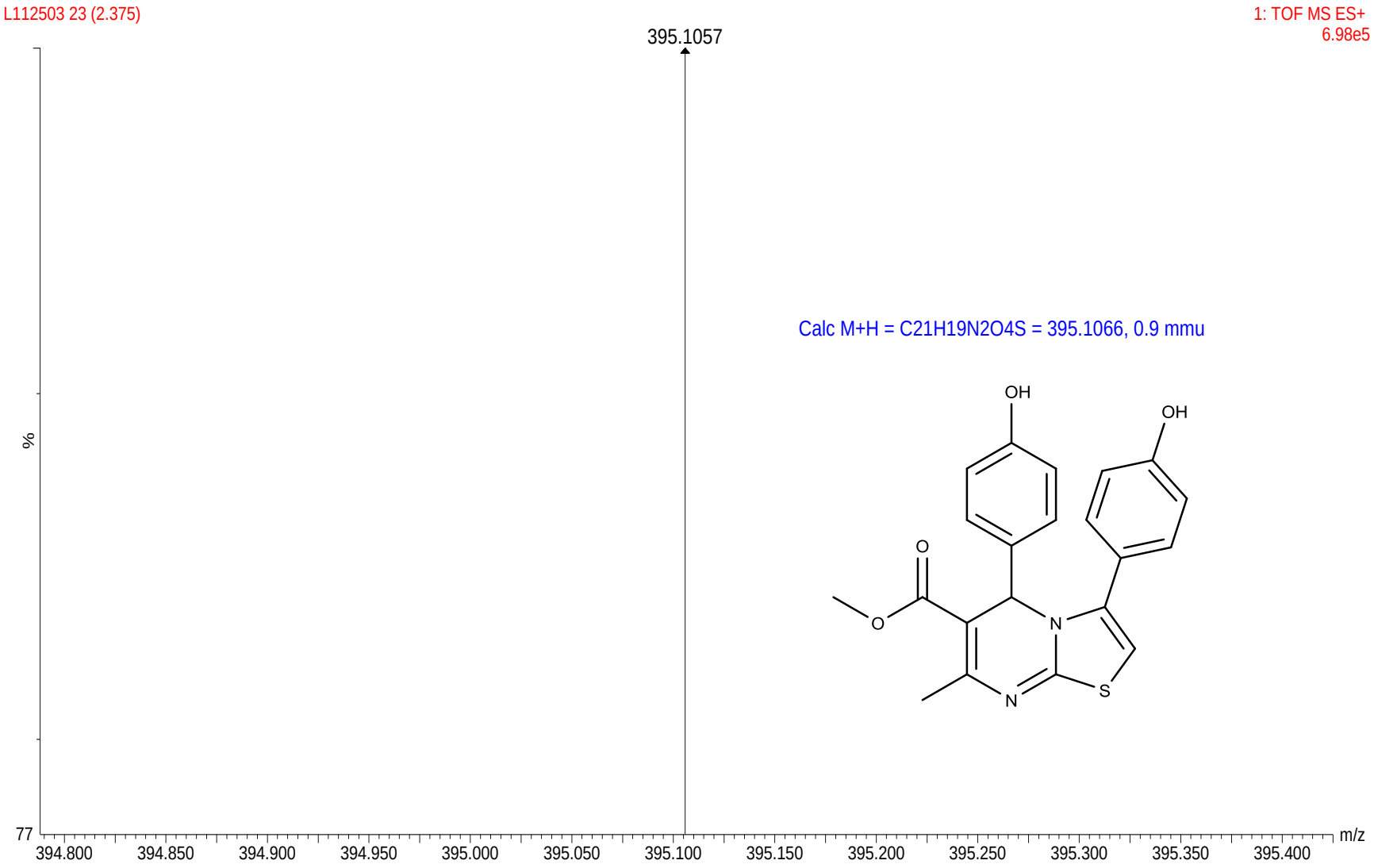
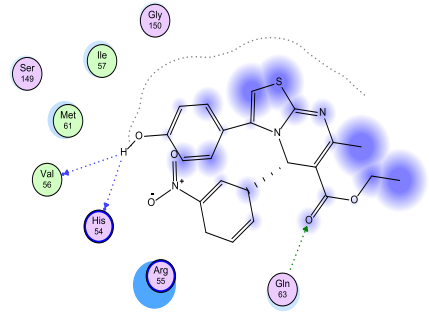
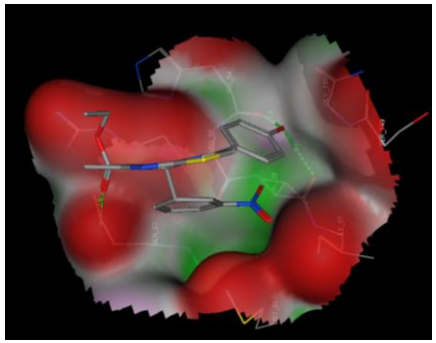
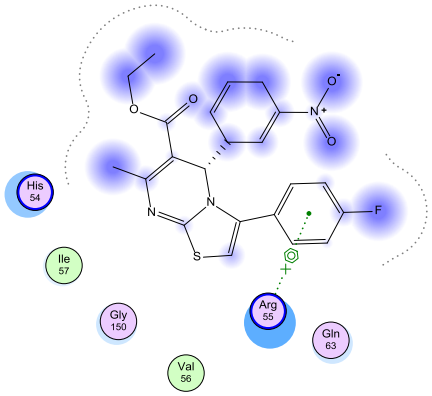
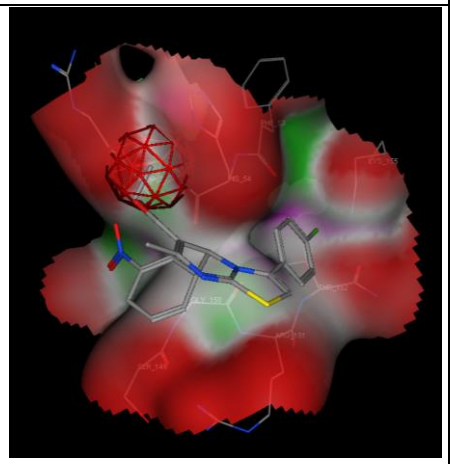
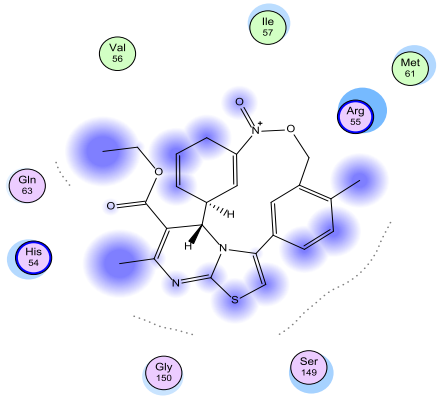
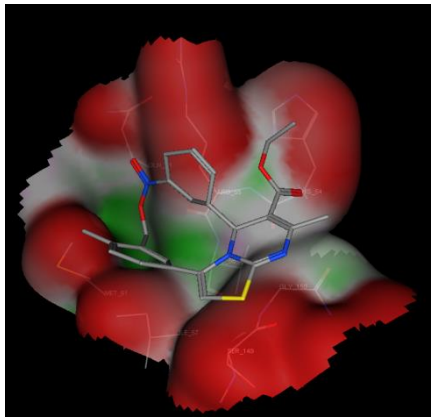
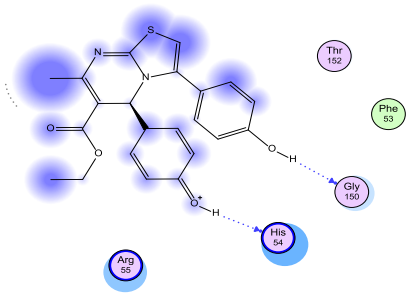
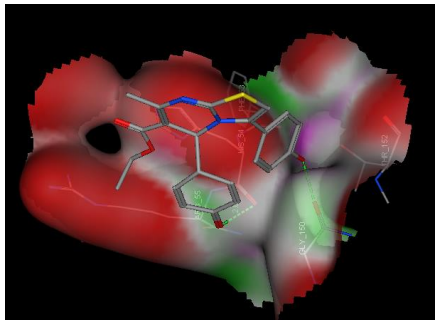
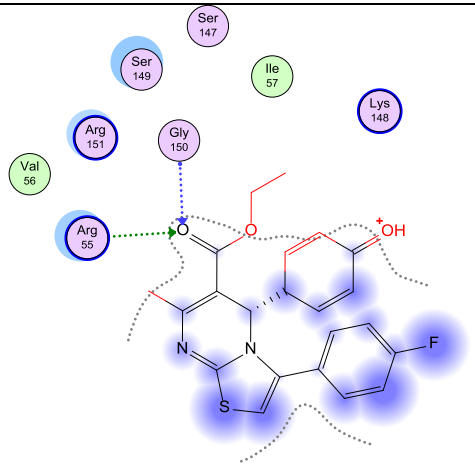
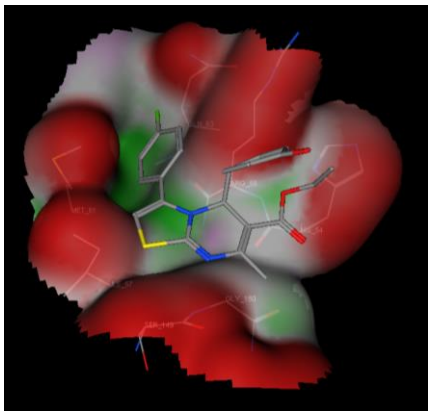
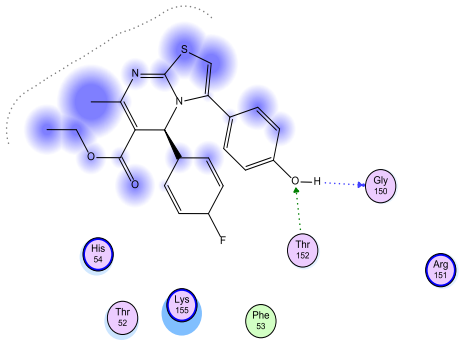
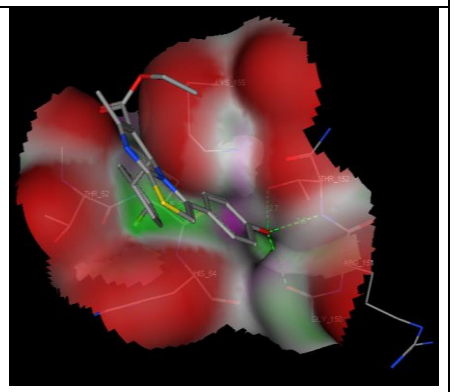
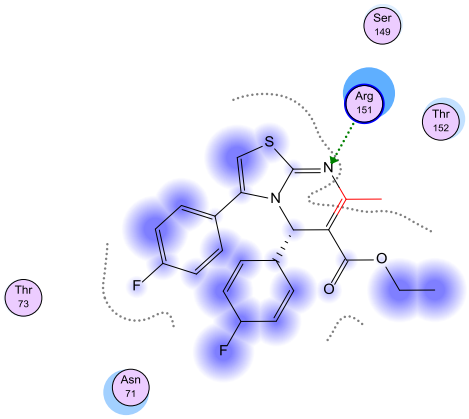
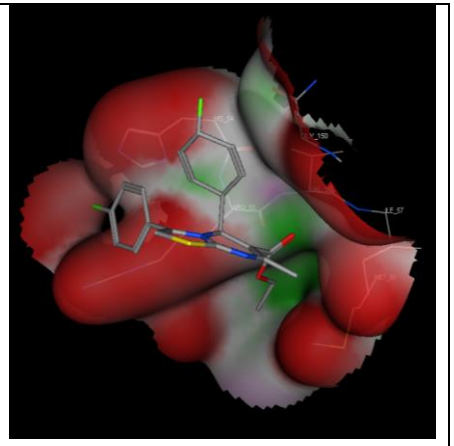
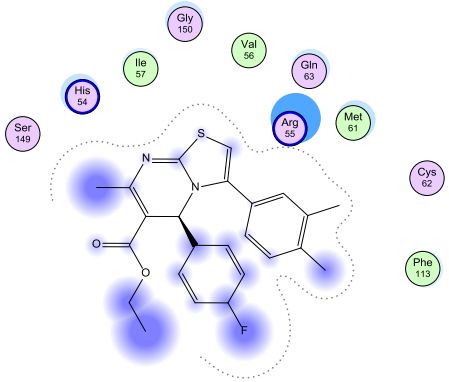
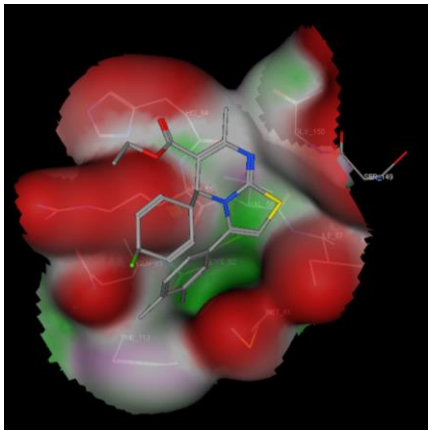
O
O
O
N
S
N
Calc M+H = C23H20FN2O5S = 455.1077, 0.6 mmu

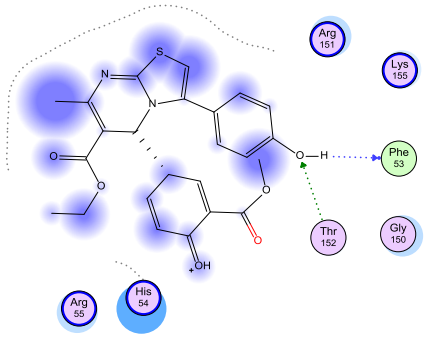
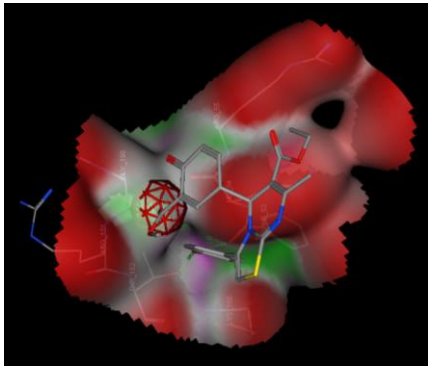
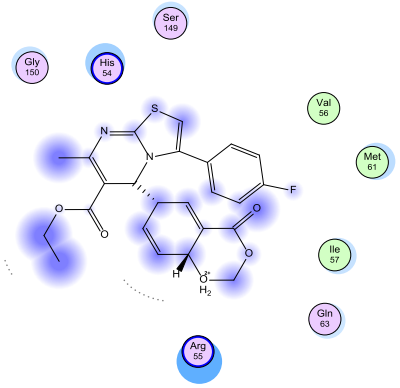
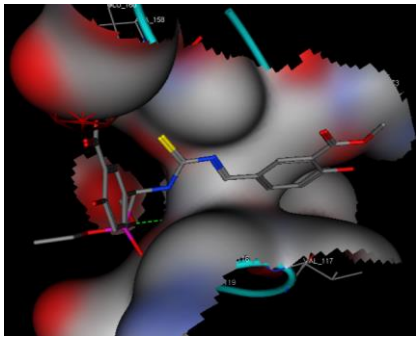
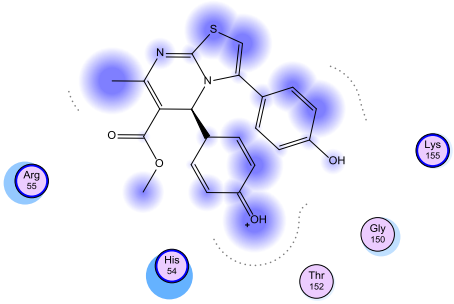
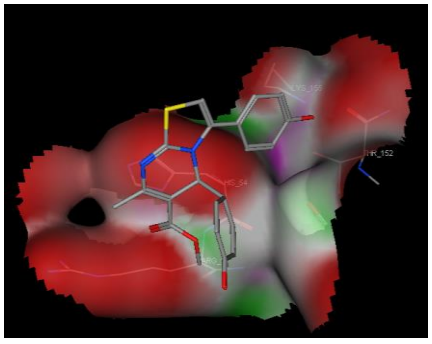

L112503 23 (2.375)
1: TOF MS ES+
6.98e5
395.1057
Calc M+H = C21H19N2O4S = 395.1066, 0.9 mmu
OH
OH
O
O
N
N
S
%
77
394.800
394.850
394.900
394.950
395.000
395.050
395.100
395.150
395.200
395.250
395.300
395.350
395.400
m/z

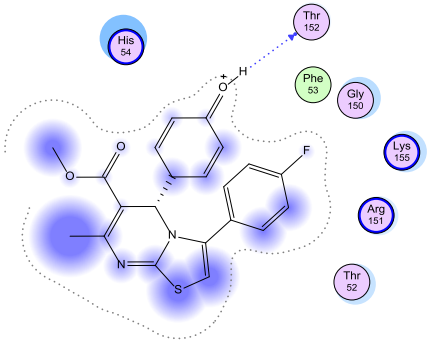
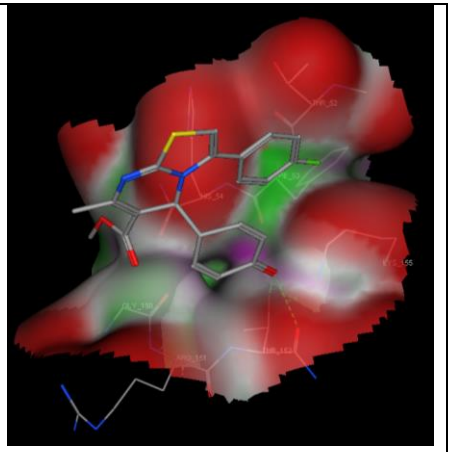
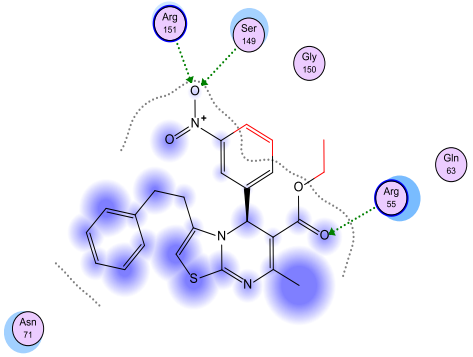
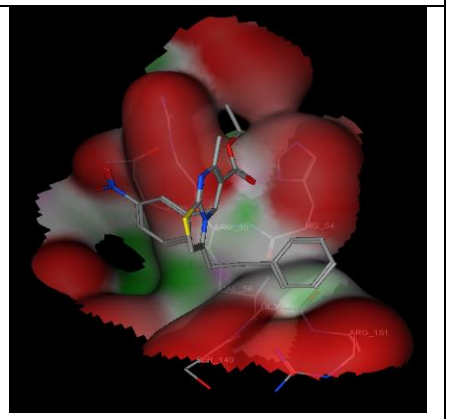
Compounds structures	Ligand Interactions with ABAD Active site	
	[a]Two Dimensional Image	[b]Three Dimensional Image
6a		
6b		

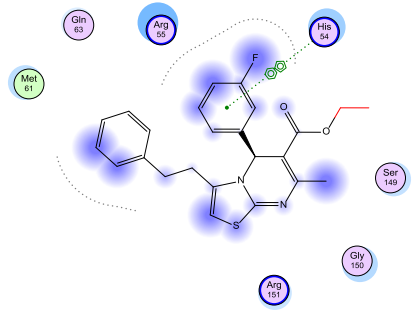
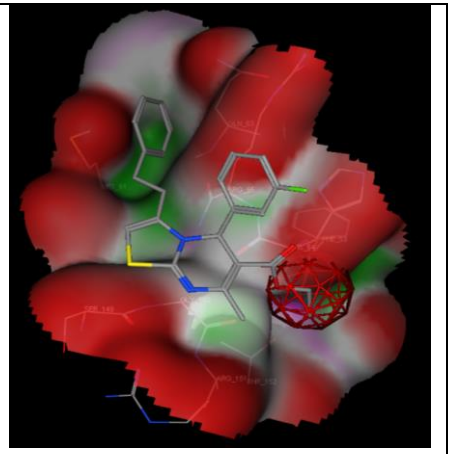
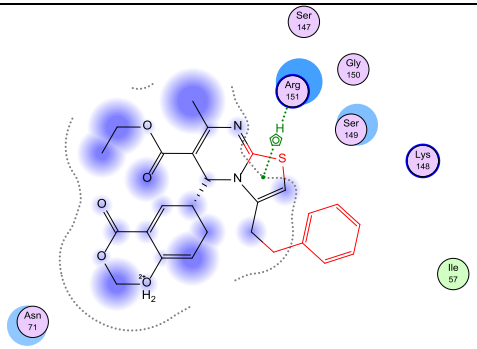
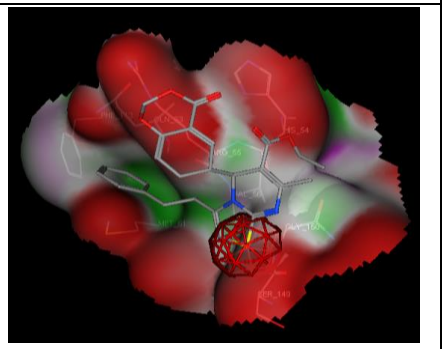
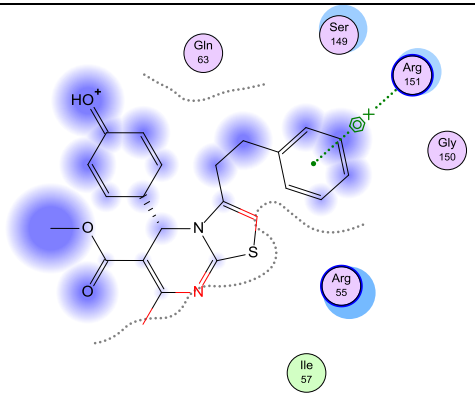
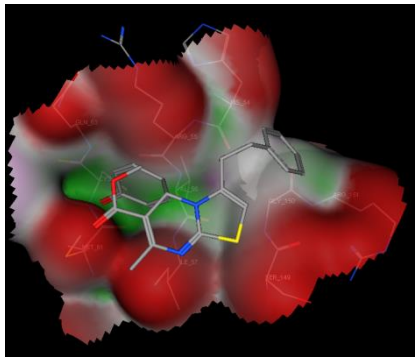
6c	 Ile 57 Val 56 Met 61 Arg 55 Gln 63 His 54 Gly 150 Ser 149	
6d	 Thr 152 Phe 53 Gly 150 His 54 Arg 55	

6e	 Ser 147 Ser 149 Ile 57 Lys 148 Arg 151 Gly 150 Val 56 Arg 55 O O +OH N N F S	
6g	 S N N O O O—H Gly 150 F His 54 Thr 152 Arg 151 Thr 52 Lys 155 Phe 53	

6h	 Ser 149 Arg 151 Thr 152 Thr 73 Asn 71 S N N O O F F	
6i	 Gly 150 Val 56 Ile 57 Gln 63 His 54 Arg 55 Met 61 Ser 149 Cys 62 Phe 113 S N N O O F	

6j	 Arg 151 Lys 155 Phe 53 Thr 152 Gly 150 His 54 Arg 55	
6k	 Ser 149 Gly 150 His 54 Val 56 Met 61 Ile 57 Gln 63 Arg 55	
6l	 Arg 55 Lys 155 Gly 150 His 54 Thr 152	

6m	 His 54 Thr 152 Phe 53 Gly 150 Lys 155 Arg 151 Thr 52 F O N S	
6n	 Arg 151 Ser 149 Gly 150 Gln 63 Arg 55 Asn 71 O N S	

6p	 Gln 63 Arg 55 His 64 Met 61 Ser 149 Gly 150 Arg 151	
6q	 Ser 147 Gly 150 Arg 151 Ser 149 Lys 148 Ile 57 Asn 71	
6r	 Ser 149 Gln 63 Arg 151 Gly 150 Arg 55 Ile 57	

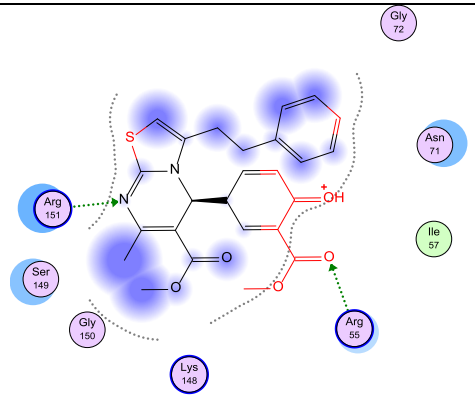
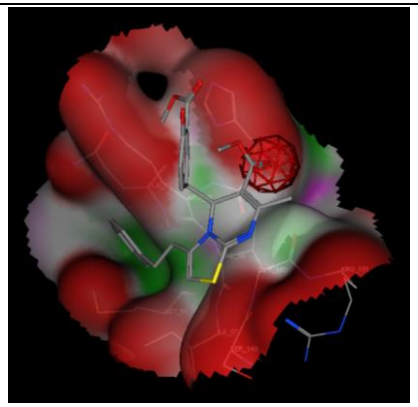
6s		

Table 1: Interaction of remaining 17 novel inhibitors with CypD active site. [a]Two-dimensional linear representations of ligand-receptor complexes. [b]Three dimensional graphical representations of ligand-receptor complexes.

Compound 6o

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nonhydrogen atoms of $[C_{24}H_{24}FN_2O_2S][Br]$ (**6o**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
S	747(1)	7908(1)	4674(1)	23(1)
F	1738(1)	4447(2)	1436(1)	42(1)
O(1)	-1398(1)	384(2)	3204(1)	25(1)
O(2)	78(1)	-577(2)	3298(1)	30(1)
N(1)	-574(1)	5496(3)	4145(1)	22(1)
N(2)	964(1)	4793(2)	4086(1)	21(1)
C(1)	320(1)	5919(3)	4270(1)	22(1)
C(2)	-878(1)	3763(3)	3860(1)	22(1)
C(3)	-264(1)	2560(3)	3656(1)	21(1)
C(4)	749(1)	3056(3)	3695(1)	22(1)
C(5)	1857(1)	5485(3)	4280(1)	22(1)
C(6)	1846(1)	7149(3)	4594(1)	24(1)
C(7)	2678(1)	4381(3)	4137(1)	24(1)
C(8)	3574(2)	5206(4)	4464(1)	30(1)
C(9)	4391(1)	4160(3)	4279(1)	27(1)
C(10)	4964(2)	5104(4)	3935(1)	33(1)
C(11)	5706(2)	4122(4)	3755(1)	39(1)
C(12)	5882(2)	2198(4)	3920(1)	40(1)
C(13)	5316(2)	1234(4)	4259(1)	38(1)
C(14)	4574(2)	2216(4)	4436(1)	34(1)

C(15)	-1891(2)	3471(3)	3836(1)	25(1)
C(16)	-496(1)	640(3)	3374(1)	24(1)
C(17)	-1689(2)	-1514(3)	2954(1)	28(1)
C(18)	-2706(2)	-1625(4)	2954(1)	32(1)
C(19)	1018(1)	3465(3)	3085(1)	23(1)
C(20)	1536(2)	2091(3)	2827(1)	29(1)
C(21)	1775(2)	2419(4)	2269(1)	33(1)
C(22)	1490(2)	4120(4)	1982(1)	30(1)
C(23)	975(2)	5523(3)	2217(1)	30(1)
C(24)	738(1)	5176(3)	2777(1)	25(1)
Br	-1926(1)	8448(1)	4673(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for $[C_{24}H_{24}FN_2O_2S][Br]$ (**6o**).

S-C(1)	1.707(2)
S-C(6)	1.735(2)
F-C(22)	1.366(2)
O(1)-C(16)	1.343(2)
O(1)-C(17)	1.452(2)
O(2)-C(16)	1.214(3)
N(1)-C(1)	1.339(3)
N(1)-C(2)	1.389(3)
N(1)-H(1N)	0.83(3)
N(2)-C(1)	1.333(3)
N(2)-C(5)	1.410(3)
N(2)-C(4)	1.488(2)
C(2)-C(3)	1.351(3)
C(2)-C(15)	1.500(3)
C(3)-C(16)	1.476(3)
C(3)-C(4)	1.522(3)
C(4)-C(19)	1.527(3)
C(4)-H(4)	0.98(3)
C(5)-C(6)	1.342(3)
C(5)-C(7)	1.498(3)
C(6)-H(6)	0.92(3)
C(7)-C(8)	1.529(3)
C(7)-H(7A)	0.95(3)
C(7)-H(7B)	0.97(3)
C(8)-C(9)	1.510(3)

C(8)-H(8A)	0.97(3)
C(8)-H(8B)	1.00(2)
C(9)-C(14)	1.387(3)
C(9)-C(10)	1.389(3)
C(10)-C(11)	1.393(3)
C(10)-H(10)	0.96(3)
C(11)-C(12)	1.376(4)
C(11)-H(11)	0.98(3)
C(12)-C(13)	1.382(4)
C(12)-H(12)	1.01(3)
C(13)-C(14)	1.390(3)
C(13)-H(13)	0.99(3)
C(14)-H(14)	0.98(3)
C(15)-H(15A)	0.96(2)
C(15)-H(15B)	0.97(3)
C(15)-H(15C)	0.95(3)
C(17)-C(18)	1.502(3)
C(17)-H(17A)	0.95(3)
C(17)-H(17B)	0.97(3)
C(18)-H(18A)	0.98(3)
C(18)-H(18B)	0.90(3)
C(18)-H(18C)	0.94(3)
C(19)-C(20)	1.389(3)
C(19)-C(24)	1.391(3)
C(20)-C(21)	1.387(3)
C(20)-H(20)	0.92(3)
C(21)-C(22)	1.366(3)

C(21)-H(21)	0.92(3)
C(22)-C(23)	1.375(3)
C(23)-C(24)	1.393(3)
C(23)-H(23)	0.92(3)
C(24)-H(24)	0.93(2)

C(1)-S-C(6)	89.2 (1)
C(16)-O(1)-C(17)	117.0 (2)
C(1)-N(1)-C(2)	121. 7(2)
C(1)-N(1)-H(1N)	116 (2)
C(2)-N(1)-H(1N)	122 (2)
C(1)-N(2)-C(5)	112.7(2)
C(1)-N(2)-C(4)	123.0(2)
C(5)-N(2)-C(4)	124.2(2)
N(2)-C(1)-N(1)	122.1(2)
N(2)-C(1)-S	113.6(2)
N(1)-C(1)-S	124.3(2)
C(3)-C(2)-N(1)	119.2(2)
C(3)-C(2)-C(15)	128.2 (2)
N(1)-C(2)-C(15)	112.6(2)
C(2)-C(3)-C(16)	124.2(2)
C(2)-C(3)-C(4)	123.1(2)
C(16)-C(3)-C(4)	112.7(2)
N(2)-C(4)-C(3)	109.5(2)
N(2)-C(4)-C(19)	110.0(2)
C(3)-C(4)-C(19)	111.6(2)

N(2)-C(4)-H(4)	108(1)
C(3)-C(4)-H(4)	108(1)
C(19)-C(4)-H(4)	110(1)
C(6)-C(5)-N(2)	111.6(2)
C(6)-C(5)-C(7)	127.6(2)
N(2)-C(5)-C(7)	120.9(2)
C(5)-C(6)-S	113.0(2)
C(5)-C(6)-H(6)	129(2)
S-C(6)-H(6)	119(2)
C(5)-C(7)-C(8)	112.3(2)
C(5)-C(7)-H(7A)	109(2)
C(8)-C(7)-H(7A)	110(2)
C(5)-C(7)-H(7B)	108(2)
C(8)-C(7)-H(7B)	111(2)
H(7A)-C(7)-H(7B)	107(2)
C(9)-C(8)-C(7)	111.1(2)
C(9)-C(8)-H(8A)	108(2)
C(7)-C(8)-H(8A)	111(2)
C(9)-C(8)-H(8B)	110(1)
C(7)-C(8)-H(8B)	110(1)
H(8A)-C(8)-H(8B)	107(2)
C(14)-C(9)-C(10)	118.4(2)
C(14)-C(9)-C(8)	120.7(2)
C(10)-C(9)-C(8)	120.8(2)
C(9)-C(10)-C(11)	120.7(2)
C(9)-C(10)-H(10)	120(2)
C(11)-C(10)-H(10)	119(2)

C(12)-C(11)-C(10)	120.1(2)
C(12)-C(11)-H(11)	122(2)
C(10)-C(11)-H(11)	118(2)
C(11)-C(12)-C(13)	120.0(2)
C(11)-C(12)-H(12)	121(2)
C(13)-C(12)-H(12)	119(2)
C(12)-C(13)-C(14)	119.8(2)
C(12)-C(13)-H(13)	123(2)
C(14)-C(13)-H(13)	117(2)
C(9)-C(14)-C(13)	121.1(2)
C(9)-C(14)-H(14)	119(2)
C(13)-C(14)-H(14)	120(2)
C(2)-C(15)-H(15A)	109(1)
C(2)-C(15)-H(15B)	111(1)
H(15A)-C(15)-H(15B)	111(2)
C(2)-C(15)-H(15C)	110(2)
H(15A)-C(15)-H(15C)	107(2)
H(15B)-C(15)-H(15C)	108(2)
O(2)-C(16)-O(1)	123.5(2)
O(2)-C(16)-C(3)	122.9(2)
O(1)-C(16)-C(3)	113.6(2)
O(1)-C(17)-C(18)	106.5(2)
O(1)-C(17)-H(17A)	108(2)
C(18)-C(17)-H(17A)	113(2)
O(1)-C(17)-H(17B)	108(1)
C(18)-C(17)-H(17B)	114(1)
H(17A)-C(17)-H(17B)	108(2)

C(17)-C(18)-H(18A)	110(2)
C(17)-C(18)-H(18B)	108(2)
H(18A)-C(18)-H(18B)	112(2)
C(17)-C(18)-H(18C)	112(2)
H(18A)-C(18)-H(18C)	108(2)
H(18B)-C(18)-H(18C)	107(2)
C(20)-C(19)-C(24)	119.4 (2)
C(20)-C(19)-C(4)	119.5 (2)
C(24)-C(19)-C(4)	121.1(2)
C(21)-C(20)-C(19)	120.4(2)
C(21)-C(20)-H(20)	121(2)
C(19)-C(20)-H(20)	119(2)
C(22)-C(21)-C(20)	118.5(2)
C(22)-C(21)-H(21)	123(2)
C(20)-C(21)-H(21)	118(2)
F-C(22)-C(21)	118.2(2)
F-C(22)-C(23)	118.5(2)
C(21)-C(22)-C(23)	123.3(2)
C(22)-C(23)-C(24)	117.7(2)
C(22)-C(23)-H(23)	121(2)
C(24)-C(23)-H(23)	121(2)
C(19)-C(24)-C(23)	120.7(2)
C(19)-C(24)-H(24)	123(1)
C(23)-C(24)-H(24)	117(1)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{24}H_{24}FN_2O_2S][Br]$ (**6o**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S	26(1)	22(1)	22(1)	-4(1)	5(1)	-1(1)
F	45(1)	62(1)	22(1)	-3(1)	13(1)	-2(1)
O(1)	28(1)	20(1)	25(1)	-4(1)	1(1)	-2(1)
O(2)	32(1)	23(1)	34(1)	-6(1)	3(1)	3(1)
N(1)	22(1)	21(1)	25(1)	-4(1)	6(1)	3(1)
N(2)	23(1)	22(1)	18(1)	-2(1)	4(1)	0(1)
C(1)	26(1)	22(1)	18(1)	0(1)	4(1)	0(1)
C(2)	27(1)	22(1)	18(1)	1(1)	2(1)	-2(1)
C(3)	25(1)	20(1)	19(1)	0(1)	2(1)	0(1)
C(4)	25(1)	20(1)	22(1)	-4(1)	3(1)	1(1)
C(5)	23(1)	25(1)	19(1)	0(1)	4(1)	-1(1)
C(6)	24(1)	26(1)	24(1)	-1(1)	4(1)	-1(1)
C(7)	23(1)	27(1)	22(1)	-2(1)	5(1)	1(1)
C(8)	26(1)	36(1)	30(1)	-5(1)	4(1)	-2(1)
C(9)	22(1)	32(1)	27(1)	-4(1)	0(1)	-1(1)
C(10)	27(1)	33(1)	38(1)	0(1)	3(1)	-3(1)
C(11)	28(1)	45(1)	44(1)	-2(1)	10(1)	-5(1)
C(12)	27(1)	44(1)	49(2)	-10(1)	4(1)	3(1)
C(13)	36(1)	31(1)	46(1)	0(1)	-1(1)	4(1)
C(14)	34(1)	36(1)	33(1)	1(1)	3(1)	-3(1)
C(15)	25(1)	25(1)	25(1)	-3(1)	4(1)	-1(1)
C(16)	30(1)	23(1)	18(1)	1(1)	3(1)	-2(1)

C(17)	36(1)	22(1)	23(1)	-4(1)	1(1)	-4(1)
C(18)	38(1)	31(1)	28(1)	-5(1)	3(1)	-8(1)
C(19)	21(1)	26(1)	21(1)	-6(1)	3(1)	-2(1)
C(20)	30(1)	29(1)	28(1)	-5(1)	4(1)	5(1)
C(21)	32(1)	41(1)	28(1)	-12(1)	8(1)	5(1)
C(22)	29(1)	44(1)	19(1)	-5(1)	7(1)	-5(1)
C(23)	32(1)	32(1)	25(1)	1(1)	5(1)	-1(1)
C(24)	27(1)	25(1)	25(1)	-4(1)	6(1)	1(1)
Br	31(1)	22(1)	26(1)	-3(1)	9(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[C_{24}H_{24}FN_2O_2S][Br]$ (**6o**).

	x	y	z	U_{eq}
H(1N)	-932(18)	6290(40)	4269(11)	30(7)
H(4)	1099(17)	1930(40)	3877(11)	31(6)
H(6)	2334(18)	7890(40)	4765(11)	33(6)
H(7A)	2615(16)	3030(40)	4239(11)	30(6)
H(7B)	2674(17)	4430(40)	3713(11)	33(6)
H(8A)	3628(17)	6600(40)	4380(11)	32(7)
H(8B)	3584(16)	5070(40)	4899(11)	33(6)
H(10)	4863(19)	6460(40)	3831(12)	41(7)
H(11)	6085(18)	4820(40)	3505(12)	41(7)
H(12)	6430(20)	1470(40)	3808(13)	53(9)
H(13)	5410(20)	-150(50)	4383(14)	59(9)
H(14)	4171(19)	1530(40)	4674(12)	44(8)
H(15A)	-2135(15)	4510(40)	4054(10)	24(6)
H(15B)	-2027(16)	2190(40)	3991(10)	25(6)
H(15C)	-2187(17)	3550(30)	3440(12)	30(6)
H(17A)	-1524(18)	-1570(40)	2567(13)	36(7)
H(17B)	-1350(16)	-2530(40)	3192(11)	29(6)
H(18A)	-3009(18)	-530(40)	2722(12)	39(7)
H(18B)	-2813(19)	-1610(40)	3331(14)	43(8)
H(18C)	-2950(20)	-2800(50)	2786(13)	48(8)
H(20)	1699(17)	940(40)	3027(11)	31(6)
H(21)	2112(19)	1470(40)	2108(12)	40(7)

H(23)	809(18)	6670(40)	2015(12)	38(7)
H(24)	414(16)	6170(30)	2938(10)	25(6)

Table 6. Torsion angles [°] for $[C_{24}H_{24}FN_2O_2S][Br]$ (**6o**).

C(5)-N(2)-C(1)-N(1)	-178.6(2)
C(4)-N(2)-C(1)-N(1)	4.3(3)
C(5)-N(2)-C(1)-S	1.2(2)
C(4)-N(2)-C(1)-S	-175.9 (1)
C(2)-N(1)-C(1)-N(2)	5.7(3)
C(2)-N(1)-C(1)-S	-174.0 (2)
C(6)-S-C(1)-N(2)	-0.6(2)
C(6)-S-C(1)-N(1)	179.2(2)
C(1)-N(1)-C(2)-C(3)	-6.1(3)
C(1)-N(1)-C(2)-C(15)	172.5 (2)
N(1)-C(2)-C(3)-C(16)	176.9(2)
C(15)-C(2)-C(3)-C(16)	-1.5(3)
N(1)-C(2)-C(3)-C(4)	-3.2(3)
C(15)-C(2)-C(3)-C(4)	178.4 (2)
C(1)-N(2)-C(4)-C(3)	-11.8(3)
C(5)-N(2)-C(4)-C(3)	171.4(2)
C(1)-N(2)-C(4)-C(19)	111.1(2)
C(5)-N(2)-C(4)-C(19)	-65.7(2)
C(2)-C(3)-C(4)-N(2)	11.3(3)
C(16)-C(3)-C(4)-N(2)	-168.8 (2)
C(2)-C(3)-C(4)-C(19)	-110.8(2)
C(16)-C(3)-C(4)-C(19)	69.2(2)
C(1)-N(2)-C(5)-C(6)	-1.4(2)
C(4)-N(2)-C(5)-C(6)	175.7(2)
C(1)-N(2)-C(5)-C(7)	177.8(2)

C(4)-N(2)-C(5)-C(7)	-5.1(3)
N(2)-C(5)-C(6)-S	0.9(2)
C(7)-C(5)-C(6)-S	-178.2(2)
C(1)-S-C(6)-C(5)	-0.21(2)
C(6)-C(5)-C(7)-C(8)	7.6(3)
N(2)-C(5)-C(7)-C(8)	-171.4(2)
C(5)-C(7)-C(8)-C(9)	-175.9(2)
C(7)-C(8)-C(9)-C(14)	-69.2(3)
C(7)-C(8)-C(9)-C(10)	109.1(2)
C(14)-C(9)-C(10)-C(11)	-0.3(3)
C(8)-C(9)-C(10)-C(11)	-178.7(2)
C(9)-C(10)-C(11)-C(12)	-0.2(4)
C(10)-C(11)-C(12)-C(13)	0.5(4)
C(11)-C(12)-C(13)-C(14)	-0.3(4)
C(10)-C(9)-C(14)-C(13)	0.6(3)
C(8)-C(9)-C(14)-C(13)	178.9(2)
C(12)-C(13)-C(14)-C(9)	-0.2(4)
C(17)-O(1)-C(16)-O(2)	4.3(3)
C(17)-O(1)-C(16)-C(3)	-176.5(2)
C(2)-C(3)-C(16)-O(2)	-165.4(2)
C(4)-C(3)-C(16)-O(2)	14.7(3)
C(2)-C(3)-C(16)-O(1)	15.3(3)
C(4)-C(3)-C(16)-O(1)	-164.6(2)
C(16)-O(1)-C(17)-C(18)	165.2 (2)
N(2)-C(4)-C(19)-C(20)	131.1(2)
C(3)-C(4)-C(19)-C(20)	-107.2(2)
N(2)-C(4)-C(19)-C(24)	-50.2(2)

C(3)-C(4)-C(19)-C(24)	71.6(2)
C(24)-C(19)-C(20)-C(21)	0.1(3)
C(4)-C(19)-C(20)-C(21)	178.9(2)
C(19)-C(20)-C(21)-C(22)	0.1(3)
C(20)-C(21)-C(22)-F	179.1(2)
C(20)-C(21)-C(22)-C(23)	-0.3(3)
F-C(22)-C(23)-C(24)	-179.2(2)
C(21)-C(22)-C(23)-C(24)	0.2(3)
C(20)-C(19)-C(24)-C(23)	-0.2(3)
C(4)-C(19)-C(24)-C(23)	-178.9(2)
C(22)-C(23)-C(24)-C(19)	0.1(3)

Table 7. Hydrogen bonds for [C24H24FN2O2S][Br] (**6o**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Br	0.83(3)	2.35(3)	3.185(2)	177(2)

Compound 6p

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nonhydrogen atoms of $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
S	7246(1)	525(1)	558(1)	21(1)
O(1)	3158(2)	355(1)	3591(1)	22(1)
O(2)	6131(2)	-182(1)	3995(1)	31(1)
O(3)	4012(2)	3629(1)	3547(1)	27(1)
N(1)	7985(3)	63(1)	1916(1)	21(1)
N(2)	5125(2)	810(1)	1595(1)	18(1)
C(1)	6794(3)	452(1)	1436(1)	19(1)
C(2)	7358(3)	-92(1)	2584(1)	21(1)
C(3)	5684(3)	246(1)	2792(1)	19(1)
C(4)	4359(3)	785(1)	2321(1)	18(1)
C(5)	4100(3)	1172(1)	1000(1)	20(1)
C(6)	5067(3)	1069(1)	411(1)	21(1)
C(7)	2209(3)	1620(1)	1076(1)	21(1)
C(8)	1220(3)	1908(1)	368(1)	22(1)
C(9)	-690(3)	2370(1)	428(1)	21(1)
C(10)	-1938(3)	2538(1)	-196(1)	23(1)
C(11)	-3678(3)	2970(1)	-179(1)	26(1)
C(12)	-4237(3)	3240(1)	466(1)	27(1)

C(13)	-3020(4)	3079(1)	1086(1)	31(1)
C(14)	-1262(3)	2649(1)	1069(1)	28(1)
C(15)	8714(4)	-654(1)	2977(1)	26(1)
C(16)	5067(3)	107(1)	3516(1)	21(1)
C(17)	2524(4)	305(1)	4314(1)	27(1)
C(18)	806(4)	843(1)	4374(1)	31(1)
C(19)	4311(3)	1554(1)	2635(1)	18(1)
C(20)	2492(3)	1825(1)	2868(1)	21(1)
C(21)	2410(3)	2518(1)	3167(1)	22(1)
C(22)	4165(3)	2957(1)	3234(1)	21(1)
C(23)	5980(3)	2700(1)	2988(1)	21(1)
C(24)	6046(3)	1998(1)	2698(1)	20(1)
Br	11695(1)	-599(1)	1138(1)	23(1)

Table 9. Bond lengths [Å] and angles [°] for $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**).

S-C(1)	1.714(2)
S-C(6)	1.733(2)
O(1)-C(16)	1.346(2)
O(1)-C(17)	1.465(2)
O(2)-C(16)	1.207(2)
O(3)-C(22)	1.361(2)
O(3)-H(3O)	0.79(3)
N(1)-C(1)	1.339(3)
N(1)-C(2)	1.389(3)
N(1)-H(1N)	0.78(3)
N(2)-C(1)	1.326(3)
N(2)-C(5)	1.414(2)
N(2)-C(4)	1.501(2)
C(2)-C(3)	1.344(3)
C(2)-C(15)	1.502(3)
C(3)-C(16)	1.481(3)
C(3)-C(4)	1.533(3)
C(4)-C(19)	1.517(3)
C(4)-H(4)	0.95(2)
C(5)-C(6)	1.341(3)
C(5)-C(7)	1.496(3)
C(6)-H(6)	0.90(2)
C(7)-C(8)	1.521(3)
C(7)-H(7A)	0.93(3)
C(7)-H(7B)	0.95(3)

C(8)-C(9)	1.516(3)
C(8)-H(8A)	0.98(3)
C(8)-H(8B)	0.96(3)
C(9)-C(14)	1.393(3)
C(9)-C(10)	1.401(3)
C(10)-C(11)	1.384(3)
C(10)-H(10)	0.98(3)
C(11)-C(12)	1.390(3)
C(11)-H(11)	0.95(3)
C(12)-C(13)	1.383(3)
C(12)-H(12)	1.00(3)
C(13)-C(14)	1.391(3)
C(13)-H(13)	0.92(3)
C(14)-H(14)	0.98(3)
C(15)-H(15B)	0.91(4)
C(15)-H(15A)	0.93(5)
C(15)-H(15C)	0.97(4)
C(17)-C(18)	1.499(3)
C(17)-H(17A)	0.96(3)
C(17)-H(17B)	0.93(3)
C(18)-H(18A)	0.97(3)
C(18)-H(18B)	0.96(3)
C(18)-H(18C)	0.96(3)
C(19)-C(24)	1.387(3)
C(19)-C(20)	1.394(3)
C(20)-C(21)	1.382(3)
C(20)-H(20)	0.94(2)

C(21)-C(22)	1.392(3)
C(21)-H(21)	0.94(3)
C(22)-C(23)	1.393(3)
C(23)-C(24)	1.387(3)
C(23)-H(23)	0.93(2)
C(24)-H(24)	0.95(2)

C(1)-S-C(6)	89.2(1)
C(16)-O(1)-C(17)	115.0(2)
C(22)-O(3)-H(3O)	110(2)
C(1)-N(1)-C(2)	121.1(2)
C(1)-N(1)-H(1N)	115(2)
C(2)-N(1)-H(1N)	121(2)
C(1)-N(2)-C(5)	112.8(2)
C(1)-N(2)-C(4)	122.8(2)
C(5)-N(2)-C(4)	124.3(2)
N(2)-C(1)-N(1)	123.0(2)
N(2)-C(1)-S	113.5(2)
N(1)-C(1)-S	123.5(2)
C(3)-C(2)-N(1)	119.4(2)
C(3)-C(2)-C(15)	128.6(2)
N(1)-C(2)-C(15)	112.0(2)
C(2)-C(3)-C(16)	119.4(2)
C(2)-C(3)-C(4)	123.5(2)
C(16)-C(3)-C(4)	117.1(2)
N(2)-C(4)-C(19)	110.5(2)

N(2)-C(4)-C(3)	109.2(2)
C(19)-C(4)-C(3)	112.9(2)
N(2)-C(4)-H(4)	107(1)
C(19)-C(4)-H(4)	109(1)
C(3)-C(4)-H(4)	108(1)
C(6)-C(5)-N(2)	111.5(2)
C(6)-C(5)-C(7)	127.8(2)
N(2)-C(5)-C(7)	120.8(2)
C(5)-C(6)-S	113.0(2)
C(5)-C(6)-H(6)	128(1)
S-C(6)-H(6)	119(1)
C(5)-C(7)-C(8)	112.9(2)
C(5)-C(7)-H(7A)	108(1)
C(8)-C(7)-H(7A)	111(1)
C(5)-C(7)-H(7B)	109(1)
C(8)-C(7)-H(7B)	111(1)
H(7A)-C(7)-H(7B)	106(2)
C(9)-C(8)-C(7)	114.2(2)
C(9)-C(8)-H(8A)	108(2)
C(7)-C(8)-H(8A)	108(1)
C(9)-C(8)-H(8B)	108(1)
C(7)-C(8)-H(8B)	111(1)
H(8A)-C(8)-H(8B)	108(2)
C(14)-C(9)-C(10)	117.8(2)
C(14)-C(9)-C(8)	123.7(2)
C(10)-C(9)-C(8)	118.5(2)
C(11)-C(10)-C(9)	121.3(2)

C(11)-C(10)-H(10)	120(1)
C(9)-C(10)-H(10)	119(1)
C(10)-C(11)-C(12)	120.2(2)
C(10)-C(11)-H(11)	120(2)
C(12)-C(11)-H(11)	120(2)
C(13)-C(12)-C(11)	119.2(2)
C(13)-C(12)-H(12)	119(2)
C(11)-C(12)-H(12)	122(2)
C(12)-C(13)-C(14)	120.7(2)
C(12)-C(13)-H(13)	119(2)
C(14)-C(13)-H(13)	120(2)
C(13)-C(14)-C(9)	120.9(2)
C(13)-C(14)-H(14)	119(2)
C(9)-C(14)-H(14)	120(2)
C(2)-C(15)-H(15B)	113(2)
C(2)-C(15)-H(15A)	112(3)
H(15B)-C(15)-H(15A)	103(3)
C(2)-C(15)-H(15C)	107(2)
H(15B)-C(15)-H(15C)	107(3)
H(15A)-C(15)-H(15C)	115(4)
O(2)-C(16)-O(1)	122.8(2)
O(2)-C(16)-C(3)	125.2(2)
O(1)-C(16)-C(3)	112.0(2)
O(1)-C(17)-C(18)	108.0(2)
O(1)-C(17)-H(17A)	109(2)
C(18)-C(17)-H(17A)	113(2)
O(1)-C(17)-H(17B)	108(2)

C(18)-C(17)-H(17B)	110(2)
H(17A)-C(17)-H(17B)	109(2)
C(17)-C(18)-H(18A)	109(2)
C(17)-C(18)-H(18B)	108(2)
H(18A)-C(18)-H(18B)	108(2)
C(17)-C(18)-H(18C)	112(2)
H(18A)-C(18)-H(18C)	108(2)
H(18B)-C(18)-H(18C)	111(2)
C(24)-C(19)-C(20)	118.8(2)
C(24)-C(19)-C(4)	121.4(2)
C(20)-C(19)-C(4)	119.8(2)
C(21)-C(20)-C(19)	121.1(2)
C(21)-C(20)-H(20)	121(1)
C(19)-C(20)-H(20)	118(1)
C(20)-C(21)-C(22)	119.6(2)
C(20)-C(21)-H(21)	122(2)
C(22)-C(21)-H(21)	119(2)
O(3)-C(22)-C(21)	117.2(2)
O(3)-C(22)-C(23)	122.9(2)
C(21)-C(22)-C(23)	119.9(2)
C(24)-C(23)-C(22)	119.8(2)
C(24)-C(23)-H(23)	122(1)
C(22)-C(23)-H(23)	119(1)
C(23)-C(24)-C(19)	120.8(2)
C(23)-C(24)-H(24)	119(2)
C(19)-C(24)-H(24)	121(2)

Table 10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S	26(1)	21(1)	15(1)	0(1)	5(1)	-1(1)
O(1)	26(1)	26(1)	16(1)	2(1)	5(1)	0(1)
O(2)	34(1)	38(1)	20(1)	9(1)	4(1)	7(1)
O(3)	28(1)	20(1)	33(1)	-7(1)	5(1)	1(1)
N(1)	24(1)	21(1)	18(1)	-1(1)	5(1)	4(1)
N(2)	23(1)	18(1)	14(1)	0(1)	3(1)	-2(1)
C(1)	24(1)	17(1)	17(1)	-1(1)	3(1)	-4(1)
C(2)	27(1)	19(1)	16(1)	-2(1)	2(1)	-4(1)
C(3)	24(1)	15(1)	16(1)	0(1)	1(1)	-3(1)
C(4)	22(1)	20(1)	14(1)	1(1)	4(1)	-1(1)
C(5)	25(1)	18(1)	16(1)	1(1)	0(1)	-3(1)
C(6)	25(1)	21(1)	16(1)	1(1)	1(1)	-2(1)
C(7)	24(1)	22(1)	18(1)	1(1)	2(1)	0(1)
C(8)	24(1)	24(1)	18(1)	0(1)	0(1)	-1(1)
C(9)	26(1)	19(1)	20(1)	3(1)	2(1)	-4(1)
C(10)	27(1)	23(1)	20(1)	1(1)	0(1)	-3(1)
C(11)	31(1)	22(1)	23(1)	2(1)	-3(1)	0(1)
C(12)	31(1)	21(1)	29(1)	2(1)	2(1)	3(1)
C(13)	40(1)	31(1)	22(1)	-3(1)	4(1)	6(1)
C(14)	35(1)	30(1)	19(1)	2(1)	0(1)	5(1)
C(15)	31(1)	24(1)	21(1)	2(1)	2(1)	7(1)
C(16)	25(1)	19(1)	18(1)	0(1)	3(1)	-3(1)

C(17)	35(1)	28(1)	18(1)	3(1)	11(1)	-2(1)
C(18)	34(1)	31(1)	29(1)	0(1)	13(1)	0(1)
C(19)	24(1)	19(1)	12(1)	2(1)	0(1)	1(1)
C(20)	22(1)	23(1)	17(1)	1(1)	1(1)	-1(1)
C(21)	22(1)	24(1)	22(1)	1(1)	5(1)	4(1)
C(22)	28(1)	19(1)	16(1)	0(1)	2(1)	3(1)
C(23)	23(1)	22(1)	18(1)	0(1)	1(1)	-2(1)
C(24)	21(1)	22(1)	16(1)	0(1)	4(1)	3(1)
Br	27(1)	22(1)	21(1)	-1(1)	6(1)	2(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**).

	x	y	z	U_{eq}
H(3O)	5090(50)	3833(16)	3572(15)	36(8)
H(1N)	8850(40)	-162(15)	1761(14)	31(7)
H(4)	3000(40)	593(12)	2259(12)	18(6)
H(6)	4730(30)	1253(12)	-26(13)	17(5)
H(7A)	2570(40)	2006(14)	1384(13)	23(6)
H(7B)	1260(40)	1327(13)	1310(13)	23(6)
H(8A)	2230(40)	2217(14)	154(13)	29(6)
H(8B)	850(40)	1508(14)	51(13)	25(6)
H(10)	-1550(40)	2348(14)	-650(14)	27(6)
H(11)	-4500(40)	3080(15)	-606(15)	34(7)
H(12)	-5520(40)	3533(15)	500(14)	33(7)
H(13)	-3400(40)	3250(15)	1510(15)	36(7)
H(14)	-420(40)	2542(14)	1512(14)	31(6)
H(15B)	8010(60)	-960(20)	3250(20)	69(1)
H(15A)	9690(70)	-440(30)	3300(30)	100(2)
H(15C)	9270(60)	-960(20)	2620(20)	79(11)
H(17A)	3700(50)	397(16)	4649(16)	40(7)
H(17B)	2070(40)	-173(16)	4380(14)	32(7)
H(18A)	350(40)	814(16)	4847(16)	41(7)
H(18B)	1320(40)	1330(16)	4312(14)	37(7)
H(18C)	-360(50)	742(16)	4037(16)	42(8)

H(20)	1320(40)	1519(13)	2816(12)	23(6)
H(21)	1180(40)	2712(14)	3314(13)	28(6)
H(23)	7130(40)	3002(13)	3037(12)	19(5)
H(24)	7310(40)	1822(13)	2558(12)	25(6)

Table 12. Torsion angles [°] for $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**).

C(5)-N(2)-C(1)-N(1)	-179.1(2)
C(4)-N(2)-C(1)-N(1)	-2.7(3)
C(5)-N(2)-C(1)-S	-0.2(2)
C(4)-N(2)-C(1)-S	176.2(1)
C(2)-N(1)-C(1)-N(2)	10.7(3)
C(2)-N(1)-C(1)-S	-168.1(1)
C(6)-S-C(1)-N(2)	0.3(2)
C(6)-S-C(1)-N(1)	179.2(2)
C(1)-N(1)-C(2)-C(3)	-10.1(3)
C(1)-N(1)-C(2)-C(15)	168.7(2)
N(1)-C(2)-C(3)-C(16)	-177.4(2)
C(15)-C(2)-C(3)-C(16)	4.1(3)
N(1)-C(2)-C(3)-C(4)	1.9(3)
C(15)-C(2)-C(3)-C(4)	-176.6 (2)
C(1)-N(2)-C(4)-C(19)	120.1 (2)
C(5)-N(2)-C(4)-C(19)	-63.9(2)
C(1)-N(2)-C(4)-C(3)	-4.7(2)
C(5)-N(2)-C(4)-C(3)	171.3(2)
C(2)-C(3)-C(4)-N(2)	5.0(3)
C(16)-C(3)-C(4)-N(2)	-175.8(2)
C(2)-C(3)-C(4)-C(19)	-118.4(2)
C(16)-C(3)-C(4)-C(19)	60.9(2)
C(1)-N(2)-C(5)-C(6)	0.0(2)
C(4)-N(2)-C(5)-C(6)	-176.4(2)
C(1)-N(2)-C(5)-C(7)	-178.6 (2)

C(4)-N(2)-C(5)-C(7)	5.1(3)
N(2)-C(5)-C(6)-S	0.2(2)
C(7)-C(5)-C(6)-S	178.7(1)
C(1)-S-C(6)-C(5)	-0.3(1)
C(6)-C(5)-C(7)-C(8)	6.9(3)
N(2)-C(5)-C(7)-C(8)	-174.8(2)
C(5)-C(7)-C(8)-C(9)	-179.5(2)
C(7)-C(8)-C(9)-C(14)	13.6(3)
C(7)-C(8)-C(9)-C(10)	-167.5(2)
C(14)-C(9)-C(10)-C(11)	0.3(3)
C(8)-C(9)-C(10)-C(11)	-178.6(2)
C(9)-C(10)-C(11)-C(12)	-0.7(3)
C(10)-C(11)-C(12)-C(13)	0.7(3)
C(11)-C(12)-C(13)-C(14)	-0.2(3)
C(12)-C(13)-C(14)-C(9)	-0.2(4)
C(10)-C(9)-C(14)-C(13)	0.2(3)
C(8)-C(9)-C(14)-C(13)	179.0(2)
C(17)-O(1)-C(16)-O(2)	5.0(3)
C(17)-O(1)-C(16)-C(3)	-173.9(2)
C(2)-C(3)-C(16)-O(2)	14.2(3)
C(4)-C(3)-C(16)-O(2)	-165.1(2)
C(2)-C(3)-C(16)-O(1)	-166.9(2)
C(4)-C(3)-C(16)-O(1)	13.8(2)
C(16)-O(1)-C(17)-C(18)	158.6(2)
N(2)-C(4)-C(19)-C(24)	-54.8(2)
C(3)-C(4)-C(19)-C(24)	67.9(2)
N(2)-C(4)-C(19)-C(20)	125.2(2)

C(3)-C(4)-C(19)-C(20)	-112.1 (2)
C(24)-C(19)-C(20)-C(21)	-1.0(3)
C(4)-C(19)-C(20)-C(21)	179.0(2)
C(19)-C(20)-C(21)-C(22)	0.4(3)
C(20)-C(21)-C(22)-O(3)	-178.6(2)
C(20)-C(21)-C(22)-C(23)	1.2(3)
O(3)-C(22)-C(23)-C(24)	177.6(2)
C(21)-C(22)-C(23)-C(24)	-2.1(3)
C(22)-C(23)-C(24)-C(19)	1.5(3)
C(20)-C(19)-C(24)-C(23)	0.1(3)
C(4)-C(19)-C(24)-C(23)	-179.9(2)

Table 13. Hydrogen bonds for $[C_{24}H_{25}N_2O_3S][Br]$ (**6p**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3O)...Br#1	0.79(3)	2.36(3)	3.144(2)	170(3)
N(1)-H(1N)...Br	0.78(3)	2.42(3)	3.183(2)	167(3)

Symmetry transformations used to generate equivalent atoms: #1: -x+2,y+1/2,-z+1/2.

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Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nonhydrogen atoms of $C_{22}H_{22}N_4O_4S_2$ (**9**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
S(1)	9114(1)	3484(1)	1384(1)	27(1)
S(2)	13898(1)	-94(1)	2809(1)	26(1)
O(1)	6304(1)	7040(1)	627(1)	36(1)
O(2)	9698(1)	814(1)	1216(1)	27(1)
O(3)	13775(1)	-943(1)	3156(1)	30(1)
O(4)	14563(1)	560(1)	3215(1)	36(1)
N(1)	7674(1)	2826(2)	498(1)	27(1)
N(2)	10600(1)	2040(2)	1733(1)	24(1)
N(3)	8362(2)	7764(2)	1436(1)	39(1)
N(4)	14071(2)	-422(2)	2119(1)	34(1)
C(1)	8037(2)	3605(2)	833(1)	25(1)
C(2)	9067(2)	2311(2)	1123(1)	23(1)
C(3)	8242(2)	2092(2)	652(1)	25(1)
C(4)	9808(2)	1664(2)	1362(1)	22(1)
C(5)	7910(2)	1156(2)	295(2)	35(1)
C(6)	7586(2)	4508(2)	757(1)	27(1)
C(7)	8025(2)	5356(2)	1008(1)	27(1)
C(8)	7570(2)	6191(2)	944(1)	29(1)

C(9)	6670(2)	6199(2)	633(2)	31(1)
C(10)	6241(2)	5356(2)	357(2)	37(1)
C(11)	6693(2)	4529(2)	424(2)	34(1)
C(12)	8013(2)	7067(2)	1217(1)	30(1)
C(13)	5386(2)	7084(2)	383(2)	36(1)
C(14)	5252(5)	8103(5)	557(4)	39(2)
C(15)	5532(8)	8222(9)	1370(6)	81(4)
C(16)	4300(3)	8297(3)	178(3)	43(1)
C(14')	4999(8)	7961(9)	631(7)	19(3)
C(15')	5159(6)	8839(5)	273(4)	28(2)
C(16')	5480(10)	8095(12)	1457(6)	11(2)
C(17)	11368(2)	1511(2)	1988(1)	24(1)
C(18)	11400(2)	563(2)	2196(2)	32(1)
C(19)	12168(2)	81(2)	2442(2)	32(1)
C(20)	12917(2)	541(2)	2502(1)	26(1)
C(21)	12896(2)	1495(2)	2322(1)	26(1)
C(22)	12121(2)	1975(2)	2063(1)	24(1)
S(31)	4261(1)	3402(1)	1512(1)	24(1)
S(32)	9061(1)	-90(1)	2742(1)	23(1)
O(31)	1407(1)	6944(1)	739(1)	25(1)
O(32)	4814(1)	730(1)	1371(1)	38(1)
O(33)	8938(1)	-916(1)	3117(1)	27(1)
O(34)	9718(1)	580(1)	3132(1)	32(1)
N(31)	2800(1)	2745(1)	660(1)	25(1)
N(32)	5734(1)	1973(1)	1678(1)	23(1)
N(33)	3447(2)	7701(2)	1524(1)	31(1)
N(34)	9252(1)	-483(2)	2071(1)	27(1)

C(31)	3173(2)	3514(2)	1005(1)	24(1)
C(32)	4201(2)	2236(2)	1230(1)	22(1)
C(33)	3369(2)	2013(2)	781(1)	25(1)
C(34)	4941(2)	1588(2)	1440(1)	22(1)
C(35)	3021(2)	1094(2)	408(2)	35(1)
C(36)	2718(2)	4406(2)	956(1)	25(1)
C(37)	3145(2)	5267(2)	1188(1)	24(1)
C(38)	2682(2)	6096(2)	1108(1)	23(1)
C(39)	1782(2)	6092(2)	792(1)	23(1)
C(40)	1358(2)	5232(2)	562(2)	27(1)
C(41)	1821(2)	4407(2)	642(2)	27(1)
C(42)	3111(2)	6990(2)	1336(1)	25(1)
C(43)	484(2)	7004(2)	440(1)	24(1)
C(44)	262(2)	8033(2)	467(1)	26(1)
C(45)	581(2)	8382(2)	1244(2)	50(1)
C(46)	-703(2)	8175(2)	77(2)	33(1)
C(47)	6513(2)	1459(2)	1905(1)	26(1)
C(48)	6553(2)	475(2)	1936(3)	79(2)
C(49)	7332(2)	20(2)	2188(3)	71(2)
C(50)	8078(2)	527(2)	2409(1)	26(1)
C(51)	8053(2)	1504(2)	2372(1)	23(1)
C(52)	7268(2)	1968(2)	2116(1)	22(1)

Table 15. Bond lengths [Å] and angles [°] for $C_{22}H_{22}N_4O_4S_2$ (**9**).

S(1)-C(2)	1.728(2)
S(1)-C(1)	1.731(3)
S(2)-O(4)	1.435(2)
S(2)-O(3)	1.441(2)
S(2)-N(4)	1.589(3)
S(2)-C(20)	1.777(3)
O(1)-C(9)	1.340(3)
O(1)-C(13)	1.443(4)
O(2)-C(4)	1.232(3)
N(1)-C(1)	1.307(3)
N(1)-C(3)	1.367(3)
N(2)-C(4)	1.362(3)
N(2)-C(17)	1.415(3)
N(2)-H(2N)	0.89(3)
N(3)-C(12)	1.142(4)
N(4)-H(4N1)	0.81(4)
N(4)-H(4N2)	0.91(4)
C(1)-C(6)	1.465(3)
C(2)-C(3)	1.380(3)
C(2)-C(4)	1.475(3)
C(3)-C(5)	1.500(3)
C(5)-H(5A)	0.96(4)
C(5)-H(5B)	1.00(4)
C(5)-H(5C)	0.98(5)
C(6)-C(7)	1.395(3)

C(6)-C(11)	1.397(4)
C(7)-C(8)	1.388(4)
C(7)-H(7)	0.91(3)
C(8)-C(9)	1.407(4)
C(8)-C(12)	1.438(3)
C(9)-C(10)	1.390(4)
C(10)-C(11)	1.376(4)
C(10)-H(10)	0.93(4)
C(11)-H(11)	1.00(3)
C(13)-C(14)	1.519(8)
C(13)-C(14')	1.573(13)
C(13)-H(13A)	0.97(3)
C(13)-H(13B)	1.04(4)
C(14)-C(15)	1.509(11)
C(14)-C(16)	1.516(8)
C(14)-H(14A)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(14')-C(15')	1.508(13)
C(14')-C(16')	1.534(16)
C(14')-H(14B)	1.0000
C(15')-H(15D)	0.9800
C(15')-H(15E)	0.9800

C(15')-H(15F)	0.9800
C(16')-H(16D)	0.9800
C(16')-H(16E)	0.9800
C(16')-H(16F)	0.9800
C(17)-C(18)	1.395(4)
C(17)-C(22)	1.395(3)
C(18)-C(19)	1.381(4)
C(18)-H(18)	1.00(4)
C(19)-C(20)	1.394(4)
C(19)-H(19)	0.99(3)
C(20)-C(21)	1.390(3)
C(21)-C(22)	1.388(3)
C(21)-H(21)	0.89(3)
C(22)-H(22)	0.95(3)
S(31)-C(31)	1.729(2)
S(31)-C(32)	1.730(2)
S(32)-O(34)	1.435(2)
S(32)-O(33)	1.446(2)
S(32)-N(34)	1.598(2)
S(32)-C(50)	1.767(2)
O(31)-C(39)	1.346(3)
O(31)-C(43)	1.446(3)
O(32)-C(34)	1.228(3)
N(31)-C(31)	1.308(3)
N(31)-C(33)	1.370(3)
N(32)-C(34)	1.356(3)
N(32)-C(47)	1.419(3)

N(32)-H(32N)	0.85(3)
N(33)-C(42)	1.143(3)
N(34)-H(341)	0.80(4)
N(34)-H(342)	0.91(4)
C(31)-C(36)	1.461(3)
C(32)-C(33)	1.378(3)
C(32)-C(34)	1.478(3)
C(33)-C(35)	1.496(3)
C(35)-H(35A)	1.00(4)
C(35)-H(35B)	0.89(4)
C(35)-H(35C)	1.10(4)
C(36)-C(37)	1.397(3)
C(36)-C(41)	1.402(3)
C(37)-C(38)	1.385(3)
C(37)-H(37)	0.98(3)
C(38)-C(39)	1.408(3)
C(38)-C(42)	1.438(3)
C(39)-C(40)	1.393(3)
C(40)-C(41)	1.381(3)
C(40)-H(40)	0.94(3)
C(41)-H(41)	1.02(4)
C(43)-C(44)	1.508(3)
C(43)-H(43A)	0.93(3)
C(43)-H(43B)	0.95(3)
C(44)-C(45)	1.508(4)
C(44)-C(46)	1.527(3)
C(44)-H(44)	1.01(3)

C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.96(3)
C(46)-H(46B)	0.97(4)
C(46)-H(46C)	1.06(4)
C(47)-C(52)	1.384(3)
C(47)-C(48)	1.391(4)
C(48)-C(49)	1.378(4)
C(48)-H(48)	1.00(5)
C(49)-C(50)	1.370(4)
C(49)-H(49)	0.9500
C(50)-C(51)	1.380(3)
C(51)-C(52)	1.392(3)
C(51)-H(51)	0.84(4)
C(52)-H(52)	0.96(4)

C(2)-S(1)-C(1)	89.6(1)
O(4)-S(2)-O(3)	119.8(1)
O(4)-S(2)-N(4)	107.4(1)
O(3)-S(2)-N(4)	106.6(1)
O(4)-S(2)-C(20)	107.1(1)
O(3)-S(2)-C(20)	106.7(1)
N(4)-S(2)-C(20)	108.9(1)
C(9)-O(1)-C(13)	118.7(2)
C(1)-N(1)-C(3)	112.0(2)
C(4)-N(2)-C(17)	124.4(2)

C(4)-N(2)-H(2N)	123.2(2)
C(17)-N(2)-H(2N)	111.0(2)
S(2)-N(4)-H(4N1)	122(2)
S(2)-N(4)-H(4N2)	121(2)
H(4N1)-N(4)-H(4N2)	116(3)
N(1)-C(1)-C(6)	123.8(2)
N(1)-C(1)-S(1)	114.1(2)
C(6)-C(1)-S(1)	122.1(2)
C(3)-C(2)-C(4)	126.2(2)
C(3)-C(2)-S(1)	109.4(2)
C(4)-C(2)-S(1)	124.4(2)
N(1)-C(3)-C(2)	114.9(2)
N(1)-C(3)-C(5)	117.5(2)
C(2)-C(3)-C(5)	127.6(2)
O(2)-C(4)-N(2)	122.2(2)
O(2)-C(4)-C(2)	119.8(2)
N(2)-C(4)-C(2)	118.1(2)
C(3)-C(5)-H(5A)	111(2)
C(3)-C(5)-H(5B)	105(2)
H(5A)-C(5)-H(5B)	106(3)
C(3)-C(5)-H(5C)	111(3)
H(5A)-C(5)-H(5C)	111(3)
H(5B)-C(5)-H(5C)	112(3)
C(7)-C(6)-C(11)	118.6(2)
C(7)-C(6)-C(1)	121.7(2)
C(11)-C(6)-C(1)	119.7(2)
C(8)-C(7)-C(6)	119.7(2)

C(8)-C(7)-H(7)	122(2)
C(6)-C(7)-H(7)	119(2)
C(7)-C(8)-C(9)	121.2(2)
C(7)-C(8)-C(12)	120.3(2)
C(9)-C(8)-C(12)	118.4(2)
O(1)-C(9)-C(10)	125.9(3)
O(1)-C(9)-C(8)	115.6(2)
C(10)-C(9)-C(8)	118.5(2)
C(11)-C(10)-C(9)	120.1(3)
C(11)-C(10)-H(10)	122(3)
C(9)-C(10)-H(10)	118(3)
C(10)-C(11)-C(6)	121.7(2)
C(10)-C(11)-H(11)	118.1(2)
C(6)-C(11)-H(11)	120.0(2)
N(3)-C(12)-C(8)	179.6(3)
O(1)-C(13)-C(14)	101.9(3)
O(1)-C(13)-C(14')	117.6(5)
O(1)-C(13)-H(13A)	106.3(2)
C(14)-C(13)-H(13A)	117.4(2)
C(14')-C(13)-H(13A)	99(2)
O(1)-C(13)-H(13B)	108(2)
C(14)-C(13)-H(13B)	110(2)
C(14')-C(13)-H(13B)	113(2)
H(13A)-C(13)-H(13B)	112(3)
C(15)-C(14)-C(16)	109.5(6)
C(15)-C(14)-C(13)	109.8(7)
C(16)-C(14)-C(13)	106.6(5)

C(15)-C(14)-H(14A)	110.3
C(16)-C(14)-H(14A)	110.3
C(13)-C(14)-H(14A)	110.3
C(15')-C(14')-C(16')	106.7(9)
C(15')-C(14')-C(13)	108.6(8)
C(16')-C(14')-C(13)	108.9(10)
C(15')-C(14')-H(14B)	110.8
C(16')-C(14')-H(14B)	110.8
C(13)-C(14')-H(14B)	110.8
C(14')-C(15')-H(15D)	109.5
C(14')-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(14')-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5
H(15E)-C(15')-H(15F)	109.5
C(14')-C(16')-H(16D)	109.5
C(14')-C(16')-H(16E)	109.5
H(16D)-C(16')-H(16E)	109.5
C(14')-C(16')-H(16F)	109.5
H(16D)-C(16')-H(16F)	109.5
H(16E)-C(16')-H(16F)	109.5
C(18)-C(17)-C(22)	119.6(2)
C(18)-C(17)-N(2)	122.3(2)
C(22)-C(17)-N(2)	118.1(2)
C(19)-C(18)-C(17)	119.8(2)
C(19)-C(18)-H(18)	117(2)
C(17)-C(18)-H(18)	123(2)

C(18)-C(19)-C(20)	120.5(2)
C(18)-C(19)-H(19)	120(2)
C(20)-C(19)-H(19)	120(2)
C(21)-C(20)-C(19)	120.0(2)
C(21)-C(20)-S(2)	120.1(2)
C(19)-C(20)-S(2)	119.9(2)
C(22)-C(21)-C(20)	119.5(2)
C(22)-C(21)-H(21)	120(2)
C(20)-C(21)-H(21)	121(2)
C(21)-C(22)-C(17)	120.6(2)
C(21)-C(22)-H(22)	121(2)
C(17)-C(22)-H(22)	118(2)
C(31)-S(31)-C(32)	89.2(1)
O(34)-S(32)-O(33)	119.6(1)
O(34)-S(32)-N(34)	107.9(1)
O(33)-S(32)-N(34)	105.9(1)
O(34)-S(32)-C(50)	107.3(1)
O(33)-S(32)-C(50)	106.3(1)
N(34)-S(32)-C(50)	109.6(1)
C(39)-O(31)-C(43)	119.3(1)
C(31)-N(31)-C(33)	111.8(2)
C(34)-N(32)-C(47)	125.6(2)
C(34)-N(32)-H(32N)	119(2)
C(47)-N(32)-H(32N)	116(2)
S(32)-N(34)-H(341)	113(2)
S(32)-N(34)-H(342)	112(2)
H(341)-N(34)-H(342)	118(3)

N(31)-C(31)-C(36)	123.1(2)
N(31)-C(31)-S(31)	114.5(2)
C(36)-C(31)-S(31)	122.4(18)
C(33)-C(32)-C(34)	125.8(2)
C(33)-C(32)-S(31)	109.9(2)
C(34)-C(32)-S(31)	124.3(2)
N(31)-C(33)-C(32)	114.6(2)
N(31)-C(33)-C(35)	117.0(2)
C(32)-C(33)-C(35)	128.5(2)
O(32)-C(34)-N(32)	122.8(2)
O(32)-C(34)-C(32)	119.1(2)
N(32)-C(34)-C(32)	118.1(2)
C(33)-C(35)-H(35A)	108(2)
C(33)-C(35)-H(35B)	110(2)
H(35A)-C(35)-H(35B)	105(3)
C(33)-C(35)-H(35C)	106(2)
H(35A)-C(35)-H(35C)	110(3)
H(35B)-C(35)-H(35C)	117(3)
C(37)-C(36)-C(41)	118.6(2)
C(37)-C(36)-C(31)	122.3(2)
C(41)-C(36)-C(31)	119.1(2)
C(38)-C(37)-C(36)	119.9(2)
C(38)-C(37)-H(37)	121(2)
C(36)-C(37)-H(37)	119(2)
C(37)-C(38)-C(39)	121.2(2)
C(37)-C(38)-C(42)	120.7(2)
C(39)-C(38)-C(42)	118.1(2)

O(31)-C(39)-C(40)	125.8(2)
O(31)-C(39)-C(38)	115.5(2)
C(40)-C(39)-C(38)	118.8(2)
C(41)-C(40)-C(39)	119.9(2)
C(41)-C(40)-H(40)	123(2)
C(39)-C(40)-H(40)	117(2)
C(40)-C(41)-C(36)	121.6(2)
C(40)-C(41)-H(41)	117(2)
C(36)-C(41)-H(41)	122(2)
N(33)-C(42)-C(38)	179.0(3)
O(31)-C(43)-C(44)	106.8 (2)
O(31)-C(43)-H(43A)	109(2)
C(44)-C(43)-H(43A)	110(2)
O(31)-C(43)-H(43B)	110(2)
C(44)-C(43)-H(43B)	108(2)
H(43A)-C(43)-H(43B)	112(2)
C(45)-C(44)-C(43)	111.1(2)
C(45)-C(44)-C(46)	110.9(2)
C(43)-C(44)-C(46)	110.0(2)
C(45)-C(44)-H(44)	107(2)
C(43)-C(44)-H(44)	111(2)
C(46)-C(44)-H(44)	107(2)
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5

H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	109(2)
C(44)-C(46)-H(46B)	109(2)
H(46A)-C(46)-H(46B)	105(3)
C(44)-C(46)-H(46C)	114(2)
H(46A)-C(46)-H(46C)	109(3)
H(46B)-C(46)-H(46C)	110(3)
C(52)-C(47)-C(48)	118.8(2)
C(52)-C(47)-N(32)	118.0(2)
C(48)-C(47)-N(32)	123.2(2)
C(49)-C(48)-C(47)	120.3(3)
C(49)-C(48)-H(48)	120(3)
C(47)-C(48)-H(48)	116(3)
C(50)-C(49)-C(48)	120.6(3)
C(50)-C(49)-H(49)	119.7
C(48)-C(49)-H(49)	119.7
C(49)-C(50)-C(51)	120.0(2)
C(49)-C(50)-S(32)	118.8(2)
C(51)-C(50)-S(32)	121.15(2)
C(50)-C(51)-C(52)	119.6(2)
C(50)-C(51)-H(51)	125(3)
C(52)-C(51)-H(51)	116(3)
C(47)-C(52)-C(51)	120.6(2)
C(47)-C(52)-H(52)	118(2)
C(51)-C(52)-H(52)	122(2)

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{22}H_{22}N_4O_4S_2$ (**9**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	20(1)	23(1)	36(1)	-13(1)	10(1)	-6(1)
S(2)	23(1)	15(1)	35(1)	-5(1)	5(1)	0(1)
O(1)	41(1)	22(1)	55(1)	-6(1)	29(1)	0(1)
O(2)	27(1)	19(1)	32(1)	-3(1)	10(1)	-5(1)
O(3)	29(1)	19(1)	37(1)	1(1)	9(1)	2(1)
O(4)	24(1)	20(1)	52(1)	-10(1)	4(1)	0(1)
N(1)	24(1)	21(1)	34(1)	-6(1)	11(1)	-6(1)
N(2)	22(1)	17(1)	26(1)	-1(1)	4(1)	-3(1)
N(3)	57(2)	26(1)	39(1)	-11(1)	23(1)	-16(1)
N(4)	43(1)	19(1)	44(1)	-2(1)	21(1)	-6(1)
C(1)	23(1)	26(1)	30(1)	-8(1)	12(1)	-8(1)
C(2)	25(1)	19(1)	25(1)	-4(1)	11(1)	-5(1)
C(3)	26(1)	21(1)	27(1)	-2(1)	9(1)	-4(1)
C(4)	25(1)	22(1)	19(1)	-1(1)	9(1)	-5(1)
C(5)	30(2)	20(1)	41(2)	-7(1)	-1(1)	-4(1)
C(6)	26(1)	23(1)	36(1)	-11(1)	17(1)	-5(1)
C(7)	24(1)	27(1)	33(1)	-8(1)	16(1)	-8(1)
C(8)	33(1)	24(1)	36(1)	-11(1)	21(1)	-10(1)
C(9)	36(1)	23(1)	44(2)	-7(1)	25(1)	-3(1)
C(10)	25(1)	31(1)	60(2)	-12(1)	22(1)	-5(1)
C(11)	26(1)	27(1)	54(2)	-16(1)	21(1)	-9(1)
C(12)	40(2)	24(1)	31(1)	-5(1)	19(1)	-7(1)

C(13)	40(2)	32(2)	36(2)	0(1)	16(1)	12(1)
C(14)	31(4)	32(3)	57(4)	11(2)	22(3)	11(2)
C(15)	59(6)	76(7)	83(7)	-36(5)	0(5)	27(5)
C(16)	31(2)	49(3)	51(3)	14(2)	20(2)	19(2)
C(14')	23(7)	16(6)	20(5)	1(4)	10(5)	14(5)
C(15')	51(6)	14(4)	22(4)	5(3)	16(4)	16(4)
C(16')	11(4)	16(4)	5(3)	0(3)	4(3)	9(3)
C(17)	24(1)	20(1)	24(1)	-2(1)	4(1)	-1(1)
C(18)	23(1)	27(1)	36(1)	3(1)	3(1)	-5(1)
C(19)	27(1)	21(1)	39(1)	1(1)	3(1)	-3(1)
C(20)	24(1)	19(1)	30(1)	-5(1)	5(1)	-1(1)
C(21)	23(1)	21(1)	34(1)	-4(1)	12(1)	-3(1)
C(22)	26(1)	15(1)	29(1)	-2(1)	11(1)	-1(1)
S(31)	18(1)	18(1)	33(1)	-7(1)	8(1)	1(1)
S(32)	18(1)	14(1)	29(1)	-2(1)	2(1)	2(1)
O(31)	18(1)	16(1)	42(1)	-4(1)	13(1)	2(1)
O(32)	25(1)	16(1)	79(2)	-2(1)	25(1)	1(1)
O(33)	24(1)	21(1)	35(1)	4(1)	9(1)	6(1)
O(34)	22(1)	18(1)	43(1)	-9(1)	1(1)	0(1)
N(31)	17(1)	17(1)	42(1)	-6(1)	12(1)	0(1)
N(32)	17(1)	14(1)	31(1)	-1(1)	1(1)	2(1)
N(33)	35(1)	21(1)	39(1)	-8(1)	18(1)	-7(1)
N(34)	29(1)	18(1)	33(1)	0(1)	9(1)	-3(1)
C(31)	19(1)	19(1)	35(1)	-4(1)	12(1)	-1(1)
C(32)	21(1)	16(1)	32(1)	-3(1)	13(1)	1(1)
C(33)	20(1)	16(1)	40(1)	-3(1)	14(1)	1(1)
C(34)	21(1)	18(1)	28(1)	1(1)	13(1)	2(1)

C(35)	20(1)	18(1)	63(2)	-11(1)	11(1)	1(1)
C(36)	19(1)	19(1)	38(1)	-8(1)	12(1)	0(1)
C(37)	16(1)	20(1)	35(1)	-7(1)	12(1)	-1(1)
C(38)	21(1)	18(1)	33(1)	-7(1)	13(1)	-2(1)
C(39)	21(1)	18(1)	33(1)	-4(1)	15(1)	2(1)
C(40)	16(1)	21(1)	44(1)	-6(1)	13(1)	-1(1)
C(41)	20(1)	19(1)	44(1)	-7(1)	15(1)	-2(1)
C(42)	24(1)	21(1)	31(1)	-4(1)	13(1)	0(1)
C(43)	20(1)	22(1)	30(1)	-1(1)	12(1)	3(1)
C(44)	24(1)	19(1)	35(1)	2(1)	11(1)	6(1)
C(45)	39(2)	46(2)	48(2)	-21(1)	0(1)	20(1)
C(46)	24(1)	32(2)	40(2)	5(1)	12(1)	10(1)
C(47)	20(1)	18(1)	28(1)	0(1)	-1(1)	3(1)
C(48)	20(2)	18(2)	152(4)	-2(2)	-15(2)	-1(1)
C(49)	20(2)	16(1)	136(4)	2(2)	-13(2)	0(1)
C(50)	19(1)	16(1)	32(1)	-1(1)	-2(1)	4(1)
C(51)	22(1)	16(1)	34(1)	-1(1)	13(1)	0(1)
C(52)	24(1)	14(1)	32(1)	1(1)	14(1)	3(1)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{22}H_{22}N_4O_4S_2$ (**9**).

	x	y	z	U_{eq}
H(2N)	10707(19)	2660(20)	1753(16)	29(7)
H(4N1)	14270(20)	-70(20)	1909(19)	36(9)
H(4N2)	13840(20)	-970(30)	1885(17)	35(8)
H(5A)	8360(20)	800(30)	229(18)	43(9)
H(5B)	7760(20)	790(30)	660(20)	49(1)
H(5C)	7410(30)	1240(30)	-170(30)	86(2)
H(7)	8604(19)	5340(20)	1223(15)	24(7)
H(10)	5650(30)	5380(30)	130(20)	66(1)
H(11)	6360(20)	3930(20)	264(18)	41(9)
H(13A)	5230(20)	6590(20)	643(18)	36(8)
H(13B)	5120(20)	6980(30)	-180(20)	48(1)
H(14A)	5578	8544	370	47
H(15A)	6157	8169	1610	122
H(15B)	5269	7728	1557	122
H(15C)	5355	8847	1473	122
H(16A)	3992	7905	398	64
H(16B)	4104	8143	-342	64
H(16C)	4190	8967	233	64
H(14B)	4373	7871	499	23
H(15D)	4840	8796	-257	43
H(15E)	5772	8893	386	43

H(15F)	4969	9398	458	43
H(16D)	6095	8142	1578	16
H(16E)	5370	7552	1713	16
H(16F)	5282	8677	1609	16
H(18)	10880(20)	180(30)	2130(20)	50(1)
H(19)	12190(20)	-600(20)	2568(18)	47(9)
H(21)	13370(20)	1800(20)	2365(16)	26(7)
H(22)	12092(19)	2630(20)	1947(16)	31(8)
H(32N)	5783(19)	2570(20)	1723(16)	26(7)
H(341)	9310(20)	-70(30)	1821(19)	38(9)
H(342)	8910(20)	-980(30)	1844(18)	39(9)
H(35A)	2550(30)	1240(30)	-80(20)	54(1)
H(35B)	3410(20)	800(30)	297(18)	43(9)
H(35C)	2770(20)	720(30)	761(19)	48(1)
H(37)	3772(19)	5270(20)	1403(15)	26(7)
H(40)	750(20)	5240(20)	367(18)	43(9)
H(41)	1480(20)	3790(20)	479(18)	44(9)
H(43A)	283(18)	6640(20)	726(16)	24(7)
H(43B)	250(19)	6810(20)	-59(17)	27(7)
H(44)	537(19)	8440(20)	208(17)	36(8)
H(45A)	305	8023	1510	75
H(45B)	445	9056	1247	75
H(45C)	1202	8294	1482	75
H(46A)	-830(20)	8840(20)	77(18)	42(9)
H(46B)	-990(20)	7880(20)	358(19)	49(9)
H(46C)	-960(30)	7920(30)	-460(20)	66(1)
H(48)	6040(30)	140(30)	1940(30)	95

H(49)	7352	-652	2209	86
H(51)	8480(20)	1850(30)	2479(19)	47(1)
H(52)	7230(20)	2650(30)	2090(20)	52(1)

Table 18. Torsion angles [°] for $C_{22}H_{22}N_4O_4S_2$ (**9**).

C(3)-N(1)-C(1)-C(6)	178.7(2)
C(3)-N(1)-C(1)-S(1)	-1.3(3)
C(2)-S(1)-C(1)-N(1)	1.4(2)
C(2)-S(1)-C(1)-C(6)	-178.7(2)
C(1)-S(1)-C(2)-C(3)	-1.1(2)
C(1)-S(1)-C(2)-C(4)	177.6(2)
C(1)-N(1)-C(3)-C(2)	0.4(3)
C(1)-N(1)-C(3)-C(5)	-179.3(2)
C(4)-C(2)-C(3)-N(1)	-178.0(2)
S(1)-C(2)-C(3)-N(1)	0.6(3)
C(4)-C(2)-C(3)-C(5)	1.7(4)
S(1)-C(2)-C(3)-C(5)	-179.7(2)
C(17)-N(2)-C(4)-O(2)	-0.3(4)
C(17)-N(2)-C(4)-C(2)	-179.3(2)
C(3)-C(2)-C(4)-O(2)	-9.6(4)
S(1)-C(2)-C(4)-O(2)	171.9(2)
C(3)-C(2)-C(4)-N(2)	169.3(2)
S(1)-C(2)-C(4)-N(2)	-9.1(3)
N(1)-C(1)-C(6)-C(7)	-167.6(2)
S(1)-C(1)-C(6)-C(7)	12.5(3)
N(1)-C(1)-C(6)-C(11)	12.4(4)
S(1)-C(1)-C(6)-C(11)	-167.6(2)
C(11)-C(6)-C(7)-C(8)	2.0(4)
C(1)-C(6)-C(7)-C(8)	-178.1(2)
C(6)-C(7)-C(8)-C(9)	0.4(4)

C(6)-C(7)-C(8)-C(12)	178.5(2)
C(13)-O(1)-C(9)-C(10)	6.6(4)
C(13)-O(1)-C(9)-C(8)	-174.0(2)
C(7)-C(8)-C(9)-O(1)	177.5(2)
C(12)-C(8)-C(9)-O(1)	-0.6(4)
C(7)-C(8)-C(9)-C(10)	-3.0(4)
C(12)-C(8)-C(9)-C(10)	178.9(3)
O(1)-C(9)-C(10)-C(11)	-177.4(3)
C(8)-C(9)-C(10)-C(11)	3.2(4)
C(9)-C(10)-C(11)-C(6)	-0.9(5)
C(7)-C(6)-C(11)-C(10)	-1.8(4)
C(1)-C(6)-C(11)-C(10)	178.3(3)
C(9)-O(1)-C(13)-C(14)	172.6(4)
C(9)-O(1)-C(13)-C(14')	158.9(6)
O(1)-C(13)-C(14)-C(15)	-73.3(7)
O(1)-C(13)-C(14)-C(16)	168.2(4)
C(14')-C(13)-C(14)-C(16)	-49.2(2)
O(1)-C(13)-C(14')-C(15')	66.9(9)
C(14)-C(13)-C(14')-C(15')	24.8(2)
O(1)-C(13)-C(14')-C(16')	-48.9(1)
C(4)-N(2)-C(17)-C(18)	-30.4(4)
C(4)-N(2)-C(17)-C(22)	152.5(2)
C(22)-C(17)-C(18)-C(19)	-2.9(4)
N(2)-C(17)-C(18)-C(19)	-180.0(2)
C(17)-C(18)-C(19)-C(20)	1.6(4)
C(18)-C(19)-C(20)-C(21)	0.7(4)
C(18)-C(19)-C(20)-S(2)	-179.2(2)

O(4)-S(2)-C(20)-C(21)	33.4(2)
O(3)-S(2)-C(20)-C(21)	162.9(2)
N(4)-S(2)-C(20)-C(21)	-82.3(2)
O(4)-S(2)-C(20)-C(19)	-146.6(2)
O(3)-S(2)-C(20)-C(19)	-17.1(2)
N(4)-S(2)-C(20)-C(19)	97.6(2)
C(19)-C(20)-C(21)-C(22)	-1.8(4)
S(2)-C(20)-C(21)-C(22)	178.2(2)
C(20)-C(21)-C(22)-C(17)	0.5(4)
C(18)-C(17)-C(22)-C(21)	1.8(4)
N(2)-C(17)-C(22)-C(21)	179.0(2)
C(33)-N(31)-C(31)-C(36)	178.5(2)
C(33)-N(31)-C(31)-S(31)	-0.1(3)
C(32)-S(31)-C(31)-N(31)	0.4(2)
C(32)-S(31)-C(31)-C(36)	-178.3(2)
C(31)-S(31)-C(32)-C(33)	-0.5(2)
C(31)-S(31)-C(32)-C(34)	179.0(2)
C(31)-N(31)-C(33)-C(32)	-0.3(3)
C(31)-N(31)-C(33)-C(35)	-179.3(2)
C(34)-C(32)-C(33)-N(31)	-178.9(2)
S(31)-C(32)-C(33)-N(31)	0.5(3)
C(34)-C(32)-C(33)-C(35)	-0.1(4)
S(31)-C(32)-C(33)-C(35)	179.4(2)
C(47)-N(32)-C(34)-O(32)	-2.7(4)
C(47)-N(32)-C(34)-C(32)	179.6(2)
C(33)-C(32)-C(34)-O(32)	-18.8(4)
S(31)-C(32)-C(34)-O(32)	161.9(2)

C(33)-C(32)-C(34)-N(32)	159.0(2)
S(31)-C(32)-C(34)-N(32)	-20.4(3)
N(31)-C(31)-C(36)-C(37)	-165.4(2)
S(31)-C(31)-C(36)-C(37)	13.1(4)
N(31)-C(31)-C(36)-C(41)	12.4(4)
S(31)-C(31)-C(36)-C(41)	-169.1(2)
C(41)-C(36)-C(37)-C(38)	0.2(4)
C(31)-C(36)-C(37)-C(38)	178.0(2)
C(36)-C(37)-C(38)-C(39)	-0.3(4)
C(36)-C(37)-C(38)-C(42)	-179.3(2)
C(43)-O(31)-C(39)-C(40)	2.0(4)
C(43)-O(31)-C(39)-C(38)	-178.3(2)
C(37)-C(38)-C(39)-O(31)	-179.4(2)
C(42)-C(38)-C(39)-O(31)	-0.4(3)
C(37)-C(38)-C(39)-C(40)	0.3(4)
C(42)-C(38)-C(39)-C(40)	179.3(2)
O(31)-C(39)-C(40)-C(41)	179.4(2)
C(38)-C(39)-C(40)-C(41)	-0.3(4)
C(39)-C(40)-C(41)-C(36)	0.2(4)
C(37)-C(36)-C(41)-C(40)	-0.2(4)
C(31)-C(36)-C(41)-C(40)	-178.0(2)
C(39)-O(31)-C(43)-C(44)	178.8(2)
O(31)-C(43)-C(44)-C(45)	-63.6(3)
O(31)-C(43)-C(44)-C(46)	173.3(2)
C(34)-N(32)-C(47)-C(52)	178.5(2)
C(34)-N(32)-C(47)-C(48)	-2.7(5)
C(52)-C(47)-C(48)-C(49)	1.3(7)

N(32)-C(47)-C(48)-C(49)	-177.5(4)
C(47)-C(48)-C(49)-C(50)	-0.2(8)
C(48)-C(49)-C(50)-C(51)	-0.9(7)
C(48)-C(49)-C(50)-S(32)	179.0(4)
O(34)-S(32)-C(50)-C(49)	-162.8(3)
O(33)-S(32)-C(50)-C(49)	-33.8(3)
N(34)-S(32)-C(50)-C(49)	80.2(3)
O(34)-S(32)-C(50)-C(51)	17.0(3)
O(33)-S(32)-C(50)-C(51)	146.0(2)
N(34)-S(32)-C(50)-C(51)	-99.9(2)
C(49)-C(50)-C(51)-C(52)	0.7(5)
S(32)-C(50)-C(51)-C(52)	-179.11(2)
C(48)-C(47)-C(52)-C(51)	-1.5(5)
N(32)-C(47)-C(52)-C(51)	177.4(2)
C(50)-C(51)-C(52)-C(47)	0.5(4)

Table 19. Hydrogen bonds for $C_{22}H_{22}N_4O_4S_2$ (**9**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...O(33)#1	0.89(3)	2.08(3)	2.974(3)	175(3)
N(4)-H(4N1)...O(32)#2	0.81(4)	2.02(4)	2.827(3)	176(3)
N(4)-H(4N2)...N(33)#3	0.91(4)	2.03(4)	2.924(3)	170(3)
N(32)-H(32N)...O(3)#1	0.85(3)	2.21(3)	3.040(3)	166(3)
N(32)-H(32N)...S(31)	0.85(3)	2.72(3)	3.134(2)	111(2)
N(34)-H(341)...O(2)	0.80(4)	2.02(4)	2.807(3)	167(3)
N(34)-H(342)...N(3)#4	0.91(4)	2.02(4)	2.915(3)	168(3)

Symmetry transformations used to generate equivalent atoms: #1: -x+2,y+1/2,-z+1/2; #2: x+1,y,z; #3: x+1,y-1,z; and #4: x,y-1,z.