SUPPORTING INFORMATION

Acetylcholinesterase Inhibitors: Structure Based Design, Synthesis, Pharmacophore Modeling and Virtual Screening

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Ethyl 3-hydroxy-7-methyl-5-(4-nitrophenyl)-3-phenethyl-3,5-dihydro-2H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6b)

Color less solid, R_f 0.37; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 217-220 ºC; IR: 3232, 2862, 2796, 2356, 1712, 1668, 1525, 1496, 1434, 1346, 1253, 1089, 738 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 1.17 (t, 3H), 2.27 (*s*, 3H), 2.39 (s, 2H), 2.67-2.85 (m, 2H), 3.54-3.58 (m, 1H), 3.96-4.19 (m, 3H), 5.80 (s, 1H), 6.922-6.95 (m, 1H), 7.12-7.32 (m, 5H), 7.64-7.70 (m, 1H), 7.66-7.80 (m, 1H), 8.15-8.20 (m, 2H); ^{13}C NMR (DMSO-d$_6$) δ 13.8, 17.7, 28.9, 36.8, 37.7, 48.6, 54.3, 54.8, 60.7, 105.1, 122.3, 123.2, 123.7, 126.2, 127.7, 128.2, 128.4, 130.7, 140.0, 143.8, 147.4, 147.6, 163.4, 166.6. HRMS cald for $C_{24}H_{26}N_3O_5S$ (M+H) 468.1593; found 468.1574 (TOF MS ES$^+$).

Ethyl 5-(4-fluorophenyl)-3-hydroxy-7-methyl-3-phenethyl-3,5-dihydro-2H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6c)

Color less solid, R_f 0.40; (dichloromethane: ethyl acetate, 5:1 v/v). Yield: 78%; m.p.: 275-277 ºC; IR: 3143, 2918, 2867, 2360, 1710, 1654, 1593, 1539, 1446, 1338, 1265, 705 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 1.19 (t, 3H), 2.35 (*s*, 3H), 2.64-2.84 (m, 3H), 3.56-3.60 (m, 1H), 3.95-4.19 (m, 3H), 5.66 (s, 1H), 6.97 (d, 1H), 7.13-7.45 (m, 8H); HRMS cald for $C_{24}H_{26}FN_2O_3S$ (M+H) 440.1570; found 440.1581 (TOF MS ES$^+$).

Ethyl 3-hydroxy-5-(4-hydroxyphenyl)-7-methyl-3-phenethyl-3,5-dihydro-2H-thiazolo[3,2-a]pyrimidine-6-carboxylate (6d)

Color less solid, R_f 0.31; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 281-283 ºC; IR: 3271, 2972, 2815, 2366, 1716, 1668, 1527, 1442, 1265, 1093, 850, 738 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 1.19 (t, 3H), 2.26 (*s*, 3H), 2.57 (d, 1H), 4.00-4.18 (m, 3H), 5.84 (s, 1H), 6.69-6.73 (m, 2H), 7.09-7.29 (m, 6H), 9.57 (s, 1H); HRMS cald for $C_{24}H_{27}N_2O_4S$ (M+H)$^+$ 439.1692; found 439.1677 (TOF MS ES$^+$).

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

Color less solid, R_f 0.42; (dichloromethane: ethyl acetate, 2:1 v/v). Yield: 78%; m.p.: 246-248 ºC; IR: 3141, 3105, 2927, 2806, 2358, 1720, 1658, 1593, 1533, 1440, 1344, 1253, 1091, 852, 740 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 1.19 (t, 3H), 2.27 (*s*, 3H), 2.64-2.83 (m, 1H), 3.54-.358 (m, 1H), 3.90 (s, 3H), 3.95-4.17 (m, 3H), 5.61 (s, 1H), 6.94-6.98 (m, 2H), 7.14-7.29 (m, 4H), 7.41-7.44 (m, 1H), 7.50-7.76 (m, 1H), 10.52 (s, 1H); HRMS cald for $C_{26}H_{29}N_2O_6S$ $(M+H)^+$ 497.1746; found 497.1730 (TOF MS ES$^+$).

Ethyl 7-methyl-5-(4-nitrophenyl)-3-phenethyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate (7b)

Color less solid, R_f 0.33; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 85%; m.p.: 242-248 ºC; IR: 3053, 2983, 2688, 2358, 1677, 1529, 1350, 1265, 1294, 1110, 748 cm^{-1}; ^{1}H NMR (DMSO-d$_6$) δ 1.21 (*t*, 3H), 2.39 (*s*, 3H), 2.63-2.85 (m, 2H), 3.01-3.08 (m, 1H), 4.05-4.18 (m, 1H), 6.63 (s, 1H), 7.09-7.13 (m, 3H), 7.20-7.28 (m, 5H), 7.40-7.44 (m, 2H), 8.21-8.25 (m, 2H); ^{13}C NMR (DMSO-d$_6$) δ 13.9, 18.2, 27.3, 32.1, 57.6, 60.5, 102.3, 116.0 126.3, 128.2, 128.4, 129.5, 131.5, 136.5, 139.4, 140.6, 141.6, 161.2, 163.1, 163.9. HRMS cald for $C_{24}H_{24}N_3O_4S$ (M+H) 450.1488; found 450.1459 (TOF MS ES$^+$).

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

Color less solid, R_f 0.35; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 86%; m.p.: 275-276 ºC; IR: 3053, 2988, 2684, 2360, 1683, 1527, 1340, 1265, 1294, 1091, 896, 736 cm^{-1}; ^{1}H NMR (DMSO-d$_6$) δ 1.21 (*t*, 3H), 2.39 (*s*, 3H), 2.66-2.82 (m, 3H), 3.03-3.06 (m, 1H), 4.07-4.17 (m, 2H), 6.43 (s, 1H), 7.09-7.13 (m, 3H), 7.18-7.29 (m, 5H), 7.40-7.43 (m, 2H); ^{13}C NMR (DMSO-d$_6$) δ 13.9, 17.9, 28.6, 32.1, 57.6, 60.6, 102.4, 116.0 (*J* = 21.3 *Hz*), 126.3, 128.2, 128.4, 129.5 (*J* = 7.5 *Hz*), 136.5, 139.4, 140.7, 141.1, 161.2, 163.1, 163.8. HRMS cald for $C_{24}H_{24}FN_2O_2S$ (M+H) 423.1543; found 423.1545 (TOF MS ES$^+$).

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

Color less solid, R_f 0.28; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 256-258 ºC; IR: 3342, 2972, 2894, 2358, 1720, 1658, 1533, 1527, 1344, 1272, 1170, 1091, 1049, 852, 783, 740, 698, 667 cm^{-1}; ^1H NMR (DMSO-d_6) δ 1.21 (*t*, 3H), 2.39 (*s*, 3H), 2.70-2.84 (m, 3H), 2.98-3.05 (m, 1H), 4.05-4.18 (m, 2H), 6.28 (s, 1H), 6.74-6.77 (m, 2H), 7.09 (s, 1H), 7.12-7.16 (m, 4H), 7.18-7.22 (m, 1H), 7.25-7.29 (m, 2H), 9.77 (s, 1H); ^{13}C NMR (DMSO-d_6) δ 13.9, 17.8, 27.3, 32.2, 58.0, 60.4, 103.0, 108.6, 115.7, 126.3, 128.2, 128.4, 128.5, 130.6, 139.5, 140.7, 141.7, 158.1, 160.5, 163.9. HRMS cald for $C_{24}H_{25}N_2O_3S$ (M+H), 421.1586; found 421.1568 (TOF MS ES^+).

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

Color less solid, R_f 0.31; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 281-283 ºC; IR: 3292, 3147, 2923, 2808, 2362, 1710, 1654, 1593, 1539, 1265, 1016, 740 cm-1; ^1H NMR (DMSO-d_6) δ 1.21 (t, 3H), 2.39 (*s*, 3H), 2.64-2.74 (m, 2H), 2.79-2.85 (m, 1H), 2.99-3.06 (m, 1H), 3.86 (s, 3H), 4.01-4.18 (m, 2H), 6.42 (s, 1H), 7.00-7.02 (m, 1H), 7.10-7.12 (m, 3H), 7.24-7.26 (m, 2H), 7.41-7.44 (m, 2H), 7.75 (d, 1H), 10.59 (s, 1H); ^{13}C NMR (DMSO-d_6) δ 13.8, 18.1, 27.4, 52.6, 57.6, 60.5, 61.5, 102.2, 108.5, 113.6, 118.8, 126.3, 128.1, 128.3, 128.9, 129.0, 131.1, 133.7, 139.5, 140.6, 159.8, 160.9, 163.8, 168.0. HRMS cald for $C_{26}H_{27}N_2O_5S$ (M+H) 479.1641; found 479.1646 (TOF MS ES^+).

Methyl 7-methyl-5-(3-nitrophenyl)-3-phenethyl-5H-thiazolo [3, 2-a] pyrimidine-6-carboxylate (7f)

Color less solid, R_f 0.29; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 80%; m.p.: 144-146 ºC; IR: 3053, 2985, 2684, 2360, 1716, 1681, 1533, 1421, 1265, 1093, 738 cm-1; ^1H NMR (DMSO-d_6) δ 2.40 (*s*, 3H), 2.63-2.85 (m, 3H), 3.02-3.09 (m, 1H), 3.67 (s, 3H), 4.05-4.18 (m, 1H), 6.44 (s, 1H), 7.11-7.14 (m, 1H), 7.18-7.28 (m, 4H), 7.39-7.43 (m, 2H), 8.17-8.24 (m, 2H); ^{13}C NMR (DMSO-d_6) δ 17.9, 27.3, 32.1, 51.7, 57.7, 60.6, 102.4, 108.5, 116.0, 126.3, 128.2, 128.4, 129.4, 136.4, 139.4, 140.5, 142.7, 160.7, 163.1, 164.3. HRMS cald for $C_{19}H_{22}N_2O_7PS$ $(M+H)^+$ 453.0885; found 453.0900 (TOF MS ES^+).

Methyl 7-methyl-5-(4-nitrophenyl)-3-phenethyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate (7g)

Color less solid, R*f* 0.30; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 78%; m.p.: 156-158 ºC; IR: IR: 3053, 2979, 2860, 2690, 2358, 1676, 1595, 1529, 1348, 1257, 1108, 783, 736 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 2.39 (*s*, 3H), 2.61-2.72 (m, 2H), 2.78-2.85 (m, 1H), 3.67 (s, 3H), 4.05-4.19 (m, 1H), 6.63 (s, 1H), 7.09-7.26 (m, 6H), 7.69-7.72 (m, 1H), 7.78-7.81 (m, 1H), 8.14-8.25 (m, 2H); ^{13}C NMR (DMSO-d$_6$) δ 18.4, 27.2, 32.0, 51.7, 57.5, 60.6, 101.4, 108.5, 122.1, 124.1, 126.3, 128.1, 128.3, 131.1, 133.6, 139.4, 140.5, 141.8, 147.9, 161.6, 163.7, 164.3. HRMS cald for $C_{23}H_{22}N_3O_4S$ (M+H) 436.1253; found 436.1250 (TOF MS ES$^+$).

Methyl 5-(4-fluorophenyl)-7-methyl-3-phenethyl-5H-thiazolo [3, 2-a] pyrimidine-6-carboxylate (7h)

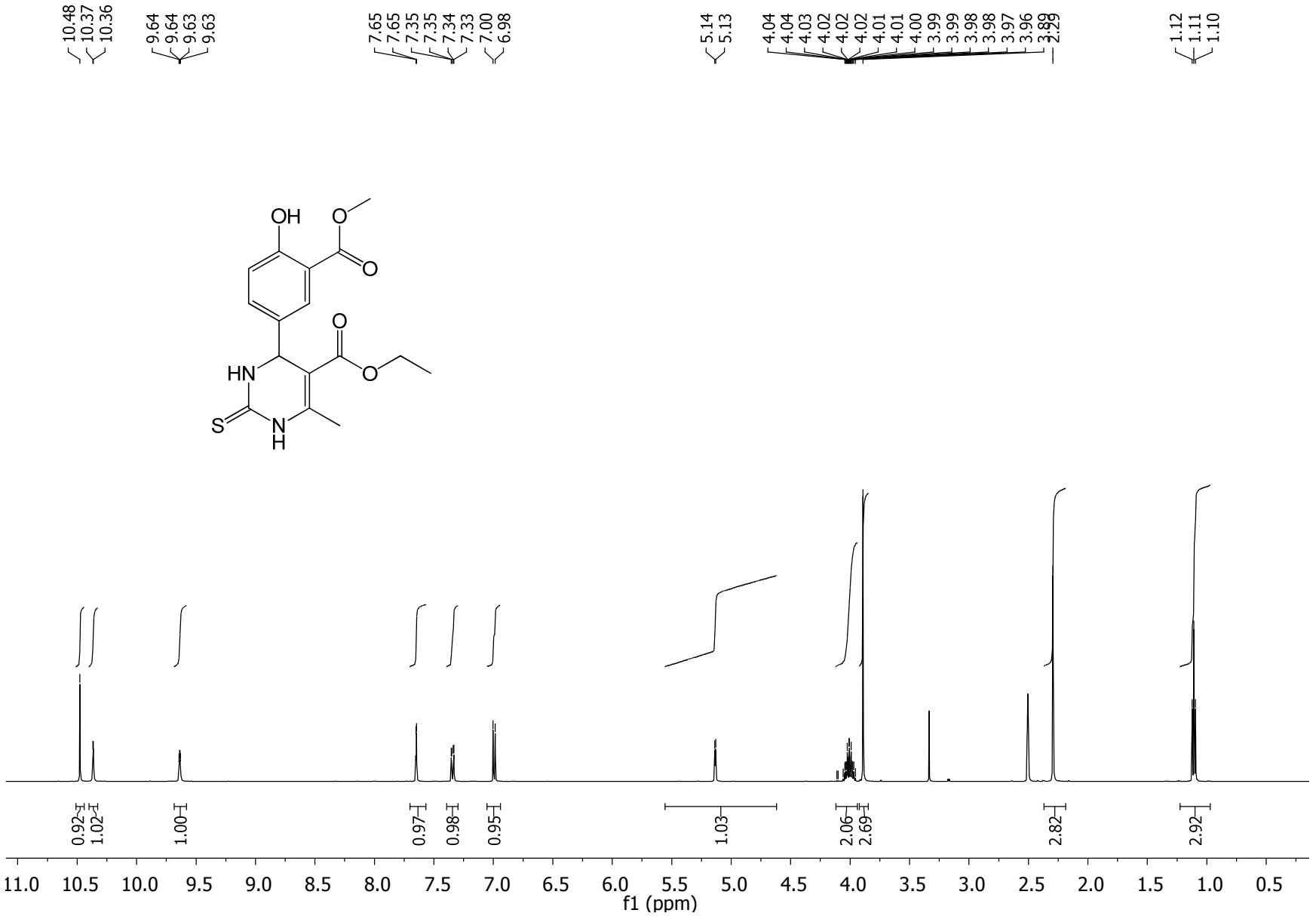
Color less solid, R*f* 0.38; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 182-184 ºC; IR: 3053, 2985, 2684, 2360, 1716, 1681, 1533, 1421, 1265, 1093, 896, 738 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 2.40 (*s*, 3H), 2.62-2.82 (m, 2H), 3.03-3.07 (m, 1H), 3.67 (s, 3H), 4.05-4.18 (m, 1H), 6.64 (s, 1H), 7.11-7.14 (m, 3H), 7.18-7.28 (m, 5H), 7.39-7.43 (m, 2H); ^{13}C NMR (DMSO-d$_6$) δ 18.5, 27.2, 32.0, 51.6, 57.5, 60.6, 101.4, 122.1, 126.3, 128.1, 128.3, 131.1, 133.5, 139.4, 140.5, 147.8, 161.6, 163.7. HRMS cald for $C_{23}H_{21}FN_2O_2S$ (M+H)$^+$ 408.1308; found 453.0900 (TOF MS ES$^+$).

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

Color less solid, R$_f$ 0.42; (dichloromethane: ethyl acetate, 1:1 v/v). Yield: 80%; m.p.: 173-175 ºC; IR: 3155, 3107, 2931, 2360, 1720, 1658, 1614, 1533, 1442, 1346, 1265, 1172, 1091, 852, 748 cm^{-1}; ^{1}H NMR (DMSO-d$_6$) δ 2.39 (*s*, 3H), 2.70-2.83 (m, 3H), 2.97-3.06 (m, 1H), 3.66 (s, 3H), 6.29 (s, 1H), 6.74-6.77 (m, 2H), 7.11-7.15 (m, 5H), 7.18-7.21 (m, 1H), 7.25-7.29 (m, 2H), 9.77 (s, 1H); ^{13}C NMR (DMSO-d$_6$) δ 17.7, 27.3, 32.2, 51.6, 58.0, 60.4, 102.3, 108.8, 115.8 126.3, 128.2, 128.4, 130.6, 139.5, 140.7, 141.8, 158.1, 160.4, 163.9, 164.4. HRMS cald for $C_{23}H_{23}N_2O_3S$ (M+H) 407.1429; found 407.1414 (TOF MS ES$^+$).

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

Color less solid, R*f* 0.36; (hexanes: ethyl acetate, 1:1 v/v). Yield: 83%; m.p.: 148-150 ºC; IR: 3155, 3107, 2931, 2360, 1720, 1699, 1658, 1537, 1442, 1346, 1265, 1172, 1091, 852, 738 cm-1; ^{1}H NMR (DMSO-d$_6$) δ 2.39 (*s*, 3H), 2.64-2.74 (m, 2H), 2.79-2.85 (m, 1H), 3.00-3.09 (m, 1H), 3.66 (s, 3H), 3.86 (s, 3H), 6.45 (s, 1H), 7.00-7.02 (m, 1H), 7.11-7.13 (m, 3H), 7.20-7.21 (m, 1H), 7.24-7.28 (m, 2H), 7.422-7.46 (m, 1H), 7.72 (d, 1H), 10.59 (s, 1H); ^{13}C NMR (DMSO-d$_6$) δ 13.8, 18.1, 27.3, 32.2, 51.6, 52.6, 57.7, 60.5, 102.2, 108.6, 113.7, 118.7, 126.3, 128.1, 128.3, 128.9, 129.2, 130.9, 140.7, 159.8, 160.9, 163.8, 164.4, 168.0. HRMS cald for $C_{25}H_{25}N_2O_5S$ (M+H) 464.1484; found 465.1461(TOF MS ES$^+$).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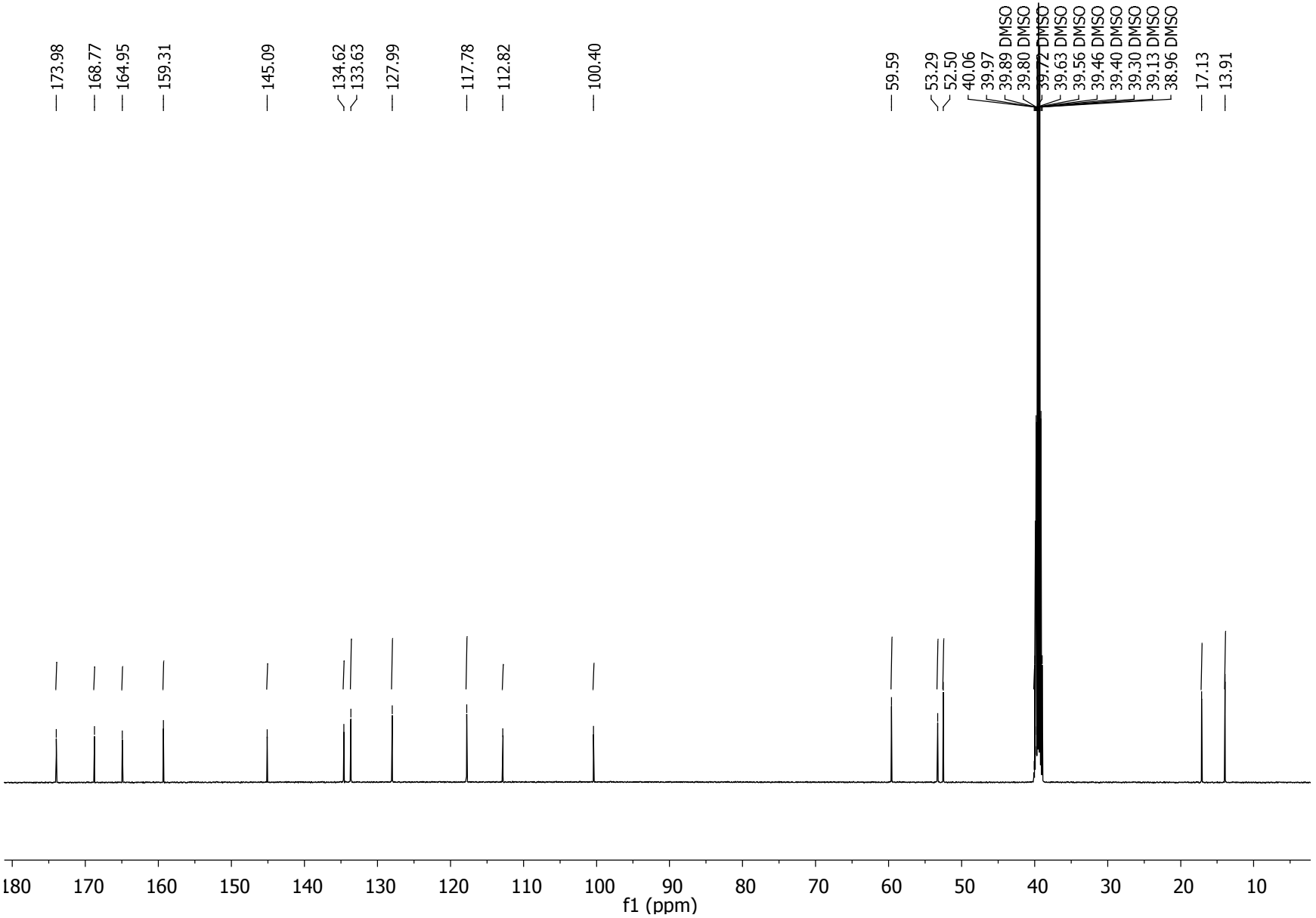
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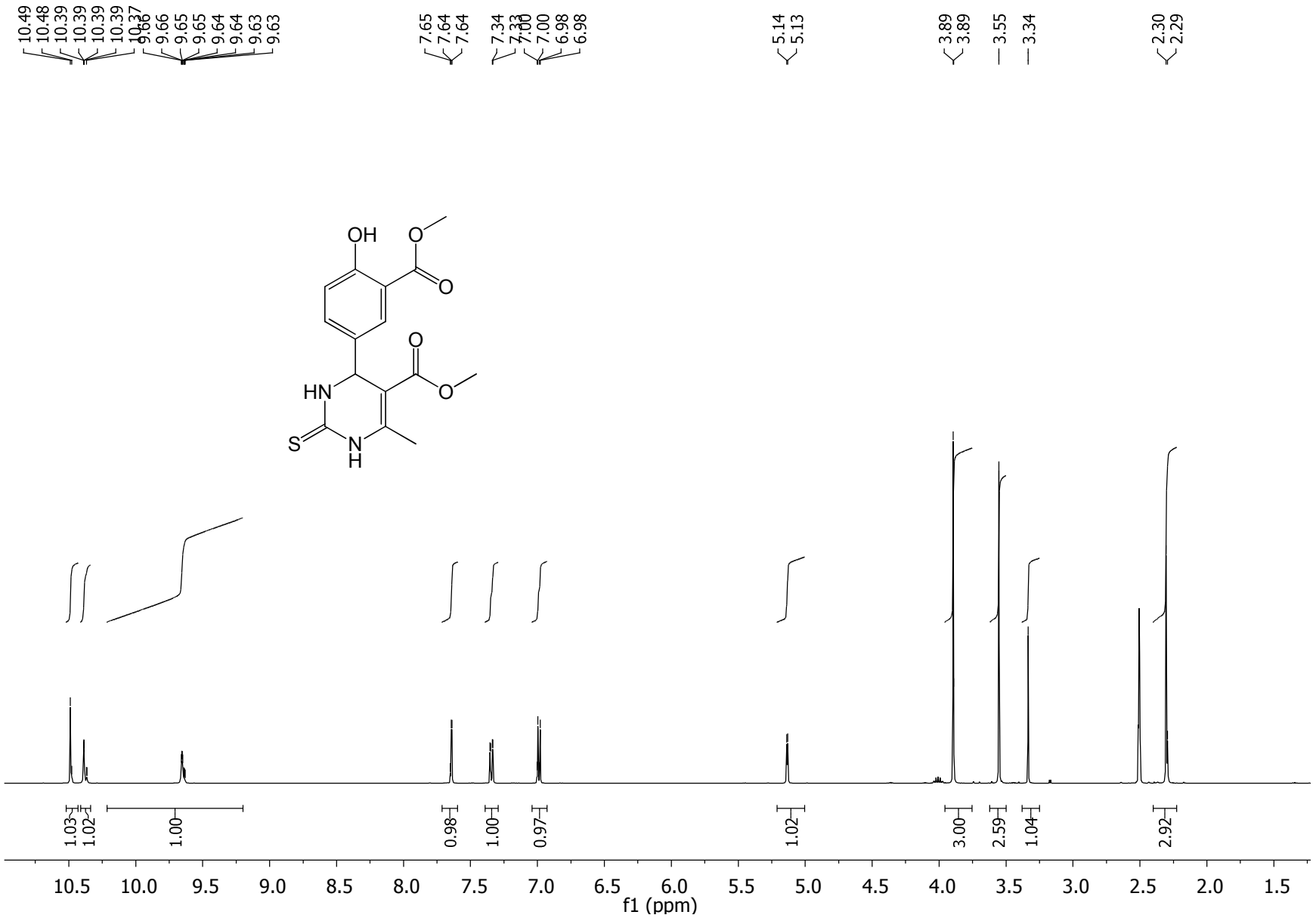
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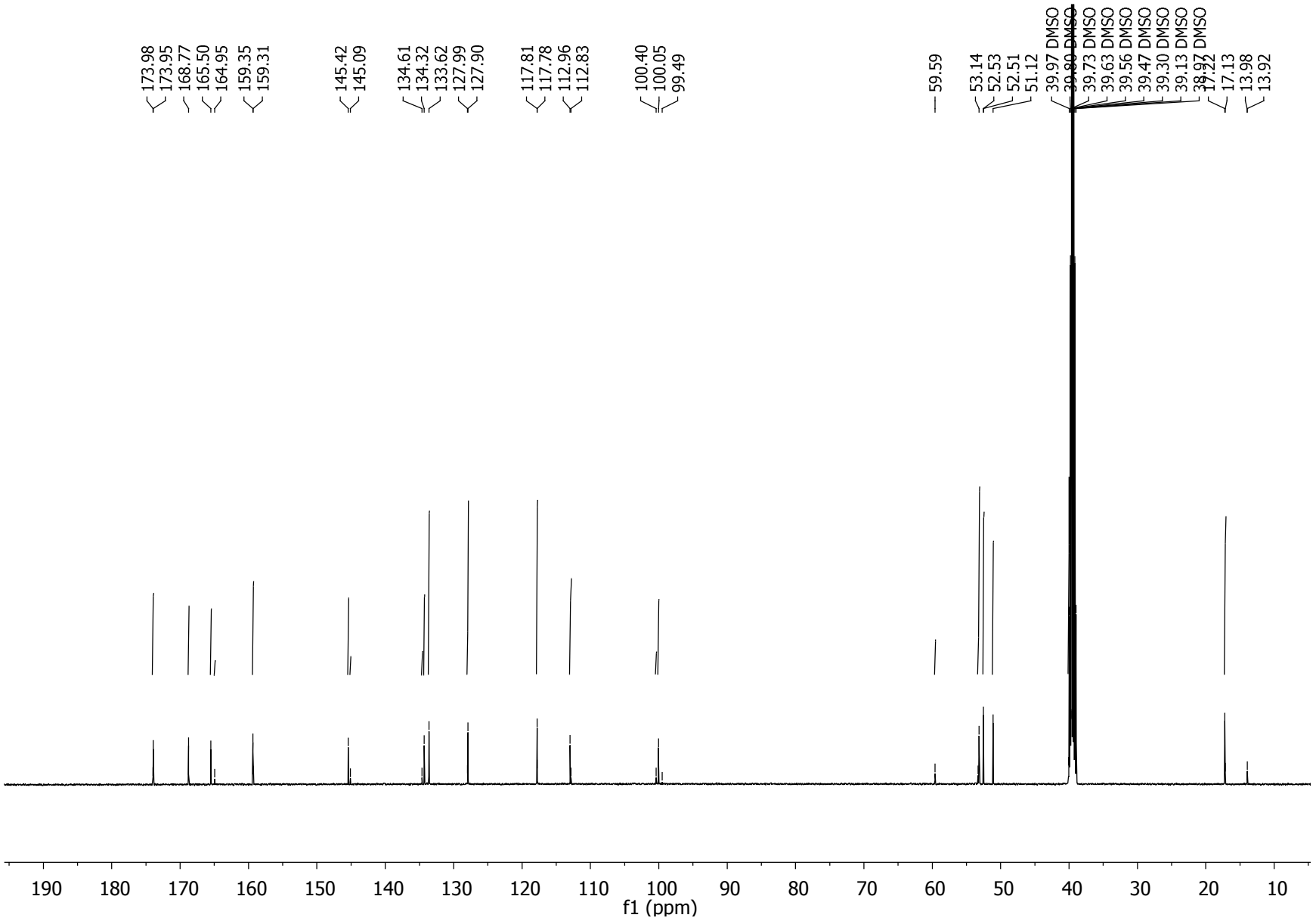
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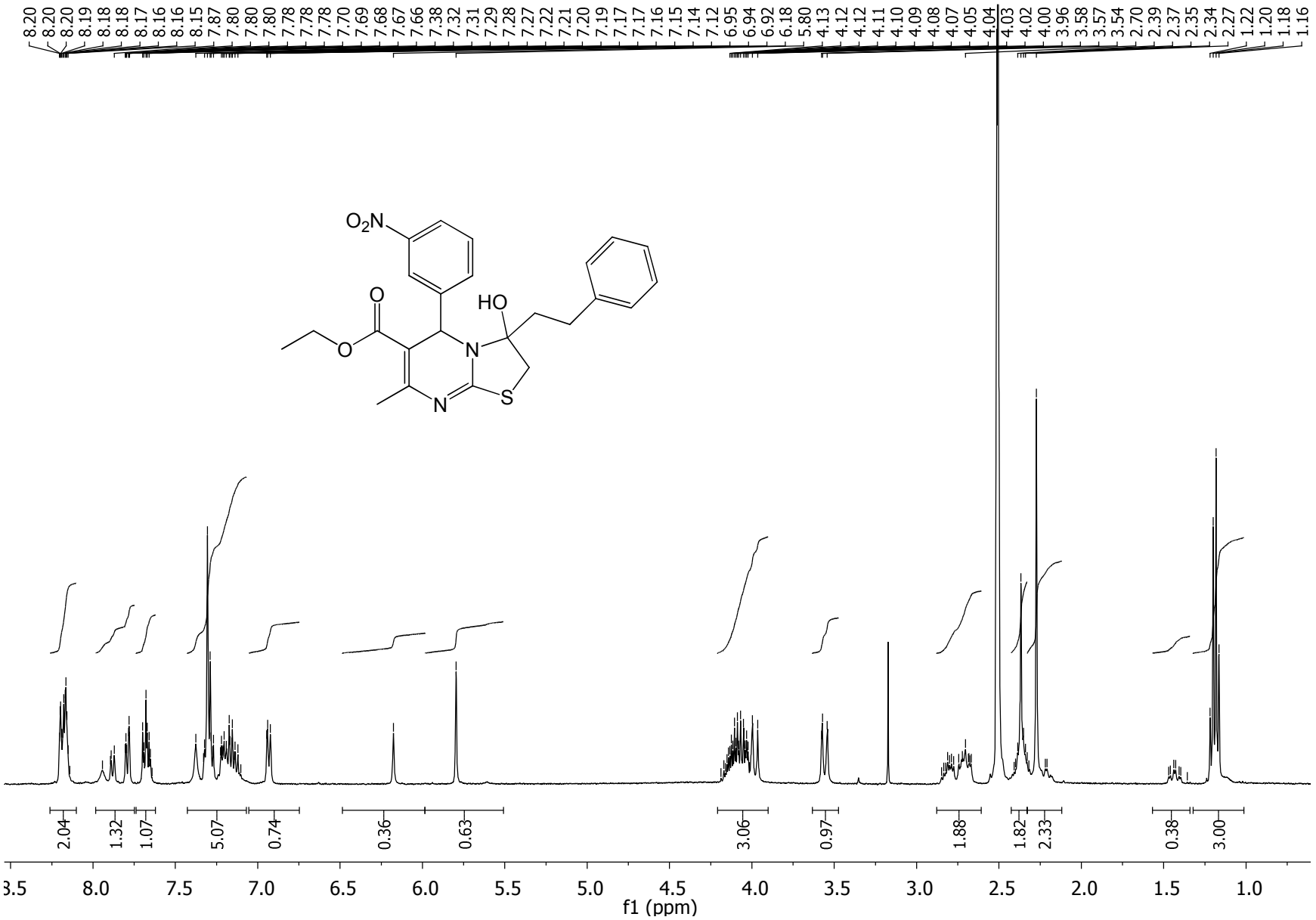
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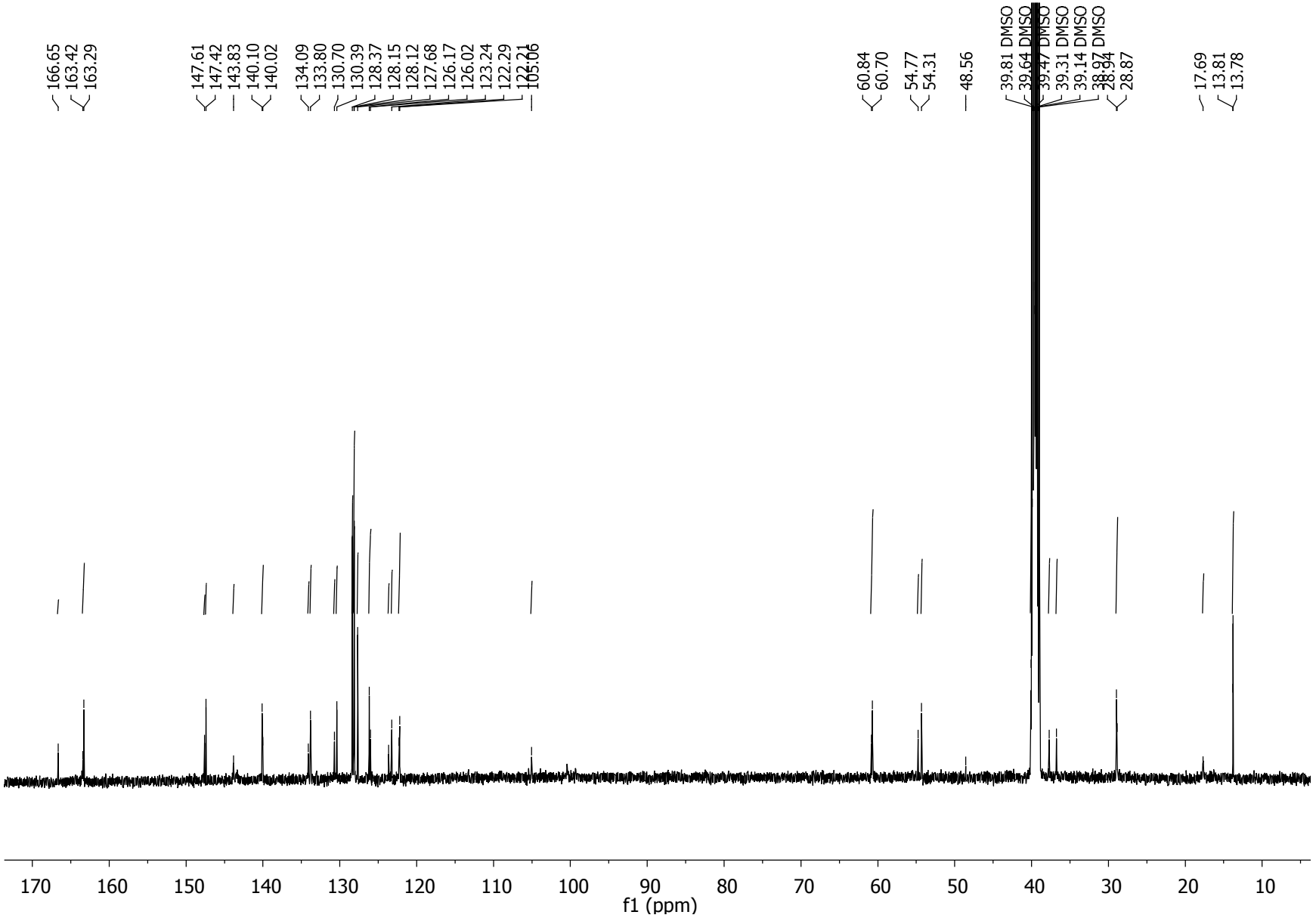
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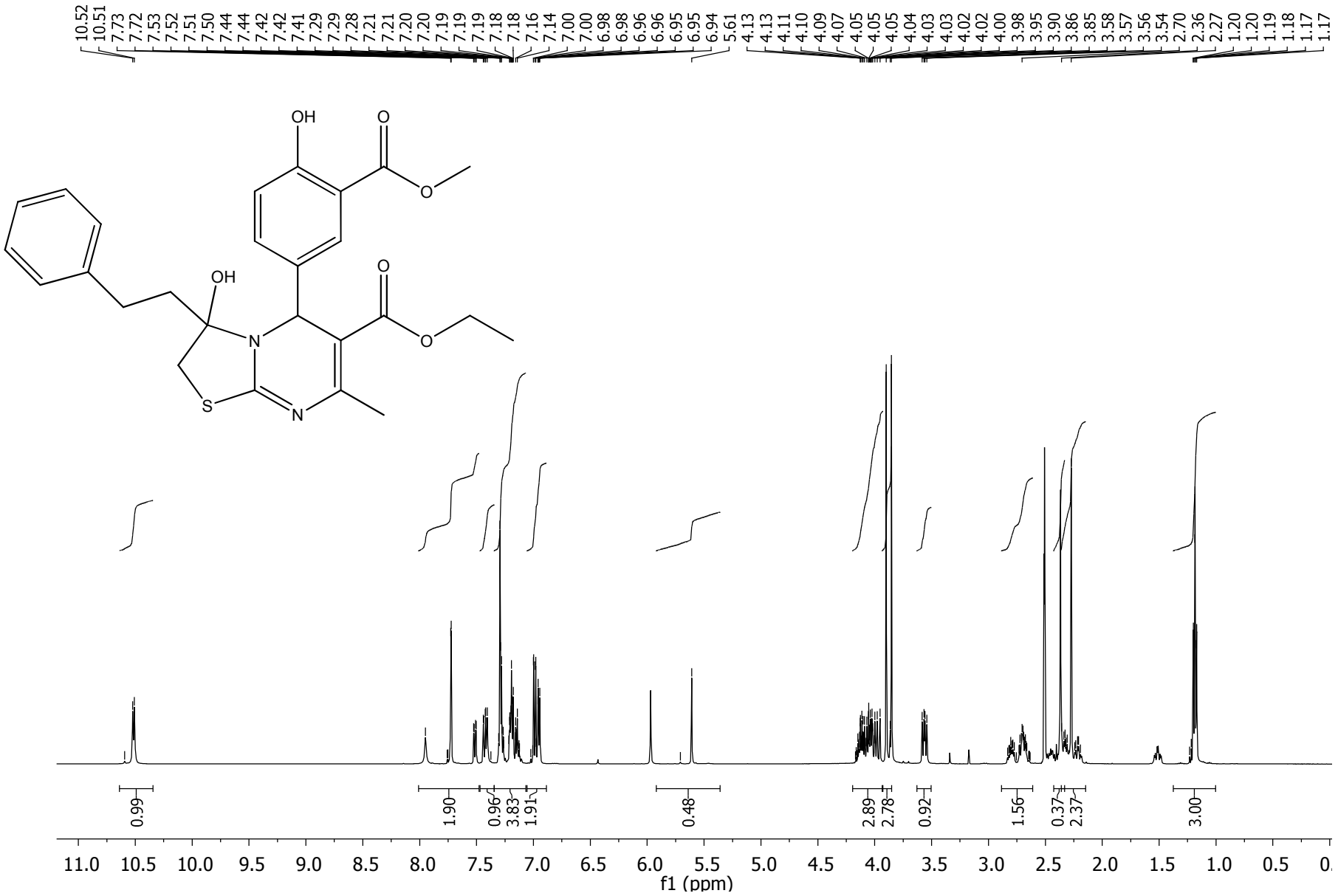
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6.98
6.96
6.96
6.95
6.95
6.94
5.61
4.13
4.13
4.11
4.10
4.09
4.07
4.05
4.05
4.05
4.04
4.03
4.03
4.02
4.02
4.00
3.98
3.95
3.90
3.86
3.85
3.58
3.57
3.56
3.54
2.70
2.36
2.27
1.20
1.20
1.19
1.18
1.17
1.17
OH
O
O
OH
O
O
N
S
N
0.99
1.90
0.96
3.83
1.91
0.48
2.89
2.78
0.92
1.56
0.37
2.37
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
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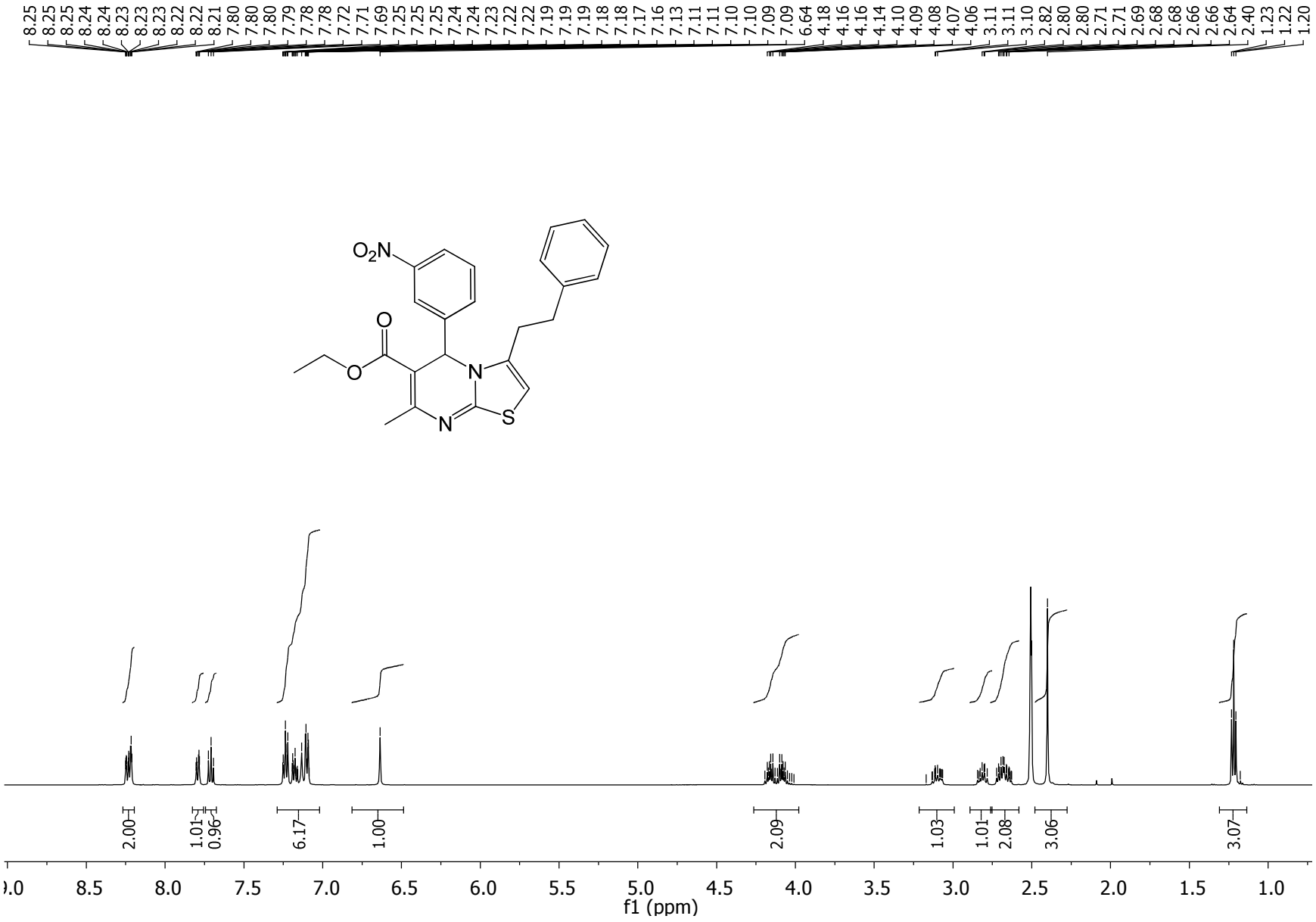
0.5
f1 (ppm)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O2N
O
O
N
N
S
2.00
1.01
0.96
6.17
1.00
2.09
1.03
1.01
2.08
3.06
3.07
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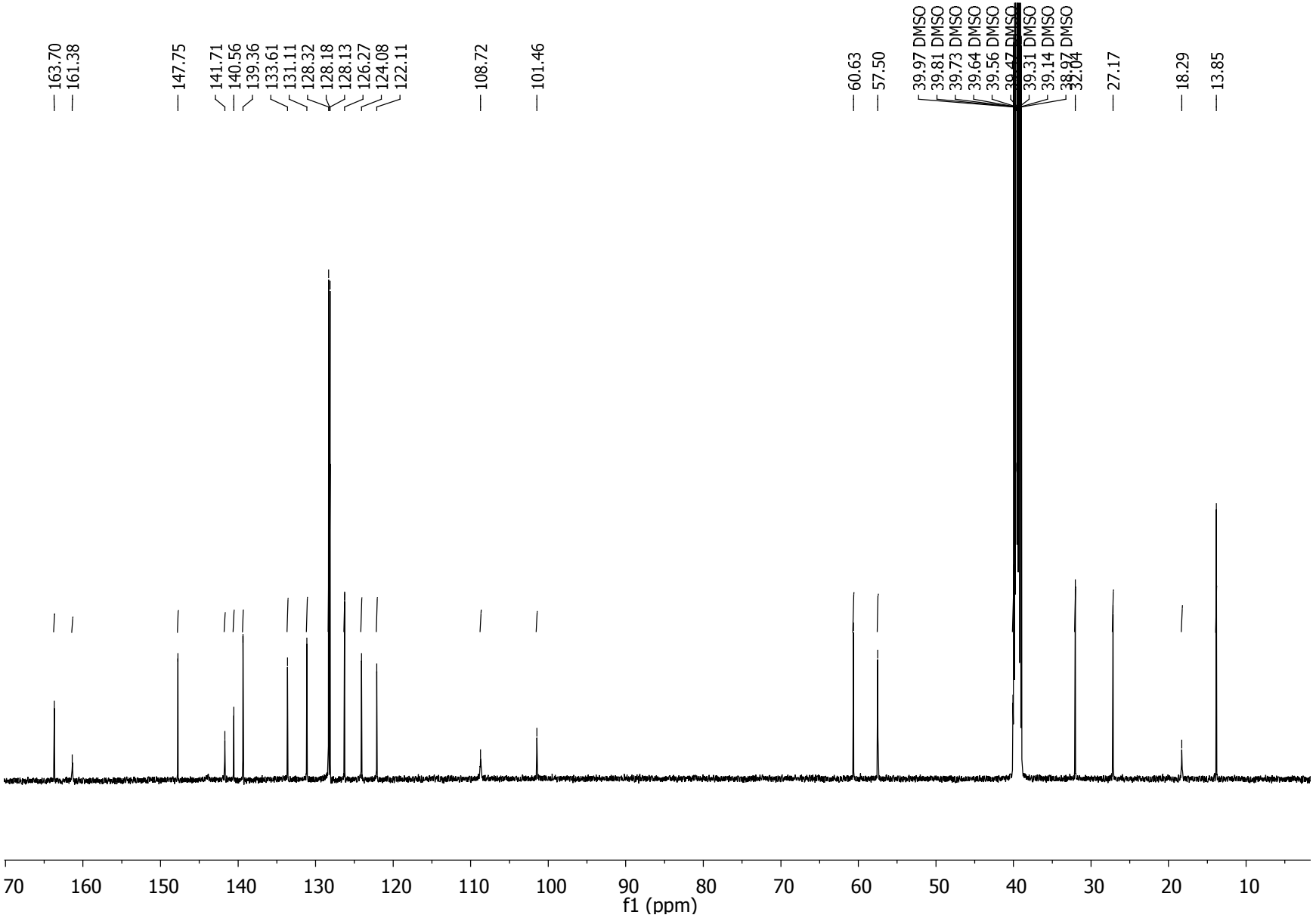
f1 (ppm)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128.32
128.18
128.13
126.27
124.08
122.11
108.72
101.46
60.63
57.50
39.97 DMSO
39.81 DMSO
39.73 DMSO
39.64 DMSO
39.56 DMSO
39.47 DMSO
39.31 DMSO
39.14 DMSO
38.97 DMSO
32.04
27.17
18.29
13.85
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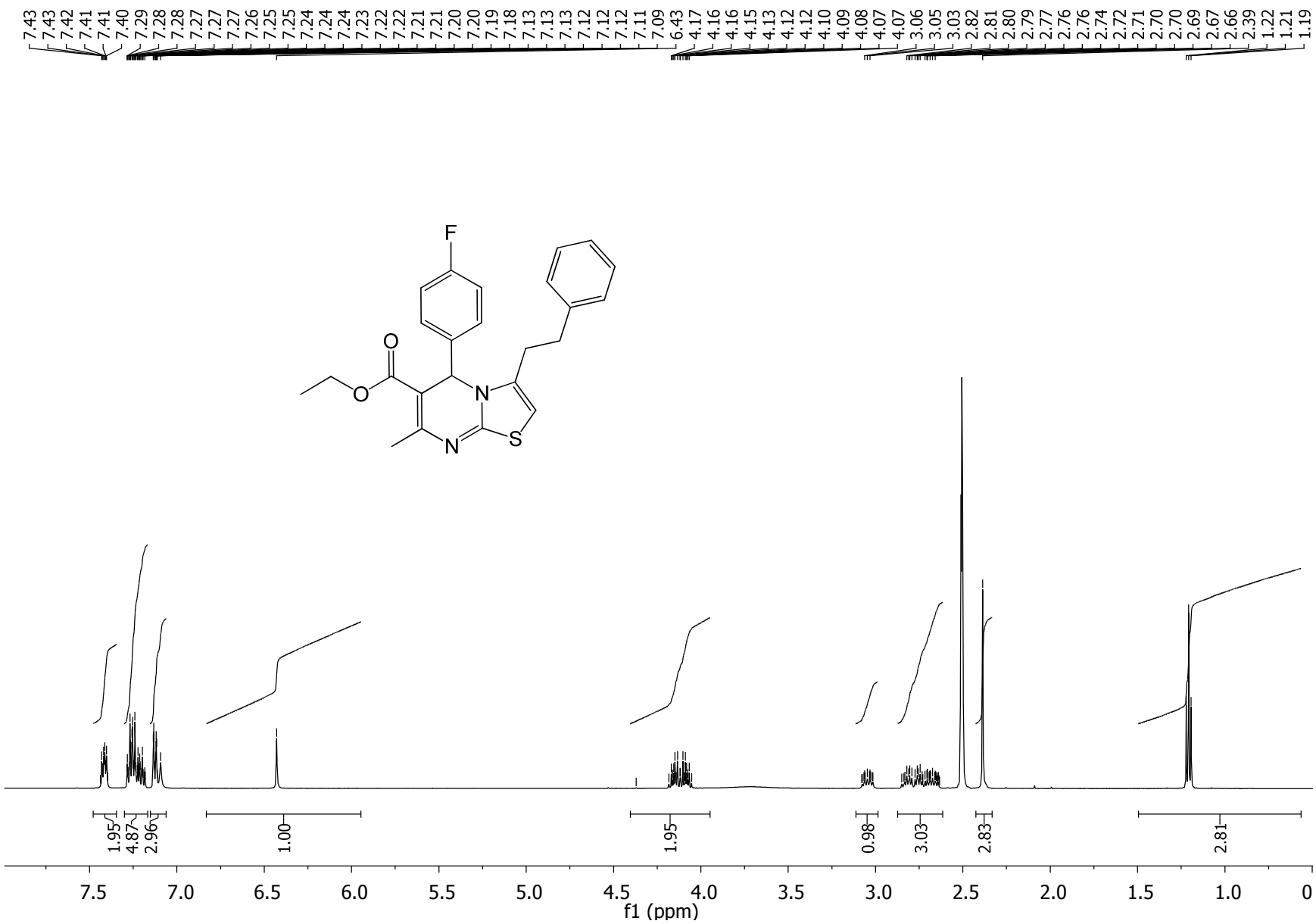
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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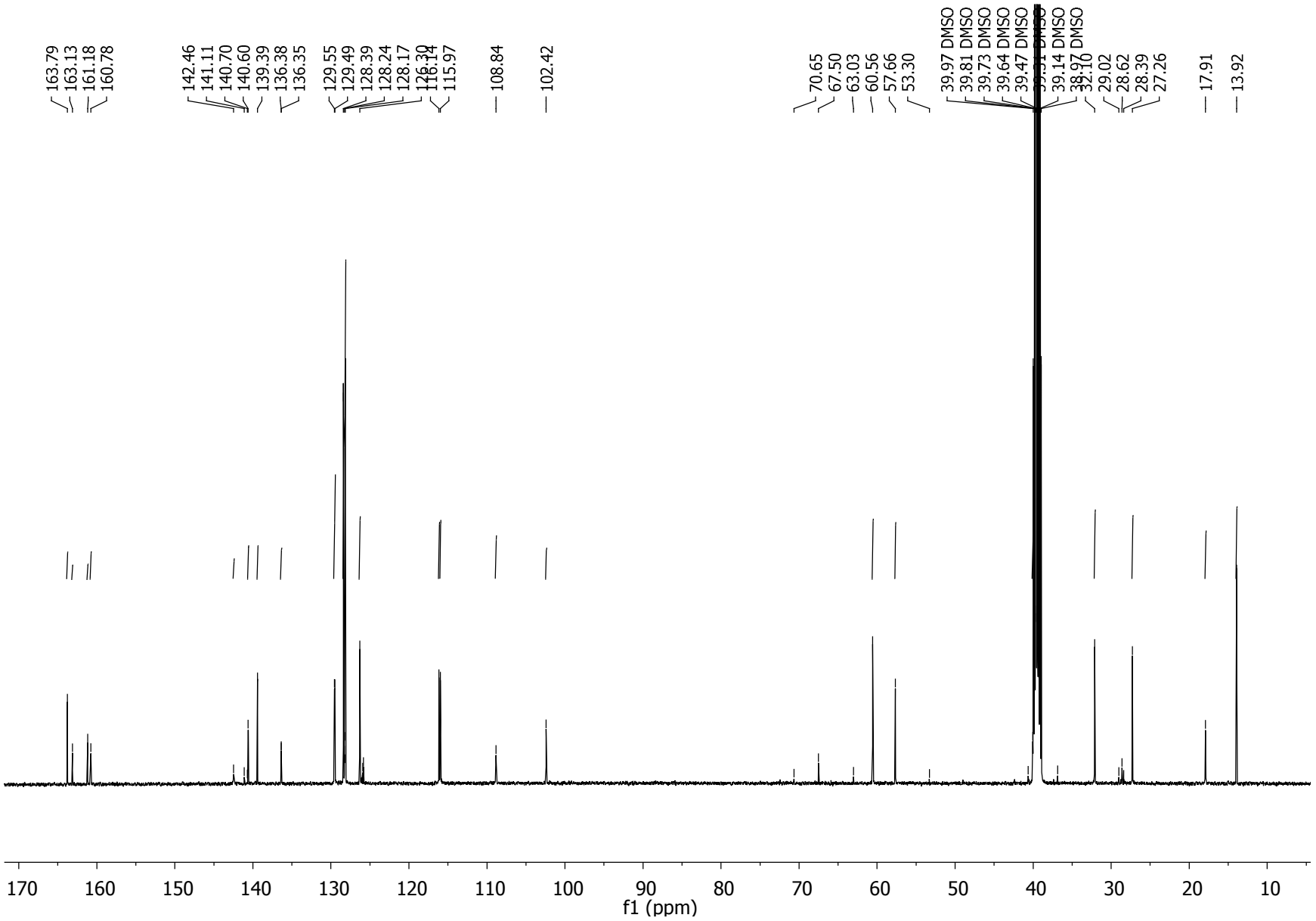
F
O
O
N
N
S
1.95
4.87
2.96
1.00
1.95
0.98
3.03
2.83
2.81
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0
f1 (ppm)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129.55
129.49
128.39
128.24
128.17
116.14
115.97
108.84
102.42
70.65
67.50
63.03
60.56
57.66
53.30
39.97 DMSO
39.81 DMSO
39.73 DMSO
39.64 DMSO
39.47 DMSO
39.14 DMSO
38.97 DMSO
32.10
29.02
28.62
28.39
27.26
17.91
13.92
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140
130
120
110
100
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80
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60
50
40
30
20
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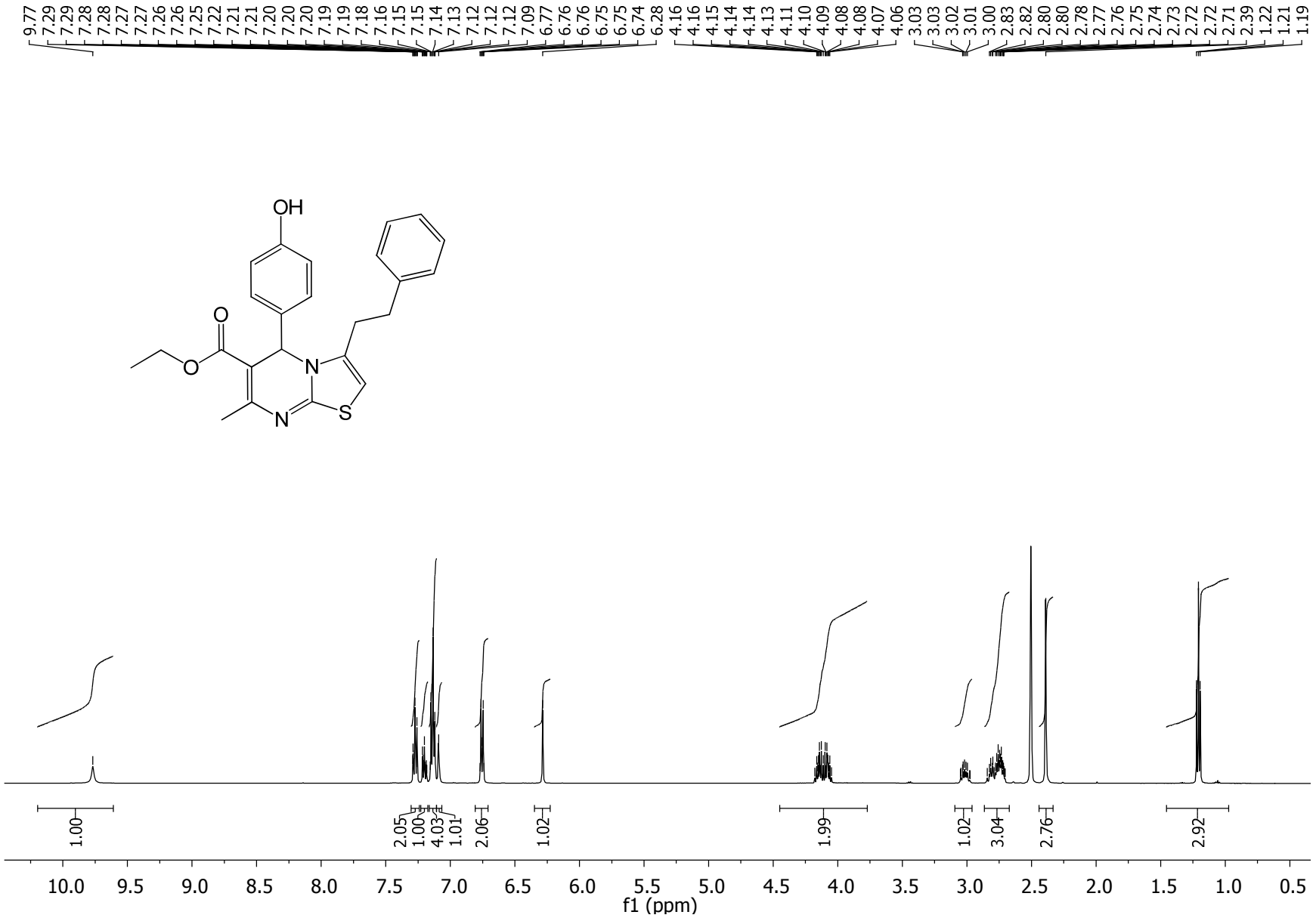
f1 (ppm)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7.27
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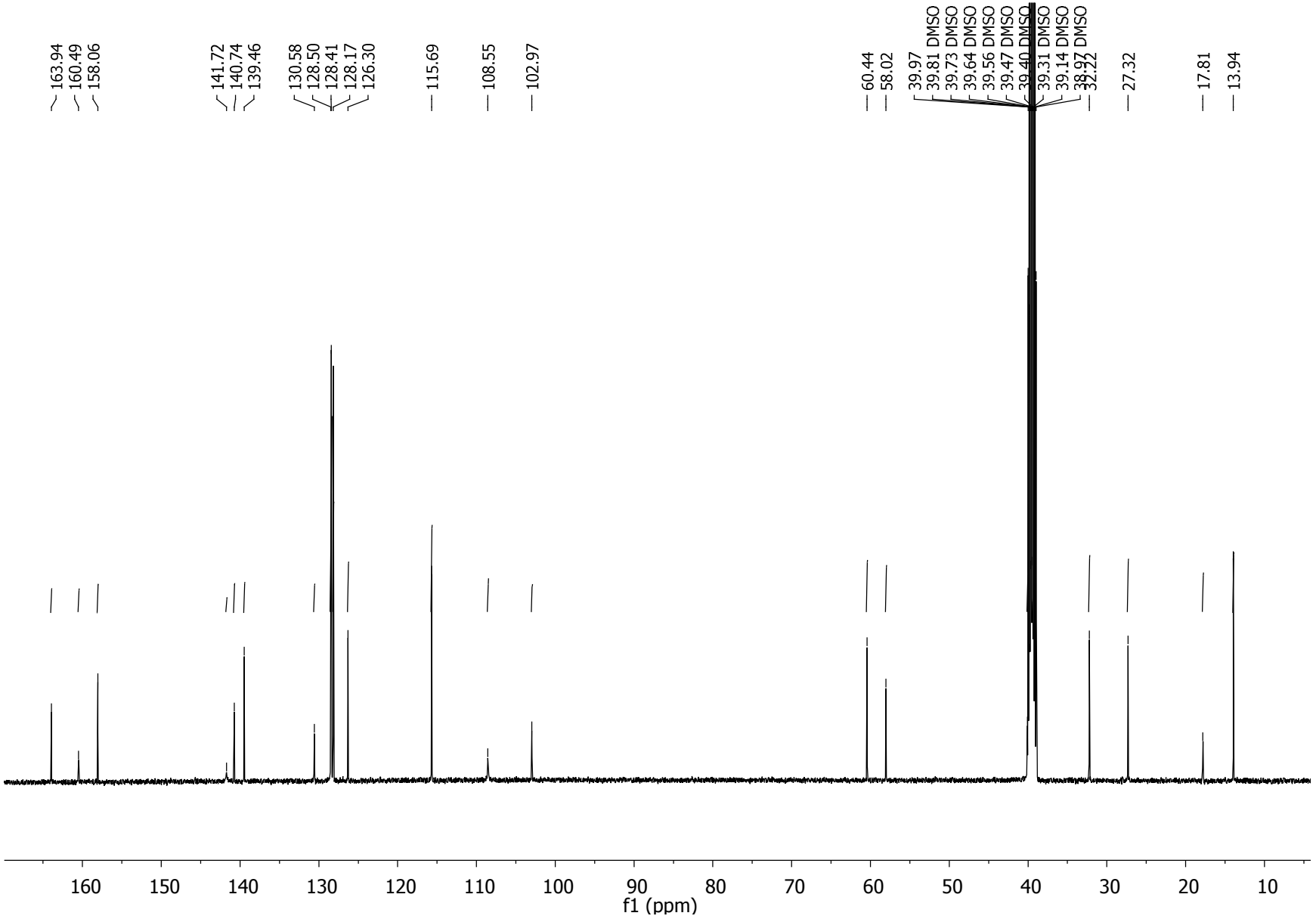
7.21
7.21
7.20
7.20
7.20
7.19
7.19
7.18
7.16
7.15
7.15
7.14
7.13
7.12
7.12
7.12
7.09
6.77
6.76
6.76
6.75
6.75
6.74
6.28
4.16
4.16
4.15
4.14
4.14
4.13
4.11
4.10
4.09
4.08
4.08
4.07
4.06
3.03
3.03
3.02
3.01
3.00
2.83
2.82
2.80
2.80
2.78
2.77
2.76
2.75
2.74
2.73
2.72
2.72
2.71
2.39
1.22
1.21
1.19
OH
O
O
N
N
S
1.00
2.05
1.00
4.03
1.01
2.06
1.02
1.99
1.02
3.04
2.76
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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139.46
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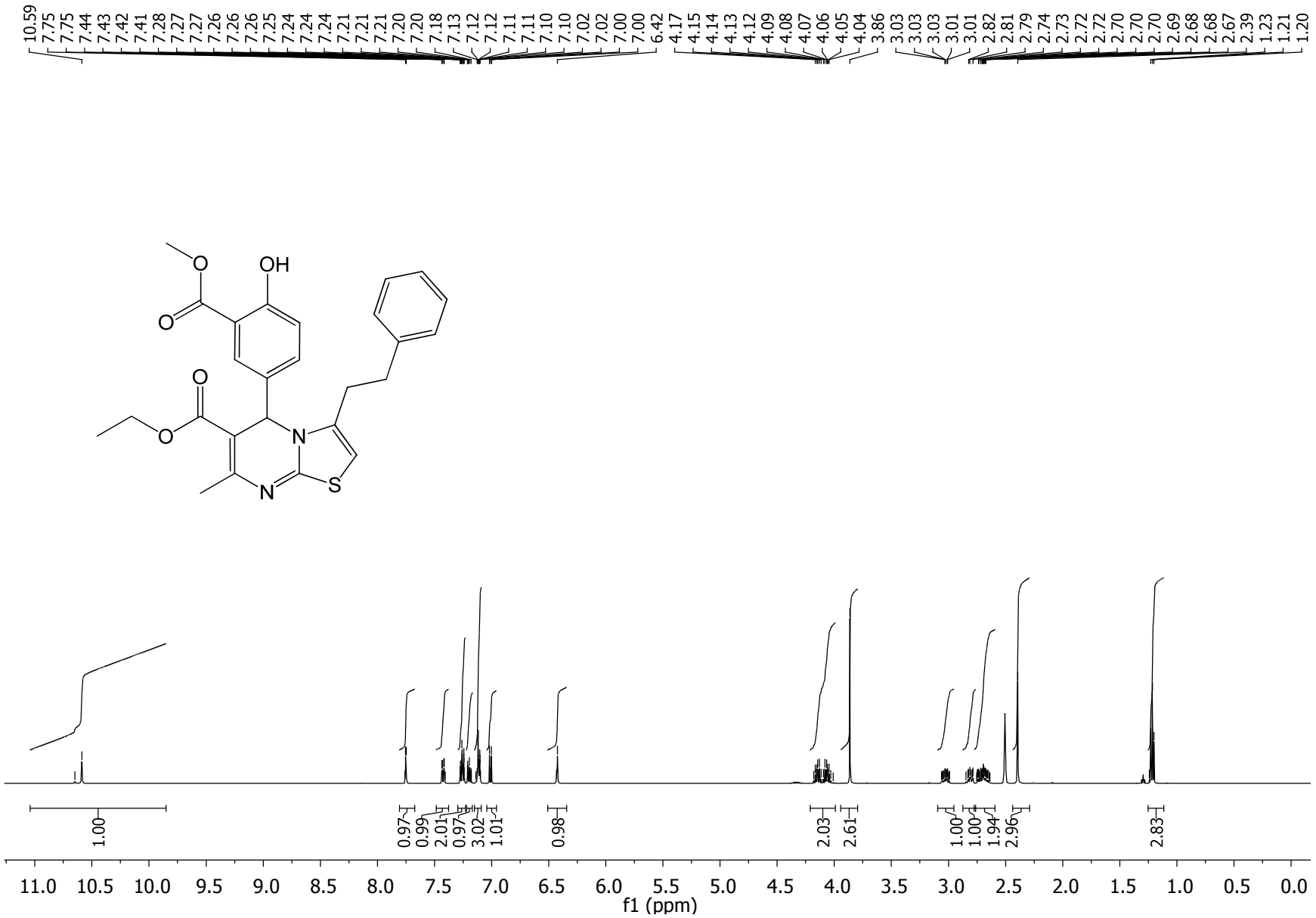
128.41
128.17
126.30
115.69
108.55
102.97
60.44
58.02
39.97
39.81 DMSO
39.73 DMSO
39.64 DMSO
39.56 DMSO
39.47 DMSO
39.40 DMSO
39.31 DMSO
39.14 DMSO
38.97 DMSO
32.22
27.32
17.81
13.94
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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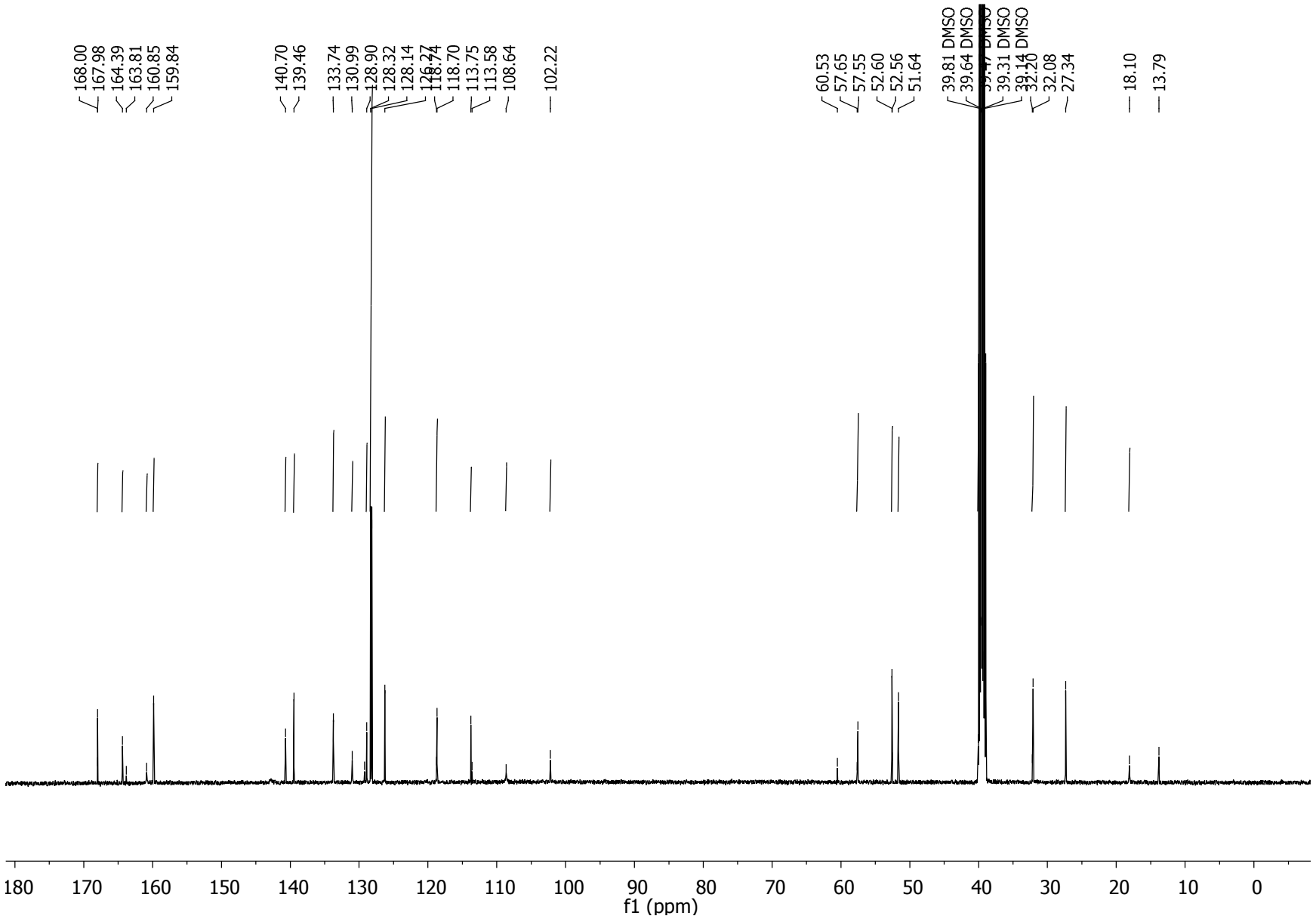
7.27
7.26
7.26
7.26
7.25
7.24
7.24
7.24
7.21
7.21
7.21
7.20
7.20
7.18
7.13
7.12
7.12
7.11
7.11
7.10
7.10
7.02
7.02
7.00
7.00
6.42
4.17
4.15
4.14
4.13
4.12
4.09
4.08
4.07
4.06
4.05
4.04
3.86
3.03
3.03
3.03
3.01
3.01
2.82
2.81
2.79
2.74
2.73
2.72
2.72
2.70
2.70
2.70
2.69
2.68
2.68
2.67
2.39
1.23
1.21
1.20
O
OH
O
O
O
N
N
S
1.00
0.97
0.99
2.01
0.97
3.02
1.01
0.98
2.03
2.61
1.00
1.00
1.94
2.96
2.83
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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139.46
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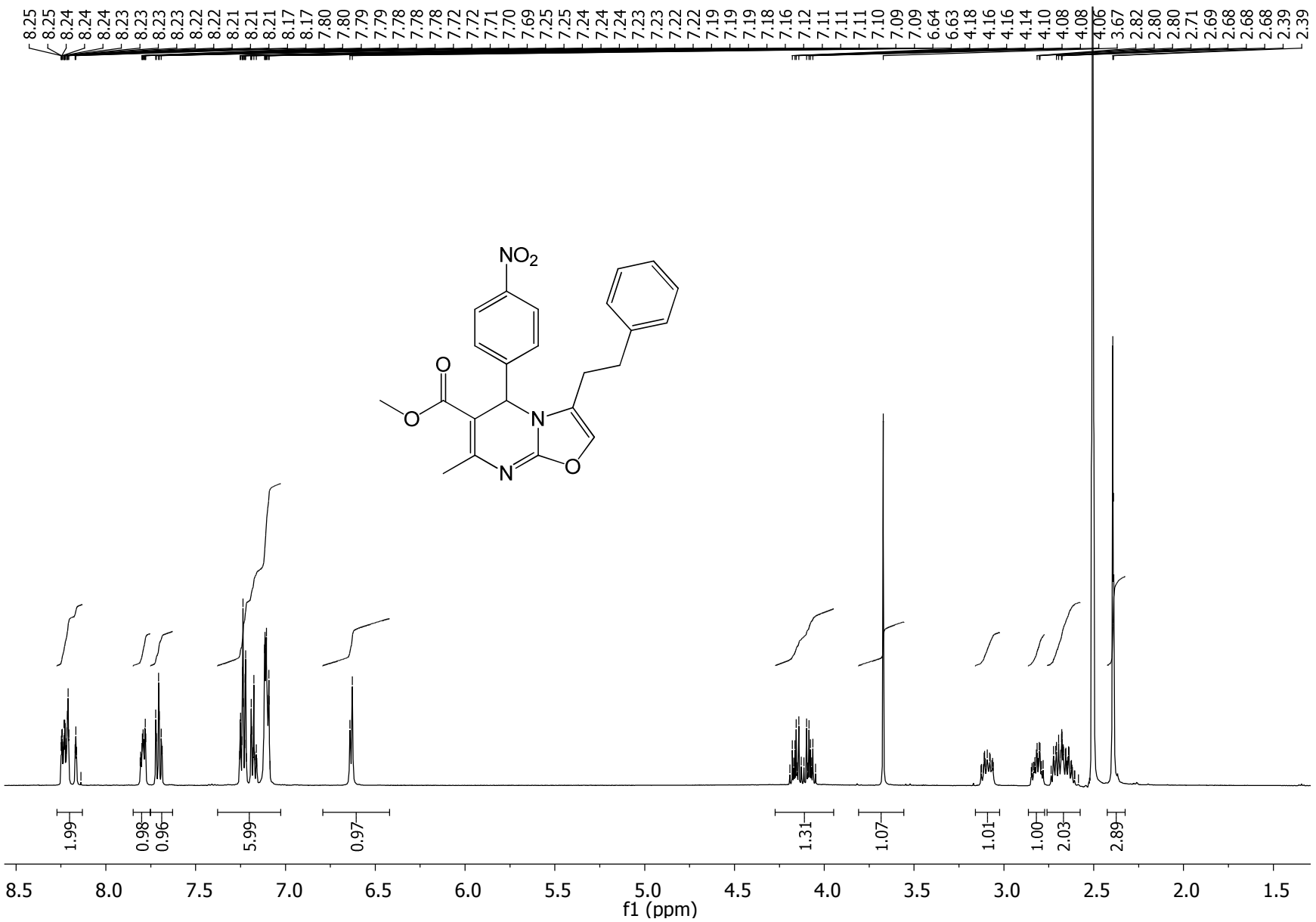
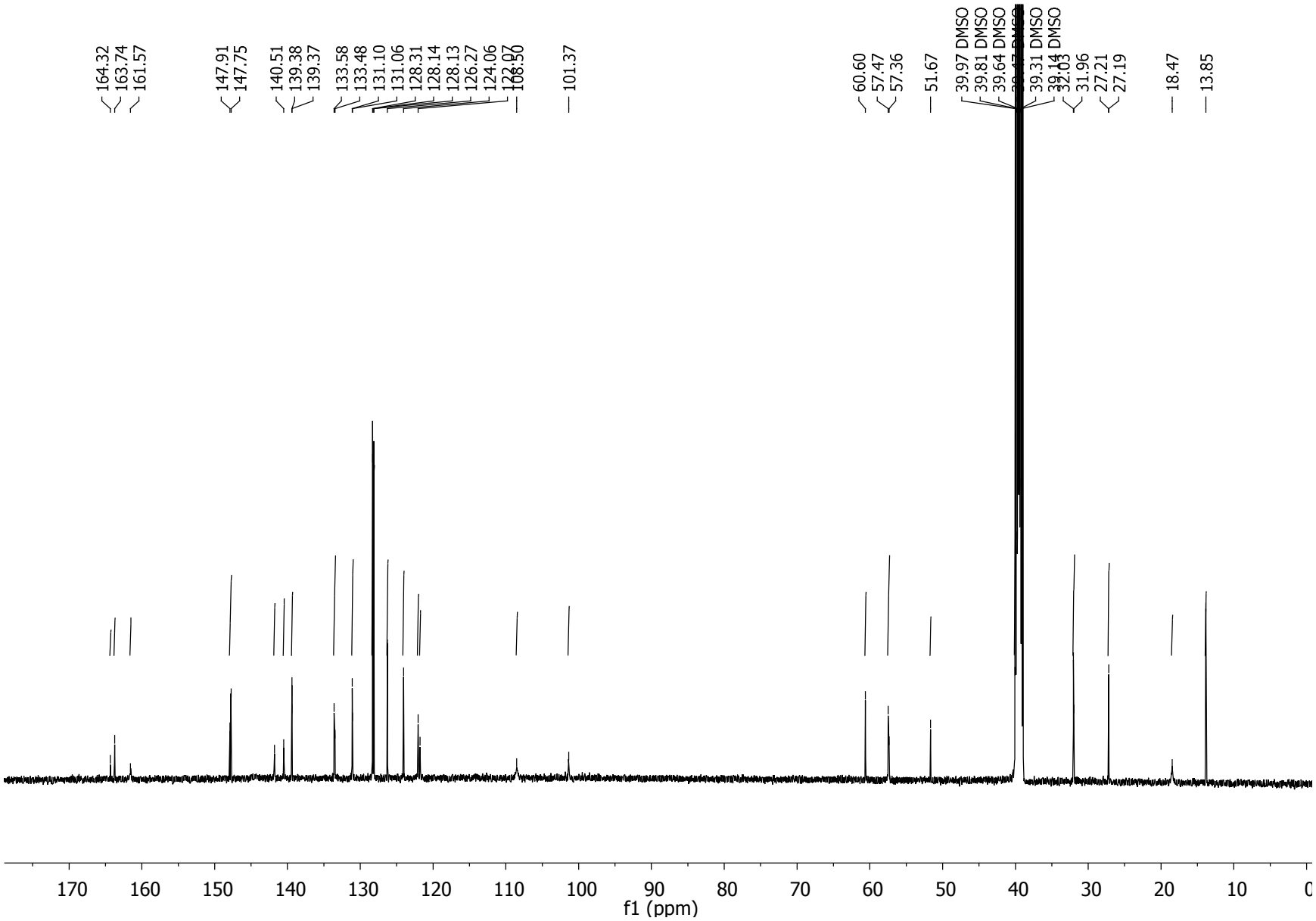
130.99
128.90
128.32
128.14
118.70
113.75
113.58
108.64
102.22
60.53
57.65
57.55
52.60
52.56
51.64
39.81 DMSO
39.64 DMSO
39.31 DMSO
39.14 DMSO
32.20
32.08
27.34
18.10
13.79
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.25 8.25 8.24 8.24 8.24 8.23 8.23 8.23 8.22 8.22 8.21 8.21 8.21 8.17 7.80 7.80 7.79 7.79 7.78 7.78 7.78 7.72 7.72 7.71 7.70 7.69 7.25 7.25 7.24 7.24 7.24 7.23 7.23 7.22 7.22 7.19 7.19 7.19 7.18 7.16 7.12 7.11 7.11 7.11 7.10 7.09 7.09 6.64 6.63 4.18 4.16 4.16 4.14 4.10 4.08 4.08 4.06 3.67 2.82 2.80 2.80 2.71 2.69 2.68 2.68 2.68 2.39 2.39
NO2
O
O
N
N
O
1.99
0.98
0.96
5.99
0.97
1.31
1.07
1.01
1.00
2.03
2.89
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)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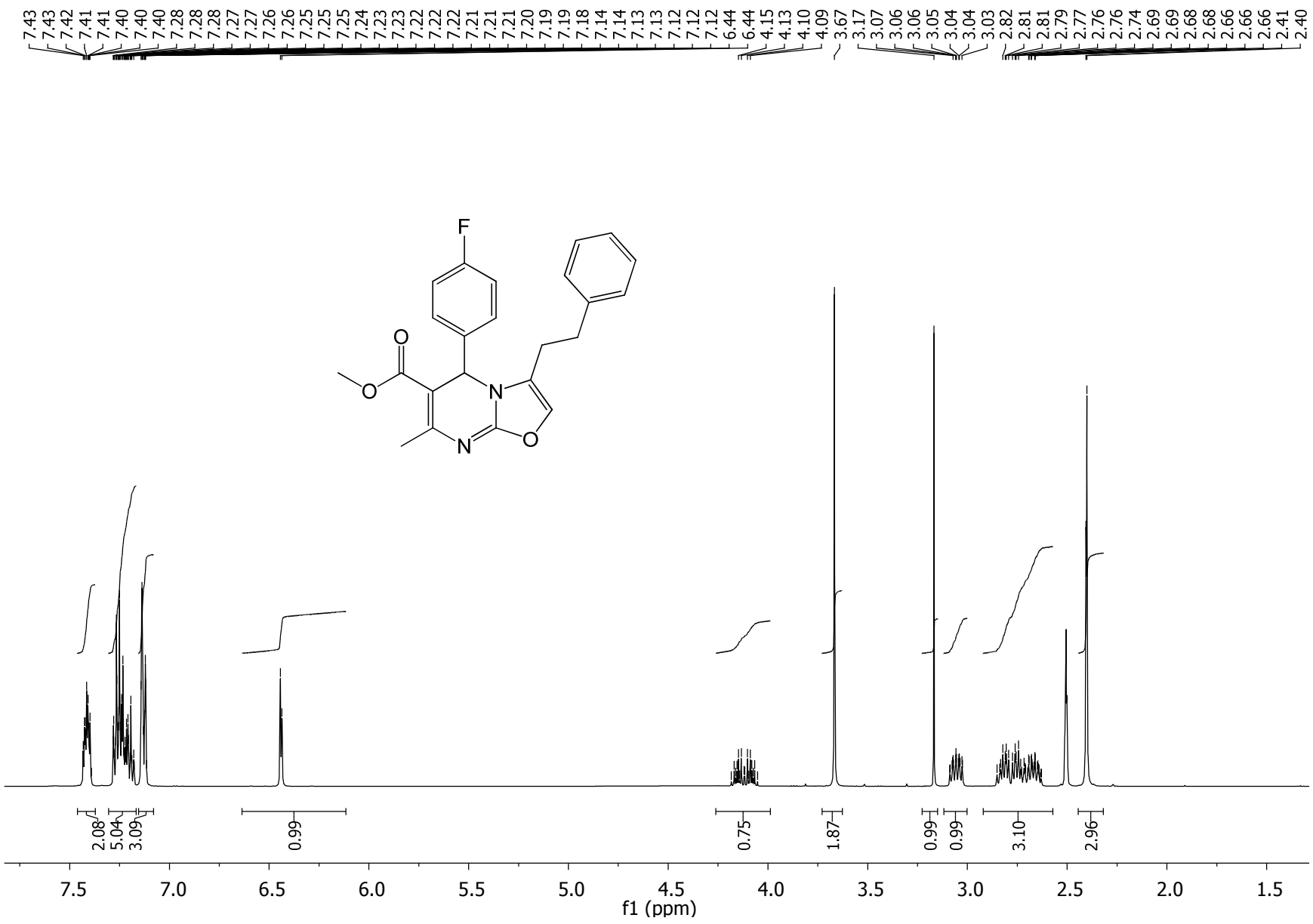
131.06
128.31
128.14
128.13
126.27
124.06
101.37
60.60
57.47
57.36
51.67
39.97 DMSO
39.81 DMSO
39.64 DMSO
39.31 DMSO
39.14 DMSO
32.03
31.96
27.21
27.19
18.47
13.85
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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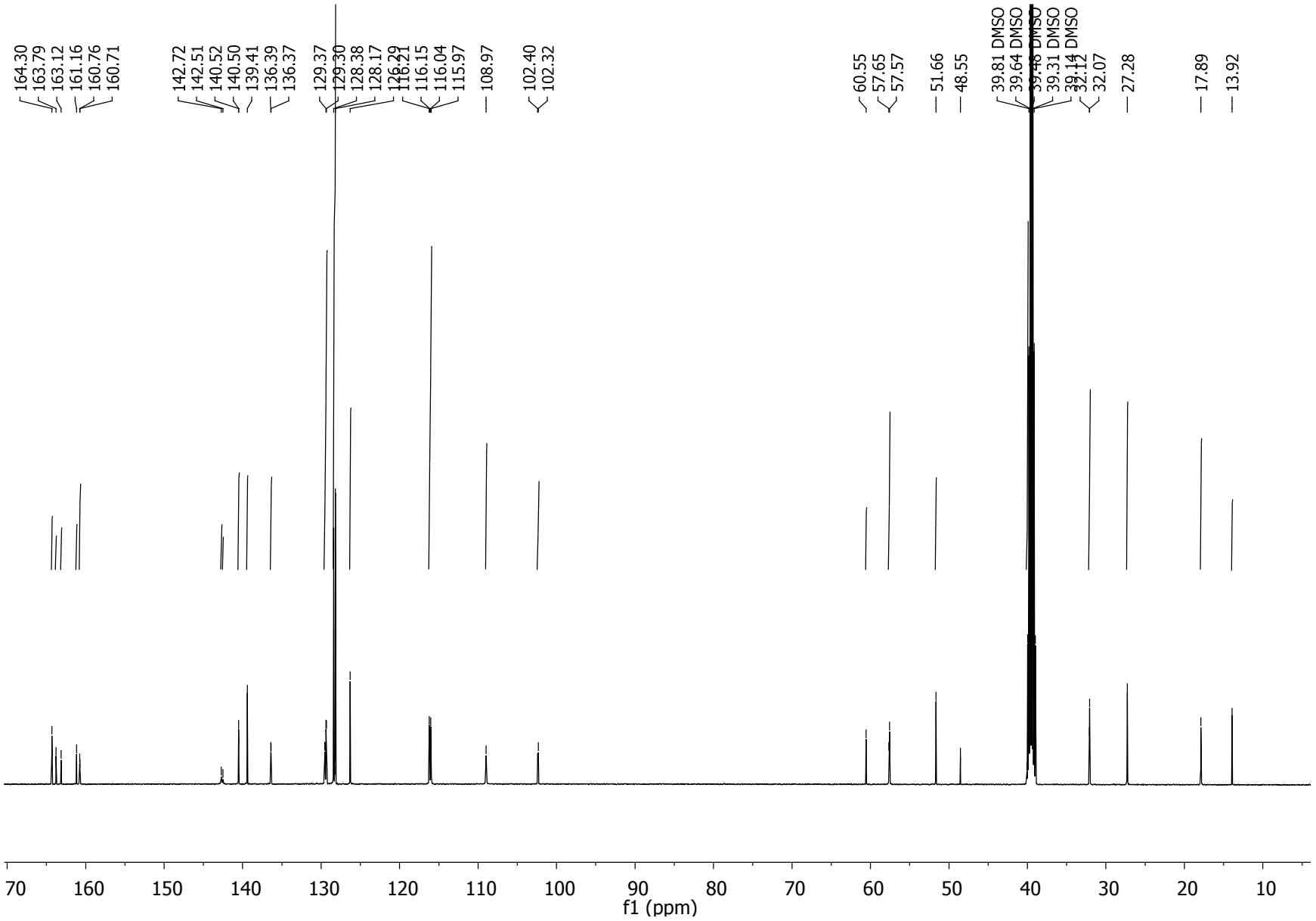
F
O
O
N
N
O
2.08
5.04
3.09
0.99
0.75
1.87
0.99
0.99
3.10
2.96
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)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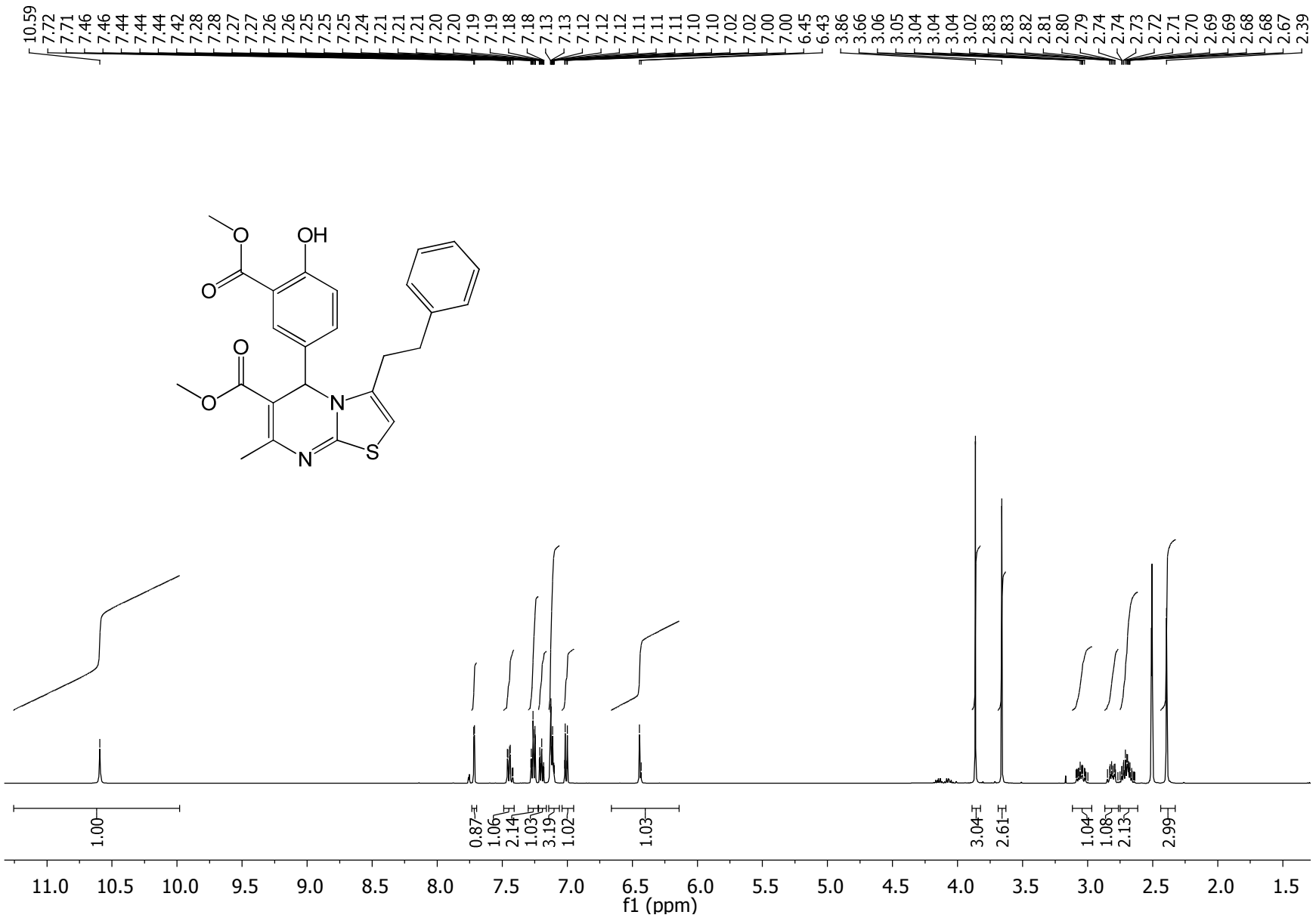
140.50
139.41
136.39
136.37
129.37
129.30
128.38
128.17
116.29
116.21
116.15
116.04
115.97
108.97
102.40
102.32
60.55
57.65
57.57
51.66
48.55
39.81 DMSO
39.64 DMSO
39.48 DMSO
39.31 DMSO
39.14 DMSO
32.12
32.07
27.28
17.89
13.92
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.27
7.27
7.26
7.26
7.25
7.25
7.25
7.24
7.21
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.13
7.13
7.12
7.12
7.12
7.11
7.11
7.11
7.10
7.10
7.02
7.02
7.00
7.00
6.45
6.43
3.86
3.66
3.06
3.05
3.04
3.04
3.04
3.02
2.83
2.83
2.82
2.81
2.80
2.79
2.74
2.74
2.73
2.72
2.71
2.70
2.69
2.69
2.68
2.68
2.67
2.39
O
OH
O
O
O
N
N
S
1.00
0.87
1.06
2.14
1.03
3.19
1.02
1.03
3.04
2.61
1.04
1.08
2.13
2.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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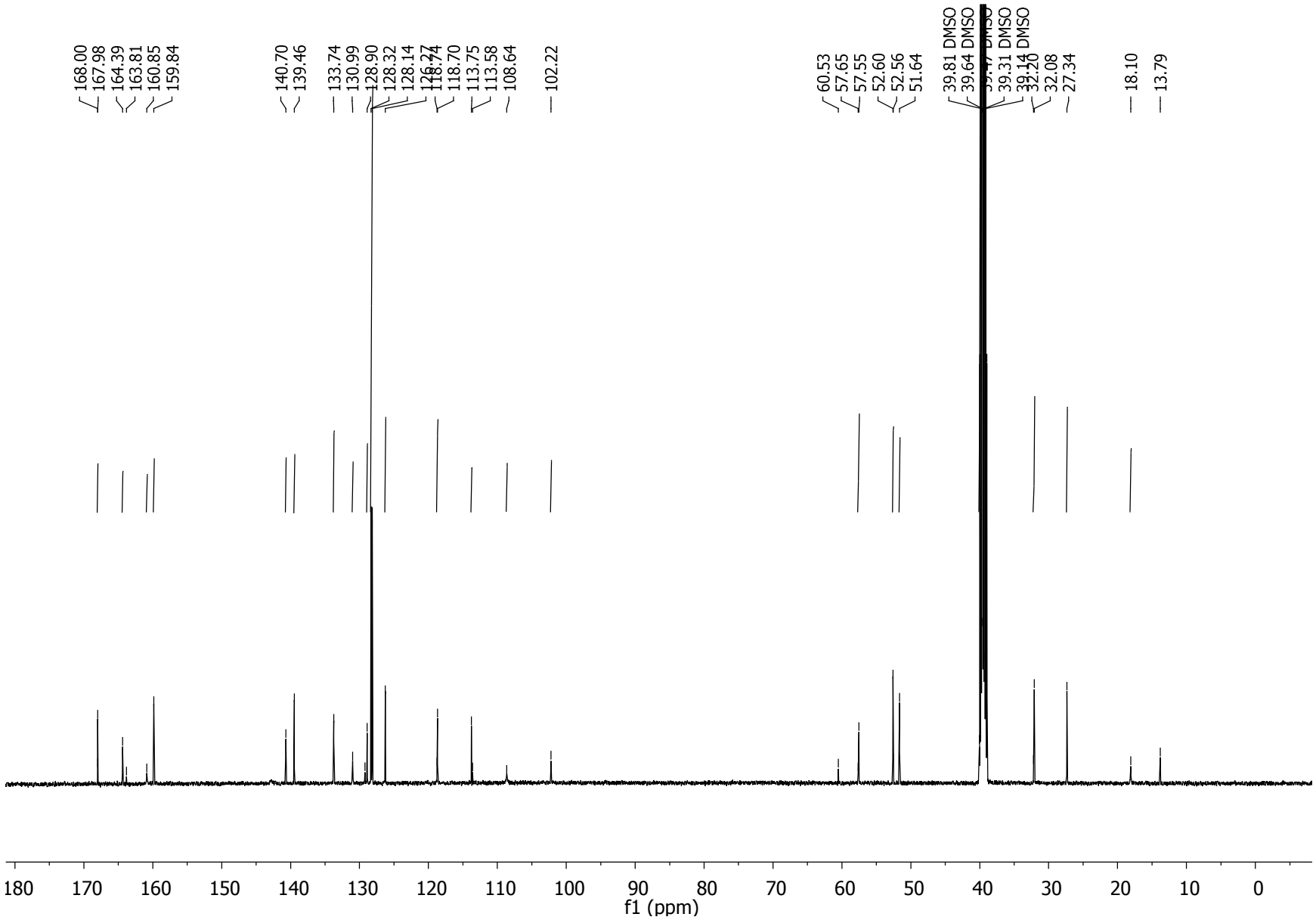
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)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133.74
130.99
128.90
128.32
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118.70
113.75
113.58
108.64
102.22
60.53
57.65
57.55
52.60
52.56
51.64
39.81 DMSO
39.64 DMSO
39.31 DMSO
39.14 DMSO
32.20
32.08
27.34
18.10
13.79
180
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150
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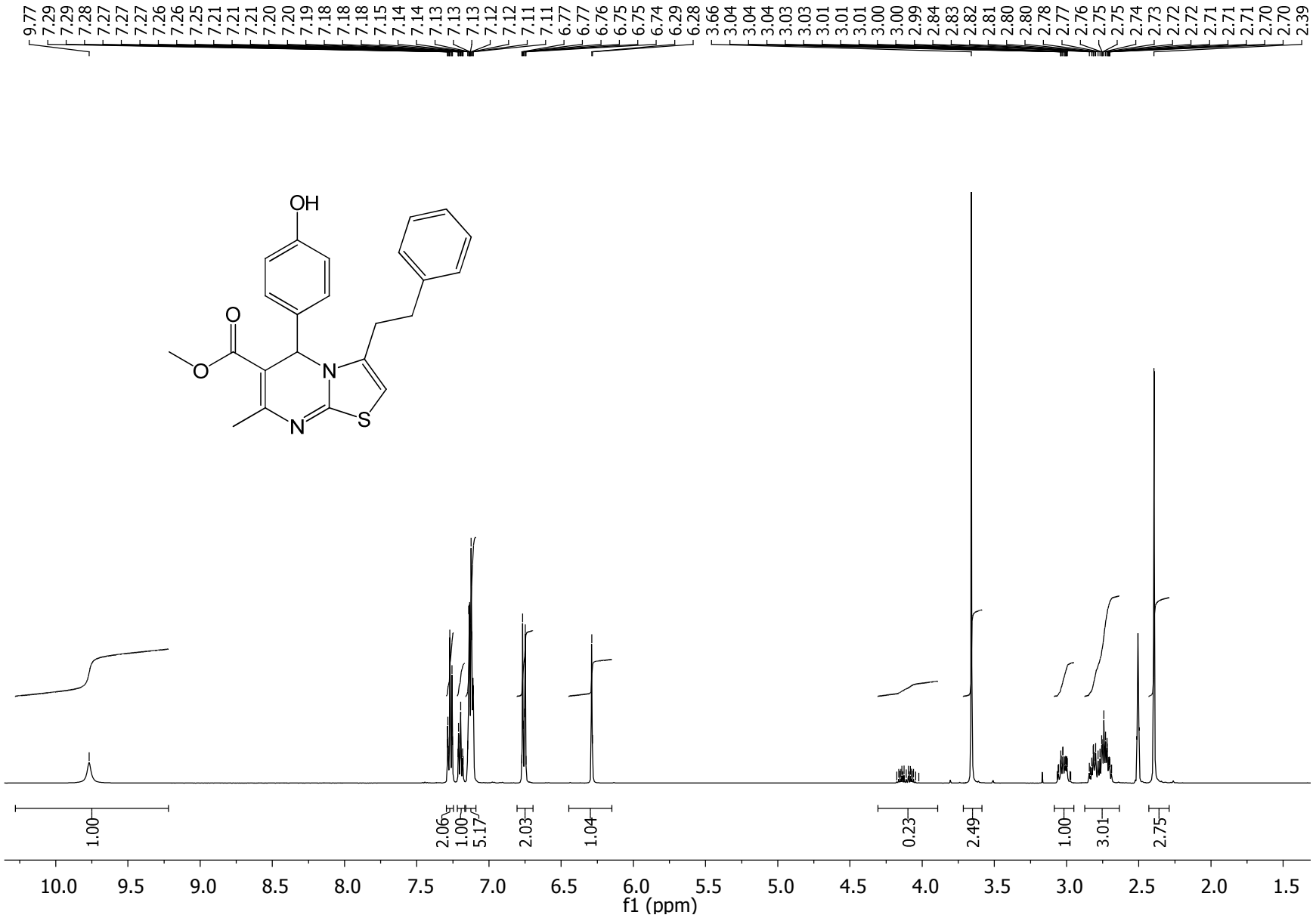
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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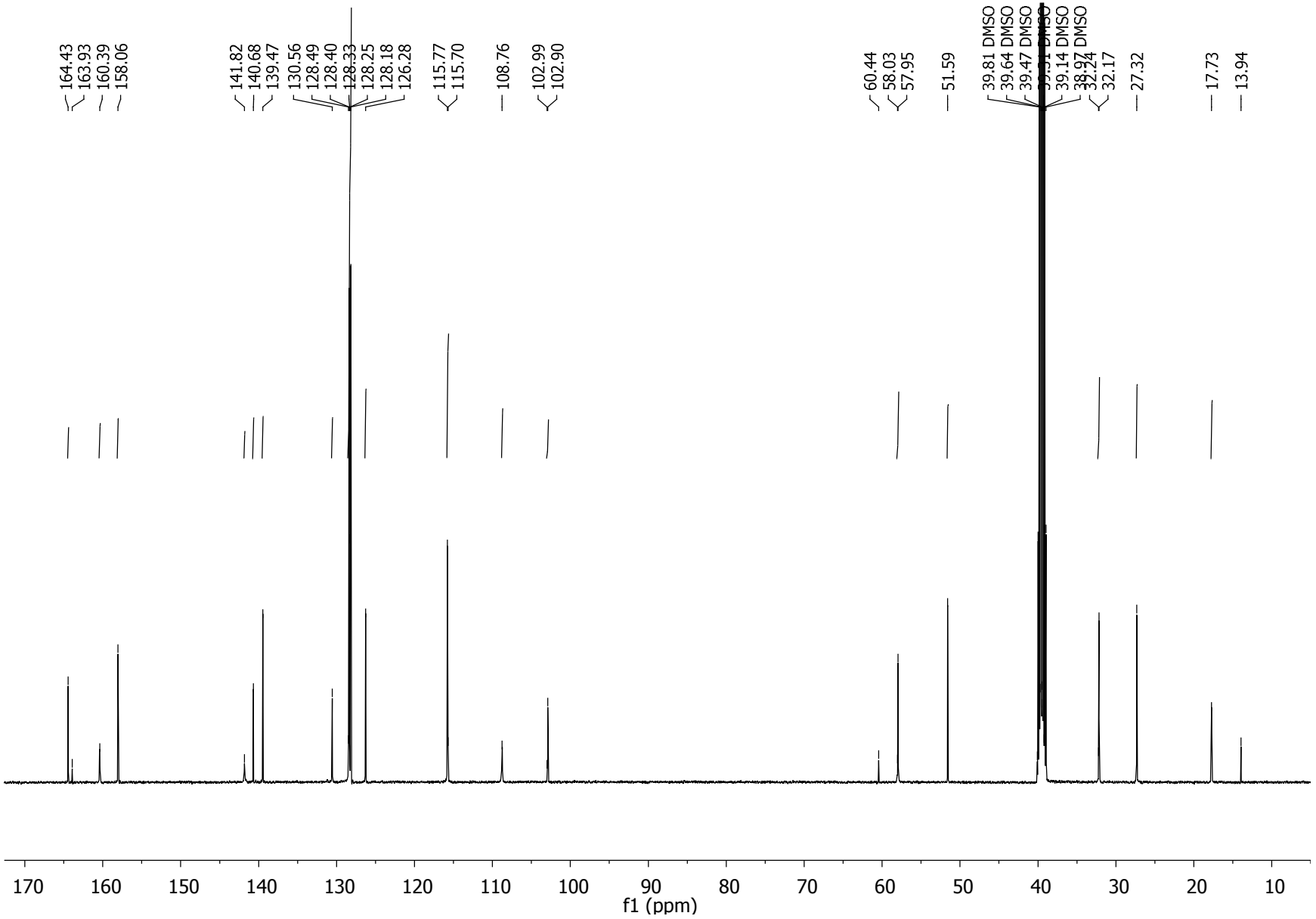
3.66 3.04 3.04 3.04 3.03 3.03 3.01 3.01 3.01 3.00 3.00 2.99 2.84 2.83 2.82 2.81 2.80 2.80 2.78 2.77 2.76 2.75 2.75 2.74 2.73 2.72 2.72 2.71 2.71 2.71 2.70 2.70 2.39
OH
O
O
N
N
S
1.00
2.06
1.00
5.17
2.03
1.04
0.23
2.49
1.00
3.01
2.75
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)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128.33
128.25
128.18
126.28
115.77
115.70
108.76
102.99
102.90
60.44
58.03
57.95
51.59
39.81 DMSO
39.64 DMSO
39.47 DMSO
39.14 DMSO
32.24
32.17
27.32
17.73
13.94
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Compound 6a

Table S-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $[C_{24}H_{26}N_3O_5S][Br]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S	-282(1)	3821(1)	709(1)	20(1)
O(1)	4494(1)	1682(1)	674(1)	21(1)
O(2)	4308(1)	2090(1)	-842(1)	28(1)
O(3)	7681(1)	5074(1)	1436(1)	32(1)
O(4)	7340(1)	3564(1)	1484(1)	33(1)
O(5)	1332(1)	2373(1)	2263(1)	21(1)
N(1)	1153(1)	3397(1)	-441(1)	20(1)
N(2)	1882(1)	3399(1)	1156(1)	16(1)
N(3)	7020(1)	4397(1)	1426(1)	23(1)
C(1)	1029(1)	3527(1)	438(1)	17(1)
C(2)	2100(1)	2892(1)	-642(1)	19(1)

C(3)	2989(1)	2710(1)	58(1)	17(1)
C(4)	3053(1)	3137(1)	1028(1)	16(1)
C(5)	1529(1)	3332(1)	2089(1)	17(1)
C(6)	372(1)	3860(1)	1945(1)	19(1)
C(7)	2429(1)	3792(1)	2854(1)	18(1)
C(8)	2036(2)	3748(2)	3795(1)	33(1)
C(9)	2864(1)	4194(1)	4598(1)	21(1)
C(10)	3080(2)	5163(1)	4638(1)	28(1)
C(11)	3832(2)	5551(2)	5400(2)	34(1)
C(12)	4352(2)	4982(2)	6132(1)	35(1)
C(13)	4140(2)	4011(2)	6099(1)	33(1)
C(14)	3409(2)	3624(1)	5334(1)	26(1)
C(15)	1946(2)	2568(1)	-1637(1)	24(1)
C(16)	3982(1)	2133(1)	-105(1)	19(1)
C(17)	5573(2)	1198(1)	619(1)	26(1)
C(18)	5892(2)	555(2)	1440(1)	28(1)
C(19)	3858(1)	3999(1)	1136(1)	16(1)

C(20)	5040(1)	3830(1)	1297(1)	17(1)
C(21)	5778(1)	4598(1)	1313(1)	19(1)
C(22)	5401(2)	5529(1)	1217(1)	21(1)
C(23)	4221(2)	5689(1)	1079(1)	22(1)
C(24)	3456(1)	4931(1)	1024(1)	19(1)
Br	-1252(1)	3642(1)	-1883(1)	22(1)

Table S-2. Bond lengths [Å] for $[C_{24}H_{26}N_3O_5S][Br]$.

S-C(1)	1.724(2)	N(2)-C(5)	1.5024(19)
S-C(6)	1.818(2)	N(3)-C(21)	1.474(2)
O(1)-C(16)	1.339(2)	C(2)-C(3)	1.339(2)
O(1)-C(17)	1.463(2)	C(2)-C(15)	1.497(2)
O(2)-C(16)	1.212(2)	C(3)-C(16)	1.485(2)
O(3)-N(3)	1.230(2)	C(3)-C(4)	1.525(2)
O(4)-N(3)	1.229(2)	C(4)-C(19)	1.530(2)
O(5)-C(5)	1.401(2)	C(4)-H(4)	1.00(2)
O(5)-H(5O)	0.80(3)	C(5)-C(7)	1.527(2)
N(1)-C(1)	1.331(2)	C(5)-C(6)	1.535(2)
N(1)-C(2)	1.405(2)	C(6)-H(6A)	0.95(2)
N(1)-H(1N)	0.82(3)	C(6)-H(6B)	0.98(2)
N(2)-C(1)	1.317(2)	C(7)-C(8)	1.535(2)
N(2)-C(4)	1.4809(19)	C(7)-H(7A)	1.02(2)

C(7)-H(7B)	0.92(2)	C(15)-H(15C)	0.93(3)
C(8)-C(9)	1.508(3)	C(17)-C(18)	1.489(3)
C(8)-H(8A)	1.00(3)	C(17)-H(17A)	0.96(3)
C(8)-H(8B)	0.96(3)	C(17)-H(17B)	0.96(3)
C(9)-C(10)	1.386(3)	C(18)-H(18A)	0.95(3)
C(9)-C(14)	1.392(3)	C(18)-H(18B)	0.94(3)
C(10)-C(11)	1.391(3)	C(18)-H(18C)	0.97(3)
C(10)-H(10)	0.97(2)	C(19)-C(24)	1.393(2)
C(11)-C(12)	1.378(3)	C(19)-C(20)	1.393(2)
C(11)-H(11)	0.91(3)	C(20)-C(21)	1.387(2)
C(12)-C(13)	1.387(3)	C(20)-H(20)	0.90(2)
C(12)-H(12)	1.10(2)	C(21)-C(22)	1.382(3)
C(13)-C(14)	1.383(3)	C(22)-C(23)	1.389(3)
C(13)-H(13)	0.92(3)	C(22)-H(22)	0.91(2)
C(14)-H(14)	0.95(3)	C(23)-C(24)	1.391(2)
C(15)-H(15A)	0.94(3)	C(23)-H(23)	0.92(2)
C(15)-H(15B)	0.92(3)	C(24)-H(24)	0.91(2)

Table S-3. Bond angles [°] for $[C_{24}H_{26}N_3O_5S][Br]$.

C(1)-S-C(6)	90.47(8)	N(1)-C(1)-S	121.90(13)
C(16)-O(1)-C(17)	115.35(13)	C(3)-C(2)-N(1)	118.49(15)
C(5)-O(5)-H(5O)	110.4(17)	C(3)-C(2)-C(15)	127.51(16)
C(1)-N(1)-C(2)	120.86(15)	N(1)-C(2)-C(15)	113.89(15)
C(1)-N(1)-H(1N)	115.3(17)	C(2)-C(3)-C(16)	120.64(15)
C(2)-N(1)-H(1N)	121.6(17)	C(2)-C(3)-C(4)	121.38(14)
C(1)-N(2)-C(4)	121.64(13)	C(16)-C(3)-C(4)	117.87(14)
C(1)-N(2)-C(5)	115.05(13)	N(2)-C(4)-C(3)	109.69(13)
C(4)-N(2)-C(5)	122.08(13)	N(2)-C(4)-C(19)	111.61(13)
O(4)-N(3)-O(3)	123.46(15)	C(3)-C(4)-C(19)	108.93(12)
O(4)-N(3)-C(21)	118.52(14)	N(2)-C(4)-H(4)	107.1(11)
O(3)-N(3)-C(21)	118.01(15)	C(3)-C(4)-H(4)	109.9(11)
N(2)-C(1)-N(1)	122.34(15)	C(19)-C(4)-H(4)	109.6(11)
N(2)-C(1)-S	115.69(12)	O(5)-C(5)-N(2)	108.07(13)

O(5)-C(5)-C(7)	113.12(14)	C(9)-C(8)-C(7)	114.37(15)
N(2)-C(5)-C(7)	110.95(13)	C(9)-C(8)-H(8A)	108.7(17)
O(5)-C(5)-C(6)	108.36(13)	C(7)-C(8)-H(8A)	110.3(17)
N(2)-C(5)-C(6)	104.17(13)	C(9)-C(8)-H(8B)	111.5(18)
C(7)-C(5)-C(6)	111.72(14)	C(7)-C(8)-H(8B)	109.7(18)
C(5)-C(6)-S	108.38(11)	H(8A)-C(8)-H(8B)	102(2)
C(5)-C(6)-H(6A)	113.5(12)	C(10)-C(9)-C(14)	118.71(17)
S-C(6)-H(6A)	105.4(12)	C(10)-C(9)-C(8)	121.91(18)
C(5)-C(6)-H(6B)	110.6(12)	C(14)-C(9)-C(8)	119.35(18)
S-C(6)-H(6B)	109.2(12)	C(9)-C(10)-C(11)	120.20(18)
H(6A)-C(6)-H(6B)	109.6(16)	C(9)-C(10)-H(10)	118.2(14)
C(5)-C(7)-C(8)	110.27(14)	C(11)-C(10)-H(10)	121.5(14)
C(5)-C(7)-H(7A)	108.4(11)	C(12)-C(11)-C(10)	120.60(19)
C(8)-C(7)-H(7A)	110.0(11)	C(12)-C(11)-H(11)	120.1(19)
C(5)-C(7)-H(7B)	109.3(13)	C(10)-C(11)-H(11)	119.2(19)
C(8)-C(7)-H(7B)	108.6(13)	C(11)-C(12)-C(13)	119.64(19)
H(7A)-C(7)-H(7B)	110.3(17)	C(11)-C(12)-H(12)	114.0(11)

C(13)-C(12)-H(12)	126.4(11)	O(1)-C(17)-H(17A)	108.2(14)
C(14)-C(13)-C(12)	119.71(19)	C(18)-C(17)-H(17A)	111.7(14)
C(14)-C(13)-H(13)	119.9(17)	O(1)-C(17)-H(17B)	105.9(15)
C(12)-C(13)-H(13)	120.4(17)	C(18)-C(17)-H(17B)	109.8(15)
C(13)-C(14)-C(9)	121.11(18)	H(17A)-C(17)-H(17B)	112(2)
C(13)-C(14)-H(14)	119.5(15)	C(17)-C(18)-H(18A)	108.6(18)
C(9)-C(14)-H(14)	119.4(15)	C(17)-C(18)-H(18B)	112.4(15)
C(2)-C(15)-H(15A)	111.4(16)	H(18A)-C(18)-H(18B)	105(2)
C(2)-C(15)-H(15B)	108.9(15)	C(17)-C(18)-H(18C)	114.2(16)
H(15A)-C(15)-H(15B)	111(2)	H(18A)-C(18)-H(18C)	110(2)
C(2)-C(15)-H(15C)	111.0(16)	H(18B)-C(18)-H(18C)	105(2)
H(15A)-C(15)-H(15C)	104(2)	C(24)-C(19)-C(20)	119.28(15)
H(15B)-C(15)-H(15C)	111(2)	C(24)-C(19)-C(4)	122.84(14)
O(2)-C(16)-O(1)	124.00(15)	C(20)-C(19)-C(4)	117.76(15)
O(2)-C(16)-C(3)	124.69(16)	C(21)-C(20)-C(19)	118.55(16)
O(1)-C(16)-C(3)	111.29(13)	C(21)-C(20)-H(20)	120.8(13)
O(1)-C(17)-C(18)	108.90(15)	C(19)-C(20)-H(20)	120.6(13)

C(22)-C(21)-C(20)	123.19(16)	C(22)-C(23)-C(24)	120.58(16)
C(22)-C(21)-N(3)	119.24(15)	C(22)-C(23)-H(23)	117.5(15)
C(20)-C(21)-N(3)	117.56(16)	C(24)-C(23)-H(23)	121.9(15)
C(21)-C(22)-C(23)	117.59(16)	C(23)-C(24)-C(19)	120.74(15)
C(21)-C(22)-H(22)	121.5(15)	C(23)-C(24)-H(24)	118.5(14)
C(23)-C(22)-H(22)	120.9(15)	C(19)-C(24)-H(24)	120.8(14)

Table S-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{24}H_{26}N_3O_5S][Br]$. 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	13(1)	27(1)	19(1)	0(1)	4(1)	1(1)
O(1)	20(1)	26(1)	20(1)	2(1)	11(1)	4(1)
O(2)	32(1)	34(1)	22(1)	2(1)	15(1)	8(1)
O(3)	20(1)	39(1)	36(1)	-3(1)	6(1)	-11(1)
O(4)	20(1)	35(1)	46(1)	10(1)	10(1)	4(1)
O(5)	17(1)	22(1)	24(1)	4(1)	5(1)	-2(1)
N(1)	16(1)	26(1)	16(1)	0(1)	2(1)	0(1)
N(2)	13(1)	20(1)	16(1)	-1(1)	6(1)	-1(1)
N(3)	16(1)	34(1)	18(1)	2(1)	5(1)	-4(1)
C(1)	15(1)	17(1)	18(1)	0(1)	5(1)	-2(1)
C(2)	20(1)	20(1)	18(1)	-1(1)	8(1)	-3(1)
C(3)	18(1)	19(1)	16(1)	-2(1)	7(1)	-3(1)

C(4)	12(1)	20(1)	15(1)	-1(1)	6(1)	1(1)
C(5)	15(1)	22(1)	17(1)	1(1)	8(1)	-1(1)
C(6)	14(1)	25(1)	18(1)	-1(1)	5(1)	0(1)
C(7)	14(1)	25(1)	15(1)	-1(1)	6(1)	0(1)
C(8)	24(1)	58(1)	18(1)	-6(1)	9(1)	-11(1)
C(9)	18(1)	32(1)	17(1)	-3(1)	9(1)	1(1)
C(10)	28(1)	30(1)	28(1)	4(1)	12(1)	9(1)
C(11)	39(1)	26(1)	40(1)	-12(1)	19(1)	-1(1)
C(12)	28(1)	52(1)	25(1)	-15(1)	8(1)	-5(1)
C(13)	24(1)	50(1)	25(1)	8(1)	3(1)	7(1)
C(14)	24(1)	25(1)	30(1)	2(1)	9(1)	3(1)
C(15)	24(1)	30(1)	17(1)	-3(1)	5(1)	-3(1)
C(16)	20(1)	20(1)	20(1)	-2(1)	8(1)	-2(1)
C(17)	24(1)	27(1)	31(1)	3(1)	14(1)	7(1)
C(18)	31(1)	31(1)	25(1)	1(1)	9(1)	6(1)
C(19)	16(1)	22(1)	11(1)	-2(1)	6(1)	-2(1)
C(20)	18(1)	22(1)	13(1)	0(1)	5(1)	0(1)

C(21)	15(1)	30(1)	12(1)	0(1)	5(1)	-2(1)
C(22)	22(1)	25(1)	17(1)	-2(1)	7(1)	-8(1)
C(23)	26(1)	20(1)	21(1)	-1(1)	9(1)	0(1)
C(24)	16(1)	25(1)	18(1)	-1(1)	7(1)	1(1)
Br	18(1)	24(1)	23(1)	-3(1)	2(1)	-1(1)

Table S-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[C_{24}H_{26}N_3O_5S][Br]$.

	x	y	z	U(eq)
H(5O)	1930(20)	2113(17)	2485(16)	29(6)
H(1N)	570(20)	3488(17)	-839(18)	30(6)
H(4)	3356(17)	2656(14)	1515(14)	16(5)
H(6A)	447(17)	4517(15)	2100(14)	19(5)
H(6B)	-145(18)	3557(14)	2304(15)	18(5)
H(7A)	2531(17)	4480(14)	2674(13)	16(5)
H(7B)	3112(19)	3470(14)	2909(14)	18(5)
H(8A)	1890(20)	3070(20)	3960(20)	55(8)
H(8B)	1280(30)	4010(20)	3730(20)	55(8)
H(10)	2740(20)	5547(17)	4105(17)	31(6)
H(11)	4010(20)	6180(20)	5390(20)	49(8)

H(12)	4899(17)	5373(14)	6707(14)	18(5)
H(13)	4480(20)	3627(18)	6580(20)	41(7)
H(14)	3280(20)	2956(18)	5308(16)	34(6)
H(15A)	2320(20)	1990(20)	-1683(18)	41(7)
H(15B)	1170(20)	2519(17)	-1884(17)	34(6)
H(15C)	2300(20)	2985(19)	-1987(18)	41(7)
H(17A)	5460(20)	851(17)	37(17)	33(6)
H(17B)	6140(20)	1691(18)	647(17)	35(6)
H(18A)	6630(30)	280(20)	1430(20)	55(8)
H(18B)	5380(20)	41(19)	1417(17)	40(7)
H(18C)	5900(20)	859(19)	2035(19)	43(7)
H(20)	5315(18)	3235(17)	1357(14)	22(5)
H(22)	5900(20)	6020(17)	1231(16)	30(6)
H(23)	3970(20)	6309(17)	1016(17)	32(6)
H(24)	2690(20)	5057(15)	915(15)	23(5)

Table S-6. Torsion angles [°] for $[C_{24}H_{26}N_3O_5S][Br]$.

C(4)-N(2)-C(1)-N(1)	2.4(2)	C(1)-N(2)-C(4)-C(3)	-20.3(2)
C(5)-N(2)-C(1)-N(1)	-165.15(15)	C(5)-N(2)-C(4)-C(3)	146.37(14)
C(4)-N(2)-C(1)-S	179.57(11)	C(1)-N(2)-C(4)-C(19)	100.51(17)
C(5)-N(2)-C(1)-S	12.01(18)	C(5)-N(2)-C(4)-C(19)	-92.80(17)
C(2)-N(1)-C(1)-N(2)	16.3(2)	C(2)-C(3)-C(4)-N(2)	22.6(2)
C(2)-N(1)-C(1)-S	-160.68(12)	C(16)-C(3)-C(4)-N(2)	-161.21(13)
C(6)-S-C(1)-N(2)	3.77(14)	C(2)-C(3)-C(4)-C(19)	-99.81(17)
C(6)-S-C(1)-N(1)	-179.07(15)	C(16)-C(3)-C(4)-C(19)	76.35(18)
C(1)-N(1)-C(2)-C(3)	-13.3(2)	C(1)-N(2)-C(5)-O(5)	91.05(16)
C(1)-N(1)-C(2)-C(15)	163.23(15)	C(4)-N(2)-C(5)-O(5)	-76.45(17)
N(1)-C(2)-C(3)-C(16)	176.61(14)	C(1)-N(2)-C(5)-C(7)	-144.40(15)
C(15)-C(2)-C(3)-C(16)	0.6(3)	C(4)-N(2)-C(5)-C(7)	48.10(19)
N(1)-C(2)-C(3)-C(4)	-7.3(2)	C(1)-N(2)-C(5)-C(6)	-24.04(18)
C(15)-C(2)-C(3)-C(4)	176.62(16)	C(4)-N(2)-C(5)-C(6)	168.46(14)

O(5)-C(5)-C(6)-S	-89.90(13)	C(8)-C(9)-C(14)-C(13)	-177.50(17)
N(2)-C(5)-C(6)-S	24.99(15)	C(17)-O(1)-C(16)-O(2)	6.4(2)
C(7)-C(5)-C(6)-S	144.83(12)	C(17)-O(1)-C(16)-C(3)	-172.06(14)
C(1)-S-C(6)-C(5)	-17.41(12)	C(2)-C(3)-C(16)-O(2)	29.2(3)
O(5)-C(5)-C(7)-C(8)	-60.30(19)	C(4)-C(3)-C(16)-O(2)	-146.95(17)
N(2)-C(5)-C(7)-C(8)	178.06(15)	C(2)-C(3)-C(16)-O(1)	-152.35(15)
C(6)-C(5)-C(7)-C(8)	62.29(19)	C(4)-C(3)-C(16)-O(1)	31.5(2)
C(5)-C(7)-C(8)-C(9)	-179.45(17)	C(16)-O(1)-C(17)-C(18)	-167.05(16)
C(7)-C(8)-C(9)-C(10)	66.8(2)	N(2)-C(4)-C(19)-C(24)	-21.7(2)
C(7)-C(8)-C(9)-C(14)	-114.9(2)	C(3)-C(4)-C(19)-C(24)	99.62(17)
C(14)-C(9)-C(10)-C(11)	0.4(3)	N(2)-C(4)-C(19)-C(20)	162.30(13)
C(8)-C(9)-C(10)-C(11)	178.69(17)	C(3)-C(4)-C(19)-C(20)	-76.42(17)
C(9)-C(10)-C(11)-C(12)	-1.5(3)	C(24)-C(19)-C(20)-C(21)	-1.8(2)
C(10)-C(11)-C(12)-C(13)	1.3(3)	C(4)-C(19)-C(20)-C(21)	174.36(14)
C(11)-C(12)-C(13)-C(14)	-0.1(3)	C(19)-C(20)-C(21)-C(22)	2.8(2)
C(12)-C(13)-C(14)-C(9)	-1.0(3)	C(19)-C(20)-C(21)-N(3)	-176.26(13)
C(10)-C(9)-C(14)-C(13)	0.9(3)	O(4)-N(3)-C(21)-C(22)	-177.97(16)

O(3)-N(3)-C(21)-C(22)	0.5(2)	C(21)-C(22)-C(23)-C(24)	-1.1(2)
O(4)-N(3)-C(21)-C(20)	1.1(2)	C(22)-C(23)-C(24)-C(19)	2.0(2)
O(3)-N(3)-C(21)-C(20)	179.63(15)	C(20)-C(19)-C(24)-C(23)	-0.5(2)
C(20)-C(21)-C(22)-C(23)	-1.4(2)	C(4)-C(19)-C(24)-C(23)	-176.46(14)
N(3)-C(21)-C(22)-C(23)	177.70(14)		

Table S-7. Hydrogen bonds for $[C_{24}H_{26}N_3O_5S][Br]$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Br	0.82(3)	2.40(3)	3.208(2)	173(2)

Compound 6e

Table S-8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[C_{26}H_{29}N_2O_6S][Br]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S	4398(1)	231(1)	731(1)	29(1)
N(1)	3008(1)	1632(2)	-103(1)	27(1)
N(2)	3264(1)	1107(2)	1276(1)	19(1)
O(1)	1667(1)	4143(2)	1385(1)	29(1)
O(2)	1321(1)	4827(2)	55(2)	47(1)
O(3)	4415(1)	1873(2)	2395(1)	28(1)
O(4)	975(1)	-1994(2)	-684(1)	26(1)
O(5)	-70(1)	-2712(2)	-292(1)	30(1)
O(6)	-136(1)	-1812(2)	1126(1)	30(1)
C(1)	3472(1)	1046(3)	609(1)	22(1)
C(2)	2417(1)	2661(3)	-125(2)	26(1)

C(3)	2218(1)	2856(3)	556(2)	23(1)
C(4)	2510(1)	1847(2)	1286(1)	19(1)
C(5)	3934(1)	680(3)	2062(1)	23(1)
C(6)	4456(2)	-331(3)	1763(2)	29(1)
C(7)	3569(1)	7(3)	2662(2)	24(1)
C(8)	4220(2)	-531(3)	3461(2)	31(1)
C(9)	3829(2)	-1005(3)	4085(2)	31(1)
C(10)	3341(2)	-2214(3)	3936(2)	41(1)
C(11)	2956(2)	-2623(4)	4487(2)	49(1)
C(12)	3068(2)	-1870(4)	5197(2)	50(1)
C(13)	3563(2)	-685(4)	5369(2)	45(1)
C(14)	3936(2)	-234(4)	4801(2)	36(1)
C(15)	2085(2)	3425(4)	-939(2)	35(1)
C(16)	1684(1)	4038(3)	613(2)	28(1)
C(17)	1169(2)	5289(3)	1521(2)	40(1)
C(18)	1191(2)	5149(4)	2393(2)	48(1)
C(19)	1829(1)	811(2)	1252(1)	18(1)

C(20)	1454(1)	842(3)	1855(1)	21(1)
C(21)	806(1)	-40(3)	1809(2)	24(1)
C(22)	504(1)	-970(3)	1147(2)	23(1)
C(23)	871(1)	-1018(2)	533(1)	20(1)
C(24)	1532(1)	-117(2)	598(1)	18(1)
C(25)	542(1)	-1991(3)	-179(2)	24(1)
C(26)	704(2)	-2975(3)	-1374(2)	32(1)
Br	3567(1)	1050(1)	-1666(1)	30(1)

Table S-9. Bond lengths [Å] for $[C_{26}H_{29}N_2O_6S][Br]$.

S-C(1)	1.728(2)	O(4)-C(26)	1.451(3)
S-C(6)	1.818(3)	O(5)-C(25)	1.220(3)
N(1)-C(1)	1.333(3)	O(6)-C(22)	1.357(3)
N(1)-C(2)	1.406(3)	O(6)-H(6O)	0.82(4)
N(1)-H(1N)	0.85(4)	C(2)-C(3)	1.341(4)
N(2)-C(1)	1.314(3)	C(2)-C(15)	1.502(4)
N(2)-C(4)	1.488(3)	C(3)-C(16)	1.477(3)
N(2)-C(5)	1.503(3)	C(3)-C(4)	1.518(3)
O(1)-C(16)	1.340(3)	C(4)-C(19)	1.521(3)
O(1)-C(17)	1.454(3)	C(4)-H(4)	1.00(3)
O(2)-C(16)	1.208(3)	C(5)-C(7)	1.521(3)
O(3)-C(5)	1.403(3)	C(5)-C(6)	1.522(3)
O(3)-H(3O)	0.85(4)	C(6)-H(6A)	0.93(3)
O(4)-C(25)	1.327(3)	C(6)-H(6B)	0.91(3)

C(7)-C(8)	1.535(3)	C(15)-H(15A)	0.96(4)
C(7)-H(7A)	0.92(2)	C(15)-H(15B)	0.94(4)
C(7)-H(7B)	0.98(3)	C(15)-H(15C)	0.92(4)
C(8)-C(9)	1.518(4)	C(17)-C(18)	1.489(5)
C(8)-H(8A)	0.98(4)	C(17)-H(17A)	1.03(3)
C(8)-H(8B)	1.04(3)	C(17)-H(17B)	0.99(4)
C(9)-C(14)	1.387(4)	C(18)-H(18A)	1.02(4)
C(9)-C(10)	1.394(4)	C(18)-H(18B)	1.00(4)
C(10)-C(11)	1.387(4)	C(18)-H(18C)	0.99(4)
C(10)-H(10)	1.05(4)	C(19)-C(24)	1.379(3)
C(11)-C(12)	1.367(6)	C(19)-C(20)	1.398(3)
C(11)-H(11)	1.12(4)	C(20)-C(21)	1.380(4)
C(12)-C(13)	1.381(5)	C(20)-H(20)	0.88(3)
C(12)-H(12)	1.03(3)	C(21)-C(22)	1.391(4)
C(13)-C(14)	1.407(4)	C(21)-H(21)	1.03(3)
C(13)-H(13)	0.94(4)	C(22)-C(23)	1.405(3)
C(14)-H(14)	1.03(3)	C(23)-C(24)	1.401(3)

C(23)-C(25)	1.481(3)	C(26)-H(26B)	0.96(4)
C(24)-H(24)	0.94(3)	C(26)-H(26C)	0.91(3)
C(26)-H(26A)	0.97(3)		

Table S-10. Bond angles [°] for $[C_{26}H_{29}N_2O_6S][Br]$.

C(1)-S-C(6)	89.31(11)	C(3)-C(2)-N(1)	118.4(2)
C(1)-N(1)-C(2)	121.2(2)	C(3)-C(2)-C(15)	127.9(2)
C(1)-N(1)-H(1N)	114(2)	N(1)-C(2)-C(15)	113.7(2)
C(2)-N(1)-H(1N)	123(2)	C(2)-C(3)-C(16)	121.1(2)
C(1)-N(2)-C(4)	122.32(19)	C(2)-C(3)-C(4)	121.4(2)
C(1)-N(2)-C(5)	114.34(18)	C(16)-C(3)-C(4)	117.5(2)
C(4)-N(2)-C(5)	121.89(18)	N(2)-C(4)-C(3)	109.43(18)
C(16)-O(1)-C(17)	115.4(2)	N(2)-C(4)-C(19)	111.68(18)
C(5)-O(3)-H(3O)	112(2)	C(3)-C(4)-C(19)	109.82(18)
C(25)-O(4)-C(26)	115.9(2)	N(2)-C(4)-H(4)	105.1(15)
C(22)-O(6)-H(6O)	108(3)	C(3)-C(4)-H(4)	111.0(16)
N(2)-C(1)-N(1)	121.5(2)	C(19)-C(4)-H(4)	109.8(15)
N(2)-C(1)-S	115.75(18)	O(3)-C(5)-N(2)	108.51(19)
N(1)-C(1)-S	122.65(18)	O(3)-C(5)-C(7)	112.8(2)

N(2)-C(5)-C(7)	110.32(18)	C(9)-C(8)-H(8A)	109(2)
O(3)-C(5)-C(6)	107.77(19)	C(7)-C(8)-H(8A)	110(2)
N(2)-C(5)-C(6)	103.45(19)	C(9)-C(8)-H(8B)	111.4(18)
C(7)-C(5)-C(6)	113.5(2)	C(7)-C(8)-H(8B)	109.9(18)
C(5)-C(6)-S	107.68(18)	H(8A)-C(8)-H(8B)	105(3)
C(5)-C(6)-H(6A)	109.8(15)	C(14)-C(9)-C(10)	118.9(3)
S-C(6)-H(6A)	105.8(16)	C(14)-C(9)-C(8)	120.9(3)
C(5)-C(6)-H(6B)	110(2)	C(10)-C(9)-C(8)	120.1(3)
S-C(6)-H(6B)	108(2)	C(11)-C(10)-C(9)	120.5(3)
H(6A)-C(6)-H(6B)	115(3)	C(11)-C(10)-H(10)	121(2)
C(5)-C(7)-C(8)	113.31(19)	C(9)-C(10)-H(10)	118(2)
C(5)-C(7)-H(7A)	107.0(14)	C(12)-C(11)-C(10)	120.5(3)
C(8)-C(7)-H(7A)	109.5(14)	C(12)-C(11)-H(11)	119.0(19)
C(5)-C(7)-H(7B)	106.4(17)	C(10)-C(11)-H(11)	120.3(19)
C(8)-C(7)-H(7B)	108.2(18)	C(11)-C(12)-C(13)	120.2(3)
H(7A)-C(7)-H(7B)	112(2)	C(11)-C(12)-H(12)	128.3(17)
C(9)-C(8)-C(7)	111.1(2)	C(13)-C(12)-H(12)	111.5(17)

C(12)-C(13)-C(14)	119.8(3)	C(18)-C(17)-H(17A)	111.9(17)
C(12)-C(13)-H(13)	120(2)	O(1)-C(17)-H(17B)	108(2)
C(14)-C(13)-H(13)	120(2)	C(18)-C(17)-H(17B)	109(2)
C(9)-C(14)-C(13)	120.0(3)	H(17A)-C(17)-H(17B)	113(3)
C(9)-C(14)-H(14)	117.4(16)	C(17)-C(18)-H(18A)	111(2)
C(13)-C(14)-H(14)	122.5(16)	C(17)-C(18)-H(18B)	115(2)
C(2)-C(15)-H(15A)	108(2)	H(18A)-C(18)-H(18B)	106(3)
C(2)-C(15)-H(15B)	110(2)	C(17)-C(18)-H(18C)	108(2)
H(15A)-C(15)-H(15B)	104(3)	H(18A)-C(18)-H(18C)	105(3)
C(2)-C(15)-H(15C)	109(2)	H(18B)-C(18)-H(18C)	110(3)
H(15A)-C(15)-H(15C)	107(3)	C(24)-C(19)-C(20)	118.5(2)
H(15B)-C(15)-H(15C)	118(3)	C(24)-C(19)-C(4)	120.7(2)
O(2)-C(16)-O(1)	123.9(2)	C(20)-C(19)-C(4)	120.6(2)
O(2)-C(16)-C(3)	125.7(3)	C(21)-C(20)-C(19)	121.4(2)
O(1)-C(16)-C(3)	110.4(2)	C(21)-C(20)-H(20)	121(2)
O(1)-C(17)-C(18)	106.4(2)	C(19)-C(20)-H(20)	117(2)
O(1)-C(17)-H(17A)	108.0(17)	C(20)-C(21)-C(22)	120.0(2)

C(20)-C(21)-H(21)	121.0(16)	C(23)-C(24)-H(24)	116.2(15)
C(22)-C(21)-H(21)	118.9(16)	O(5)-C(25)-O(4)	123.4(2)
O(6)-C(22)-C(21)	117.9(2)	O(5)-C(25)-C(23)	123.2(2)
O(6)-C(22)-C(23)	122.5(2)	O(4)-C(25)-C(23)	113.4(2)
C(21)-C(22)-C(23)	119.6(2)	O(4)-C(26)-H(26A)	103.3(19)
C(24)-C(23)-C(22)	119.2(2)	O(4)-C(26)-H(26B)	108.1(19)
C(24)-C(23)-C(25)	121.1(2)	H(26A)-C(26)-H(26B)	112(3)
C(22)-C(23)-C(25)	119.6(2)	O(4)-C(26)-H(26C)	109(2)
C(19)-C(24)-C(23)	121.3(2)	H(26A)-C(26)-H(26C)	113(3)
C(19)-C(24)-H(24)	122.5(15)	H(26B)-C(26)-H(26C)	111(3)

Table S-11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{26}H_{29}N_2O_6S][Br]$. 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	22(1)	44(1)	25(1)	1(1)	12(1)	6(1)
N(1)	27(1)	38(1)	18(1)	3(1)	10(1)	3(1)
N(2)	15(1)	26(1)	16(1)	2(1)	4(1)	3(1)
O(1)	26(1)	22(1)	35(1)	0(1)	6(1)	6(1)
O(2)	39(1)	50(1)	60(1)	37(1)	27(1)	22(1)
O(3)	19(1)	38(1)	26(1)	-6(1)	7(1)	-6(1)
O(4)	30(1)	25(1)	20(1)	-3(1)	5(1)	-1(1)
O(5)	22(1)	25(1)	36(1)	2(1)	2(1)	-1(1)
O(6)	23(1)	32(1)	37(1)	8(1)	13(1)	-2(1)
C(1)	19(1)	30(1)	18(1)	-1(1)	6(1)	-2(1)
C(2)	21(1)	30(1)	25(1)	5(1)	5(1)	-1(1)
C(3)	19(1)	24(1)	23(1)	6(1)	4(1)	0(1)

C(4)	17(1)	22(1)	18(1)	2(1)	6(1)	4(1)
C(5)	15(1)	32(1)	18(1)	3(1)	2(1)	2(1)
C(6)	20(1)	40(2)	25(1)	2(1)	7(1)	6(1)
C(7)	19(1)	29(1)	22(1)	4(1)	5(1)	1(1)
C(8)	23(1)	44(2)	23(1)	9(1)	4(1)	5(1)
C(9)	21(1)	45(2)	25(1)	15(1)	3(1)	10(1)
C(10)	39(2)	41(2)	42(2)	16(1)	13(1)	6(1)
C(11)	47(2)	47(2)	55(2)	24(2)	19(2)	5(2)
C(12)	35(2)	69(2)	48(2)	34(2)	18(1)	14(2)
C(13)	31(1)	73(2)	28(2)	12(2)	8(1)	19(2)
C(14)	21(1)	57(2)	29(1)	11(1)	5(1)	9(1)
C(15)	31(1)	45(2)	27(1)	12(1)	9(1)	2(1)
C(16)	20(1)	27(1)	37(2)	11(1)	10(1)	2(1)
C(17)	33(1)	23(1)	68(2)	-1(1)	22(2)	7(1)
C(18)	37(2)	47(2)	60(2)	-19(2)	17(2)	4(1)
C(19)	16(1)	20(1)	15(1)	5(1)	3(1)	7(1)
C(20)	23(1)	24(1)	15(1)	3(1)	6(1)	6(1)

C(21)	24(1)	30(1)	22(1)	9(1)	12(1)	8(1)
C(22)	16(1)	23(1)	28(1)	11(1)	7(1)	5(1)
C(23)	17(1)	20(1)	21(1)	5(1)	3(1)	5(1)
C(24)	15(1)	22(1)	17(1)	5(1)	5(1)	6(1)
C(25)	19(1)	21(1)	24(1)	6(1)	0(1)	6(1)
C(26)	43(2)	23(1)	22(1)	-3(1)	3(1)	1(1)
Br	25(1)	43(1)	25(1)	10(1)	13(1)	6(1)

Table S-12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[C_{26}H_{29}N_2O_6S][Br]$.

	x	y	z	U(eq)
H(1N)	3170(20)	1480(40)	-510(20)	41(9)
H(3O)	4220(20)	2360(40)	2700(20)	36(9)
H(6O)	-280(30)	-2250(40)	680(30)	57(12)
H(4)	2682(17)	2380(30)	1825(18)	21(7)
H(6A)	4228(16)	-1230(30)	1698(16)	13(6)
H(6B)	4990(20)	-270(30)	2110(20)	35(8)
H(7A)	3247(14)	-740(20)	2386(14)	3(5)
H(7B)	3248(19)	750(30)	2810(19)	30(7)
H(8A)	4520(20)	-1320(40)	3340(20)	45(9)
H(8B)	4660(20)	240(40)	3710(20)	39(8)
H(10)	3280(20)	-2800(40)	3400(30)	59(11)
H(11)	2510(20)	-3520(40)	4330(20)	52(10)

H(12)	2814(18)	-2050(30)	5653(19)	30(7)
H(13)	3680(20)	-210(40)	5880(20)	47(10)
H(14)	4274(18)	690(30)	4882(18)	24(7)
H(15A)	2380(30)	3090(40)	-1280(30)	60(11)
H(15B)	1540(20)	3140(40)	-1220(20)	45(9)
H(15C)	2190(20)	4370(40)	-850(20)	42(9)
H(17A)	590(20)	5180(30)	1104(19)	31(8)
H(17B)	1430(20)	6200(40)	1460(20)	49(10)
H(18A)	930(20)	4220(40)	2480(20)	53(10)
H(18B)	1750(30)	5180(40)	2820(30)	59(11)
H(18C)	840(20)	5900(40)	2500(20)	52(10)
H(20)	1627(19)	1490(30)	2250(20)	33(8)
H(21)	535(18)	-20(30)	2258(18)	28(7)
H(24)	1748(15)	-170(30)	168(16)	13(6)
H(26A)	1140(20)	-2930(30)	-1610(20)	37(8)
H(26B)	190(20)	-2650(30)	-1750(20)	36(8)
H(26C)	650(20)	-3850(40)	-1170(20)	36(8)

Table S-13. Torsion angles [°] for $[C_{26}H_{29}N_2O_6S][Br]$.

C(4)-N(2)-C(1)-N(1)	-0.9(4)	C(1)-N(2)-C(4)-C(3)	-18.5(3)
C(5)-N(2)-C(1)-N(1)	-167.3(2)	C(5)-N(2)-C(4)-C(3)	147.0(2)
C(4)-N(2)-C(1)-S	176.39(16)	C(1)-N(2)-C(4)-C(19)	103.3(2)
C(5)-N(2)-C(1)-S	9.9(3)	C(5)-N(2)-C(4)-C(19)	-91.2(2)
C(2)-N(1)-C(1)-N(2)	18.1(4)	C(2)-C(3)-C(4)-N(2)	23.6(3)
C(2)-N(1)-C(1)-S	-158.94(19)	C(16)-C(3)-C(4)-N(2)	-158.2(2)
C(6)-S-C(1)-N(2)	8.7(2)	C(2)-C(3)-C(4)-C(19)	-99.3(2)
C(6)-S-C(1)-N(1)	-174.0(2)	C(16)-C(3)-C(4)-C(19)	78.9(3)
C(1)-N(1)-C(2)-C(3)	-12.3(4)	C(1)-N(2)-C(5)-O(3)	87.3(2)
C(1)-N(1)-C(2)-C(15)	167.5(2)	C(4)-N(2)-C(5)-O(3)	-79.2(2)
N(1)-C(2)-C(3)-C(16)	172.0(2)	C(1)-N(2)-C(5)-C(7)	-148.7(2)
C(15)-C(2)-C(3)-C(16)	-7.7(4)	C(4)-N(2)-C(5)-C(7)	44.8(3)
N(1)-C(2)-C(3)-C(4)	-9.8(4)	C(1)-N(2)-C(5)-C(6)	-27.0(3)
C(15)-C(2)-C(3)-C(4)	170.4(2)	C(4)-N(2)-C(5)-C(6)	166.5(2)

O(3)-C(5)-C(6)-S	-83.5(2)	C(12)-C(13)-C(14)-C(9)	-2.3(4)
N(2)-C(5)-C(6)-S	31.3(2)	C(17)-O(1)-C(16)-O(2)	0.3(4)
C(7)-C(5)-C(6)-S	150.88(18)	C(17)-O(1)-C(16)-C(3)	179.1(2)
C(1)-S-C(6)-C(5)	-23.86(19)	C(2)-C(3)-C(16)-O(2)	7.7(4)
O(3)-C(5)-C(7)-C(8)	-61.6(3)	C(4)-C(3)-C(16)-O(2)	-170.5(2)
N(2)-C(5)-C(7)-C(8)	176.9(2)	C(2)-C(3)-C(16)-O(1)	-171.1(2)
C(6)-C(5)-C(7)-C(8)	61.3(3)	C(4)-C(3)-C(16)-O(1)	10.7(3)
C(5)-C(7)-C(8)-C(9)	172.1(2)	C(16)-O(1)-C(17)-C(18)	176.2(2)
C(7)-C(8)-C(9)-C(14)	-109.5(3)	N(2)-C(4)-C(19)-C(24)	-58.9(3)
C(7)-C(8)-C(9)-C(10)	69.2(3)	C(3)-C(4)-C(19)-C(24)	62.7(3)
C(14)-C(9)-C(10)-C(11)	1.2(4)	N(2)-C(4)-C(19)-C(20)	125.4(2)
C(8)-C(9)-C(10)-C(11)	-177.5(3)	C(3)-C(4)-C(19)-C(20)	-113.0(2)
C(9)-C(10)-C(11)-C(12)	-1.9(5)	C(24)-C(19)-C(20)-C(21)	0.7(3)
C(10)-C(11)-C(12)-C(13)	0.4(5)	C(4)-C(19)-C(20)-C(21)	176.5(2)
C(11)-C(12)-C(13)-C(14)	1.7(4)	C(19)-C(20)-C(21)-C(22)	-1.0(3)
C(10)-C(9)-C(14)-C(13)	0.8(4)	C(20)-C(21)-C(22)-O(6)	-179.6(2)
C(8)-C(9)-C(14)-C(13)	179.5(2)	C(20)-C(21)-C(22)-C(23)	0.9(3)

O(6)-C(22)-C(23)-C(24)	-179.9(2)	C(25)-C(23)-C(24)-C(19)	178.6(2)
C(21)-C(22)-C(23)-C(24)	-0.5(3)	C(26)-O(4)-C(25)-O(5)	-3.1(3)
O(6)-C(22)-C(23)-C(25)	1.6(3)	C(26)-O(4)-C(25)-C(23)	177.3(2)
C(21)-C(22)-C(23)-C(25)	-179.0(2)	C(24)-C(23)-C(25)-O(5)	-174.2(2)
C(20)-C(19)-C(24)-C(23)	-0.2(3)	C(22)-C(23)-C(25)-O(5)	4.3(3)
C(4)-C(19)-C(24)-C(23)	-176.1(2)	C(24)-C(23)-C(25)-O(4)	5.4(3)
C(22)-C(23)-C(24)-C(19)	0.1(3)	C(22)-C(23)-C(25)-O(4)	-176.0(2)

Table S-14. Hydrogen bonds for[$C_{26}H_{29}N_2O_6S$][Br] [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Br	0.85(4)	2.34(4)	3.196(2)	177(3)
O(3)-H(3O)...Br#1	0.85(4)	2.36(4)	3.202(2)	169(3)
O(6)-H(6O)...O(5)	0.82(4)	1.88(4)	2.620(3)	148(4)

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

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Table S-15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[C_{24}H_{24}N_3O_4][Br]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S	7779(1)	572(1)	3989(1)	15(1)
O(1)	-492(2)	3622(1)	4996(1)	17(1)
O(2)	-1287(2)	3420(1)	3640(1)	21(1)
O(3)	1362(2)	6896(1)	-783(1)	29(1)
O(4)	-984(2)	6042(1)	195(1)	22(1)
N(1)	5101(2)	1721(1)	4880(1)	15(1)
N(2)	4392(2)	1725(1)	3350(1)	12(1)
N(3)	734(2)	6188(1)	30(1)	19(1)
C(1)	5597(2)	1414(1)	4108(1)	14(1)
C(2)	3222(2)	2297(1)	4984(1)	14(1)
C(3)	1966(2)	2694(1)	4215(1)	13(1)

C(4)	2593(2)	2615(1)	3201(1)	12(1)
C(5)	5184(2)	1295(1)	2617(1)	13(1)
C(6)	6982(3)	662(2)	2864(1)	16(1)
C(7)	4006(2)	1577(2)	1717(1)	15(1)
C(8)	4946(3)	920(2)	1076(1)	18(1)
C(9)	3710(3)	1272(2)	166(1)	17(1)
C(10)	4383(3)	1916(2)	-828(1)	22(1)
C(11)	3182(3)	2312(2)	-1652(2)	29(1)
C(12)	1309(3)	2053(2)	-1501(2)	30(1)
C(13)	645(3)	1384(2)	-518(2)	29(1)
C(14)	1834(3)	997(2)	310(2)	24(1)
C(15)	2834(3)	2354(2)	6002(1)	17(1)
C(16)	-96(2)	3265(1)	4249(1)	14(1)
C(17)	-2530(3)	4100(2)	5141(2)	20(1)
C(18)	-2689(3)	4162(2)	6158(2)	28(1)
C(19)	3023(2)	3760(1)	2358(1)	13(1)
C(20)	1647(2)	4458(1)	1618(1)	14(1)

C(21)	2141(2)	5466(2)	842(1)	16(1)
C(22)	3918(3)	5810(2)	782(2)	20(1)
C(23)	5237(3)	5132(2)	1551(2)	21(1)
C(24)	4798(2)	4114(2)	2328(1)	17(1)
Br	8263(1)	883(1)	6586(1)	18(1)

Table S-16. Bond lengths [Å] for $[C_{24}H_{26}N_3O_5S][Br]$.

S-C(1)	1.715(2)	C(2)-C(3)	1.352(2)
S-C(6)	1.740(2)	C(2)-C(15)	1.499(2)
O(1)-C(16)	1.339(2)	C(3)-C(16)	1.475(2)
O(1)-C(17)	1.451(2)	C(3)-C(4)	1.522(2)
O(2)-C(16)	1.212(2)	C(4)-C(19)	1.525(2)
O(3)-N(3)	1.233(2)	C(4)-H(4)	0.94(2)
O(4)-N(3)	1.224(2)	C(5)-C(6)	1.339(2)
N(1)-C(1)	1.334(2)	C(5)-C(7)	1.496(2)
N(1)-C(2)	1.390(2)	C(6)-H(6)	0.89(2)
N(1)-H(1N)	0.80(2)	C(7)-C(8)	1.533(2)
N(2)-C(1)	1.333(2)	C(7)-H(7A)	0.95(2)
N(2)-C(5)	1.415(2)	C(7)-H(7B)	0.91(2)
N(2)-C(4)	1.485(2)	C(8)-C(9)	1.511(2)
N(3)-C(21)	1.472(2)	C(8)-H(8A)	0.94(2)

C(8)-H(8B)	0.95(2)	C(17)-H(17A)	0.95(2)
C(9)-C(10)	1.390(3)	C(17)-H(17B)	0.95(2)
C(9)-C(14)	1.391(3)	C(18)-H(18A)	0.95(3)
C(10)-C(11)	1.387(3)	C(18)-H(18B)	0.94(3)
C(10)-H(10)	0.94(2)	C(18)-H(18C)	1.00(3)
C(11)-C(12)	1.380(3)	C(19)-C(20)	1.391(2)
C(11)-H(11)	0.93(3)	C(19)-C(24)	1.395(2)
C(12)-C(13)	1.385(3)	C(20)-C(21)	1.386(2)
C(12)-H(12)	0.97(3)	C(20)-H(20)	0.93(2)
C(13)-C(14)	1.387(3)	C(21)-C(22)	1.382(3)
C(13)-H(13)	0.92(3)	C(22)-C(23)	1.387(3)
C(14)-H(14)	0.94(3)	C(22)-H(22)	0.86(3)
C(15)-H(15A)	0.91(2)	C(23)-C(24)	1.382(3)
C(15)-H(15B)	0.94(3)	C(23)-H(23)	0.92(2)
C(15)-H(15C)	0.94(2)	C(24)-H(24)	0.91(2)
C(17)-C(18)	1.504(3)		

Table S-17. Bond angles [°] for $[C_{24}H_{26}N_3O_5S][Br]$.

C(1)-S-C(6)	89.21(8)	N(2)-C(1)-S	113.08(12)
C(16)-O(1)-C(17)	116.69(13)	N(1)-C(1)-S	124.69(13)
C(1)-N(1)-C(2)	121.29(15)	C(3)-C(2)-N(1)	119.14(15)
C(1)-N(1)-H(1N)	115.7(16)	C(3)-C(2)-C(15)	127.92(15)
C(2)-N(1)-H(1N)	122.7(16)	N(1)-C(2)-C(15)	112.90(14)
C(1)-N(2)-C(5)	113.30(14)	C(2)-C(3)-C(16)	124.61(15)
C(1)-N(2)-C(4)	121.79(13)	C(2)-C(3)-C(4)	122.14(14)
C(5)-N(2)-C(4)	123.89(14)	C(16)-C(3)-C(4)	113.23(14)
O(4)-N(3)-O(3)	123.87(15)	N(2)-C(4)-C(3)	108.96(13)
O(4)-N(3)-C(21)	118.24(14)	N(2)-C(4)-C(19)	109.20(13)
O(3)-N(3)-C(21)	117.89(14)	C(3)-C(4)-C(19)	111.75(13)
N(2)-C(1)-N(1)	122.22(15)	N(2)-C(4)-H(4)	108.8(12)

C(3)-C(4)-H(4)	108.6(12)	C(9)-C(8)-H(8B)	111.4(14)
C(19)-C(4)-H(4)	109.6(12)	C(7)-C(8)-H(8B)	109.3(14)
C(6)-C(5)-N(2)	111.16(15)	H(8A)-C(8)-H(8B)	107.1(18)
C(6)-C(5)-C(7)	129.32(15)	C(10)-C(9)-C(14)	118.45(17)
N(2)-C(5)-C(7)	119.52(14)	C(10)-C(9)-C(8)	121.04(16)
C(5)-C(6)-S	113.25(13)	C(14)-C(9)-C(8)	120.46(16)
C(5)-C(6)-H(6)	128.6(14)	C(11)-C(10)-C(9)	120.74(18)
S-C(6)-H(6)	118.2(14)	C(11)-C(10)-H(10)	118.4(14)
C(5)-C(7)-C(8)	112.99(14)	C(9)-C(10)-H(10)	120.8(14)
C(5)-C(7)-H(7A)	108.1(13)	C(12)-C(11)-C(10)	120.48(19)
C(8)-C(7)-H(7A)	110.7(13)	C(12)-C(11)-H(11)	120.5(18)
C(5)-C(7)-H(7B)	109.2(14)	C(10)-C(11)-H(11)	119.0(18)
C(8)-C(7)-H(7B)	107.3(13)	C(11)-C(12)-C(13)	119.21(18)
H(7A)-C(7)-H(7B)	108.4(18)	C(11)-C(12)-H(12)	123.4(15)
C(9)-C(8)-C(7)	110.09(14)	C(13)-C(12)-H(12)	117.4(15)
C(9)-C(8)-H(8A)	110.2(13)	C(12)-C(13)-C(14)	120.47(19)
C(7)-C(8)-H(8A)	108.6(13)	C(12)-C(13)-H(13)	119.1(18)

C(14)-C(13)-H(13)	120.4(18)	C(18)-C(17)-H(17B)	111.7(13)
C(13)-C(14)-C(9)	120.60(18)	H(17A)-C(17)-H(17B)	111.2(19)
C(13)-C(14)-H(14)	119.1(15)	C(17)-C(18)-H(18A)	109.5(15)
C(9)-C(14)-H(14)	120.3(15)	C(17)-C(18)-H(18B)	111.9(15)
C(2)-C(15)-H(15A)	109.2(13)	H(18A)-C(18)-H(18B)	108(2)
C(2)-C(15)-H(15B)	110.3(15)	C(17)-C(18)-H(18C)	109.4(15)
H(15A)-C(15)-H(15B)	109.6(19)	H(18A)-C(18)-H(18C)	111(2)
C(2)-C(15)-H(15C)	110.7(13)	H(18B)-C(18)-H(18C)	107(2)
H(15A)-C(15)-H(15C)	109.4(19)	C(20)-C(19)-C(24)	119.77(15)
H(15B)-C(15)-H(15C)	107.6(19)	C(20)-C(19)-C(4)	120.16(14)
O(2)-C(16)-O(1)	123.75(15)	C(24)-C(19)-C(4)	120.07(15)
O(2)-C(16)-C(3)	122.95(15)	C(21)-C(20)-C(19)	118.03(15)
O(1)-C(16)-C(3)	113.27(14)	C(21)-C(20)-H(20)	120.5(13)
O(1)-C(17)-C(18)	106.53(15)	C(19)-C(20)-H(20)	121.4(13)
O(1)-C(17)-H(17A)	107.5(13)	C(22)-C(21)-C(20)	122.91(16)
C(18)-C(17)-H(17A)	111.5(13)	C(22)-C(21)-N(3)	118.46(15)
O(1)-C(17)-H(17B)	108.3(13)	C(20)-C(21)-N(3)	118.61(15)

C(21)-C(22)-C(23)	118.36(16)	C(22)-C(23)-H(23)	122.1(15)
C(21)-C(22)-H(22)	119.7(16)	C(23)-C(24)-C(19)	120.80(16)
C(23)-C(22)-H(22)	121.9(16)	C(23)-C(24)-H(24)	119.3(13)
C(24)-C(23)-C(22)	120.04(16)	C(19)-C(24)-H(24)	119.8(13)
C(24)-C(23)-H(23)	117.8(15)		

Table S-18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{24}H_{26}N_3O_5S][Br]$. 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	13(1)	17(1)	14(1)	-7(1)	-4(1)	1(1)
O(1)	14(1)	20(1)	19(1)	-10(1)	-1(1)	0(1)
O(2)	15(1)	30(1)	19(1)	-11(1)	-5(1)	0(1)
O(3)	37(1)	22(1)	14(1)	3(1)	0(1)	-4(1)
O(4)	22(1)	20(1)	19(1)	-5(1)	-5(1)	0(1)
N(1)	13(1)	20(1)	13(1)	-7(1)	-6(1)	-1(1)
N(2)	14(1)	12(1)	11(1)	-4(1)	-3(1)	-2(1)
N(3)	24(1)	14(1)	14(1)	-5(1)	-2(1)	0(1)
C(1)	14(1)	13(1)	14(1)	-4(1)	-3(1)	-3(1)
C(2)	14(1)	13(1)	15(1)	-5(1)	0(1)	-5(1)
C(3)	14(1)	12(1)	13(1)	-5(1)	-1(1)	-4(1)
C(4)	11(1)	13(1)	12(1)	-5(1)	-3(1)	-2(1)

C(5)	17(1)	12(1)	11(1)	-5(1)	0(1)	-5(1)
C(6)	19(1)	16(1)	14(1)	-7(1)	-2(1)	-2(1)
C(7)	17(1)	14(1)	13(1)	-5(1)	-3(1)	-2(1)
C(8)	20(1)	19(1)	16(1)	-9(1)	-3(1)	-1(1)
C(9)	22(1)	16(1)	16(1)	-10(1)	-3(1)	-1(1)
C(10)	29(1)	24(1)	20(1)	-14(1)	0(1)	-9(1)
C(11)	46(1)	29(1)	14(1)	-10(1)	-2(1)	-10(1)
C(12)	34(1)	37(1)	22(1)	-18(1)	-11(1)	4(1)
C(13)	22(1)	45(1)	28(1)	-22(1)	-3(1)	-4(1)
C(14)	25(1)	31(1)	18(1)	-12(1)	0(1)	-6(1)
C(15)	16(1)	20(1)	15(1)	-8(1)	-4(1)	-1(1)
C(16)	15(1)	12(1)	14(1)	-4(1)	0(1)	-4(1)
C(17)	15(1)	19(1)	24(1)	-9(1)	-2(1)	2(1)
C(18)	22(1)	33(1)	33(1)	-22(1)	2(1)	0(1)
C(19)	15(1)	13(1)	12(1)	-7(1)	0(1)	-2(1)
C(20)	14(1)	16(1)	14(1)	-7(1)	-1(1)	-2(1)
C(21)	20(1)	15(1)	12(1)	-6(1)	-1(1)	0(1)

C(22)	25(1)	15(1)	18(1)	-5(1)	4(1)	-8(1)
C(23)	18(1)	22(1)	25(1)	-10(1)	2(1)	-9(1)
C(24)	15(1)	18(1)	18(1)	-7(1)	-3(1)	-3(1)
Br	14(1)	21(1)	15(1)	-4(1)	-4(1)	-2(1)

Table S-19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[C_{24}H_{26}N_3O_5S][Br]$.

	x	y	z	U(eq)
H(1N)	5910(30)	1499(19)	5300(18)	18(5)
H(4)	1570(30)	2390(17)	3004(15)	11(4)
H(6)	7780(30)	300(19)	2533(17)	20(5)
H(7A)	3850(30)	2380(20)	1308(17)	20(5)
H(7B)	2800(30)	1386(18)	1944(16)	18(5)
H(8A)	5040(30)	120(20)	1495(17)	19(5)
H(8B)	6250(40)	1060(20)	864(17)	25(6)
H(10)	5670(40)	2080(20)	-960(18)	27(6)
H(11)	3660(40)	2750(30)	-2310(20)	48(8)
H(12)	400(40)	2330(20)	-2050(20)	36(6)
H(13)	-580(40)	1180(20)	-420(20)	49(8)
H(14)	1340(40)	560(20)	970(20)	31(6)

H(15A)	3880(30)	1936(18)	6404(16)	16(5)
H(15B)	2640(30)	3120(20)	5912(18)	28(6)
H(15C)	1690(30)	2060(18)	6331(16)	17(5)
H(17A)	-2810(30)	4850(20)	4590(18)	23(5)
H(17B)	-3340(30)	3607(19)	5136(17)	22(5)
H(18A)	-2450(40)	3400(20)	6690(20)	32(6)
H(18B)	-3940(40)	4530(20)	6282(19)	34(6)
H(18C)	-1710(40)	4630(20)	6160(20)	40(7)
H(20)	440(30)	4245(17)	1626(16)	15(5)
H(22)	4160(40)	6440(20)	290(20)	31(6)
H(23)	6410(40)	5340(20)	1570(18)	26(6)
H(24)	5700(30)	3658(18)	2812(16)	16(5)

Table S-20. Torsion angles [°] for $[C_{24}H_{26}N_3O_5S][Br]$.

C(5)-N(2)-C(1)-N(1)	-179.03(15)	C(1)-N(2)-C(4)-C(3)	-23.1(2)
C(4)-N(2)-C(1)-N(1)	12.1(2)	C(5)-N(2)-C(4)-C(3)	169.20(13)
C(5)-N(2)-C(1)-S	-0.17(18)	C(1)-N(2)-C(4)-C(19)	99.17(17)
C(4)-N(2)-C(1)-S	-169.03(11)	C(5)-N(2)-C(4)-C(19)	-68.49(18)
C(2)-N(1)-C(1)-N(2)	6.0(3)	C(2)-C(3)-C(4)-N(2)	19.6(2)
C(2)-N(1)-C(1)-S	-172.74(12)	C(16)-C(3)-C(4)-N(2)	-161.85(13)
C(6)-S-C(1)-N(2)	-0.01(13)	C(2)-C(3)-C(4)-C(19)	-101.18(18)
C(6)-S-C(1)-N(1)	178.83(16)	C(16)-C(3)-C(4)-C(19)	77.40(16)
C(1)-N(1)-C(2)-C(3)	-9.4(2)	C(1)-N(2)-C(5)-C(6)	0.3(2)
C(1)-N(1)-C(2)-C(15)	168.43(15)	C(4)-N(2)-C(5)-C(6)	168.90(14)
N(1)-C(2)-C(3)-C(16)	176.71(15)	C(1)-N(2)-C(5)-C(7)	-179.70(14)
C(15)-C(2)-C(3)-C(16)	-0.8(3)	C(4)-N(2)-C(5)-C(7)	-11.1(2)
N(1)-C(2)-C(3)-C(4)	-4.9(2)	N(2)-C(5)-C(6)-S	-0.31(19)
C(15)-C(2)-C(3)-C(4)	177.66(16)	C(7)-C(5)-C(6)-S	179.70(14)

C(1)-S-C(6)-C(5)	0.19(14)	C(4)-C(3)-C(16)-O(2)	15.5(2)
C(6)-C(5)-C(7)-C(8)	7.6(3)	C(2)-C(3)-C(16)-O(1)	16.1(2)
N(2)-C(5)-C(7)-C(8)	-172.39(14)	C(4)-C(3)-C(16)-O(1)	-162.48(13)
C(5)-C(7)-C(8)-C(9)	-178.39(14)	C(16)-O(1)-C(17)-C(18)	166.40(15)
C(7)-C(8)-C(9)-C(10)	110.26(18)	N(2)-C(4)-C(19)-C(20)	137.18(15)
C(7)-C(8)-C(9)-C(14)	-67.1(2)	C(3)-C(4)-C(19)-C(20)	-102.20(17)
C(14)-C(9)-C(10)-C(11)	2.4(3)	N(2)-C(4)-C(19)-C(24)	-42.9(2)
C(8)-C(9)-C(10)-C(11)	-174.97(17)	C(3)-C(4)-C(19)-C(24)	77.76(18)
C(9)-C(10)-C(11)-C(12)	-1.3(3)	C(24)-C(19)-C(20)-C(21)	2.8(2)
C(10)-C(11)-C(12)-C(13)	-0.5(3)	C(4)-C(19)-C(20)-C(21)	-177.19(14)
C(11)-C(12)-C(13)-C(14)	1.2(3)	C(19)-C(20)-C(21)-C(22)	-0.8(2)
C(12)-C(13)-C(14)-C(9)	-0.1(3)	C(19)-C(20)-C(21)-N(3)	177.52(14)
C(10)-C(9)-C(14)-C(13)	-1.7(3)	O(4)-N(3)-C(21)-C(22)	-163.39(15)
C(8)-C(9)-C(14)-C(13)	175.70(17)	O(3)-N(3)-C(21)-C(22)	17.5(2)
C(17)-O(1)-C(16)-O(2)	7.4(2)	O(4)-N(3)-C(21)-C(20)	18.2(2)
C(17)-O(1)-C(16)-C(3)	-174.67(14)	O(3)-N(3)-C(21)-C(20)	-160.95(15)
C(2)-C(3)-C(16)-O(2)	-165.97(17)	C(20)-C(21)-C(22)-C(23)	-2.0(3)

N(3)-C(21)-C(22)-C(23)	179.65(15)	C(20)-C(19)-C(24)-C(23)	-2.1(3)
C(21)-C(22)-C(23)-C(24)	2.8(3)	C(4)-C(19)-C(24)-C(23)	177.97(16)
C(22)-C(23)-C(24)-C(19)	-0.8(3)		

Table S-21. Hydrogen bonds for $[C_{24}H_{26}N_3O_5S][Br]$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Br	0.80(2)	2.39(3)	3.186(2)	178(2)

Compound 7i

Table S-22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[C_{23}H_{23}N_2O_3S][Br]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S(1)	-3646(1)	555(1)	-557(1)	25(1)
O(1)	-930(1)	681(1)	-3522(1)	32(1)
O(2)	-2130(1)	59(1)	-4116(1)	42(1)
O(3)	-2310(1)	3891(1)	-3401(1)	30(1)
N(1)	-3723(1)	257(1)	-2058(1)	24(1)
N(2)	-2398(1)	919(1)	-1550(1)	22(1)
C(1)	-3252(2)	571(1)	-1470(1)	23(1)
C(2)	-3233(2)	131(1)	-2729(1)	24(1)
C(3)	-2362(2)	470(1)	-2848(1)	24(1)
C(4)	-1922(2)	1018(1)	-2296(1)	22(1)

C(5)	-2015(2)	1198(1)	-866(1)	24(1)
C(6)	-2608(2)	1050(1)	-288(1)	27(1)
C(7)	-1072(2)	1622(1)	-867(1)	28(1)
C(8)	-790(2)	1936(1)	-98(1)	33(1)
C(9)	85(2)	2447(1)	-122(1)	32(1)
C(10)	788(2)	2445(1)	464(1)	33(1)
C(11)	1565(2)	2937(2)	480(2)	40(1)
C(12)	1672(2)	3437(2)	-98(2)	40(1)
C(13)	983(2)	3444(2)	-684(2)	48(1)
C(14)	189(2)	2963(2)	-692(2)	45(1)
C(15)	-3746(2)	-402(1)	-3238(1)	30(1)
C(16)	-1831(2)	365(1)	-3558(1)	28(1)
C(17)	-402(2)	686(2)	-4226(2)	41(1)
C(19)	-2040(2)	1793(1)	-2574(1)	23(1)
C(20)	-1213(2)	2203(1)	-2758(1)	26(1)
C(21)	-1315(2)	2906(1)	-3031(1)	28(1)
C(22)	-2253(2)	3200(1)	-3127(1)	25(1)

C(23)	-3086(2)	2797(1)	-2949(1)	29(1)
C(24)	-2972(2)	2095(1)	-2677(1)	27(1)
S(31)	1346(1)	4453(1)	4530(1)	28(1)
O(31)	3168(1)	4846(1)	1071(1)	39(1)
O(32)	4402(1)	4363(1)	1759(1)	38(1)
O(33)	2679(1)	1107(1)	1713(1)	29(1)
N(31)	1383(2)	4664(1)	3012(1)	27(1)
N(32)	2691(1)	4070(1)	3627(1)	25(1)
C(31)	1820(2)	4398(1)	3639(1)	26(1)
C(32)	1939(2)	4786(1)	2364(1)	27(1)
C(33)	2830(2)	4468(1)	2312(1)	27(1)
C(34)	3204(2)	3933(1)	2907(1)	25(1)
C(35)	3040(2)	3847(1)	4343(1)	28(1)
C(36)	2390(2)	4010(1)	4878(1)	30(1)
C(37)	4021(2)	3484(1)	4455(1)	33(1)
C(38)	3971(2)	2650(2)	4495(2)	40(1)
C(39)	4982(2)	2315(1)	4570(2)	39(1)

C(40)	5410(5)	2147(4)	5246(2)	126(3)
C(41)	6344(5)	1849(4)	5319(3)	150(4)
C(42)	6891(3)	1720(2)	4704(3)	77(1)
C(43)	6504(4)	1888(3)	4035(3)	102(2)
C(44)	5558(3)	2179(3)	3961(2)	81(1)
C(45)	1442(1)	5305(1)	1824(1)	35(1)
C(46)	3546(1)	4560(1)	1701(1)	30(1)
C(47)	3860(1)	4910(1)	456(1)	48(1)
C(49)	3059(2)	3156(1)	2643(1)	25(1)
C(50)	3827(2)	2802(1)	2276(1)	27(1)
C(51)	3689(2)	2114(1)	1973(1)	27(1)
C(52)	2775(2)	1776(1)	2033(1)	25(1)
C(53)	2009(2)	2114(1)	2413(1)	28(1)
C(54)	2155(2)	2804(1)	2712(1)	28(1)
Br(1)	-5536(1)	-549(1)	-1249(1)	28(1)
Br(31)	-556(1)	5478(1)	3597(1)	29(1)

Table S-23. Bond angles [°] for $[C_{23}H_{23}N_2O_3S][Br]$.

S(1)-C(1)	1.711(2)	C(2)-C(15)	1.499(3)
S(1)-C(6)	1.736(2)	C(3)-C(16)	1.469(3)
O(1)-C(16)	1.351(3)	C(3)-C(4)	1.523(3)
O(1)-C(17)	1.445(3)	C(4)-C(19)	1.518(3)
O(2)-C(16)	1.204(3)	C(4)-H(4)	0.91(3)
O(3)-C(22)	1.364(3)	C(5)-C(6)	1.337(3)
O(3)-H(3O)	0.78(3)	C(5)-C(7)	1.494(3)
N(1)-C(1)	1.345(3)	C(6)-H(6)	0.95(3)
N(1)-C(2)	1.389(3)	C(7)-C(8)	1.527(3)
N(1)-H(1N)	0.85(3)	C(7)-H(7A)	0.96(3)
N(2)-C(1)	1.329(3)	C(7)-H(7B)	1.00(3)
N(2)-C(5)	1.410(3)	C(8)-C(9)	1.513(3)
N(2)-C(4)	1.490(3)	C(8)-H(8A)	1.01(3)
C(2)-C(3)	1.352(3)	C(8)-H(8B)	0.95(3)

C(9)-C(14)	1.396(4)	C(22)-C(23)	1.388(3)
C(9)-C(10)	1.400(4)	C(23)-C(24)	1.389(3)
C(10)-C(11)	1.388(4)	C(23)-H(23)	0.90(3)
C(10)-H(10)	1.03(3)	C(24)-H(24)	0.96(3)
C(11)-C(12)	1.387(4)	S(31)-C(31)	1.715(2)
C(11)-H(11)	1.01(4)	S(31)-C(36)	1.737(3)
C(12)-C(13)	1.386(4)	O(31)-C(46)	1.333(2)
C(12)-H(12)	1.02(3)	O(31)-C(47)	1.451(2)
C(13)-C(14)	1.393(4)	O(32)-C(46)	1.216(2)
C(13)-H(13)	0.98(3)	O(33)-C(52)	1.362(3)
C(14)-H(14)	0.95(3)	O(33)-H(33O)	0.77(3)
C(19)-C(24)	1.388(3)	N(31)-C(31)	1.345(3)
C(19)-C(20)	1.392(3)	N(31)-C(32)	1.397(3)
C(20)-C(21)	1.388(3)	N(31)-H(31N)	0.87(3)
C(20)-H(20)	0.98(3)	N(32)-C(31)	1.324(3)
C(21)-C(22)	1.388(3)	N(32)-C(35)	1.412(3)
C(21)-H(21)	0.92(3)	N(32)-C(34)	1.481(3)

C(32)-C(33)	1.345(3)	C(40)-C(41)	1.382(7)
C(32)-C(45)	1.506(3)	C(40)-H(40)	0.88(5)
C(33)-C(46)	1.471(3)	C(41)-C(42)	1.346(8)
C(33)-C(34)	1.525(3)	C(41)-H(41)	0.71(8)
C(34)-C(49)	1.520(3)	C(42)-C(43)	1.328(6)
C(34)-H(34)	0.88(3)	C(42)-H(42)	1.06(4)
C(35)-C(36)	1.335(3)	C(43)-C(44)	1.390(5)
C(35)-C(37)	1.496(3)	C(43)-H(43)	0.93(5)
C(36)-H(36)	0.94(3)	C(44)-H(44)	0.87(6)
C(37)-C(38)	1.541(4)	C(49)-C(54)	1.391(3)
C(37)-H(37A)	1.02(3)	C(49)-C(50)	1.394(3)
C(37)-H(37B)	1.00(3)	C(50)-C(51)	1.388(3)
C(38)-C(39)	1.504(4)	C(50)-H(50)	0.93(3)
C(38)-H(38A)	1.02(3)	C(51)-C(52)	1.389(3)
C(38)-H(38B)	0.98(3)	C(51)-H(51)	0.92(3)
C(39)-C(44)	1.361(5)	C(52)-C(53)	1.389(3)
C(39)-C(40)	1.362(5)	C(53)-C(54)	1.390(3)

C(53)-H(53)	0.92(3)	C(54)-H(54)	0.97(3)

Table S-24. Bond angles [°] for $[C_{23}H_{23}N_2O_3S][Br]$.

C(16)-O(1)-C(17)	114.59(19)	C(2)-C(3)-C(16)	120.5(2)
C(22)-O(3)-H(3O)	112(2)	C(2)-C(3)-C(4)	122.7(2)
C(1)-N(1)-C(2)	120.68(19)	C(16)-C(3)-C(4)	116.6(2)
C(1)-N(1)-H(1N)	116.7(19)	N(2)-C(4)-C(19)	111.02(17)
C(2)-N(1)-H(1N)	119.5(19)	N(2)-C(4)-C(3)	108.71(17)
C(1)-N(2)-C(5)	113.32(18)	C(19)-C(4)-C(3)	112.11(17)
C(1)-N(2)-C(4)	122.53(18)	N(2)-C(4)-H(4)	105.4(15)
C(5)-N(2)-C(4)	124.13(17)	C(19)-C(4)-H(4)	109.6(16)
N(2)-C(1)-N(1)	121.9(2)	C(3)-C(4)-H(4)	109.7(16)
N(2)-C(1)-S(1)	112.92(16)	C(6)-C(5)-N(2)	111.5(2)
N(1)-C(1)-S(1)	125.12(17)	C(6)-C(5)-C(7)	128.8(2)
C(3)-C(2)-N(1)	118.8(2)	N(2)-C(5)-C(7)	119.62(18)
C(3)-C(2)-C(15)	127.3(2)	C(5)-C(6)-S(1)	112.79(17)
N(1)-C(2)-C(15)	113.86(19)	C(5)-C(6)-H(6)	127.0(16)

S(1)-C(6)-H(6)	120.2(16)	C(11)-C(10)-H(10)	119.8(16)
C(5)-C(7)-C(8)	113.67(19)	C(9)-C(10)-H(10)	118.9(16)
C(5)-C(7)-H(7A)	107.7(15)	C(12)-C(11)-C(10)	120.3(3)
C(8)-C(7)-H(7A)	108.9(16)	C(12)-C(11)-H(11)	120(2)
C(5)-C(7)-H(7B)	107.8(16)	C(10)-C(11)-H(11)	120(2)
C(8)-C(7)-H(7B)	110.4(16)	C(13)-C(12)-C(11)	119.0(2)
H(7A)-C(7)-H(7B)	108(2)	C(13)-C(12)-H(12)	123.7(16)
C(9)-C(8)-C(7)	113.5(2)	C(11)-C(12)-H(12)	117.3(16)
C(9)-C(8)-H(8A)	108.8(17)	C(12)-C(13)-C(14)	120.8(3)
C(7)-C(8)-H(8A)	107.9(17)	C(12)-C(13)-H(13)	121.4(18)
C(9)-C(8)-H(8B)	112.2(16)	C(14)-C(13)-H(13)	117.8(18)
C(7)-C(8)-H(8B)	110.7(16)	C(13)-C(14)-C(9)	120.7(3)
H(8A)-C(8)-H(8B)	103(2)	C(13)-C(14)-H(14)	121(2)
C(14)-C(9)-C(10)	117.8(2)	C(9)-C(14)-H(14)	119(2)
C(14)-C(9)-C(8)	122.0(2)	O(2)-C(16)-O(1)	122.3(2)
C(10)-C(9)-C(8)	120.1(2)	O(2)-C(16)-C(3)	127.1(2)
C(11)-C(10)-C(9)	121.3(2)	O(1)-C(16)-C(3)	110.59(19)

C(24)-C(19)-C(20)	118.8(2)	C(23)-C(24)-H(24)	121.0(17)
C(24)-C(19)-C(4)	120.8(2)	C(31)-S(31)-C(36)	89.36(11)
C(20)-C(19)-C(4)	120.36(19)	C(46)-O(31)-C(47)	114.71(16)
C(21)-C(20)-C(19)	120.7(2)	C(52)-O(33)-H(33O)	114(3)
C(21)-C(20)-H(20)	121.7(16)	C(31)-N(31)-C(32)	120.2(2)
C(19)-C(20)-H(20)	117.6(16)	C(31)-N(31)-H(31N)	114.9(18)
C(22)-C(21)-C(20)	119.6(2)	C(32)-N(31)-H(31N)	119.6(19)
C(22)-C(21)-H(21)	117.2(16)	C(31)-N(32)-C(35)	113.99(18)
C(20)-C(21)-H(21)	123.1(16)	C(31)-N(32)-C(34)	121.15(19)
O(3)-C(22)-C(21)	117.1(2)	C(35)-N(32)-C(34)	124.81(19)
O(3)-C(22)-C(23)	122.5(2)	N(32)-C(31)-N(31)	122.3(2)
C(21)-C(22)-C(23)	120.4(2)	N(32)-C(31)-S(31)	112.58(17)
C(22)-C(23)-C(24)	119.3(2)	N(31)-C(31)-S(31)	125.08(18)
C(22)-C(23)-H(23)	119.0(18)	C(33)-C(32)-N(31)	118.5(2)
C(24)-C(23)-H(23)	121.7(18)	C(33)-C(32)-C(45)	128.8(2)
C(19)-C(24)-C(23)	121.1(2)	N(31)-C(32)-C(45)	112.66(18)
C(19)-C(24)-H(24)	117.9(17)	C(32)-C(33)-C(46)	126.7(2)

C(32)-C(33)-C(34)	121.6(2)	C(35)-C(37)-H(37B)	107.6(16)
C(46)-C(33)-C(34)	111.61(18)	C(38)-C(37)-H(37B)	109.4(16)
N(32)-C(34)-C(49)	111.47(18)	H(37A)-C(37)-H(37B)	111(2)
N(32)-C(34)-C(33)	109.35(18)	C(39)-C(38)-C(37)	111.9(2)
C(49)-C(34)-C(33)	110.84(18)	C(39)-C(38)-H(38A)	109.3(19)
N(32)-C(34)-H(34)	105.3(16)	C(37)-C(38)-H(38A)	105.4(19)
C(49)-C(34)-H(34)	110.8(17)	C(39)-C(38)-H(38B)	111.6(18)
C(33)-C(34)-H(34)	108.9(17)	C(37)-C(38)-H(38B)	108.6(18)
C(36)-C(35)-N(32)	110.9(2)	H(38A)-C(38)-H(38B)	110(3)
C(36)-C(35)-C(37)	126.7(2)	C(44)-C(39)-C(40)	114.5(3)
N(32)-C(35)-C(37)	122.4(2)	C(44)-C(39)-C(38)	122.3(3)
C(35)-C(36)-S(31)	113.15(18)	C(40)-C(39)-C(38)	123.2(3)
C(35)-C(36)-H(36)	126.3(17)	C(39)-C(40)-C(41)	123.5(4)
S(31)-C(36)-H(36)	120.5(17)	C(39)-C(40)-H(40)	113(3)
C(35)-C(37)-C(38)	114.3(2)	C(41)-C(40)-H(40)	122(3)
C(35)-C(37)-H(37A)	107.6(19)	C(42)-C(41)-C(40)	120.3(5)
C(38)-C(37)-H(37A)	106.5(19)	C(42)-C(41)-H(41)	111(7)

C(40)-C(41)-H(41)	127(7)	C(51)-C(50)-C(49)	120.7(2)
C(43)-C(42)-C(41)	118.0(4)	C(51)-C(50)-H(50)	121.0(17)
C(43)-C(42)-H(42)	122(2)	C(49)-C(50)-H(50)	118.3(17)
C(41)-C(42)-H(42)	120(2)	C(50)-C(51)-C(52)	119.7(2)
C(42)-C(43)-C(44)	121.7(4)	C(50)-C(51)-H(51)	121.3(17)
C(42)-C(43)-H(43)	115(3)	C(52)-C(51)-H(51)	118.9(17)
C(44)-C(43)-H(43)	123(3)	O(33)-C(52)-C(51)	117.0(2)
C(39)-C(44)-C(43)	122.1(4)	O(33)-C(52)-C(53)	122.7(2)
C(39)-C(44)-H(44)	115(4)	C(51)-C(52)-C(53)	120.3(2)
C(43)-C(44)-H(44)	121(4)	C(52)-C(53)-C(54)	119.4(2)
O(32)-C(46)-O(31)	122.96(16)	C(52)-C(53)-H(53)	118.7(17)
O(32)-C(46)-C(33)	122.53(17)	C(54)-C(53)-H(53)	121.8(17)
O(31)-C(46)-C(33)	114.45(16)	C(53)-C(54)-C(49)	120.9(2)
C(54)-C(49)-C(50)	118.9(2)	C(53)-C(54)-H(54)	119.0(16)
C(54)-C(49)-C(34)	121.5(2)	C(49)-C(54)-H(54)	120.1(16)
C(50)-C(49)-C(34)	119.4(2)		

Table S-25. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[C_{23}H_{23}N_2O_3S][Br]$. 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)	31(1)	25(1)	19(1)	1(1)	4(1)	0(1)
O(1)	38(1)	33(1)	27(1)	-3(1)	12(1)	-2(1)
O(2)	43(1)	57(1)	27(1)	-14(1)	4(1)	2(1)
O(3)	34(1)	23(1)	32(1)	7(1)	0(1)	1(1)
N(1)	26(1)	24(1)	22(1)	1(1)	2(1)	-2(1)
N(2)	27(1)	22(1)	19(1)	1(1)	2(1)	2(1)
C(1)	28(1)	19(1)	22(1)	3(1)	2(1)	5(1)
C(2)	31(1)	22(1)	20(1)	1(1)	1(1)	5(1)
C(3)	30(1)	22(1)	21(1)	0(1)	1(1)	5(1)
C(4)	26(1)	23(1)	19(1)	1(1)	2(1)	2(1)

C(5)	30(1)	22(1)	20(1)	0(1)	-1(1)	4(1)
C(6)	34(1)	26(1)	20(1)	0(1)	0(1)	2(1)
C(7)	31(1)	30(1)	24(1)	-3(1)	0(1)	-2(1)
C(8)	45(1)	30(1)	22(1)	0(1)	0(1)	-7(1)
C(9)	42(1)	28(1)	27(1)	-4(1)	5(1)	-4(1)
C(10)	33(1)	27(1)	38(1)	1(1)	1(1)	1(1)
C(11)	33(1)	35(1)	53(2)	0(1)	1(1)	1(1)
C(12)	40(1)	34(1)	48(2)	-6(1)	14(1)	-6(1)
C(13)	72(2)	39(2)	33(1)	0(1)	16(1)	-16(1)
C(14)	68(2)	40(2)	27(1)	-1(1)	-1(1)	-14(1)
C(15)	35(1)	30(1)	26(1)	-3(1)	1(1)	0(1)
C(16)	35(1)	25(1)	26(1)	0(1)	4(1)	6(1)
C(17)	48(2)	44(2)	32(1)	2(1)	18(1)	4(1)
C(19)	30(1)	23(1)	16(1)	-1(1)	2(1)	1(1)
C(20)	28(1)	26(1)	24(1)	2(1)	2(1)	2(1)
C(21)	30(1)	27(1)	26(1)	2(1)	3(1)	-4(1)
C(22)	36(1)	21(1)	20(1)	1(1)	0(1)	0(1)

C(23)	28(1)	28(1)	30(1)	4(1)	0(1)	3(1)
C(24)	29(1)	25(1)	28(1)	3(1)	3(1)	-1(1)
S(31)	35(1)	26(1)	24(1)	-3(1)	6(1)	-3(1)
O(31)	38(1)	53(1)	25(1)	4(1)	7(1)	2(1)
O(32)	34(1)	44(1)	36(1)	9(1)	7(1)	-2(1)
O(33)	34(1)	25(1)	30(1)	-5(1)	2(1)	0(1)
N(31)	30(1)	25(1)	27(1)	-2(1)	3(1)	0(1)
N(32)	29(1)	23(1)	23(1)	-2(1)	2(1)	-5(1)
C(31)	31(1)	21(1)	26(1)	-5(1)	4(1)	-6(1)
C(32)	34(1)	25(1)	23(1)	-3(1)	3(1)	-6(1)
C(33)	33(1)	24(1)	24(1)	-1(1)	1(1)	-6(1)
C(34)	25(1)	27(1)	23(1)	-3(1)	4(1)	-4(1)
C(35)	34(1)	26(1)	25(1)	-1(1)	-1(1)	-7(1)
C(36)	37(1)	31(1)	24(1)	0(1)	1(1)	-6(1)
C(37)	34(1)	33(1)	31(1)	2(1)	0(1)	-3(1)
C(38)	43(1)	36(1)	42(2)	7(1)	2(1)	-3(1)
C(39)	47(2)	34(1)	36(1)	0(1)	-2(1)	1(1)

C(40)	152(5)	183(6)	42(2)	-41(3)	-25(3)	125(5)
C(41)	167(6)	196(7)	86(3)	-89(4)	-79(4)	139(6)
C(42)	62(2)	53(2)	115(4)	-14(2)	-22(2)	19(2)
C(43)	89(3)	117(4)	103(4)	62(3)	48(3)	62(3)
C(44)	87(3)	109(3)	48(2)	37(2)	14(2)	52(3)
C(45)	38(1)	39(1)	29(1)	4(1)	-1(1)	1(1)
C(46)	34(1)	30(1)	26(1)	-1(1)	3(1)	-6(1)
C(47)	45(2)	73(2)	25(1)	9(1)	9(1)	2(1)
C(49)	29(1)	25(1)	21(1)	0(1)	2(1)	0(1)
C(50)	27(1)	30(1)	24(1)	1(1)	2(1)	-2(1)
C(51)	29(1)	30(1)	23(1)	-2(1)	3(1)	5(1)
C(52)	34(1)	23(1)	19(1)	0(1)	-1(1)	2(1)
C(53)	29(1)	28(1)	28(1)	-2(1)	4(1)	-3(1)
C(54)	29(1)	27(1)	29(1)	-4(1)	5(1)	0(1)
Br(1)	31(1)	26(1)	26(1)	-1(1)	5(1)	-4(1)
Br(31)	30(1)	24(1)	34(1)	-1(1)	4(1)	1(1)

Table S-26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[C_{23}H_{23}N_2O_3S][Br]$.

	x	y	z	U(eq)
H(3O)	-2860(30)	4017(18)	-3453(18)	46(9)
H(1N)	-4240(20)	19(16)	-1960(15)	32(7)
H(4)	-1272(19)	920(13)	-2217(13)	23(6)
H(6)	-2508(19)	1183(14)	226(15)	31(7)
H(7A)	-1151(19)	2013(15)	-1222(15)	32(7)
H(7B)	-540(20)	1295(16)	-1052(16)	37(7)
H(8A)	-1380(20)	2210(16)	99(17)	42(8)
H(8B)	-698(19)	1559(15)	263(15)	31(7)
H(10)	710(20)	2078(16)	895(16)	40(7)
H(11)	2080(30)	2912(19)	900(20)	63(10)
H(12)	2260(20)	3783(16)	-63(16)	41(8)
H(13)	1030(20)	3796(17)	-1097(18)	50(8)

H(14)	-300(20)	2983(19)	-1080(20)	60(10)
H(15A)	-3268	-763	-3413	68(11)
H(15B)	-4033	-146	-3673	63(10)
H(15C)	-4273	-647	-2961	50(9)
H(17A)	224	948	-4159	61(10)
H(17B)	-805	928	-4614	35(7)
H(17C)	-267	186	-4382	50(9)
H(20)	-560(20)	1976(15)	-2692(15)	33(7)
H(21)	-787(19)	3196(14)	-3143(14)	26(6)
H(23)	-3690(20)	2993(16)	-3028(16)	39(8)
H(24)	-3530(20)	1812(15)	-2530(16)	39(7)
H(33O)	2150(30)	952(19)	1718(19)	49(10)
H(31N)	850(20)	4920(16)	3089(16)	33(7)
H(34)	3840(20)	4023(14)	3003(14)	26(6)
H(36)	2460(20)	3910(15)	5396(17)	37(7)
H(37A)	4300(20)	3655(19)	4960(20)	60(10)
H(37B)	4450(20)	3632(15)	4026(16)	33(7)

H(38A)	3570(20)	2536(18)	4967(19)	57(9)
H(38B)	3620(20)	2471(17)	4046(18)	47(8)
H(40)	4980(40)	2150(30)	5620(30)	112(17)
H(41)	6640(60)	1820(50)	5650(50)	220(40)
H(42)	7600(30)	1480(20)	4760(20)	87(13)
H(43)	6920(30)	1820(30)	3630(30)	111(17)
H(44)	5250(40)	2190(30)	3530(30)	140(20)
H(45A)	1577	5157	1305	55(9)
H(45B)	1700	5796	1909	112(17)
H(45C)	727	5301	1906	66(10)
H(47A)	3513	5091	5	39(7)
H(47B)	4145	4432	348	47(9)
H(47C)	4390	5248	598	61(10)
H(50)	4420(20)	3048(15)	2215(15)	30(7)
H(51)	4190(20)	1874(15)	1733(15)	33(7)
H(53)	1410(20)	1882(15)	2441(15)	33(7)
H(54)	1620(20)	3039(15)	2970(15)	36(7)

Table S-27. Torsion angles [°] for $[C_{23}H_{23}N_2O_3S][Br]$.

C(5)-N(2)-C(1)-N(1)	-178.9(2)	C(1)-N(2)-C(4)-C(19)	105.3(2)
C(4)-N(2)-C(1)-N(1)	2.9(3)	C(5)-N(2)-C(4)-C(19)	-72.7(2)
C(5)-N(2)-C(1)-S(1)	-0.3(2)	C(1)-N(2)-C(4)-C(3)	-18.4(3)
C(4)-N(2)-C(1)-S(1)	-178.5(2)	C(5)-N(2)-C(4)-C(3)	163.5(2)
C(2)-N(1)-C(1)-N(2)	15.7(3)	C(2)-C(3)-C(4)-N(2)	18.7(3)
C(2)-N(1)-C(1)-S(1)	-162.8(2)	C(16)-C(3)-C(4)-N(2)	-166.1(2)
C(6)-S(1)-C(1)-N(2)	0.5(2)	C(2)-C(3)-C(4)-C(19)	-104.4(2)
C(6)-S(1)-C(1)-N(1)	179.1(2)	C(16)-C(3)-C(4)-C(19)	70.8(2)
C(1)-N(1)-C(2)-C(3)	-15.0(3)	C(1)-N(2)-C(5)-C(6)	-0.3(3)
C(1)-N(1)-C(2)-C(15)	163.3(2)	C(4)-N(2)-C(5)-C(6)	177.9(2)
N(1)-C(2)-C(3)-C(16)	-178.6(2)	C(1)-N(2)-C(5)-C(7)	-178.4(2)
C(15)-C(2)-C(3)-C(16)	3.4(3)	C(4)-N(2)-C(5)-C(7)	-0.2(3)
N(1)-C(2)-C(3)-C(4)	-3.5(3)	N(2)-C(5)-C(6)-S(1)	0.7(2)
C(15)-C(2)-C(3)-C(4)	178.5(2)	C(7)-C(5)-C(6)-S(1)	178.6(2)

C(1)-S(1)-C(6)-C(5)	-0.7(2)	C(4)-C(3)-C(16)-O(2)	-166.6(2)
C(6)-C(5)-C(7)-C(8)	-2.0(3)	C(2)-C(3)-C(16)-O(1)	-172.6(2)
N(2)-C(5)-C(7)-C(8)	175.7(2)	C(4)-C(3)-C(16)-O(1)	12.0(3)
C(5)-C(7)-C(8)-C(9)	-172.1(2)	N(2)-C(4)-C(19)-C(24)	-58.5(3)
C(7)-C(8)-C(9)-C(14)	42.5(3)	C(3)-C(4)-C(19)-C(24)	63.3(3)
C(7)-C(8)-C(9)-C(10)	-141.7(2)	N(2)-C(4)-C(19)-C(20)	124.0(2)
C(14)-C(9)-C(10)-C(11)	-0.1(4)	C(3)-C(4)-C(19)-C(20)	-114.2(2)
C(8)-C(9)-C(10)-C(11)	-176.0(2)	C(24)-C(19)-C(20)-C(21)	0.8(3)
C(9)-C(10)-C(11)-C(12)	-1.3(4)	C(4)-C(19)-C(20)-C(21)	178.3(2)
C(10)-C(11)-C(12)-C(13)	1.1(4)	C(19)-C(20)-C(21)-C(22)	-0.5(3)
C(11)-C(12)-C(13)-C(14)	0.5(4)	C(20)-C(21)-C(22)-O(3)	-179.6(2)
C(12)-C(13)-C(14)-C(9)	-1.9(5)	C(20)-C(21)-C(22)-C(23)	0.2(3)
C(10)-C(9)-C(14)-C(13)	1.6(4)	O(3)-C(22)-C(23)-C(24)	179.6(2)
C(8)-C(9)-C(14)-C(13)	177.5(3)	C(21)-C(22)-C(23)-C(24)	-0.2(3)
C(17)-O(1)-C(16)-O(2)	6.1(3)	C(20)-C(19)-C(24)-C(23)	-0.8(3)
C(17)-O(1)-C(16)-C(3)	-172.6(2)	C(4)-C(19)-C(24)-C(23)	-178.3(2)
C(2)-C(3)-C(16)-O(2)	8.8(4)	C(22)-C(23)-C(24)-C(19)	0.5(3)

C(35)-N(32)-C(31)-N(31)	178.2(2)	C(35)-N(32)-C(34)-C(33)	-159.7(2)
C(34)-N(32)-C(31)-N(31)	-4.3(3)	C(32)-C(33)-C(34)-N(32)	-23.6(3)
C(35)-N(32)-C(31)-S(31)	-0.6(2)	C(46)-C(33)-C(34)-N(32)	157.7(2)
C(34)-N(32)-C(31)-S(31)	176.9(2)	C(32)-C(33)-C(34)-C(49)	99.7(2)
C(32)-N(31)-C(31)-N(32)	-17.8(3)	C(46)-C(33)-C(34)-C(49)	-79.0(2)
C(32)-N(31)-C(31)-S(31)	160.9(2)	C(31)-N(32)-C(35)-C(36)	1.1(3)
C(36)-S(31)-C(31)-N(32)	0.0(2)	C(34)-N(32)-C(35)-C(36)	-176.3(2)
C(36)-S(31)-C(31)-N(31)	-178.8(2)	C(31)-N(32)-C(35)-C(37)	-178.3(2)
C(31)-N(31)-C(32)-C(33)	16.8(3)	C(34)-N(32)-C(35)-C(37)	4.3(3)
C(31)-N(31)-C(32)-C(45)	-160.4(2)	N(32)-C(35)-C(36)-S(31)	-1.0(3)
N(31)-C(32)-C(33)-C(46)	-176.3(2)	C(37)-C(35)-C(36)-S(31)	178.3(2)
C(45)-C(32)-C(33)-C(46)	0.4(4)	C(31)-S(31)-C(36)-C(35)	0.6(2)
N(31)-C(32)-C(33)-C(34)	5.2(3)	C(36)-C(35)-C(37)-C(38)	83.5(3)
C(45)-C(32)-C(33)-C(34)	-178.1(2)	N(32)-C(35)-C(37)-C(38)	-97.2(3)
C(31)-N(32)-C(34)-C(49)	-99.8(2)	C(35)-C(37)-C(38)-C(39)	177.2(2)
C(35)-N(32)-C(34)-C(49)	77.4(3)	C(37)-C(38)-C(39)-C(44)	-84.3(4)
C(31)-N(32)-C(34)-C(33)	23.1(3)	C(37)-C(38)-C(39)-C(40)	93.3(5)

C(44)-C(39)-C(40)-C(41)	-1.3(10)	N(32)-C(34)-C(49)-C(54)	39.9(3)
C(38)-C(39)-C(40)-C(41)	-179.1(6)	C(33)-C(34)-C(49)-C(54)	-82.1(3)
C(39)-C(40)-C(41)-C(42)	1.2(13)	N(32)-C(34)-C(49)-C(50)	-144.7(2)
C(40)-C(41)-C(42)-C(43)	0.0(11)	C(33)-C(34)-C(49)-C(50)	93.3(2)
C(41)-C(42)-C(43)-C(44)	-1.0(9)	C(54)-C(49)-C(50)-C(51)	1.0(3)
C(40)-C(39)-C(44)-C(43)	0.3(8)	C(34)-C(49)-C(50)-C(51)	-174.5(2)
C(38)-C(39)-C(44)-C(43)	178.2(4)	C(49)-C(50)-C(51)-C(52)	0.3(3)
C(42)-C(43)-C(44)-C(39)	0.8(9)	C(50)-C(51)-C(52)-O(33)	178.9(2)
C(47)-O(31)-C(46)-O(32)	-0.2(3)	C(50)-C(51)-C(52)-C(53)	-1.8(3)
C(47)-O(31)-C(46)-C(33)	-177.5(1)	O(33)-C(52)-C(53)-C(54)	-178.7(2)
C(32)-C(33)-C(46)-O(32)	166.0(2)	C(51)-C(52)-C(53)-C(54)	2.1(3)
C(34)-C(33)-C(46)-O(32)	-15.3(3)	C(52)-C(53)-C(54)-C(49)	-0.8(3)
C(32)-C(33)-C(46)-O(31)	-16.7(3)	C(50)-C(49)-C(54)-C(53)	-0.7(3)
C(34)-C(33)-C(46)-O(31)	161.9(2)	C(34)-C(49)-C(54)-C(53)	174.7(2)

Table S-28. Hydrogen bonds for $[C_{23}H_{23}N_2O_3S][Br]$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3O)...Br(1)#1	0.78(3)	2.37(3)	3.145(2)	173(3)
N(1)-H(1N)...Br(1)	0.85(3)	2.41(3)	3.218(2)	160(2)
O(33)-H(33O)...Br(31)#2	0.77(3)	2.38(4)	3.139(2)	166(3)
N(31)-H(31N)...Br(31)	0.87(3)	2.35(3)	3.203(2)	166(3)

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