Supporting Information Data for

Sulphonyl thiourea compounds containing pyrimidine as dual inhibitors for I, II, IX, XII carbonic anhydrases and cancer cell lines: Synthesis, characterization and in silico studies

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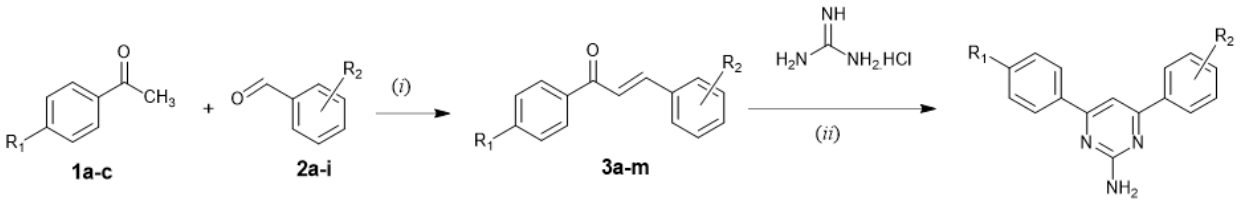
1. General procedure for synthesis of substituted 2-amino-4,6-diarylpyrimidines (4a-m)



1a-c: R_1 = H (**a**), OMe (**b**), Br (**c**).
2a-i: R_2 = H (**a**), 4-F (**b**), 3-OH (**c**), 4-OH (**d**), 4-Cl (**e**), 4-Br (**f**), 4-Me (**g**), 4-*i*Pr (**h**), 4-Me_2 (**i**).

3a-m,**4a-m**:

R_1	R_2	
H	H	(**a**)
H	4-F	(**b**)
H	3-OH	(**c**)
H	4-OH	(**d**)
OMe	4-Cl	(**e**)
OMe	4-Br	(**f**)
OMe	4-Me	(**g**)
OMe	4-^{i}Pr	(**h**)
OMe	4-NMe_2	(**i**)
Br	4-Me	(**j**)
Br	4-^{i}Pr	(**k**)
Br	4-OH	(**l**)
Br	4-NMe_2	(**m**)

These compounds were synthesized according to the literature procedure with the little modification.[1] Firstly, substituted chalcones **3a-m** were prepared by reaction between substituted acetophenones **1a-c** and corresponding substituted benzaldehydes **2a-i** according to literature

procedure and their structures were confirmed by melting points.[1, 2] Then, a reaction mixture of appropriate substituted benzylideneacetophenones (**3a-m**, 10 mmol), guanidine hydrochloride (15 mmol) and sodium hydroxide (45 mmol) were mixed carefully with a little 96% ethanol. Then it was heated under microwave-assisted and solvent-free condition for 1–2 min, the reaction mixture had become dark-yellow. Upon completion, monitored by TLC, the reaction mixture was cooled to room temperature and then triturated with water and the formed precipitate was filtered by suction and washed with water until neutral to afford the titled compounds **4a-m**, recrystallized from 1:1 EtOH-toluene to give ivory-white crystals.

2-Amino-4,6-diphenylpyrimidine (4a)

From *trans*-benzylideneacetophenone **3a** (0.005 mol, 1.04 g). M.p.: 118–119°C. Ref.:[1] 118–119°C. Yield: 0.96 g (78%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.22–8.20 (m, 4H, J=3.5 Hz, H-3' & H5' and H-3"& H-5"), 7.70 (s, 1H, H-5), 7.53–7.52 (m, 6H, J=3.0 Hz, H-2', H=4' & H-6' and H-2", H=4" & H-6"). ^{13}C NMR (150 MHz, DMSO-d_6), δ (ppm): 161.8 (C-2 pyrimidine), 158.5, 136.3, 129.5, 128.8 (4C), 127.2 (4C), 108.4 (C-5 pyrimidine).

2-Amino-4-(4-fluorophenyl)-6-phenylpyrimidine (4b)

From *trans*-2-(4-fluorobenzylidene)acetophenone **3b** (0.005 mol, 1.13 g). M.p.: 132–133°C. Ref.:[1] 132–133°C. Yield: 1.13 g (85%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.29 (dd, J= 7.0 Hz, J_{HF} =10.5 Hz, 2H, H-3" & H-5"), 8.23–8.21 (m, 2H, H-3' & H-5'), 7.71 (s, 1H, H-5), 7.53–7.52 (m, 3H, H-2', H-4' & H6'), 7.35 (t, J=7.0 Hz, J_{HF} =2.5 Hz, 2H, H-2" & H-6"), 6.73 (s, 2H, NH_2). ^{13}C NMR (150 MHz, DMSO-d_6) δ 164.6, 162.9, 162.0 (C-2 pyrimidine), 159.1, 158.5, 136.2, 130.6, 130.6, 129.6, 128.7 (2C), 127.97 & 127.92 (J_{CF} = 7.95 Hz), 127.5 (2C), 115.7 & 115.6 (J_{CF} = 19.95 Hz), 108.4 (C-5 pyrimidine).

2-Amino-4-(3-hydroxyphenyl)-6-phenylpyrimidine (4c)

From *trans*-(3-hydroxybenzylidene)acetophenone **3d** (0.005 mol, 1.34 g). M.p.: 231–232°C. Yield: 1.03 g (78%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 9.59 (s, 1H, OH), 8.20–8.18 (m, 2H, J=2.75 Hz, H-3" & H-5"), 7.61 (s, 1H, J=1.0 Hz, H-2'), 7.60 (m, 1H, J=7.5 Hz & 4.5 Hz, H-4'), 7.59 (s, 1H, H-5), 7.52-7.51 (t, 3H, J=3.25 Hz, H-2", H=4" & H-6"), 7.30 (t, 1H, J=2.75 Hz, H-6'), 6.91 (ddd, 1H, J=8.0 Hz, 2.5 Hz & 1.0 Hz, H-5'), 6.675 (s, 2H, NH_2). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.5 (C-2 pyrimidine), 158.7, 158.7, 157.7, 136.2, 134.0, 130.0, 129.6, 128.7 (2C), 127.5 (2C), 119.0, 117.4, 112.3, 108.5 (C-5 pyrimidine).

2-Amino-4-(4-Hydroxyphenyl)-6-phenylpyrimidine (4d)

From *trans*-(4-hydroxybenzylidene)acetophenone **3c** (0.005 mol, 1.34 g). M.p.: 239–240°C. Yield: 0.99 g (75%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 9.90 (s, 1H, OH), 8.19–8.17 (m, 2H, *J*=2.25 Hz, H-3" & H-5"), 8.08 (d, 2H, *J*=9.0 Hz, H-3' & H5'), 7.59 (s, 1H, H-5), 7.51–7.50 (m, 3H, *J*=2.5 Hz, H-2", H=4" & H-6"), 6.87 (d, 2H, *J*=8.5 Hz, H-2' & H6'), 6.60 (s, 2H, NH_2). ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm): 162.0 (C-2 pyrimidine), 159.1, 158.8, 158.5, 136.2, 129.6, 128.7, 128.7 (2C), 128.6 (2C), 127.5 (2C), 115.8 (2C), 108.4 (C-5 pyrimidine).

2-Amino-4-(4-chlorophenyl)-6-(4-methoxyphenyl)pyrimidine (4e)

From *trans*-2-(4-chlorobenzylidene)-4′-methoxyacetophenone **3e** (0.005 mol, 1.36 g). M.p.: 156–157°C. Yield: 1.33 g (85%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.29–8.28 (m. 2H. H-2" & H-6"). 8.22 (d. *J* =9.0 Hz, 2H, H-2' H6'), 7.72 (s, 1H, H-5), 7.57–7.54 (m, 2H, H-3" & H-5"), 7.06 (d, *J* =9.0 Hz, H-3' & H-5'), 6.71 (s, 2H, NH_2), 3.84 (s, 3H, 4'-OCH_3). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.1, 158.7, 158.6, 136.1, 131.8, 129.1, 128.7 (2C), 128.6 (2C), 128.5 (2C), 114.0 (2C), 108.9 (C-5 pyrimidine), 55.3 (4-OCH_3 phenyl).

2-Amino-4-(4-bromophenyl)-6-(4-methoxyphenyl)pyrimidine (4f)

From *trans*-2-(4-bromobenzylidene)-4′-methoxyacetophenone **3f** (0.005 mol, 1.58 g). M.p.: 170–171°C. Yield: 1.39 g (78%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.20 (d, *J* = 8.5 Hz, 2H, H-2" & H-6"), 8.17 (d, *J* =8.5 Hz, 2H, H2' & H-6'), 7.71 (d, *J* =8.5 Hz, 2H, H-3" & H-5"), 7.68 (s, 1H, H-5), 7.06 (d, *J* =8.5 Hz, 2H, H-3' & H-5'), 6.69 (s, 2H, NH_2), 3.84 (s, 3H, 4'-OCH_3). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.1, 158.5, 158.0, 132.0, 131.5 (2C), 128.6 (2C), 128.2, 127.8 (2C), 121.9, 114.0 (2C), 108.8 (C-5 pyrimidine), 55.3 (4-OCH_3 phenyl).

2-Amino-4-(4-methylphenyl)-6-(4-methoxyphenyl)pyrimidine (4g)

From *trans*-2-(4-methylbenzylidene)-4′-methoxyacetophenone **3g** (0.005 mol, 1.26 g). M.p.: 125–126°C. Yield: 1.18 g (81%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.20 (d, *J* =9.0 Hz, 2H, H-2' & H6'), 8.11 (d, *J* = 8.0 Hz, 2H, H-2" & H-6"), 7.61 (s, 1H, H-5), 7.31 (d, *J* = 8.0 Hz, 2H, H-3" & H-5"), 7.05 (d, *J* = 9.0 Hz, 2H, H-3' & H-5'), 6.60 (s, 2H, NH_2), 3.84 (s, 3H, 4'-OCH_3), 2.50 (s, 3H, 4"-CH_3). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.1, 158.6, 158.3, 140.1, 131.7, 129.1, 129.0 (2C), 128.5 (2C), 127.5 (2C), 114.0 (2C), 108.6 (C-5 pyrimidine), 55.3 (4-OCH_3 phenyl), 21.2 (4-CH_3 phenyl).

2-Amino-4-(4-isopropylphenyl)-6-(4-methoxyphenyl)pyrimidine (4h)

From *trans*-2-(4-isopropylbenzylidene)-4′-methoxyacetophenone **3h** (0.005 mol, 1.40 g). M.p.: 126–127°C. Yield: 1.29 g (81%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.18 (d, J = 9.0 Hz, 2H, H-2' & H6'), 7.05 (d, J = 9.0 Hz, 2H, H-3' & H-5'), 8.13 (d, J = 8.0 Hz, 2H, H-2" & H-6"), 7.61 (s, 1H, H-5), 7.37 (d, J = 8.0 Hz, 2H, H-3" & H-5"), 6.60 (s, 2H, NH_2), 3.84 (s, 3H, 4'-OCH_3), 2.96 [t, J = 7.0 Hz, 1H, 4"-**CH**$(CH_3)_2$], 1.24 [t, J =7.0 Hz, 6H, 4"-CH**(CH$_3$)$_2$**]. ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.2, 158.3, 158.3, 147.1, 132.8, 129.6, 128.6 (2C), 128.3 (2C), 125.6 (2C), 114.0 (2C), 108.4 (C-5 pyrimidine), 55.3 (4-OCH_3 phenyl), 33.7 [4-**CH**$(CH_3)_2$], 23.9 [4-CH**(CH$_3$)$_2$**].

2-Amino-4-(4-dimethylaminophenyl)-6-(4-methoxyphenyl)pyrimidine (4i)

From *trans*-2-(4-dimethylaminobenzylidene)-4′-methoxyacetophenone **3i** (0.005 mol, 1.41 g). M.p.: 175–176°C. Yield: 1.26 g (79%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.17 (d, J = 9.0 Hz, 2H, H-2' & H6'), 8.08 (d, J = 9.0 Hz, 2H, H-2" & H-6"), 7.51 (s,1H, H-5), 7.05 (d, J = 9.0 Hz, 2H, H-3' & H-5'), 6.79 (d, J = 9.0 Hz, 2H, H-3" & H-5"), 6.42 (s, 2H, NH_2), 3.00 [s, 6H, 4"-$N(CH_3)_2$], 3.83 (s, 3H, 4'-OCH_3). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.2, 158.3, 158.1, 151.5, 129.6, 128.8, 128.6 (2C), 128.5 (2C), 114.0 (2C), 112.2 (2C), 108.3 (C-5 pyrimidine), 55.3 (4-OCH_3 phenyl), 40.3 (4-$N(CH_3)_2$].

2-Amino-4-(4-bromophenyl)-6-(4-methylphenyl)pyrimidine (4j)

From *trans*-2-(4-methylbenzylidene)-4′-bromoacetophenone ***3J*** (0.005 mol, 1.51 g). M.p.: 152–153°C. Yield: 75%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.18 (d, J = 8.5 Hz, 2H, H-2' & H6'), 8.13 (d, J = 8.0 Hz, 2H, H-2" & H-6"), 7.71 (d, J = 8.5 Hz, 2H, H-3' & H-5'), 7.70 (s, 1H, H-5), 7.32 (d, J = 8.0 Hz, 2H, H-3" & H-5"), 6.74 (s, 2H, NH_2), 2.37 (s, 3H, 4"-CH_3). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 158.6, 158.4, 140.4, 131.9, 131.6, 131.5 (2C), 129.0 (2C), 128.1 (2C), 127.8 (2C), 121.6, 108.3 (C-5 pyrimidine), 21.2 (4-CH_3 phenyl).

2-Amino-4-(4-bromophenyl)-6-(4-isopropylphenyl)pyrimidine (4k)

From *trans*-2-(4-isopropylbenzylidene)-4′-bromoacetophenone **3k** (0.005 mol, 1.65 g). M.p.: 155-156°C. Yield: 1.31 g (71%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.14 (d, J = 8.25 Hz, 2H, H-2" & H-6"), 8.17 (d, J = 8.5 Hz, 2H, H-2' & H-6'), 7.72 (d, J = 8.5 Hz, 2H, H-3' & H-5'), 7.38 (d, J = 8.25 Hz, 2H, H-3" & H-5"), 7.69 (s, 1H, H-5), 6.74 (s, 2H, NH_2), 2.96 [t, J =7.75 Hz, 1H, 4"-**CH**$(CH_3)_2$], 1.24 [t, J = 7.75 Hz, 6H, 4"-CH**(CH$_3$)$_2$**]. ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.8 (C-2 pyrimidine), 157.3, 157.3, 147.2, 132.3, 132.3, 131.5 (2C), 128.5 (2C), 128.0 (2C), 125.6 (2C), 121.7, 108.5 (C-5 pyrimidine), 33.7 [4-**CH**$(CH_3)_2$], 23.9 [4-CH**(CH$_3$)$_2$**].

2-Amino-4-(4-bromophenyl)-6-(4-hydroxyphenyl)pyrimidine (4l)

From *trans*-2-(4-hydroxybenzylidene)-4′-bromoacetophenone **3l** (0.005 mol, 1.52 g). M.p.: 187–189°C. Yield: 1.30 g (76%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.19 (d, J = 8.5 Hz, 2H, H-2' & H6'), 7.80 (d, J = 7.5 Hz, 2H, H-2" & H-6"), 7.73 (d, J = 8.5 Hz, 2H, H-3' & H-5'), 7.72 (s, 1H, H-5), 7.43 (d, J = 7.5 Hz, 2H, H-3" & H-5"), 6.78 (s, 2H, NH_2). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.1 (C-2 pyrimidine), 159.3, 158.8, 158.6, 131.9, 131.5 (2C), 129.0 (2C), 127.8 (2C), 127.7, 121.6, 115.8 (2C), 108.4 (C-5 pyrimidine).

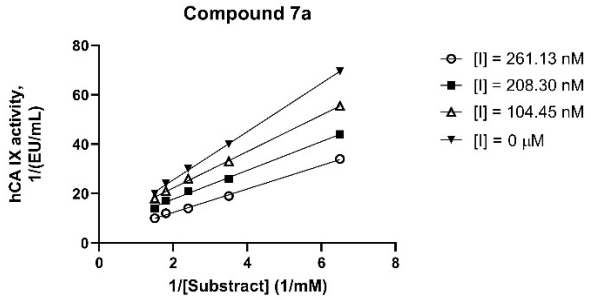
2-Amino-4-(4-bromophenyl)-6-(4-dimethylaminophenyl)pyrimidine (4m)

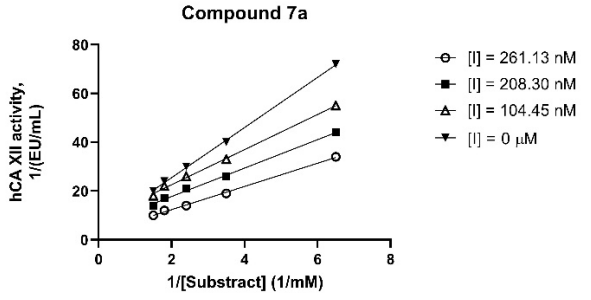
From *trans*-2-(4-dimethylaminobenzylidene)-4′-bromoacetophenone **3l** (0.005 mol, 1.65 g). M.p.: 184–186°C. Yield: 1.38 g (75%). ^{1}H NMR (500 MHz, DMSO-d_6), δ (ppm): 8.15 (d, J = 8.5 Hz, 2H, H-2' & H6'), 8.10 (d, J = 8.75 Hz, 2H, H-2" & H-6"), 7.70 (d, J = 8.5 Hz, 2H, H-3' & H-5'), 7.59 (s, 1H, H-5), 6.78 (d, , J = 8.75 Hz, 2H, H-3" & H-5"), 6.55 (s, 2H, NH_2), 3.00 [s, 6H, 4"-N(CH_3)$_2$]. ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.8 (C-2 pyrimidine), 157.9, 157.3, 151.5, 132.3, 131.5 (2C), 128.5 (2C), 128.2 (2C), 128.0, 121.7 (2C), 112.1, 108.5 (C-5 pyrimidine), 40.3 [4-N(CH_3)$_2$].

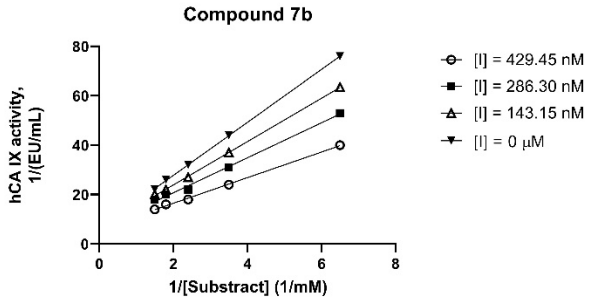
References

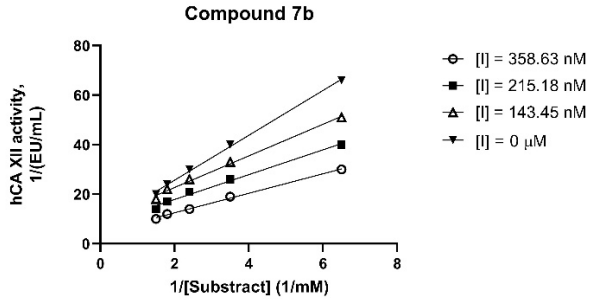
1. N. D. Thanh and N. T. T. Mai, *Carbohydrate Research*, 2009, **344**, 2399-2405.
2. N. A. A. Elkanzi, H. Hrichi, R. A. Alolayan, W. Derafa, F. M. Zahou and R. B. Bakr, *ACS Omega*, 2022, **7**, 27769-27786.

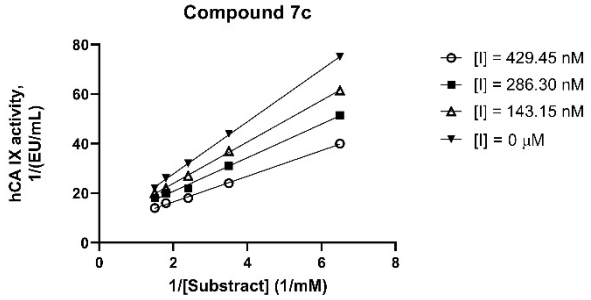
2. Lineweaver-Burk plots for sulphonyl thiourea compounds 7a-m

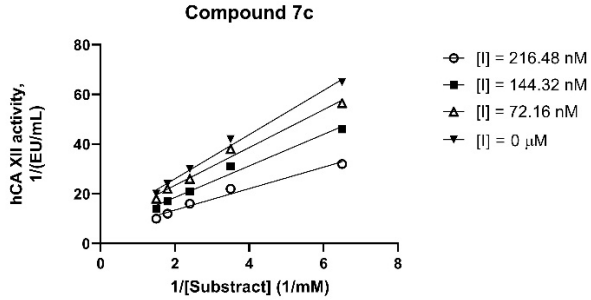


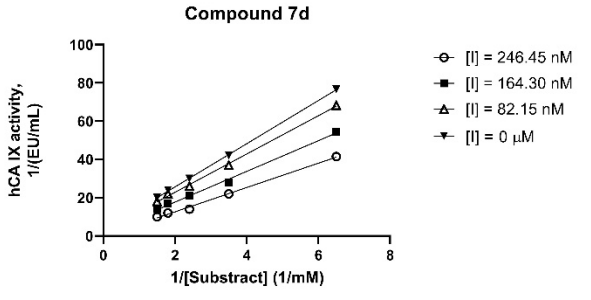


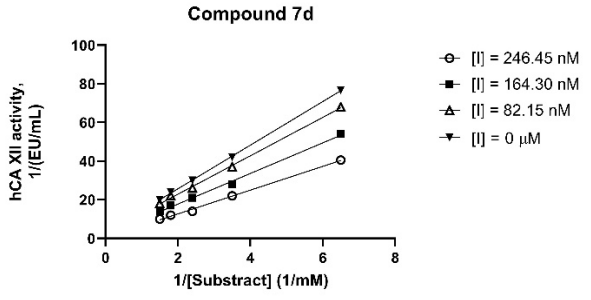


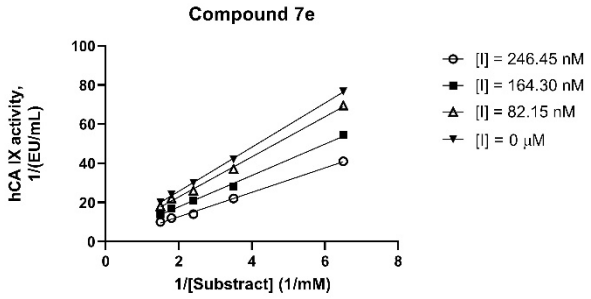











Compound 7e
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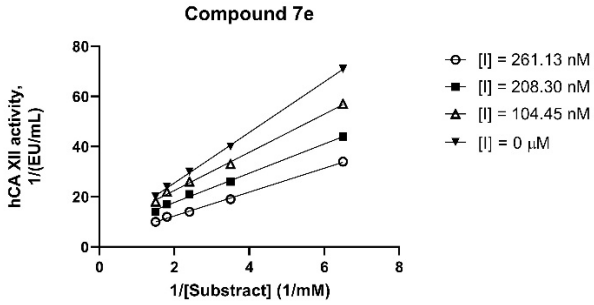
[I] = 164.30 nM
[I] = 82.15 nM
[I] = 0 μM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[I] = 104.45 nM
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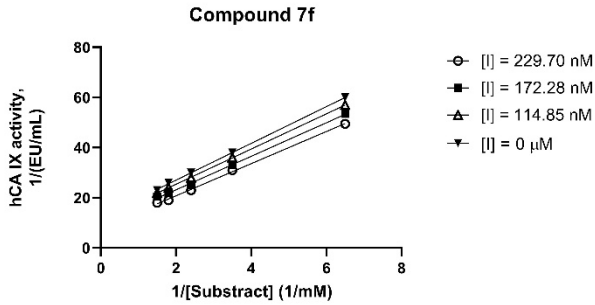
Compound 7f
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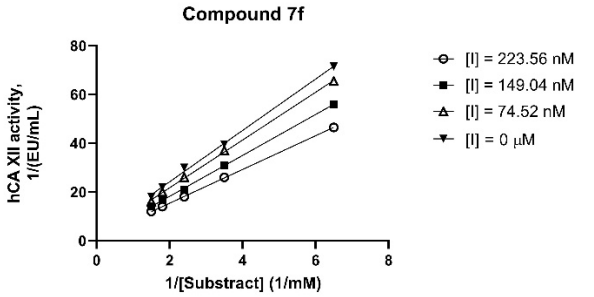
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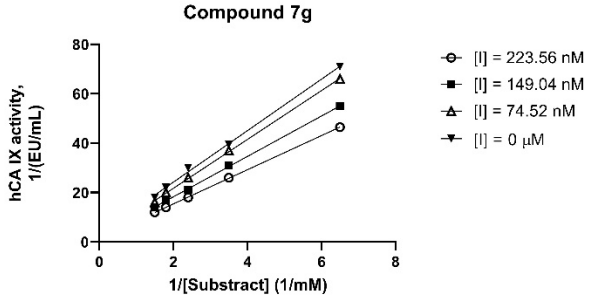
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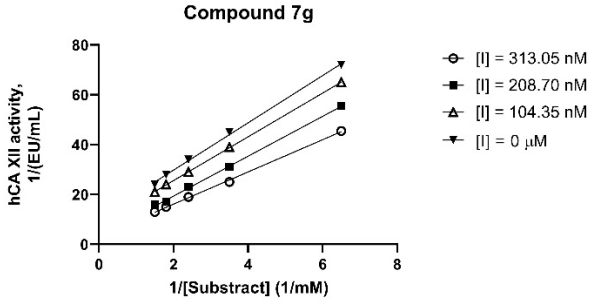
[I] = 0 μM


Compound 7g
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1/[Substract] (1/mM)
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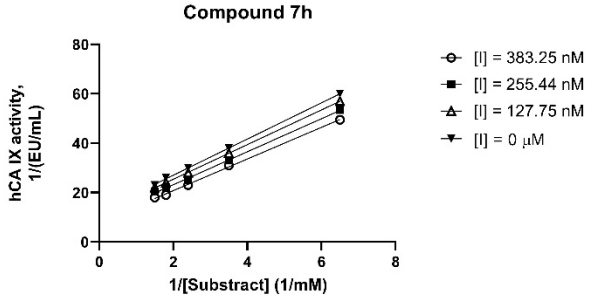
[I] = 208.70 nM
[I] = 104.35 nM
[I] = 0 μM


Compound 7h
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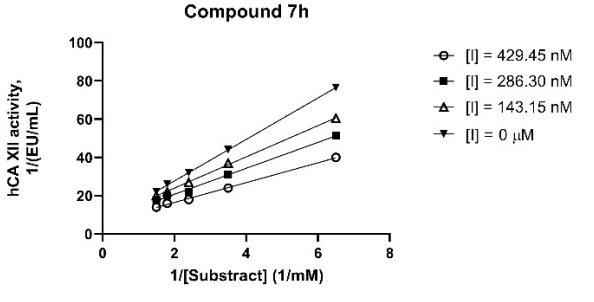
1/[Substract] (1/mM)
[I] = 383.25 nM
[I] = 255.44 nM
[I] = 127.75 nM
[I] = 0 μM


Compound 7h
hCA XII activity, 1/(EU/mL)
1/[Substract] (1/mM)
[I] = 429.45 nM
[I] = 286.30 nM
[I] = 143.15 nM
[I] = 0 μM

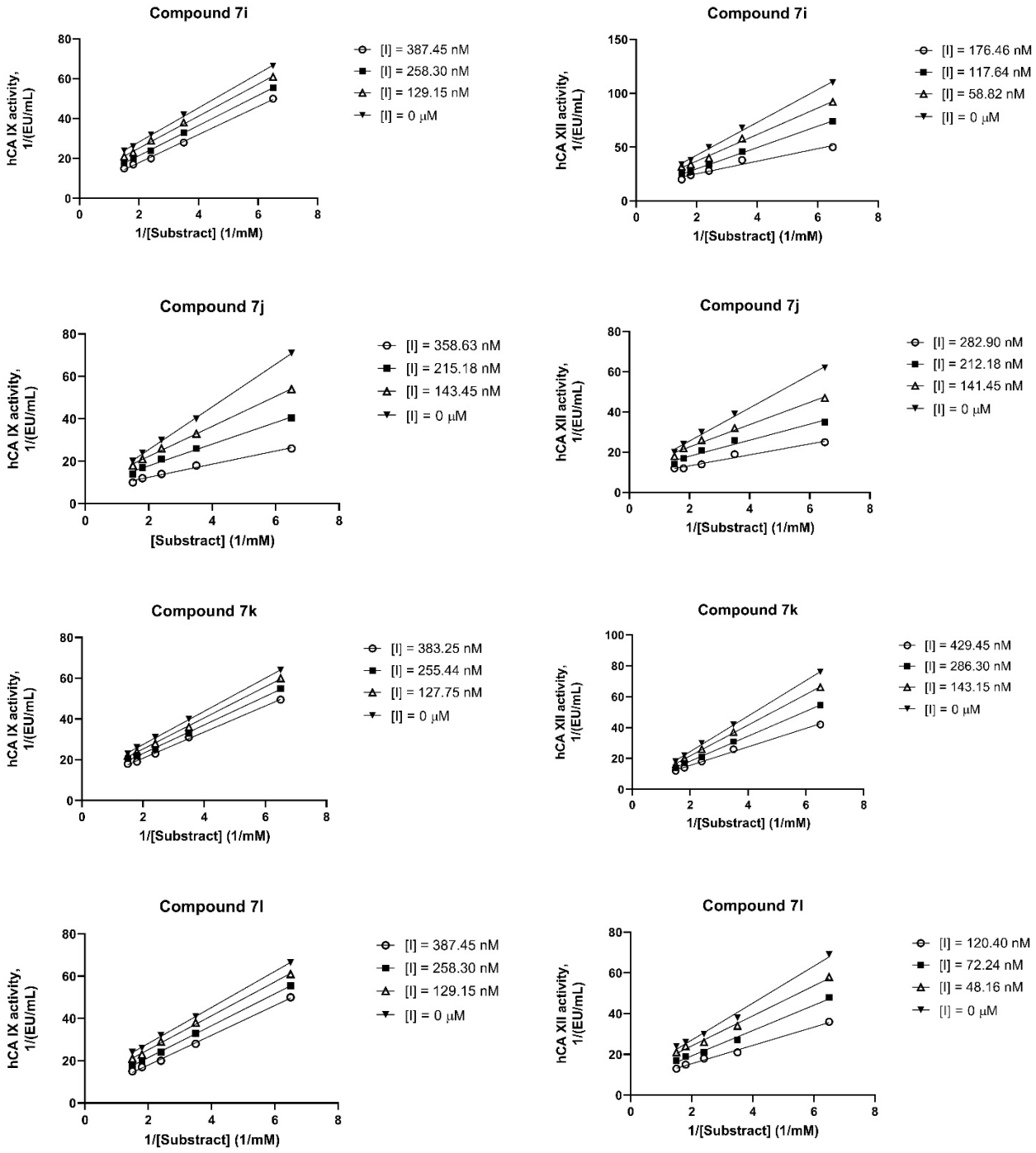


Figure S1. Lineweaver-Burk plots for compounds **7a-m.**

3. Molecular docking simulations

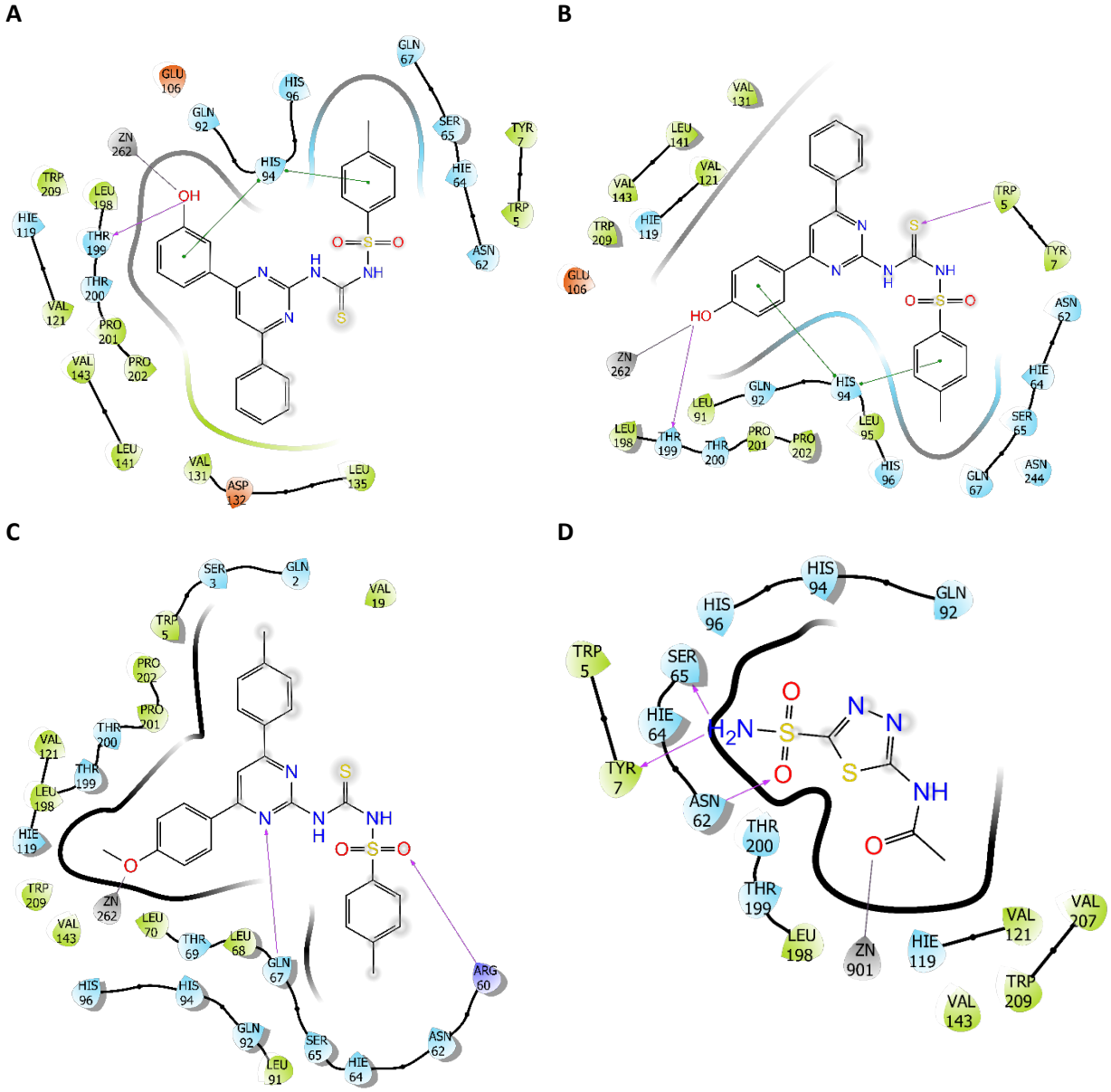


Figure S2. 2D Representations for the interacting mode and the settlement of the most potent sulphonyl thiourea ligands in the active pocket of enzyme 3IAI. The hydrogen bonds, π-π stacking and interaction with zinc(II) ion were shown. (A) **7c** (R_1 = H, R_2 = 3-OH), (B) **7d** (R_1 = H, R_2 = 4-OH), **7g** (R_1 = 4-OMe, R_2 = 4-Me), and cocrystal AZA.

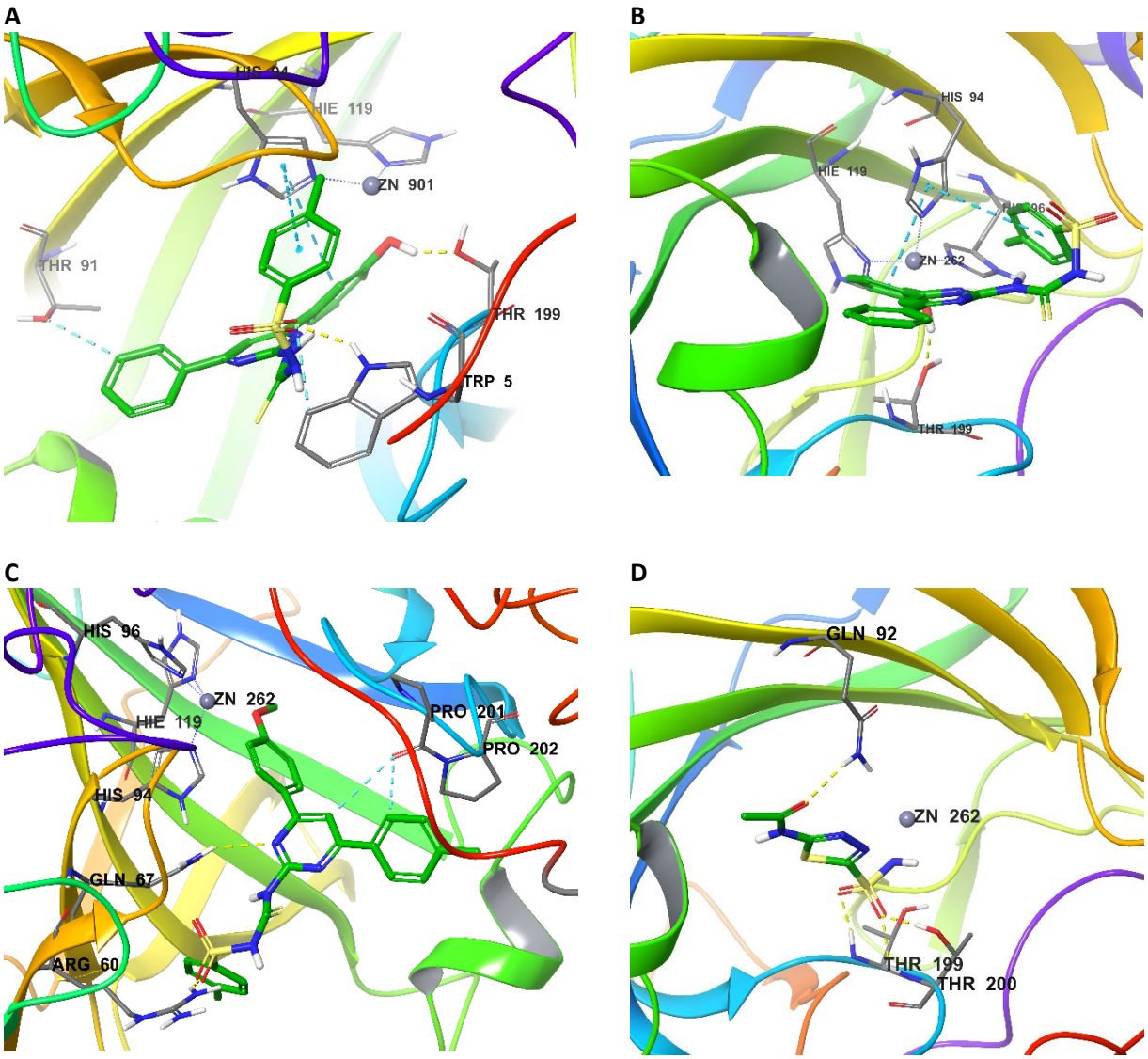


Figure S3. 3D Representation for the interacting mode and the settlement of the most potent sulphonyl thiourea ligands in the active pocket of enzyme 3IAI. The hydrogen bonds, π-π stacking and interaction with zinc(II) ion were shown. (A) **7c** (R_1 = H, R_2 = 3-OH), (B) **7d** (R_1 = H, R_2 = 4-OH), **7g** (R_1 = 4-OMe, R_2 = 4-Me), and cocrystal AZA.

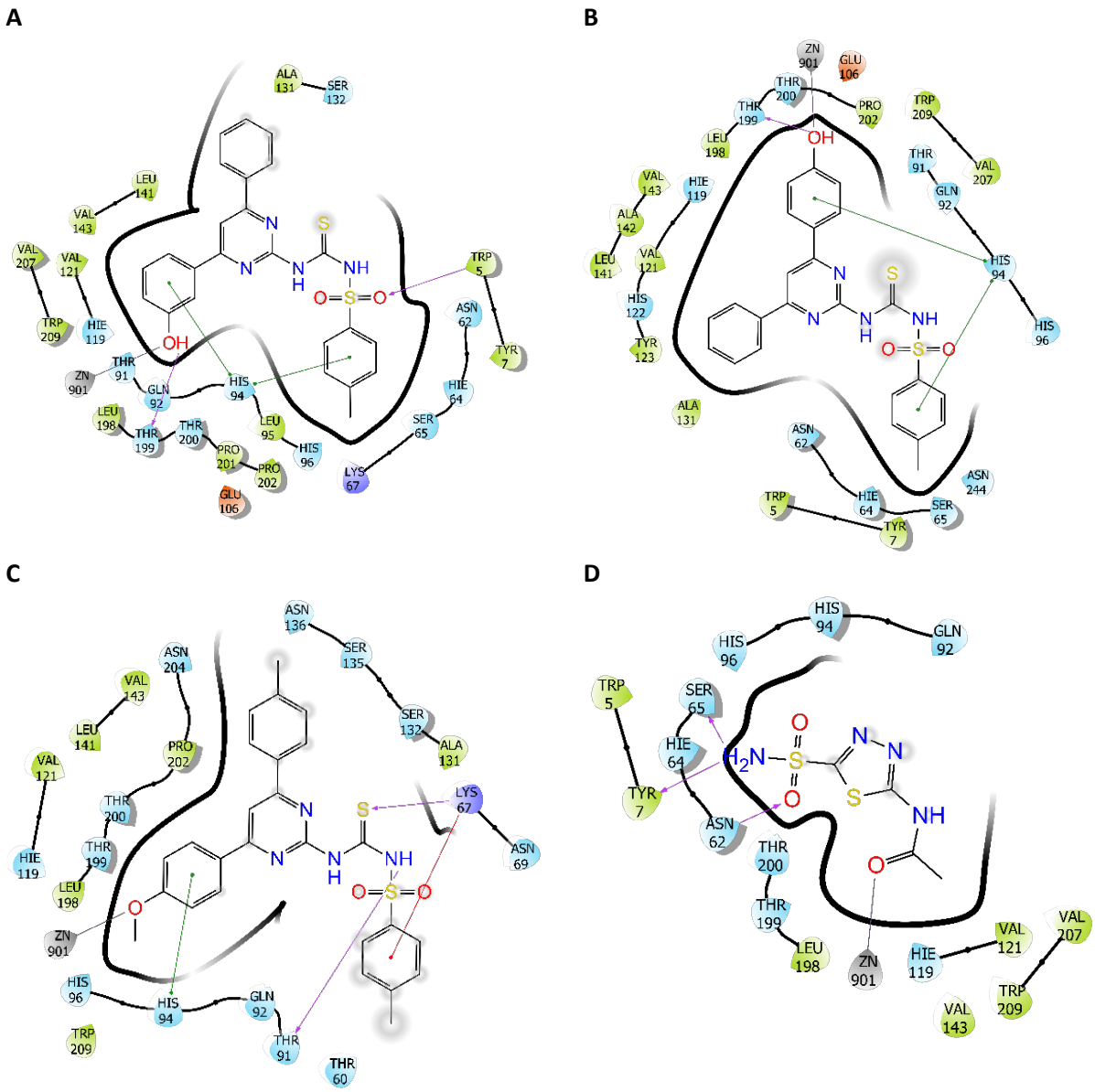


Figure S4. 2D Representations for the interacting mode and the settlement of the most potent sulphonyl thiourea ligands in the active pocket of enzyme 1JD0. The hydrogen bonds, π-π stacking and interaction with zinc(II) ion were shown. (A) **7c** (R_1 = H, R_2 = 3-OH), (B) **7d** (R_1 = H, R_2 = 4-OH), **7g** (R_1 = 4-OMe, R_2 = 4-Me), and cocrystal AZA.

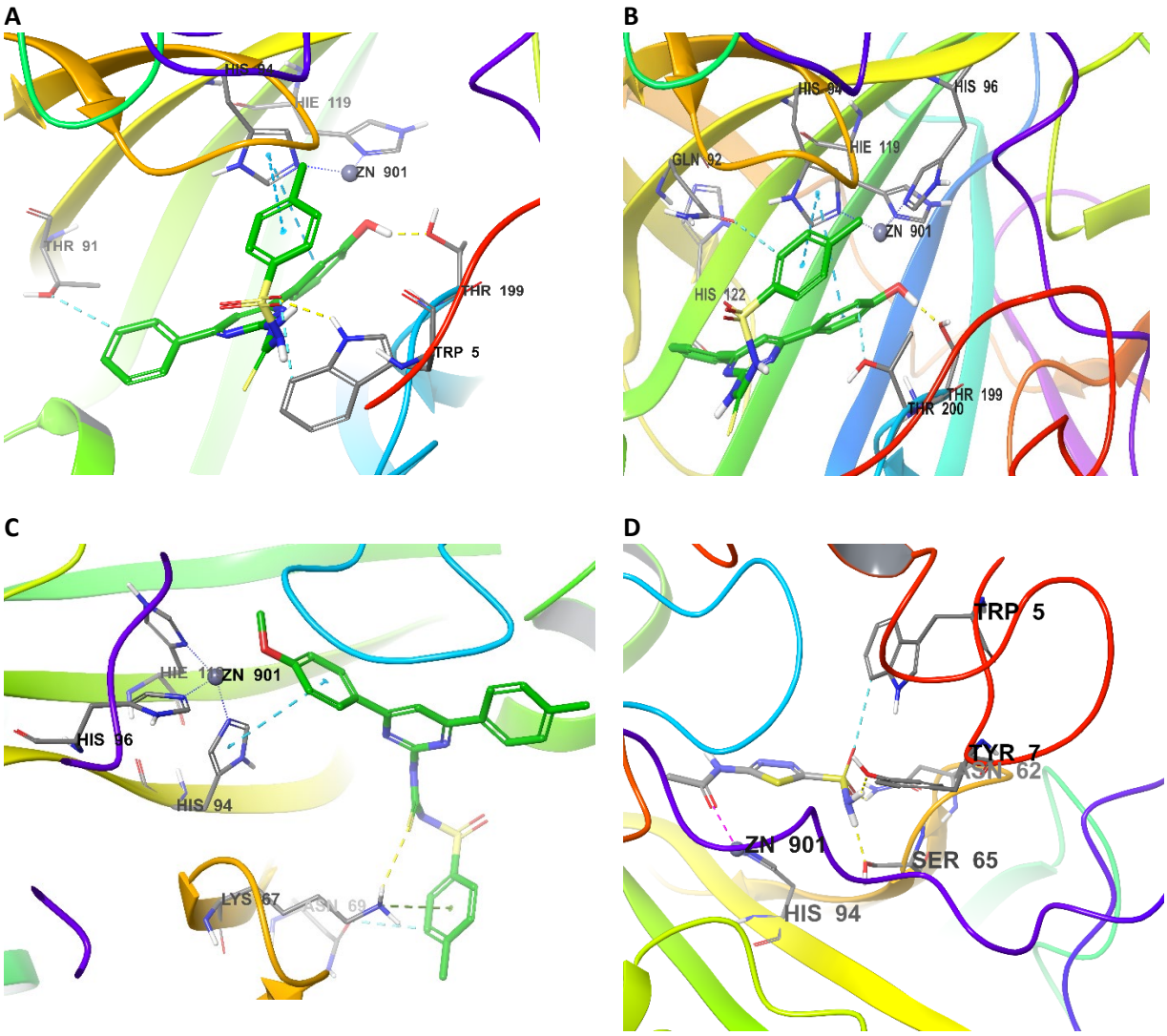
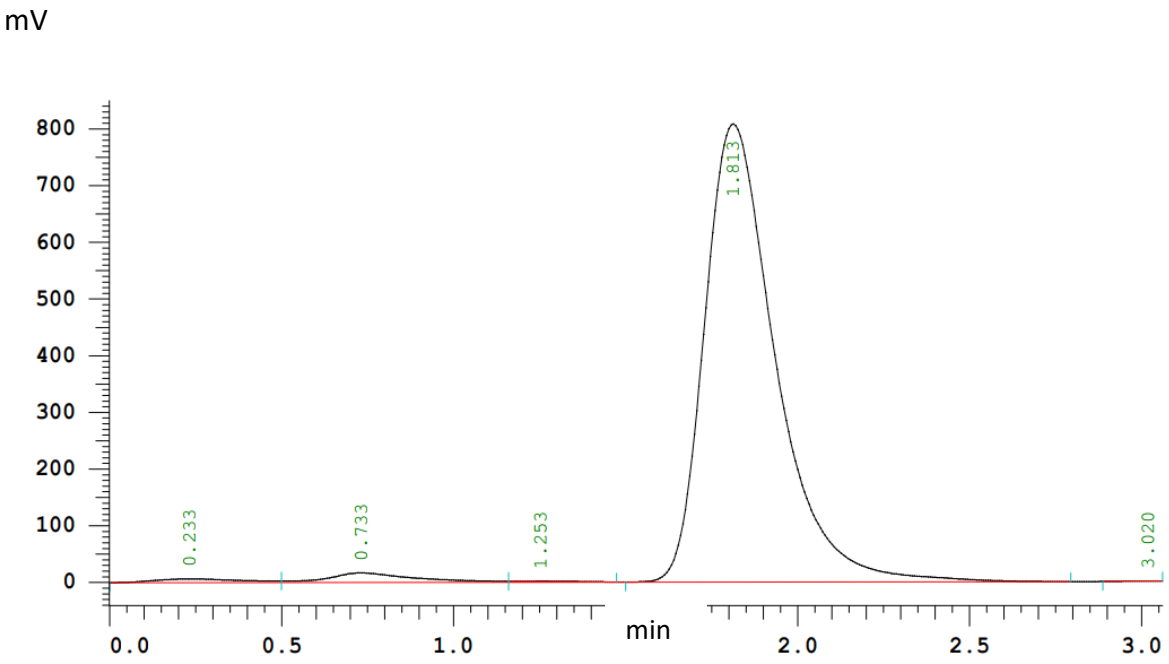


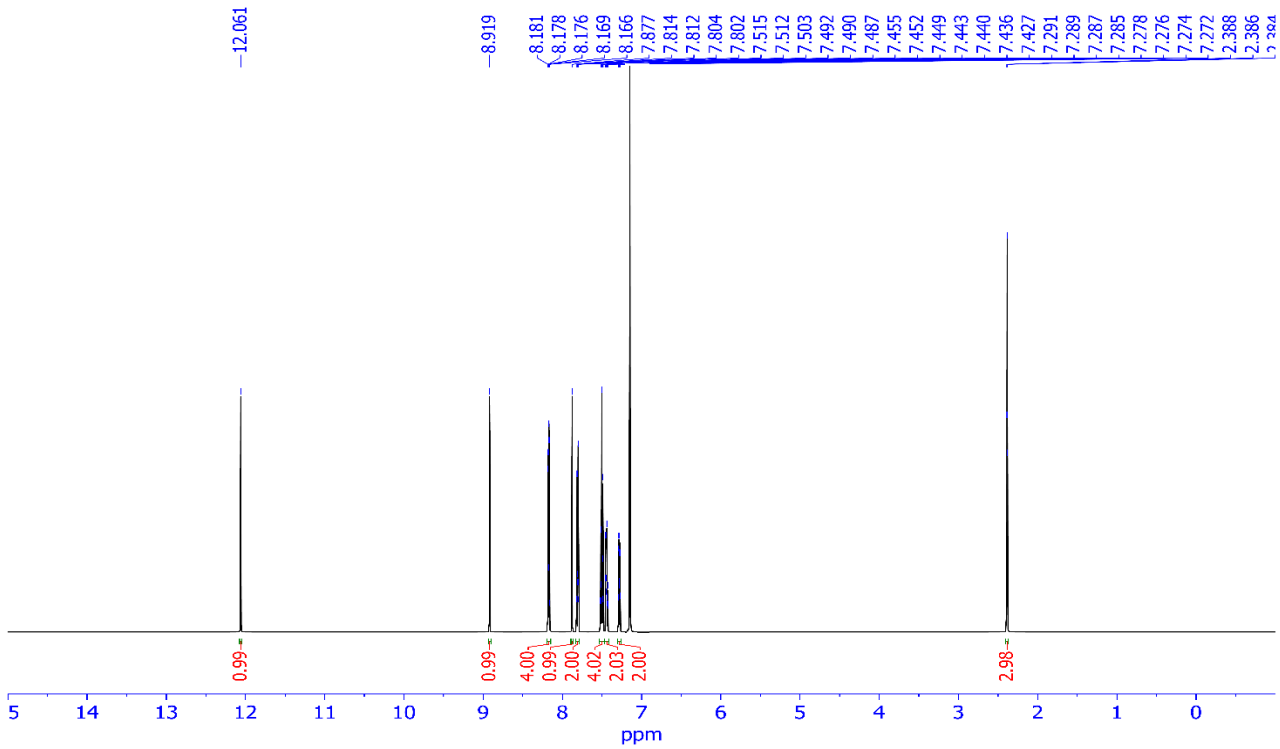
Figure S5. 3D Representation for the interacting mode and the settlement of the most potent sulphonyl thiourea ligands in the active pocket of enzyme 1JD0. The hydrogen bonds, π-π stacking and interaction with zinc(II) ion were shown. (A) **7c** (R_1 = H, R_2 = 3-OH), (B) **7d** (R_1 = H, R_2 = 4-OH), **7g** (R_1 = 4-OMe, R_2 = 4-Me), and cocrystal AZA.

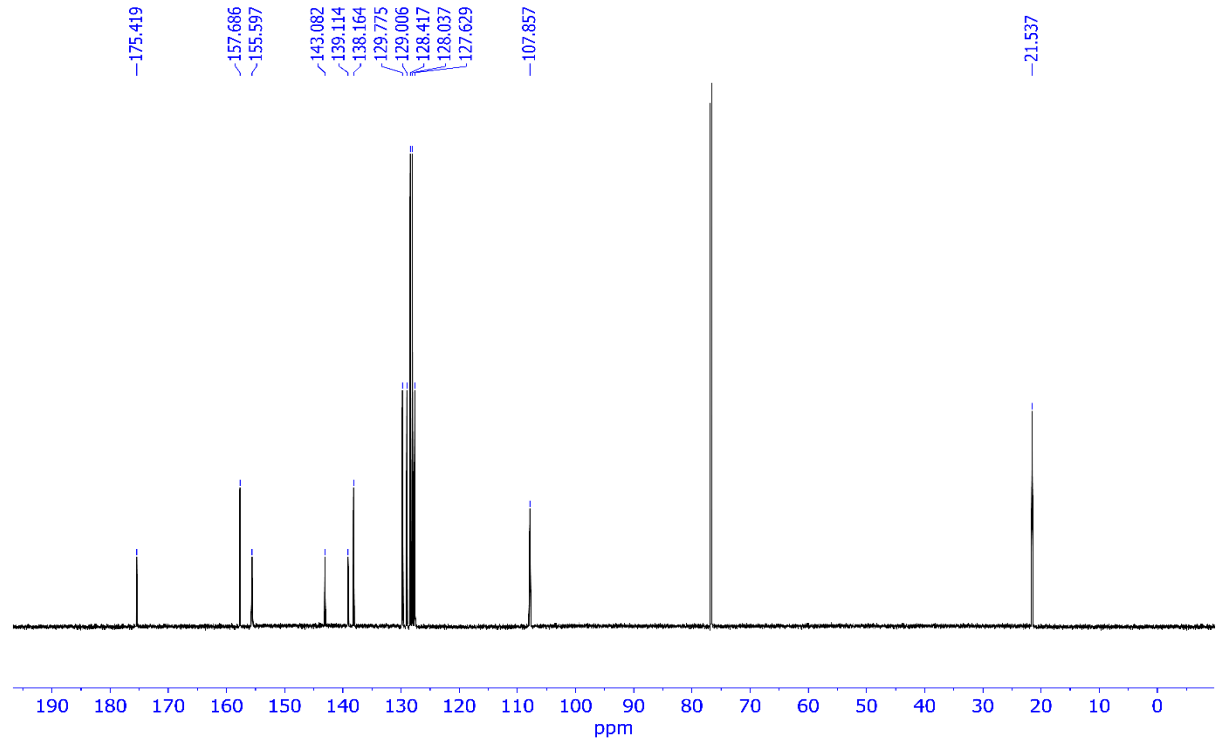
4. HPLC, NMR, and MS spectra of synthesized of 2-aminodiarylpyrimidine sulphonyl thiourea derivatives (7a-m)

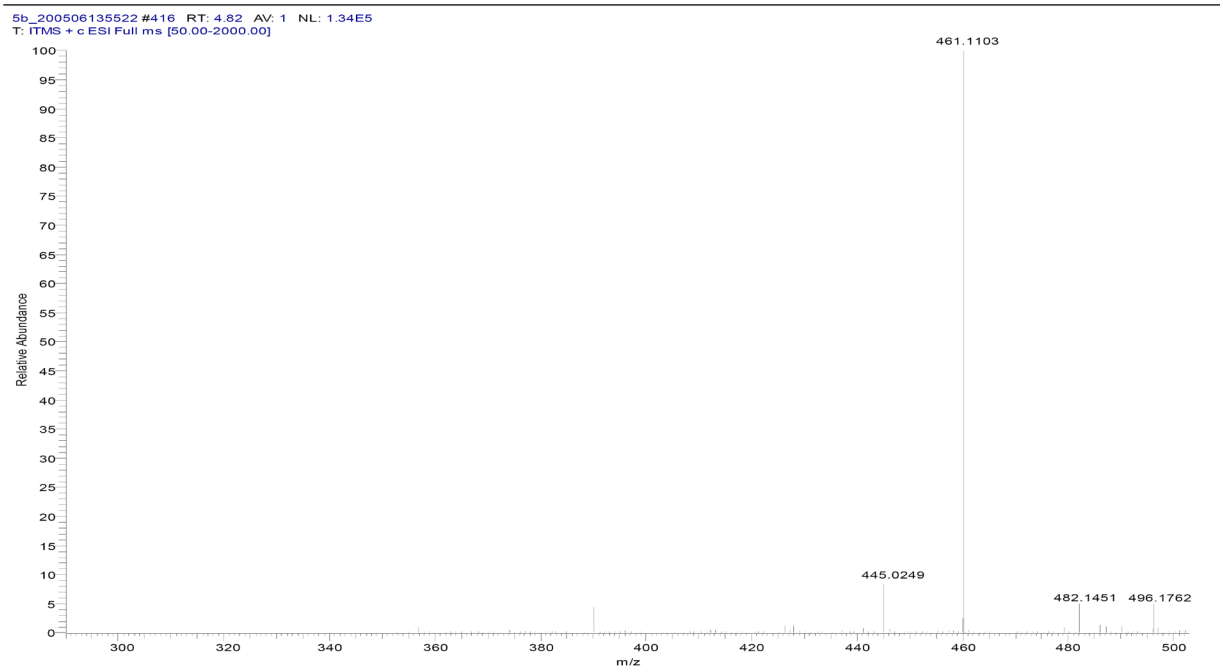
*N-((4,6-Diphenylpyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7a**)*

No.	RT	Area (%)	Concentration (%)	BC
1	0.233	117269	0.979	BV
2	0.733	310345	2.590	VV
3	1.253	6941	0.058	VB
4	1.813	11543559	96.355	TBB
5	3.020	2091	0.017	BB
		11980205	100.00	



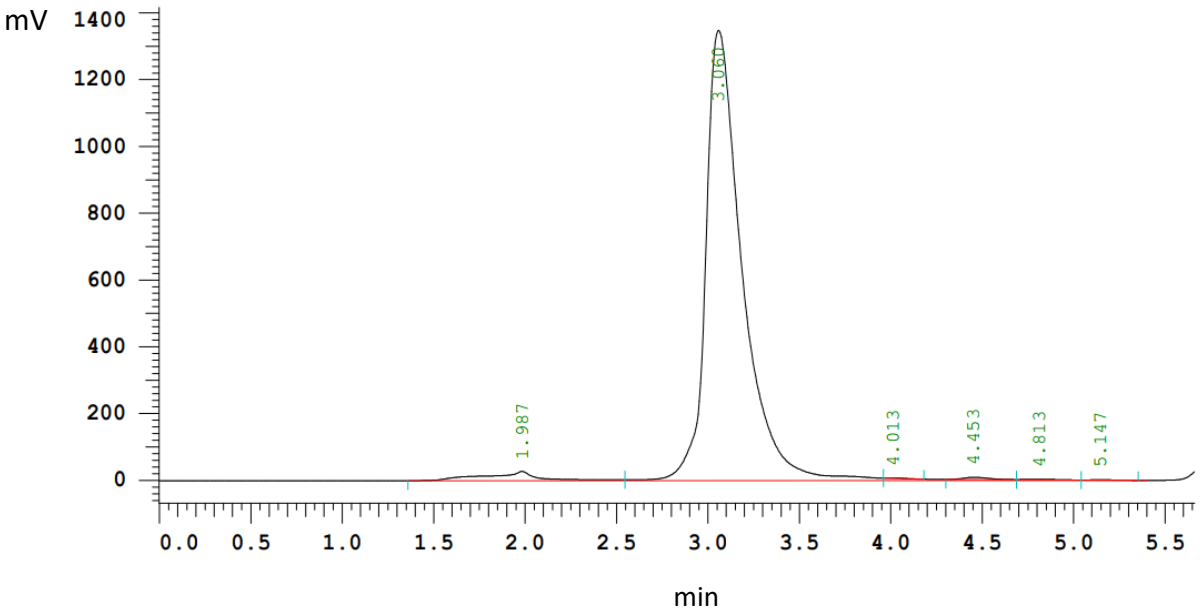

12.061
8.919
8.181
8.178
8.176
8.169
8.166
7.877
7.814
7.812
7.804
7.802
7.515
7.512
7.503
7.492
7.490
7.487
7.455
7.452
7.449
7.443
7.440
7.436
7.427
7.291
7.289
7.287
7.285
7.278
7.276
7.274
7.272
2.388
2.386
0.99
0.99
4.00
0.99
2.00
4.02
2.03
2.00
2.98
5
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

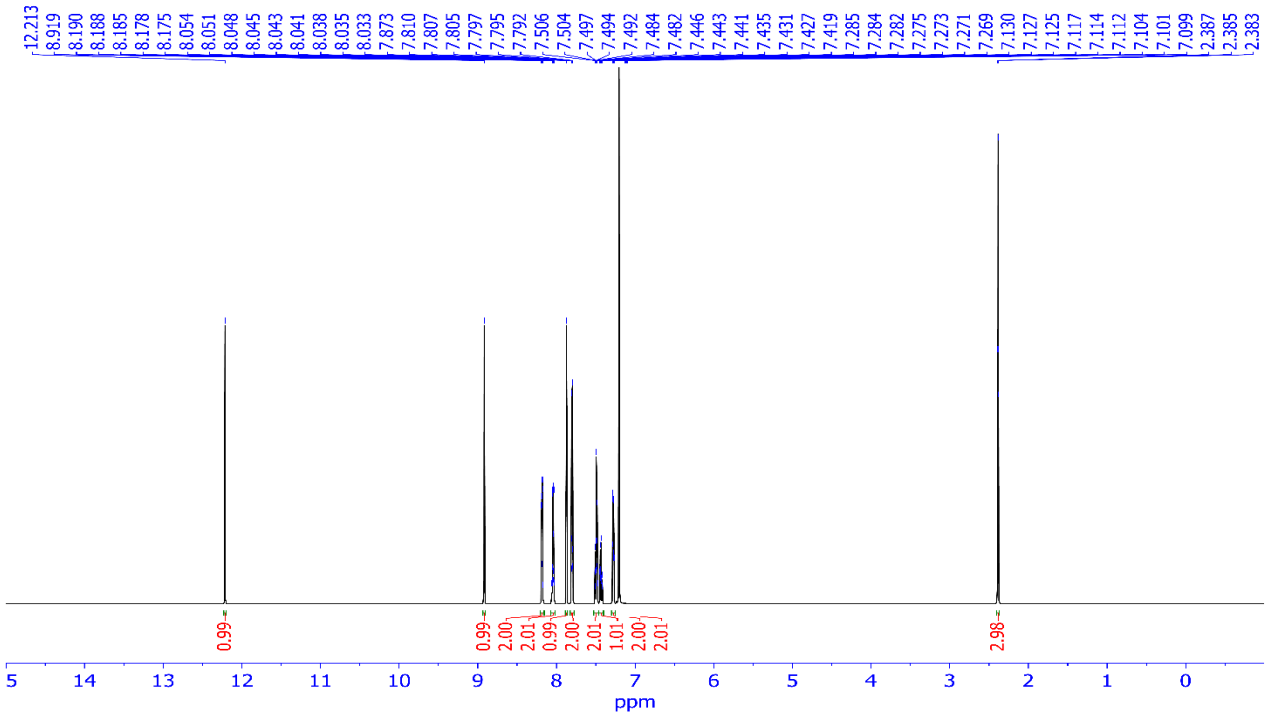

175.419
157.686
155.597
143.082
139.114
138.164
129.775
129.006
128.417
128.037
127.629
107.857
21.537
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



*N-((4-(4-Fluorophenyl)-6-phenylpyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7b**)*

No.	RT	Area (%)	Concentration (%)	BC
1	1.987	579340	2.964	BV
2	3.060	18864396	96.529	VV
3	4.013	8213	0.042	TBB
4	4.453	65138	0.333	TBV
5	4.813	16684	0.085	TVV
6	5.147	8858	0.045	TVB
		19542647	100.00	

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8.190
8.188
8.185
8.178
8.175
8.054
8.051
8.048
8.045
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8.041
8.038
8.035
8.033
7.873
7.810
7.807
7.805
7.797
7.795
7.792
7.506
7.504
7.497
7.494
7.492
7.484
7.482
7.446
7.443
7.441
7.435
7.431
7.427
7.419
7.285
7.284
7.282
7.275
7.273
7.271
7.269
7.130
7.127
7.125
7.117
7.114
7.112
7.104
7.101
7.099
2.387
2.385
2.383
0.99
0.99
2.00
2.01
0.99
2.00
2.01
1.01
2.00
2.01
2.98
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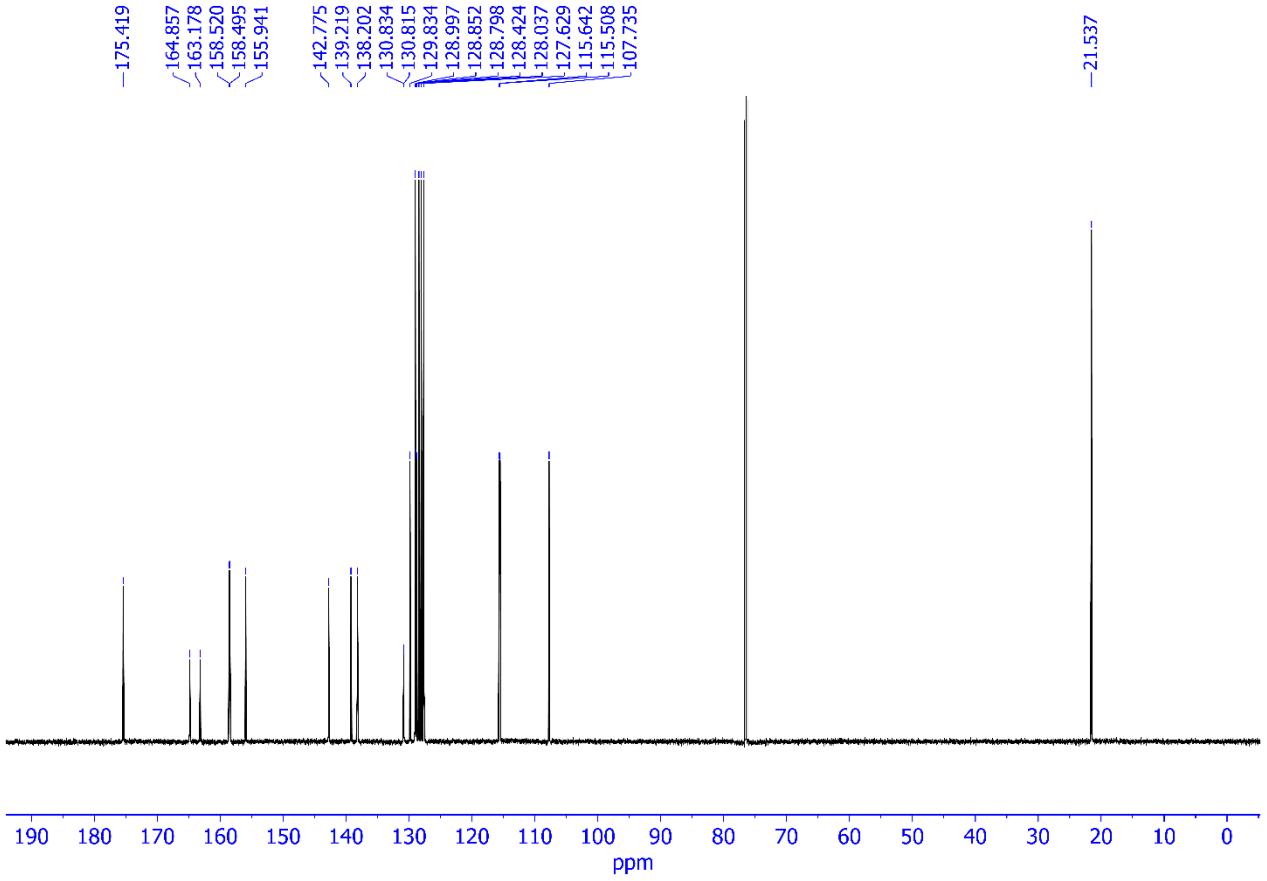
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm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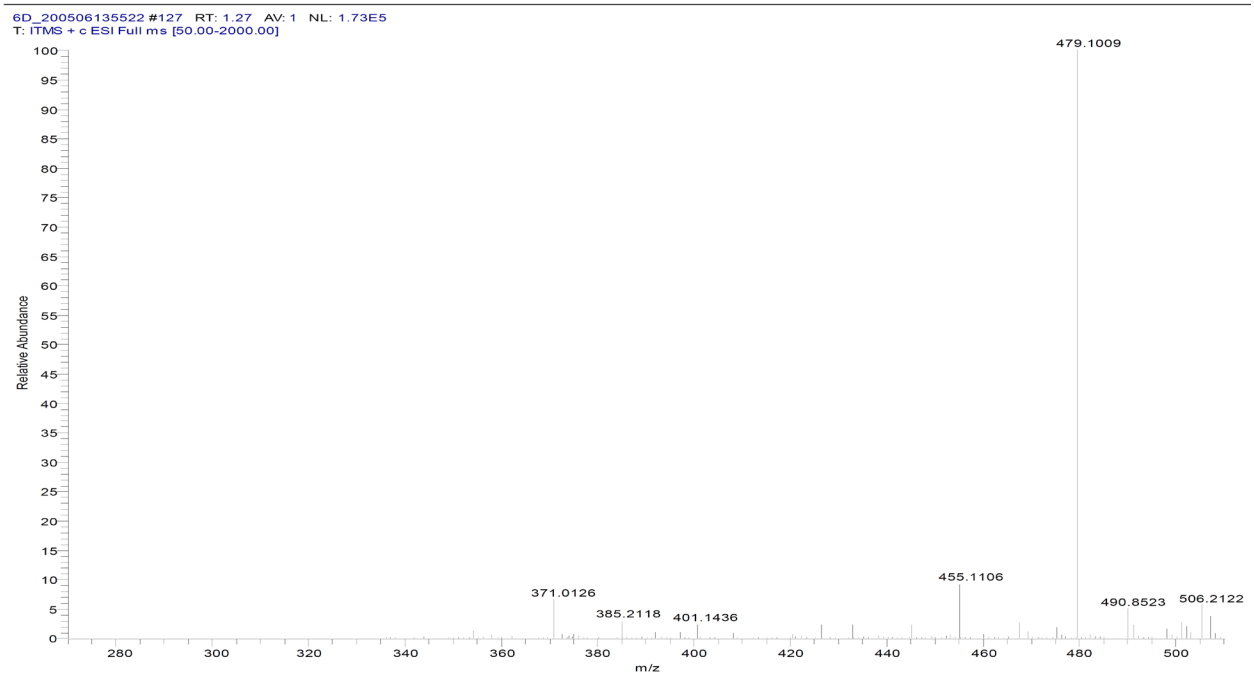
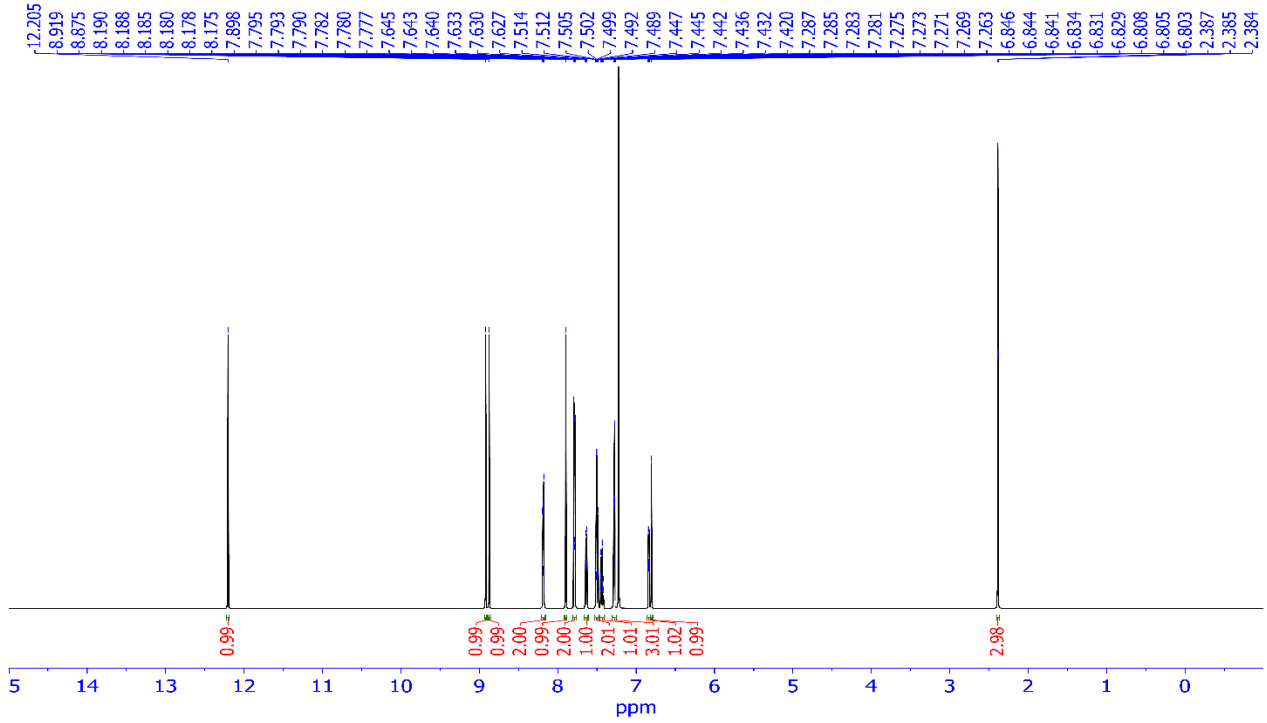
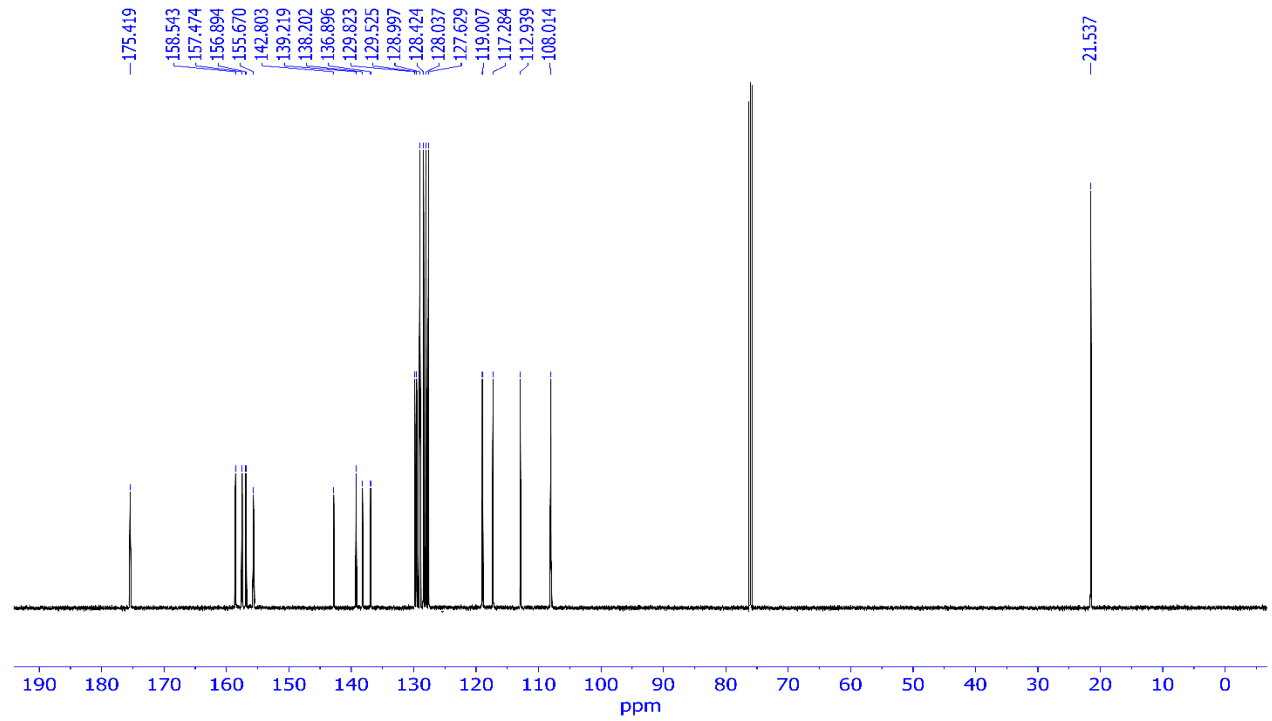
163.178
158.520
158.495
155.941
142.775
139.219
138.202
130.834
130.815
129.834
128.997
128.852
128.798
128.424
128.037
127.629
115.642
115.508
107.735
21.537
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



*N-((4-(3-Hydroxyphenyl)-6-phenylpyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7c**)*

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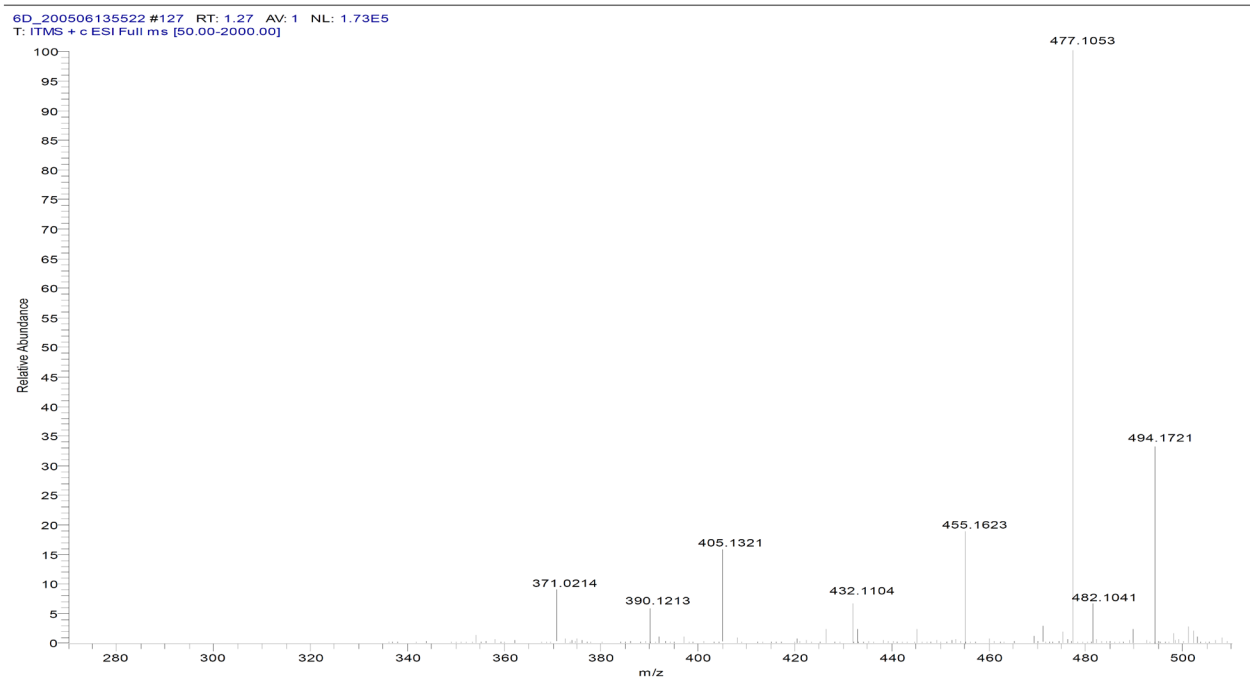
158.543
157.474
156.894
155.670
142.803
139.219
138.202
136.896
129.823
129.525
128.997
128.424
128.037
127.629
119.007
117.284
112.939
108.014
21.537
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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T: ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
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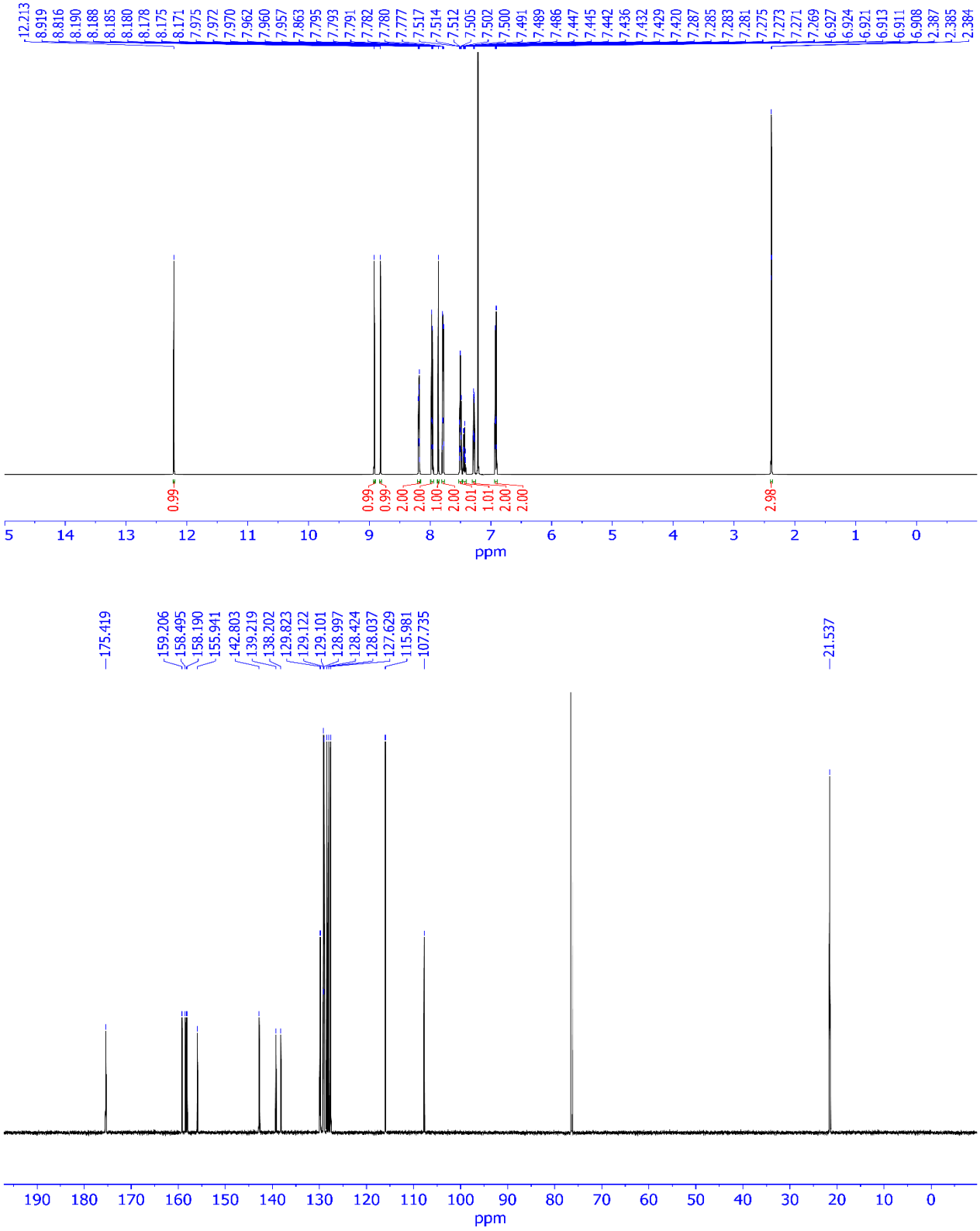
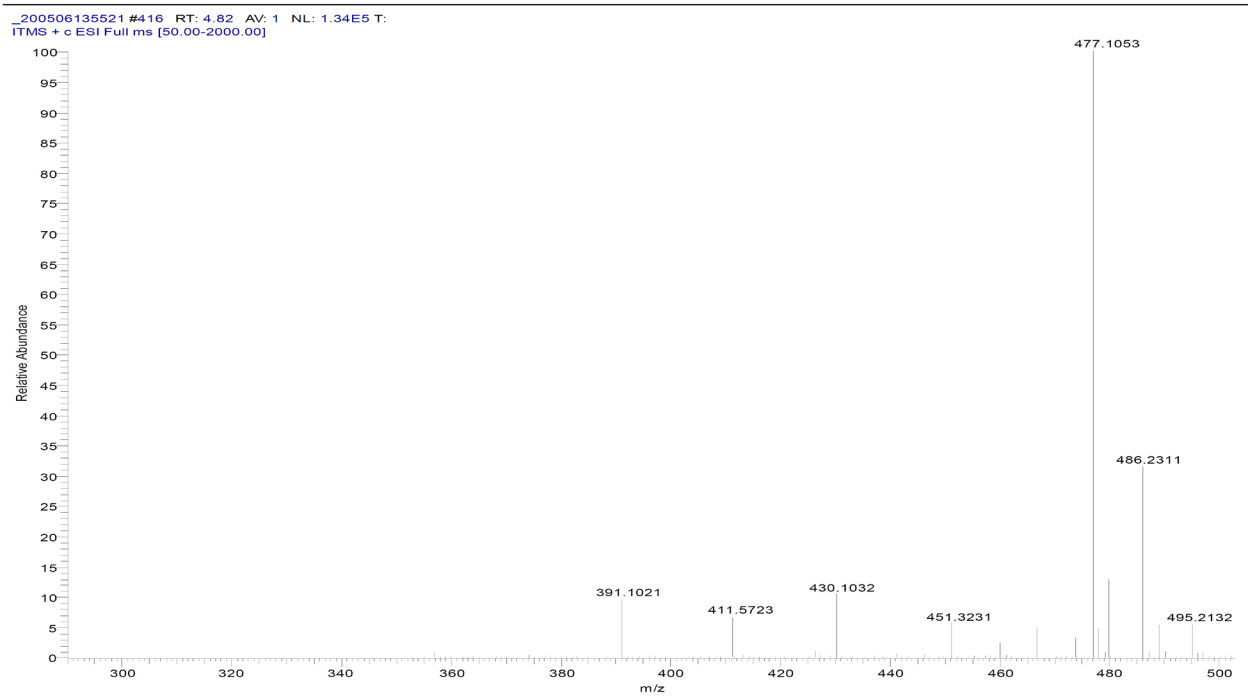
494.1721
455.1623
405.1321
371.0214
390.1213
432.1104
482.1041

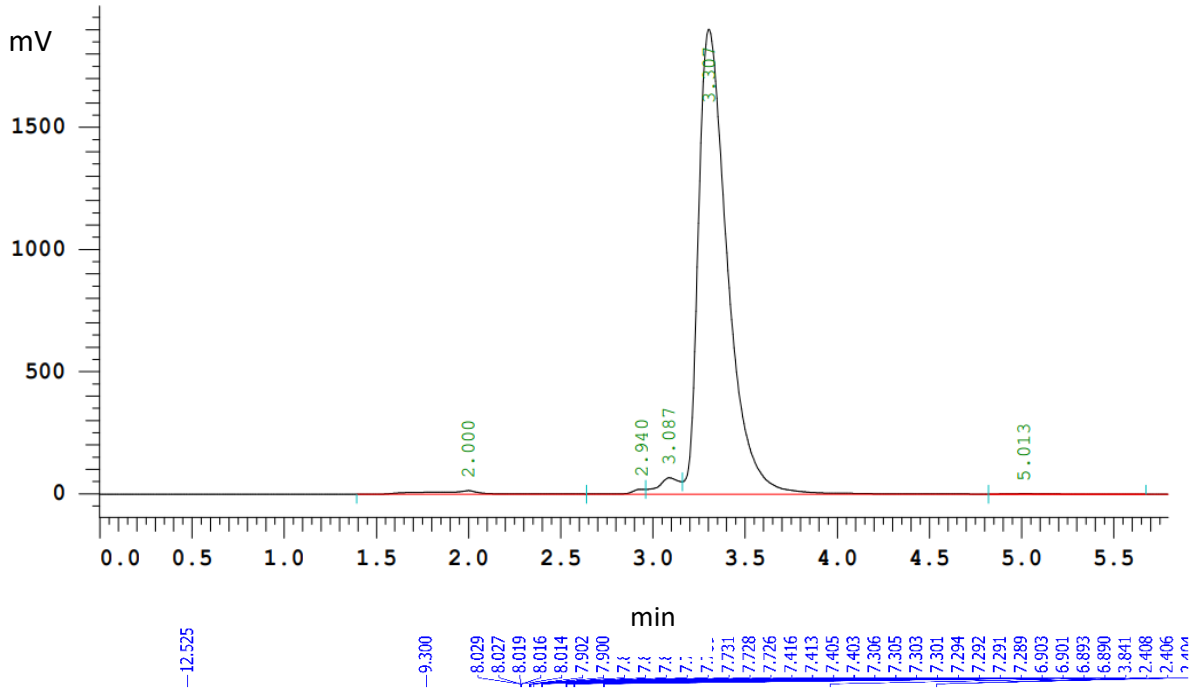
N-((4-(4-Hydroxyphenyl)-6-phenylpyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide ***(7d)***





*N-((4-(4-Chlorophenyl)-6-(4-methoxyphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7e**)*

No.	RT	Area (%)	Concentration (%)	BC
1	2.000	302963	1.384	BV
2	2.940	102967	0.470	VV
3	3.087	520051	2.421	VV
4	3.307	20931637	95.623	VV
5	5.013	22165	0.101	TBB
		21889783	100.00	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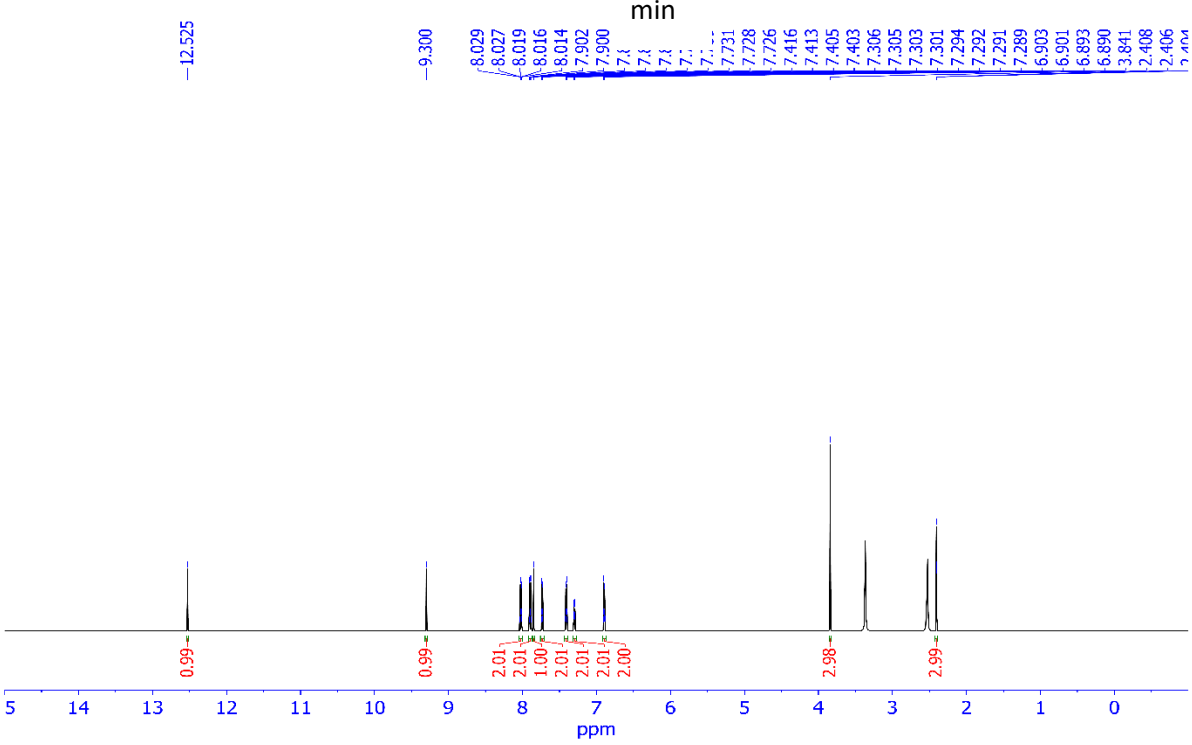
1000
500
0
2.000
2.940
3.087
3.307
5.013
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
min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0.99
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2.01
1.00
2.01
2.01
2.00
2.98
2.99
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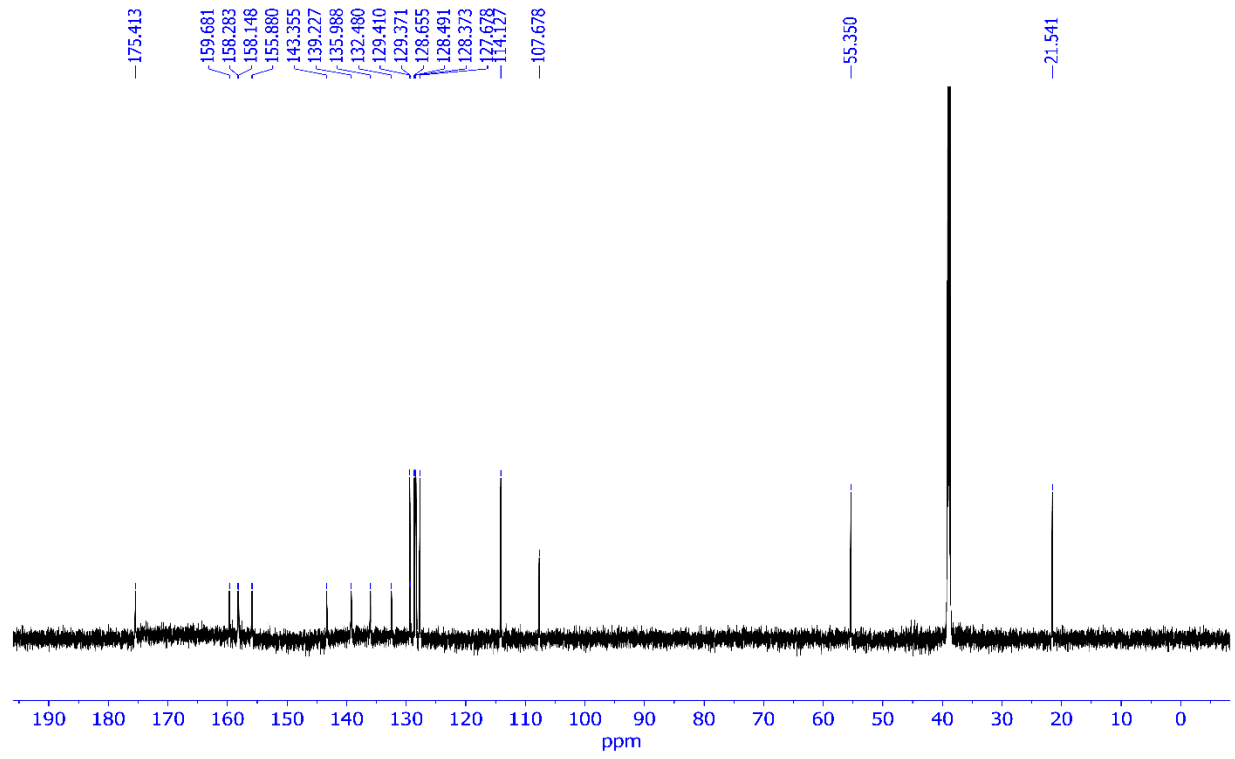
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm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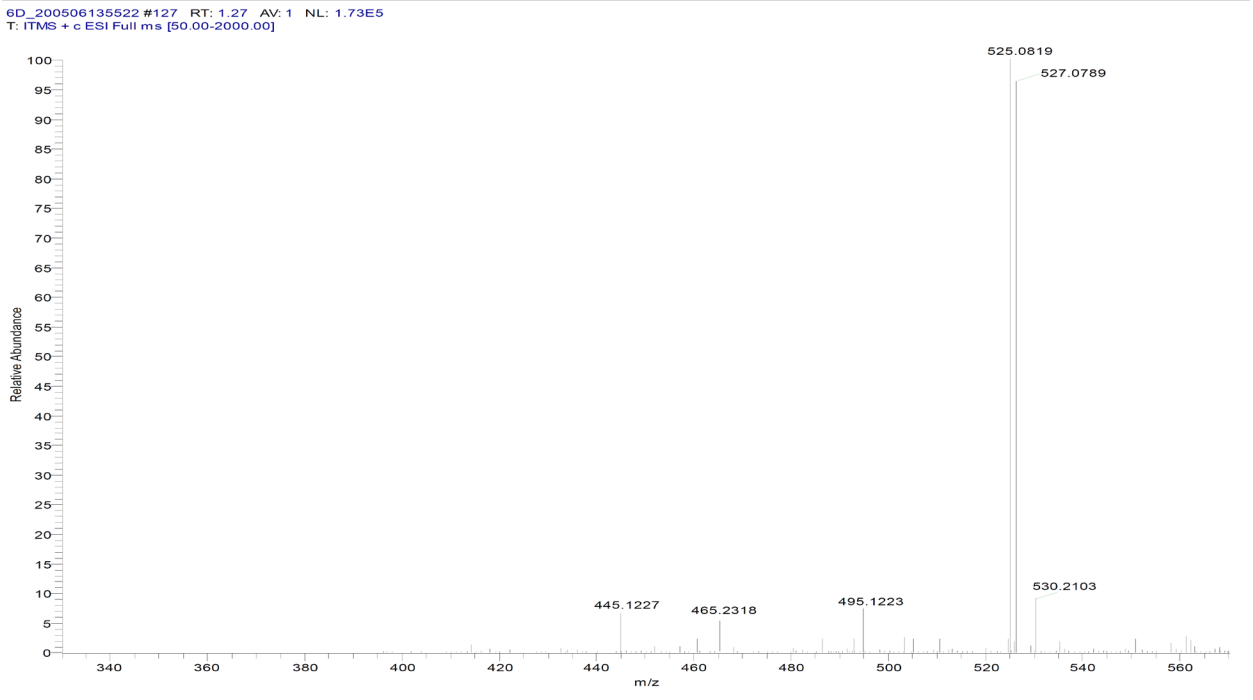
158.148
155.880
143.355
139.227
135.988
132.480
129.410
129.371
128.655
128.491
128.373
127.678
114.127
107.678
55.350
21.541
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
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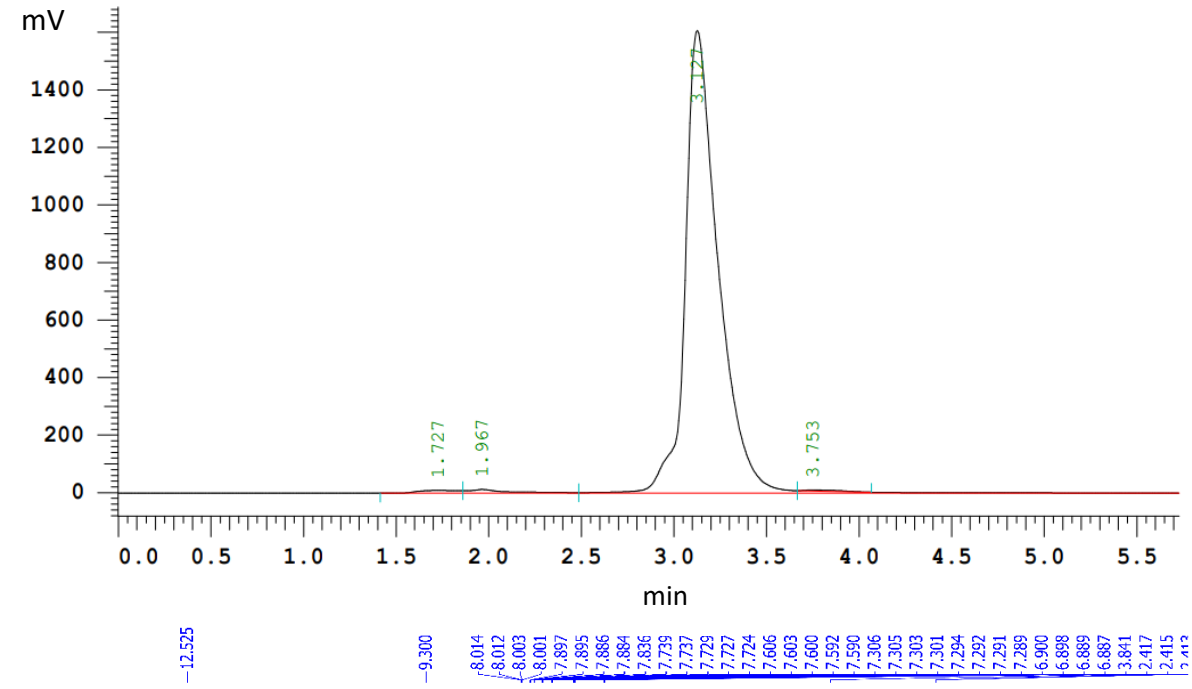
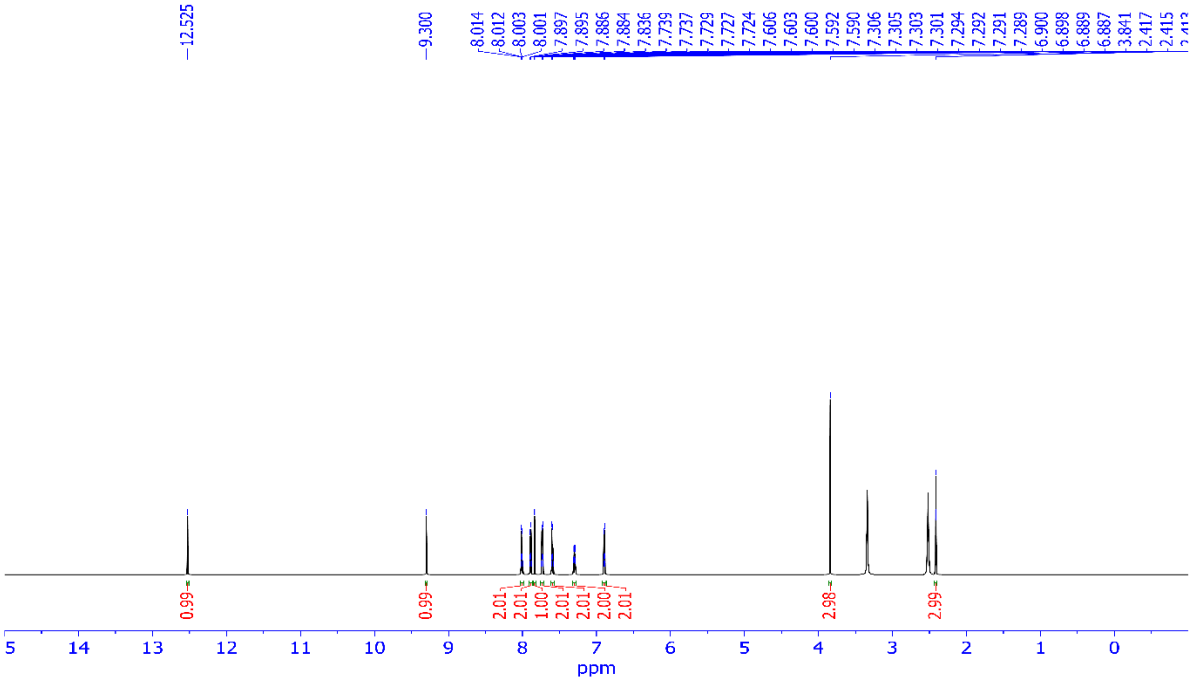
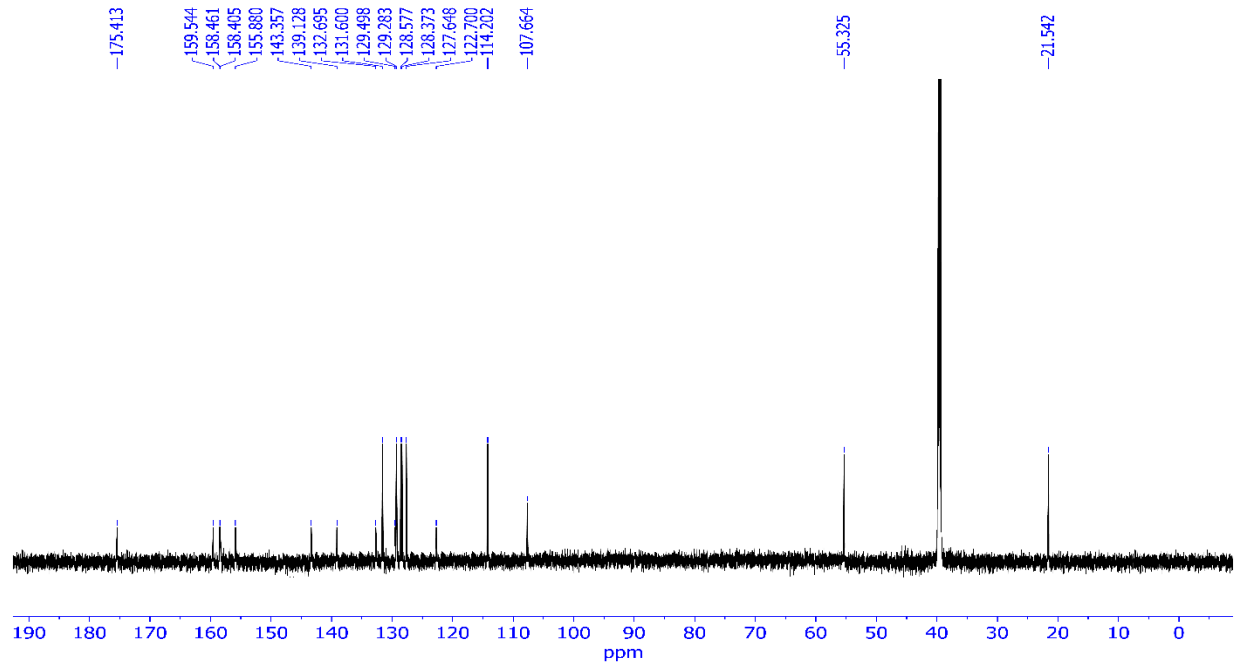
527.0789
530.2103
445.1227
465.2318
495.1223

*N-((4-(4-Bromophenyl)-6-(4-methoxyphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7f**)*

No.	RT	Area (%)	Concentration (%)	BC
1	1.727	139498	0.681	BV
2	1.967	198369	0.968	VV
3	3.127	20094728	98.101	VV
4	3.753	51104	0.249	TBB
			100.00	



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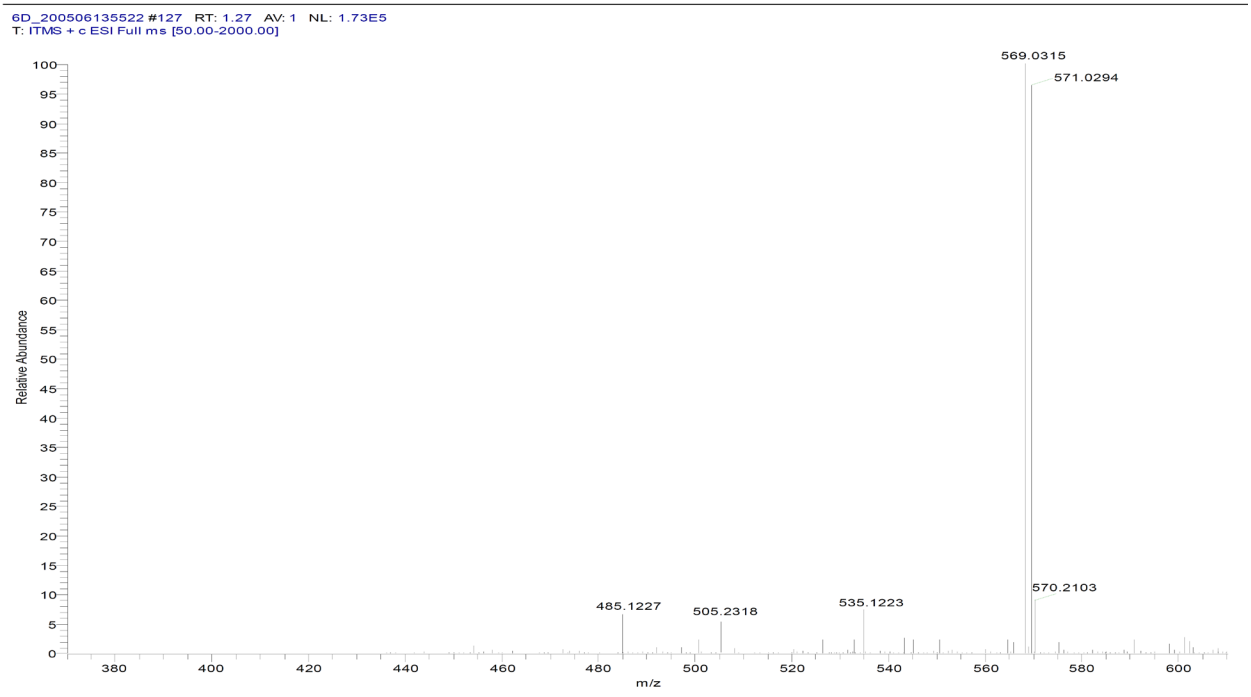
155.880
143.357
139.128
132.695
131.600
129.498
129.283
128.577
128.373
127.648
122.700
114.202
107.664
55.325
21.542
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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Relative Abundance
m/z
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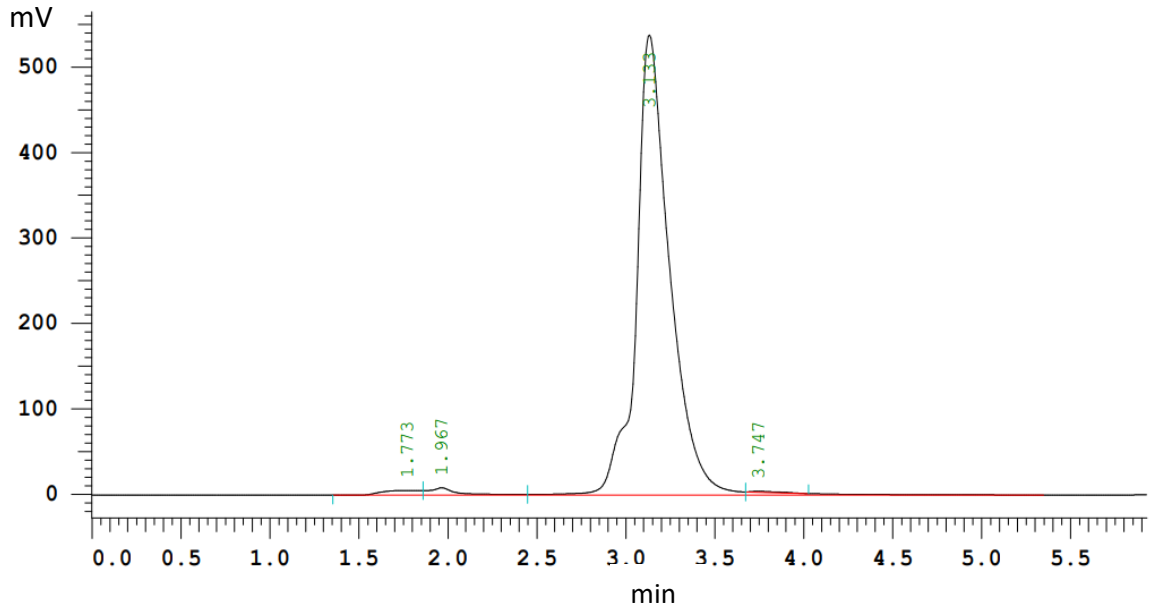
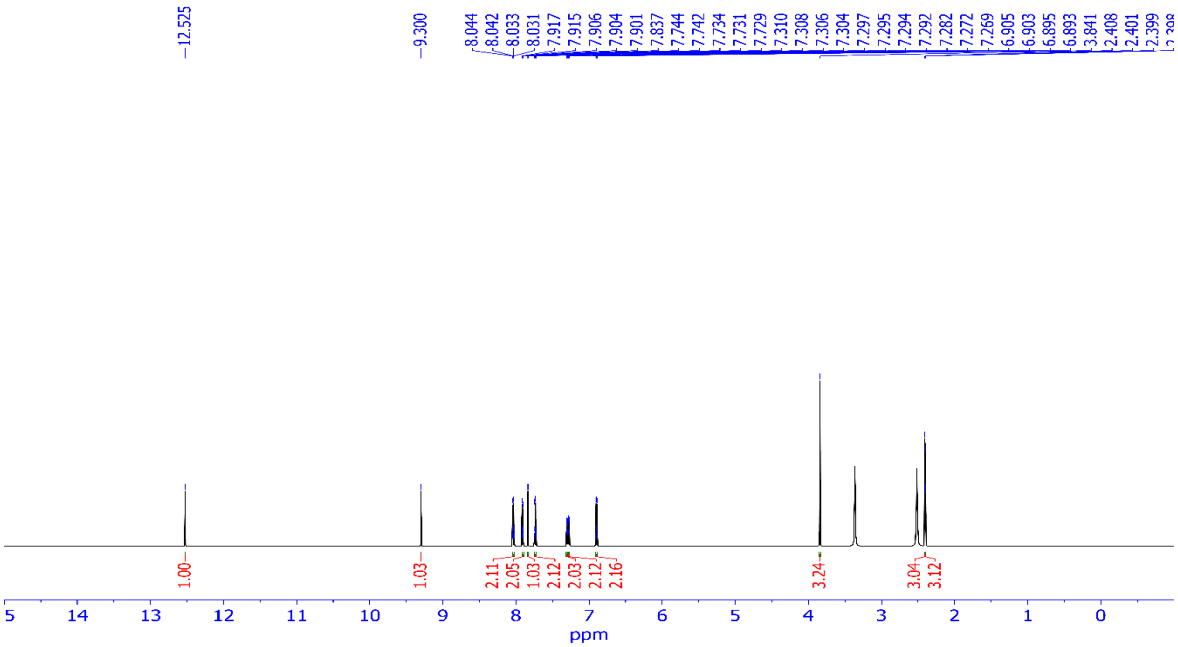
571.0294
570.2103
485.1227
505.2318
535.1223
380 400 420 440 460 480 500 520 540 560 580 600

*N-((4-(4-Methoxyphenyl)-6-(4-methylphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7g**)*

No.	RT	Area (%)	Concentration (%)	BC
1	1.773	80402	1.102	BV
2	1.967	98089	1.345	VV
3	3.133	7101267	97.364	VV
4	3.747	137930	0.189	TBB
			100.00	

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8.044
8.042
8.033
8.031
7.917
7.915
7.906
7.904
7.901
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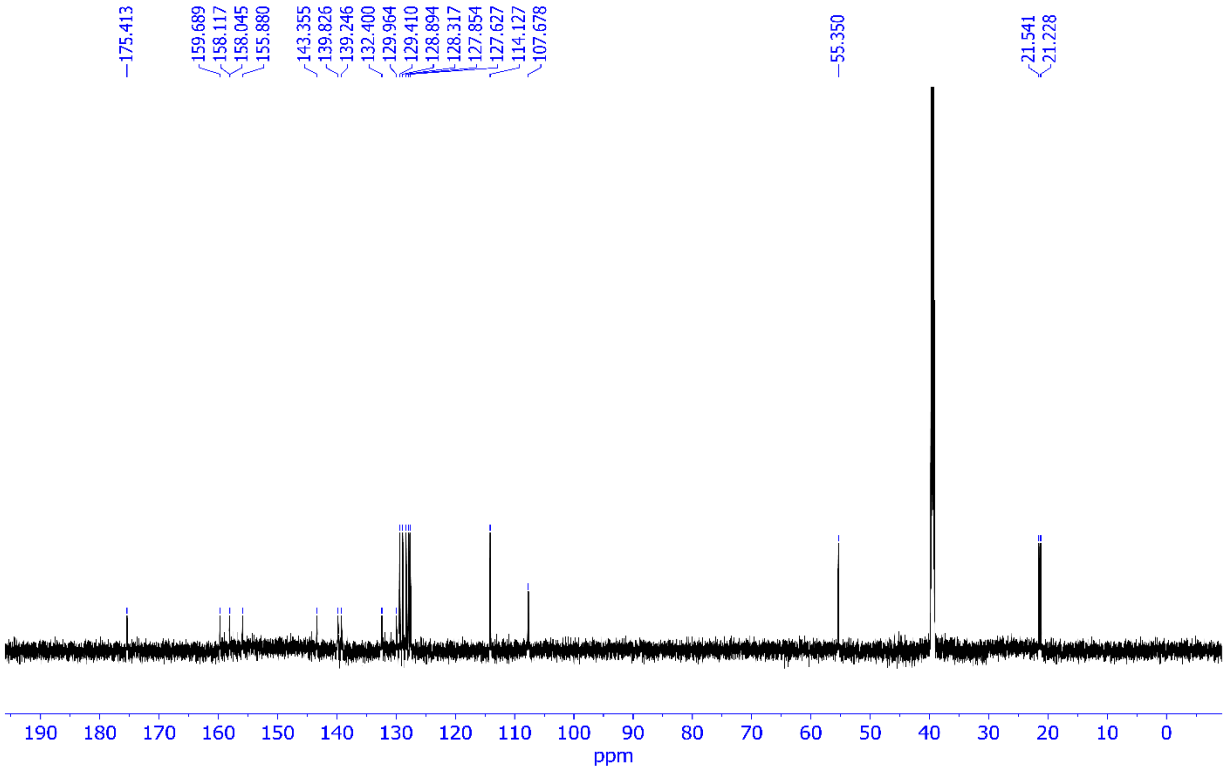
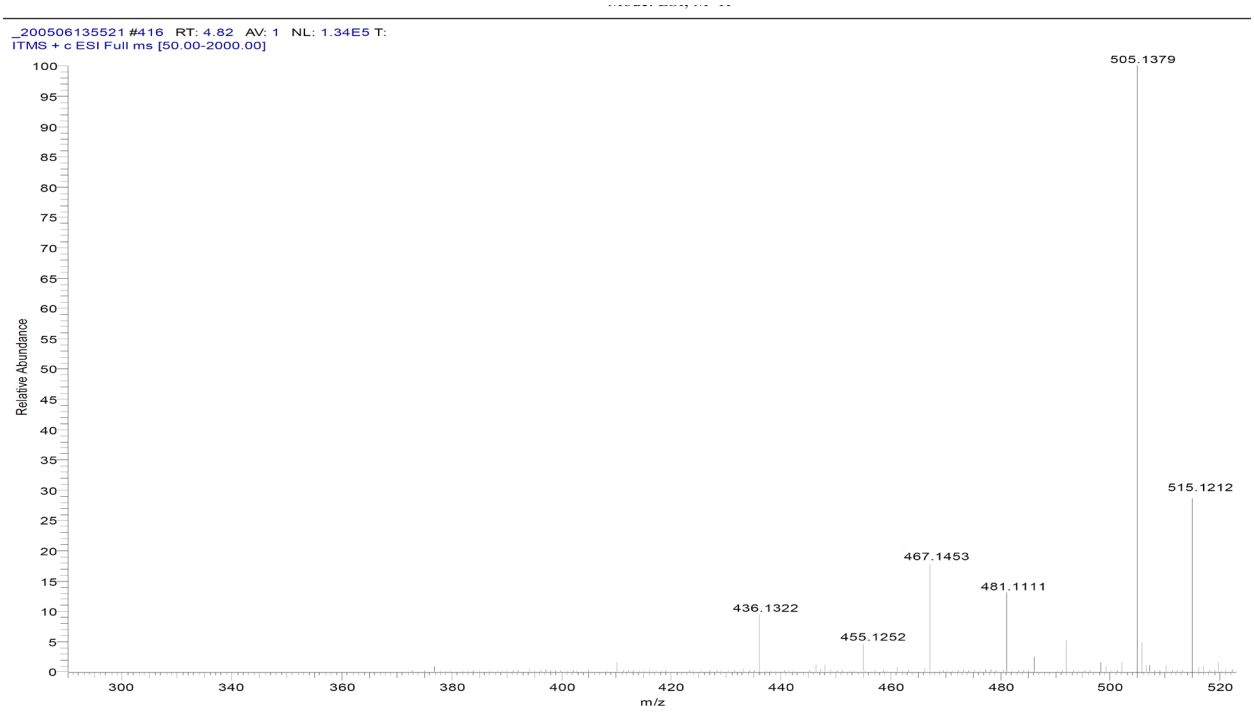
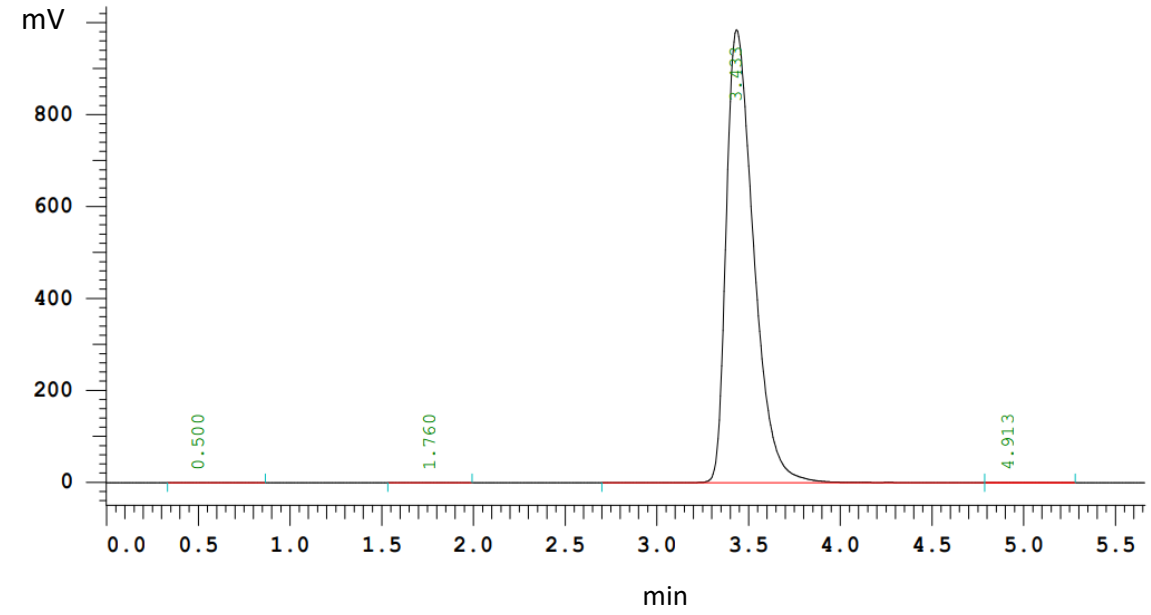
7.744
7.742
7.734
7.731
7.729
7.310
7.308
7.306
7.304
7.297
7.295
7.294
7.292
7.282
7.272
7.269
6.905
6.903
6.895
6.893
3.841
2.408
2.401
2.399
1.00
1.03
2.11
2.05
1.03
2.12
2.03
2.12
2.16
3.24
3.04
3.12
5 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
ppm


175.413
159.689
158.117
158.045
155.880
143.355
139.826
139.246
132.400
129.964
129.410
128.894
128.317
127.854
127.627
114.127
107.678
55.350
21.541
21.228
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

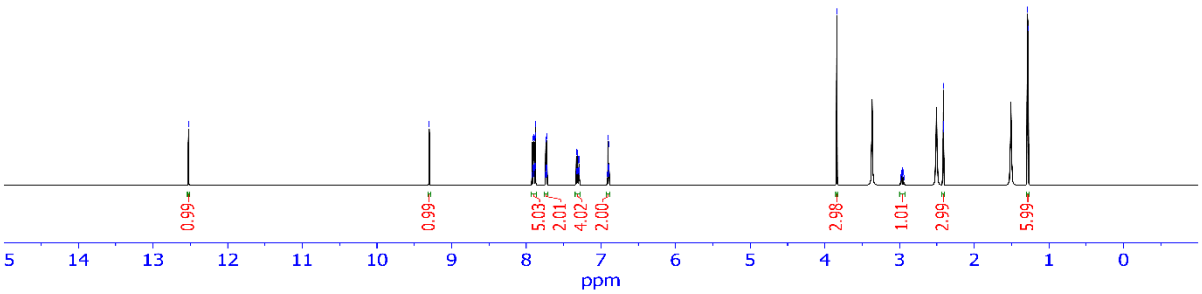


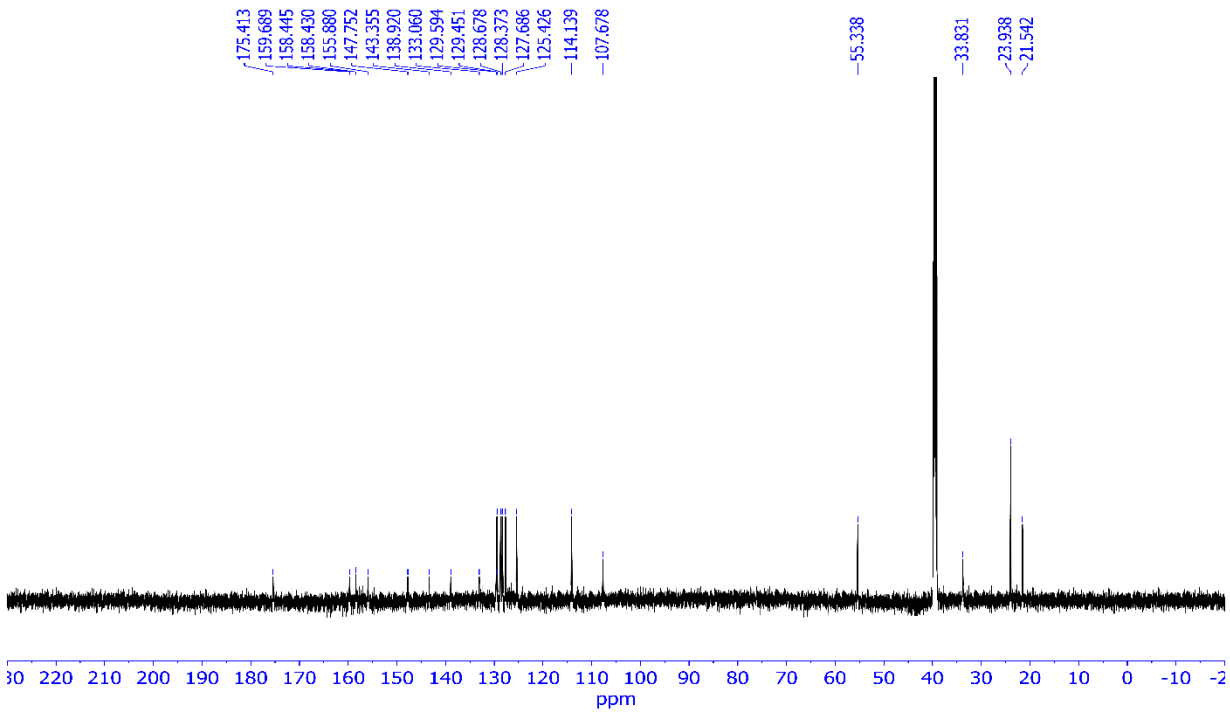
*N-((4-(4-Isopropylphenyl)-6-(4-methoxyphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7h**)*

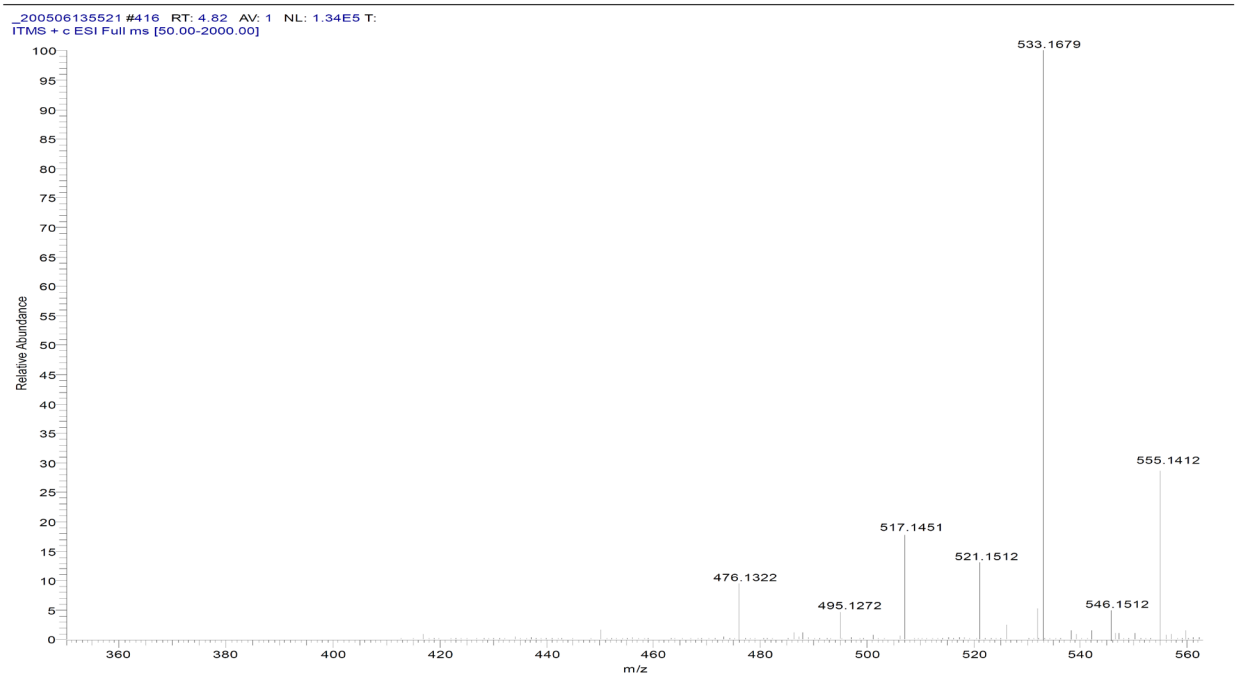
No.	RT	Area (%)	Concentration (%)	BC
1	0.500	826	0.008	BB
2	1.760	812	0.008	BB
3	3.433	10267216	99.973	BB
4	4.913	1126	0.011	TBB
		10269980	100.00	


mV
800
600
400
200
0
0.500
1.760
3.433
4.913
0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5
min


12.525
9.300
7.920
7.917
7.915
7.906
7.904
7.901
7.896
7.893
7.891
7.882
7.880
7.876
7.742
7.739
7.737
7.729
7.727
7.724
7.330
7.327
7.320
7.318
7.308
7.306
7.304
7.297
7.295
7.294
7.292
6.911
6.908
6.906
6.898
6.896
6.893
3.841
2.987
2.976
2.966
2.964
2.953
2.942
2.417
2.415
2.414
1.289
1.277

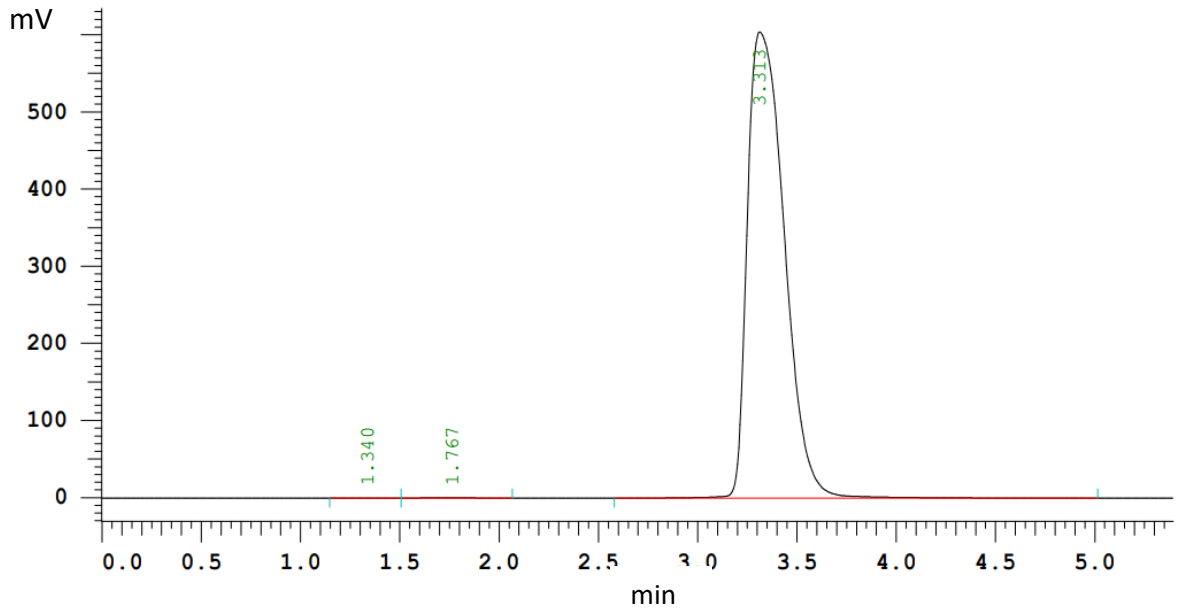

0.99
0.99
5.03
2.01
4.02
2.00
2.98
1.01
2.99
5.99
5 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
ppm

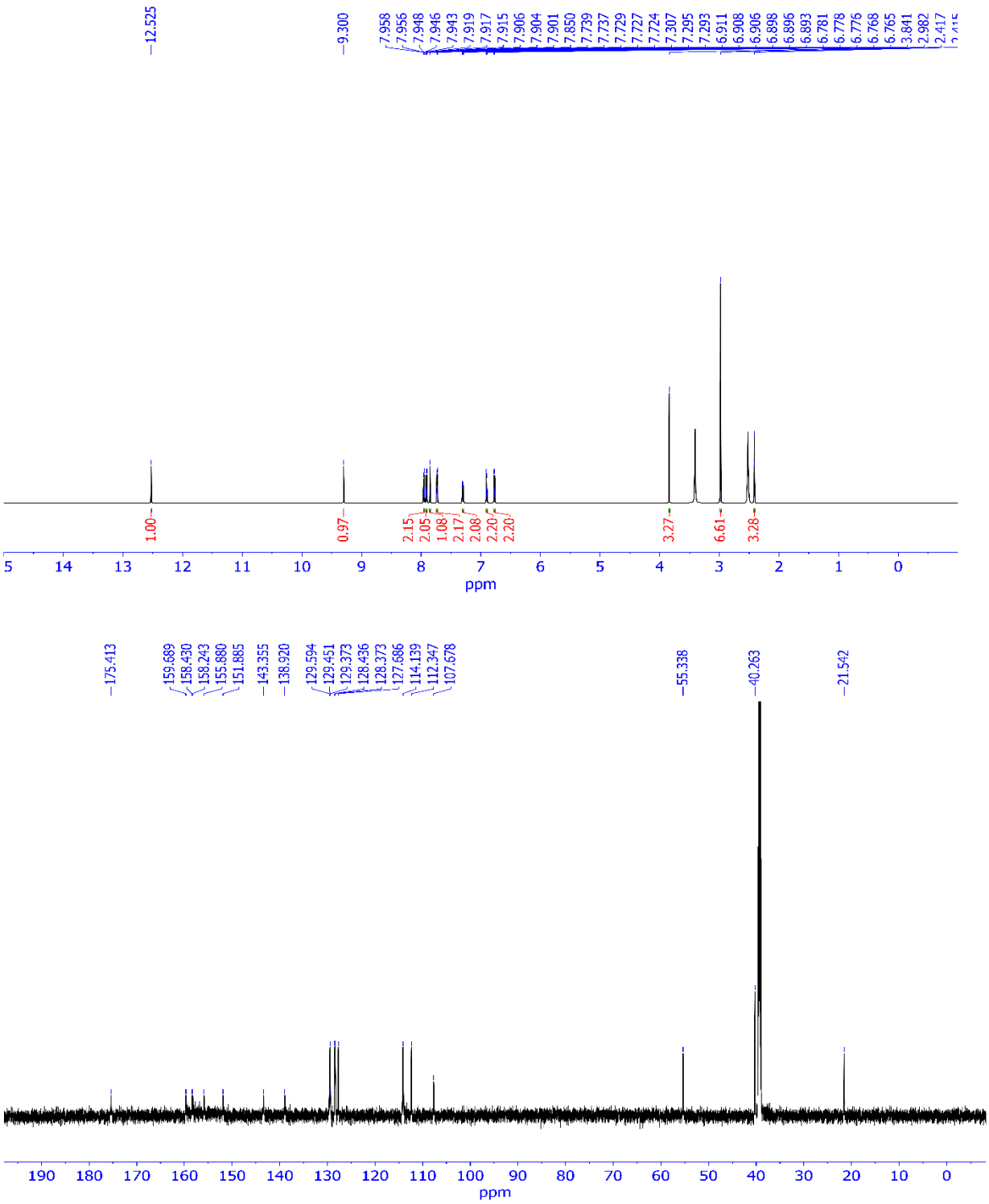

175.413
159.689
158.445
158.430
155.880
147.752
143.355
138.920
133.060
129.594
129.451
128.678
128.373
127.686
125.426
114.139
107.678
55.338
33.831
23.938
21.542
ppm

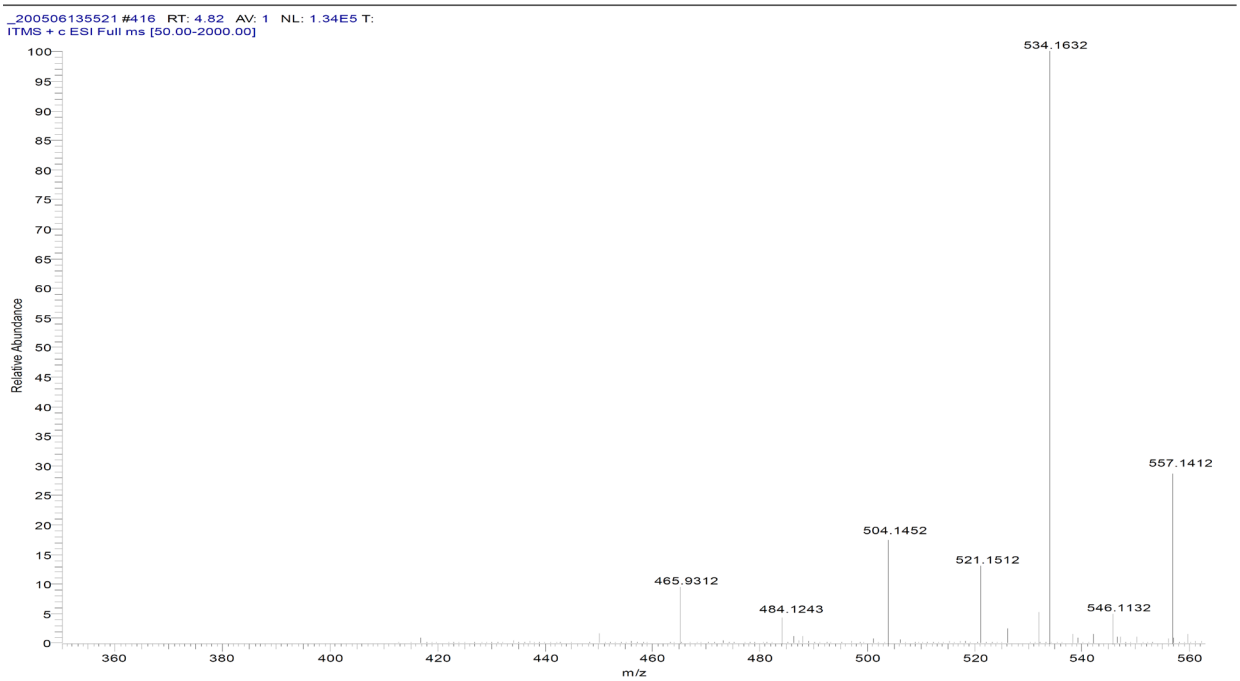

_200506135521 #416 RT: 4.82 AV: 1 NL: 1.34E5 T:
ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
533.1679
555.1412
517.1451
521.1512
476.1322
495.1272
546.1512

*N-((4-(4-(Dimethylamino)phenyl)-6-(4-methoxyphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7i**)*

No.	RT	Area (%)	Concentration (%)	BC
1	1.340	1964	0.025	BB
2	1.767	9615	0.123	BB
3	3.313	7817217	99.852	BB
		7828796	100.00	

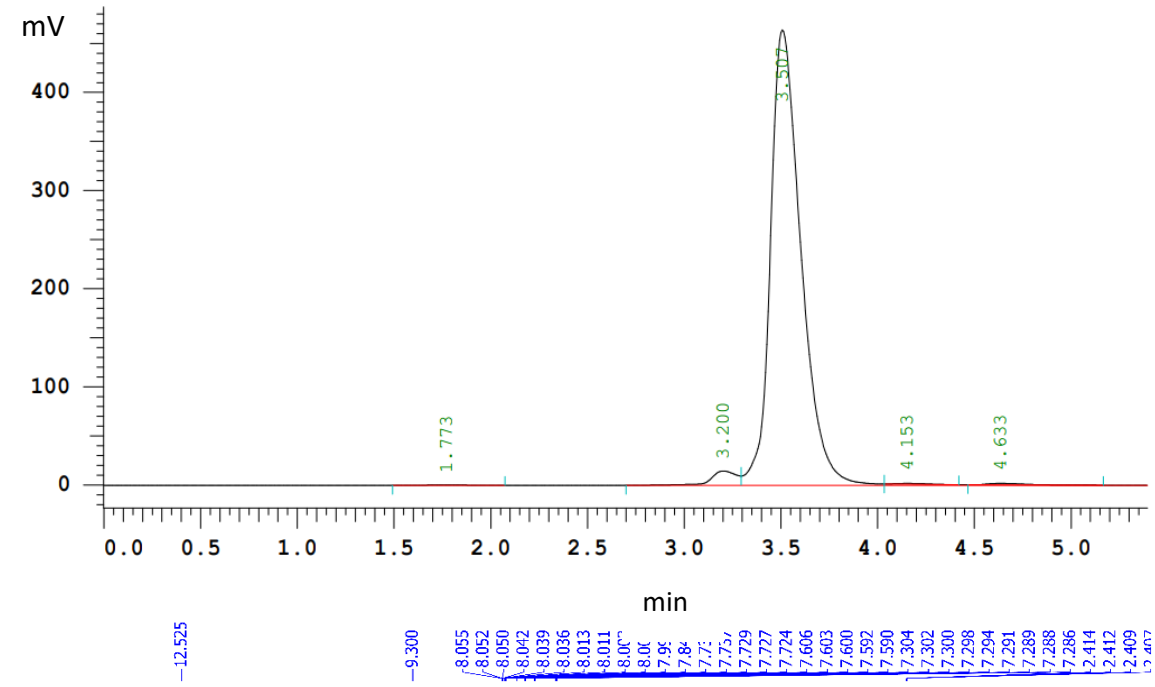


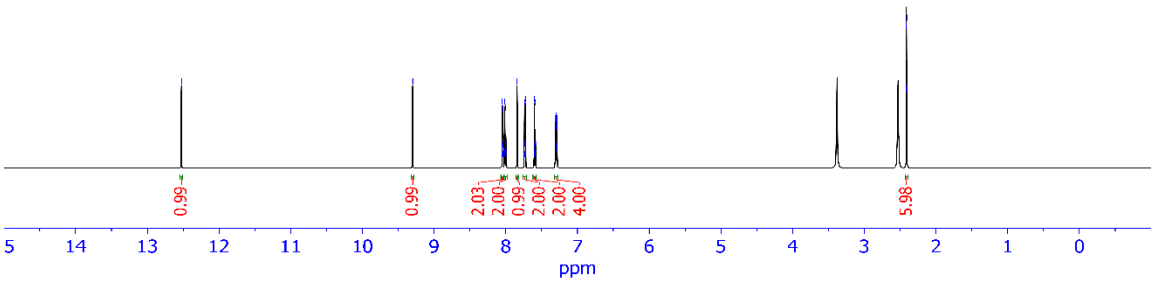

12.525
9.300
7.958
7.956
7.948
7.946
7.943
7.919
7.917
7.915
7.906
7.904
7.901
7.850
7.739
7.737
7.729
7.727
7.724
7.307
7.295
7.293
6.911
6.908
6.906
6.898
6.896
6.893
6.781
6.778
6.776
6.768
6.765
3.841
2.982
2.417
1.00
0.97
2.15
2.05
1.08
2.17
2.08
2.20
2.20
3.27
6.61
3.28
ppm
175.413
159.689
158.430
158.243
155.880
151.885
143.355
138.920
129.594
129.451
129.373
128.436
128.373
127.686
114.139
112.347
107.678
55.338
40.263
21.542
ppm

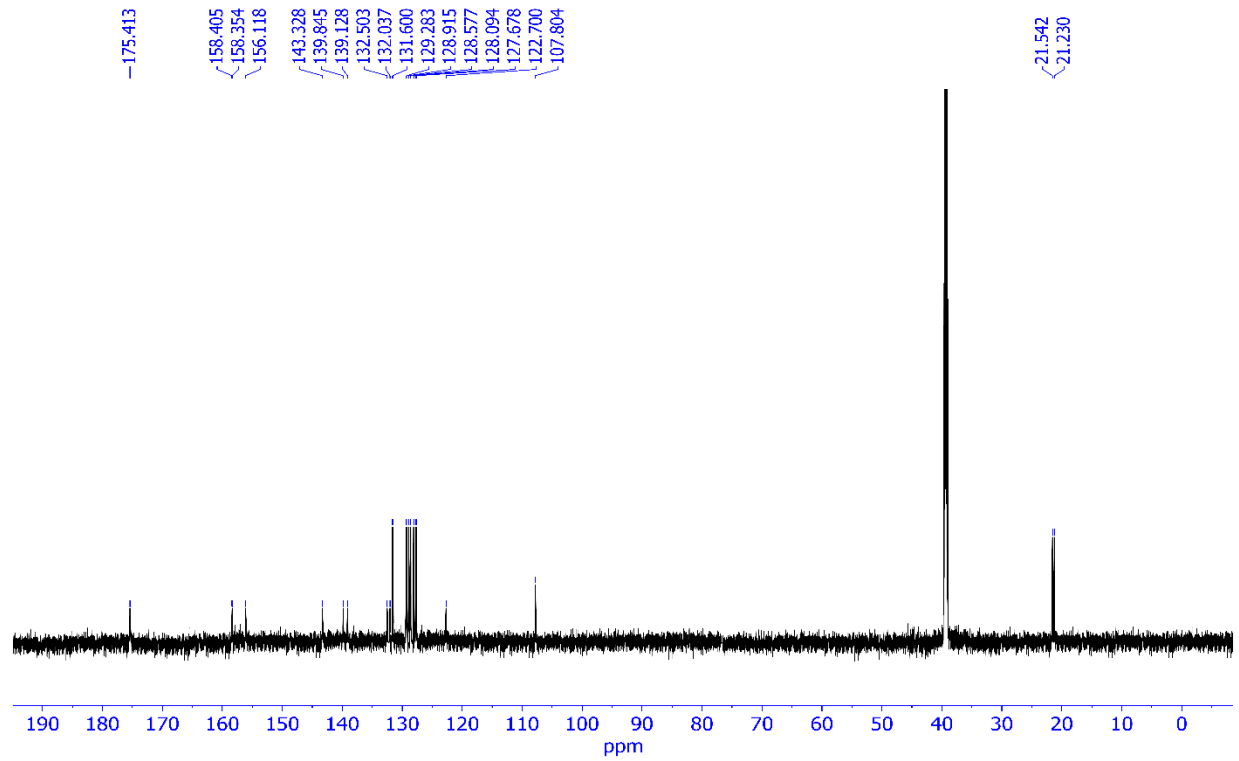


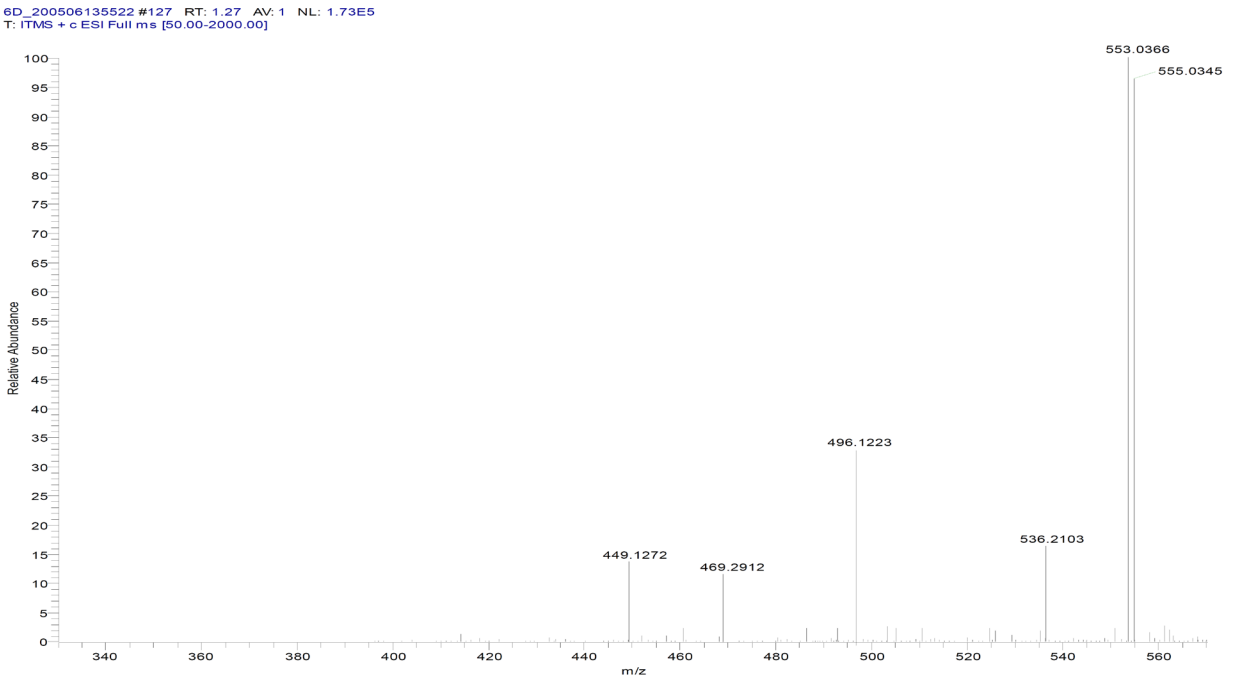
*N-((4-(4-Bromophenyl)-6-(4-methylphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7j**)*

No.	RT	Area (%)	Concentration (%)	BC
1	1.773	5537	0.105	BB
2	3.200	131857	2.494	BV
3	3.507	5119190	96.807	VV
4	4.153	10559	0.200	TBB
5	4.633	20880	0.395	TBB
			100.00	


mV
400
300
200
100
0
1.773
3.200
3.507
4.153
4.633
0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0
min

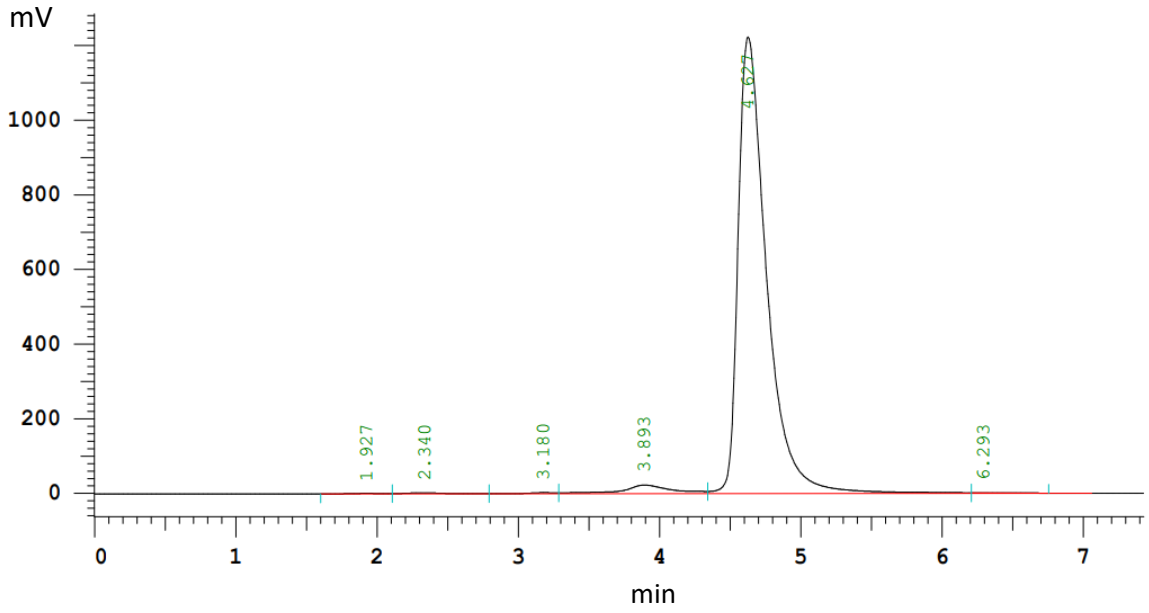

0.99
0.99
2.03
2.00
0.99
2.00
2.00
4.00
5.98
5 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
ppm

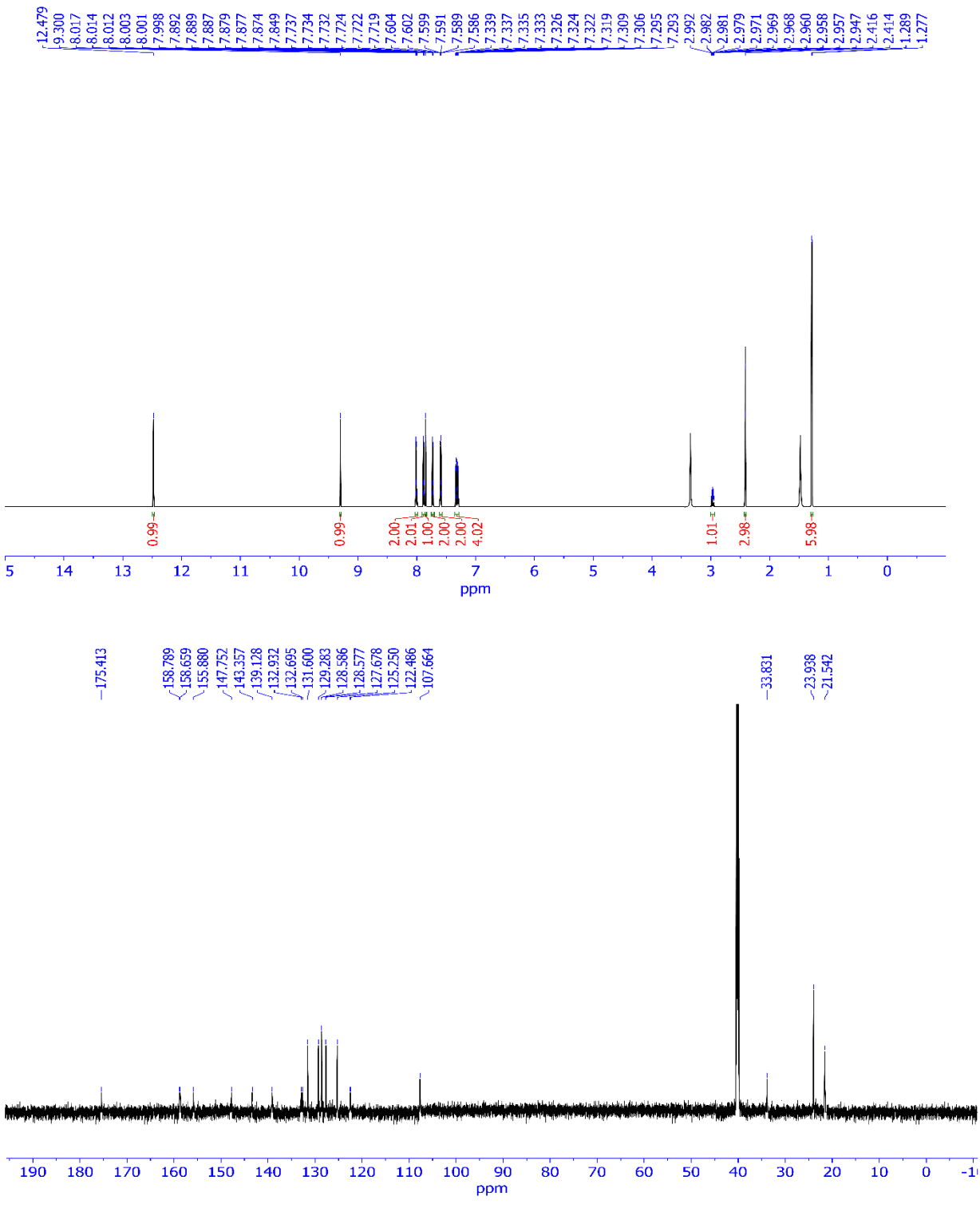

175.413
158.405
158.354
156.118
143.328
139.845
139.128
132.503
132.037
131.600
129.283
128.915
128.577
128.094
127.678
122.700
107.804
21.542
21.230
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

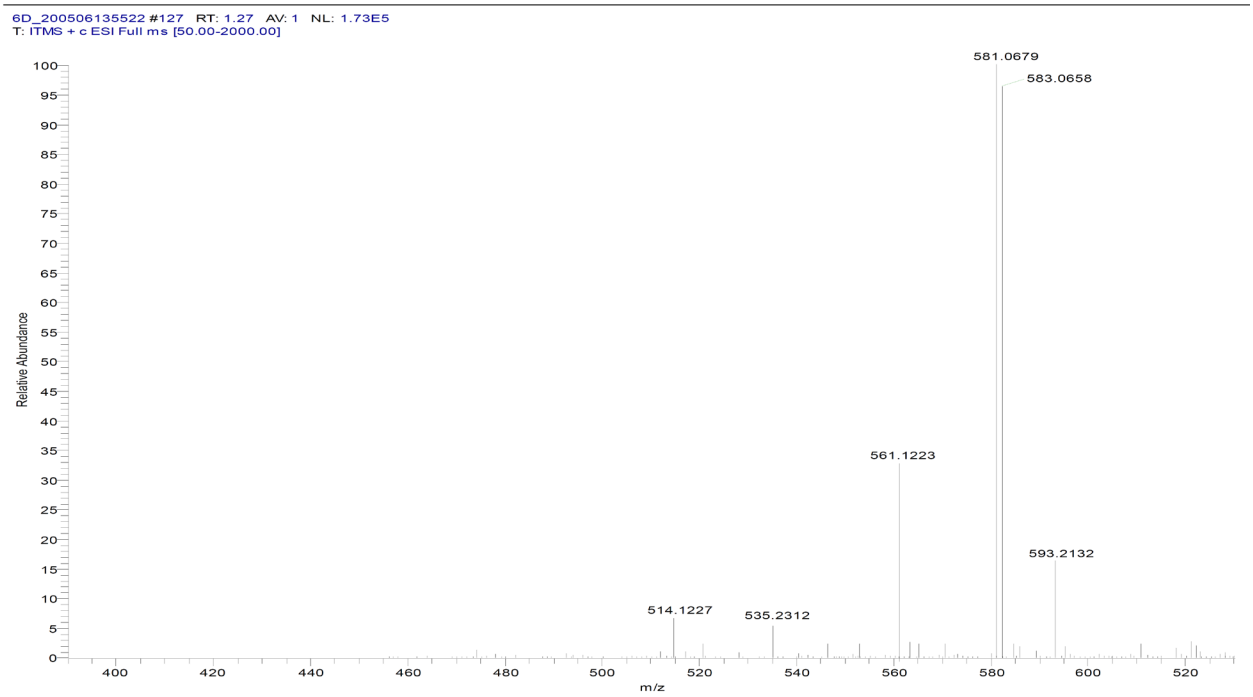

6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
553.0366
555.0345
496.1223
536.2103
449.1272
469.2912
Relative Abundance
m/z

*N-((4-(4-Bromophenyl)-6-(4-isopropylphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7k**)*

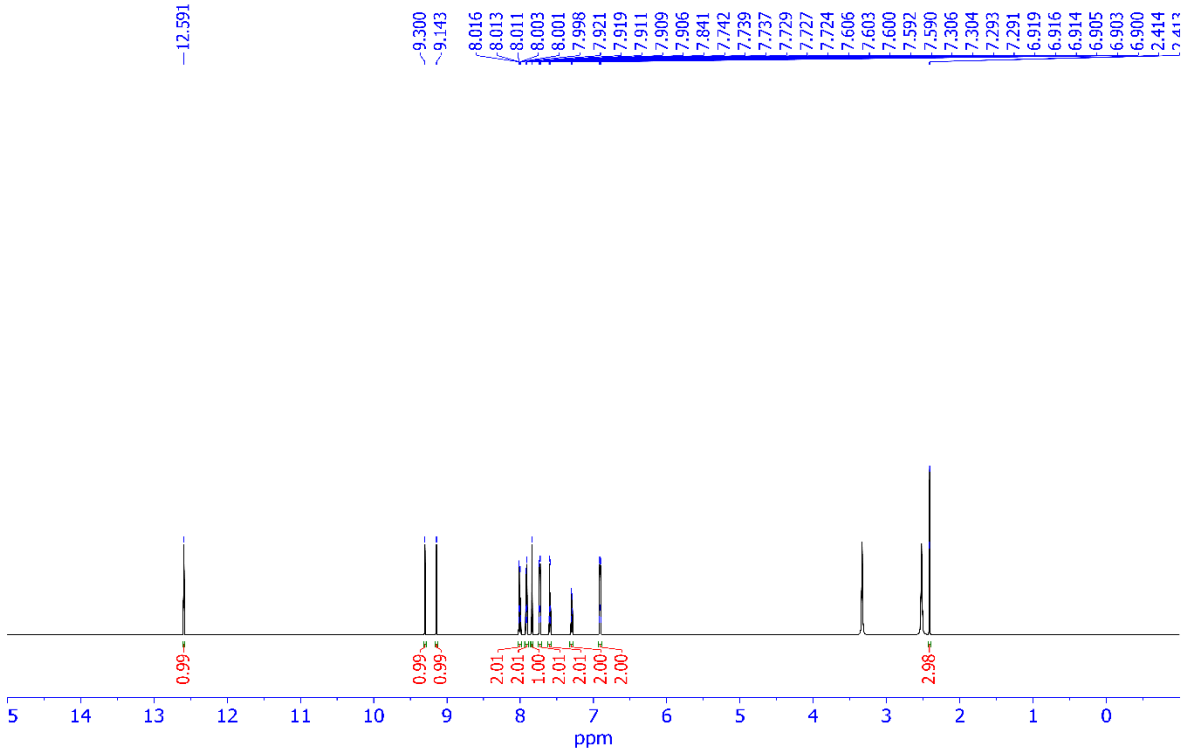
No.	RT	Area (%)	Concentration (%)	BC
1	1.927	25856	0.145	BV
2	2.340	56014	0.314	VV
3	3.180	41491	0.232	VV
4	3.893	564929	3.163	VV
5	4.627	17168353	96.126	VV
6	6.293	3631	0.020	TBB
		17860274	100.00	

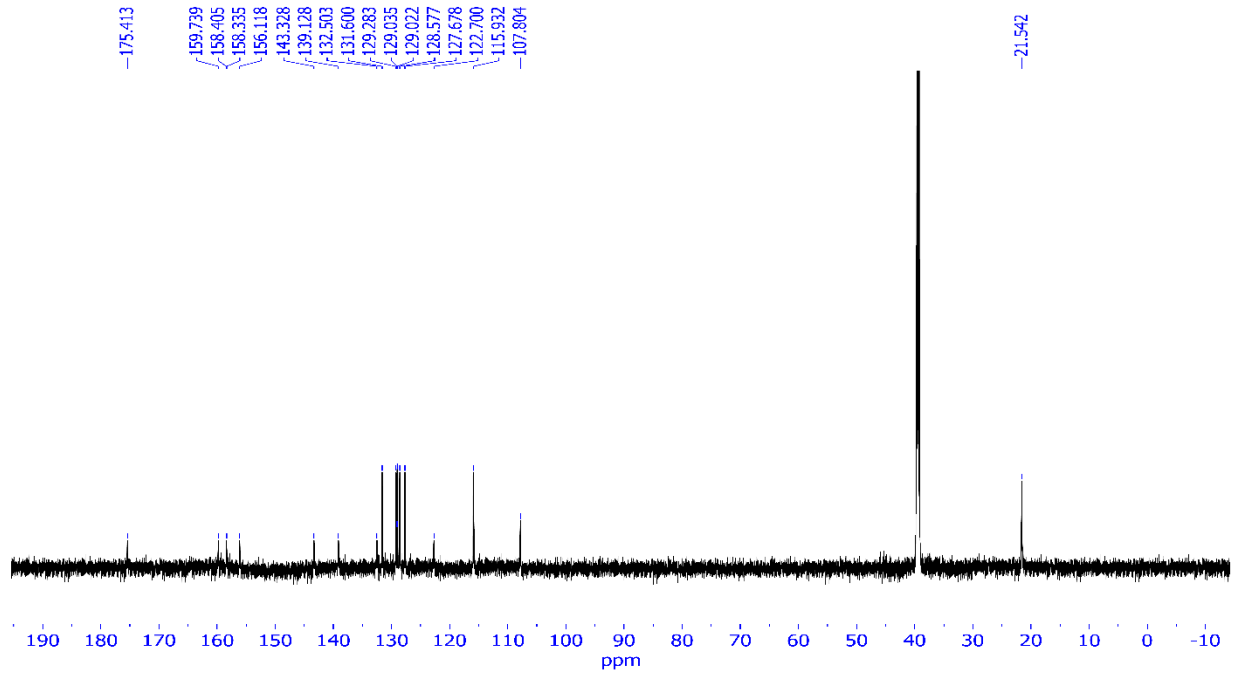


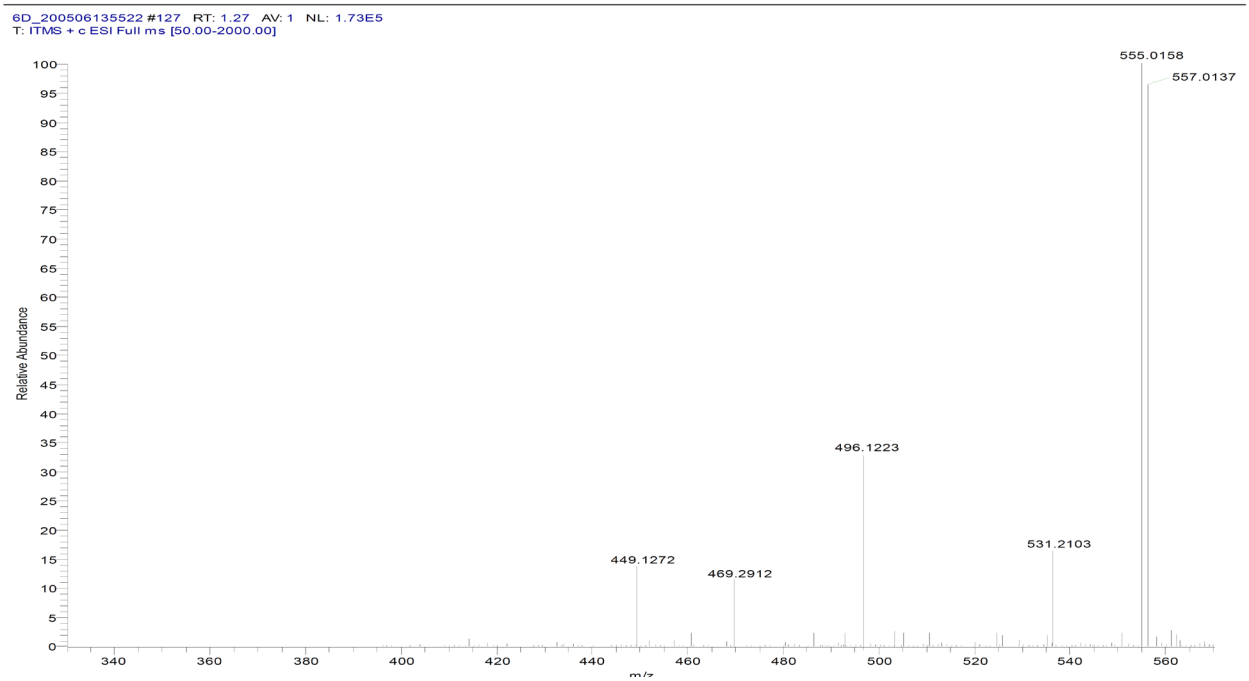

12.479
9.300
8.017
8.014
8.012
8.003
8.001
7.998
7.892
7.889
7.887
7.879
7.877
7.874
7.849
7.737
7.734
7.732
7.724
7.722
7.719
7.604
7.602
7.599
7.591
7.589
7.586
7.339
7.337
7.335
7.333
7.326
7.324
7.322
7.319
7.309
7.306
7.295
7.293
2.992
2.982
2.981
2.979
2.971
2.969
2.968
2.960
2.958
2.957
2.947
2.416
2.414
1.289
1.277
0.99
0.99
2.00
2.01
1.00
2.00
2.00
4.02
1.01
2.98
5.98
ppm
175.413
158.789
158.659
155.880
147.752
143.357
139.128
132.932
132.695
131.600
129.283
128.586
128.577
127.678
125.250
122.486
107.664
33.831
23.938
21.542
ppm



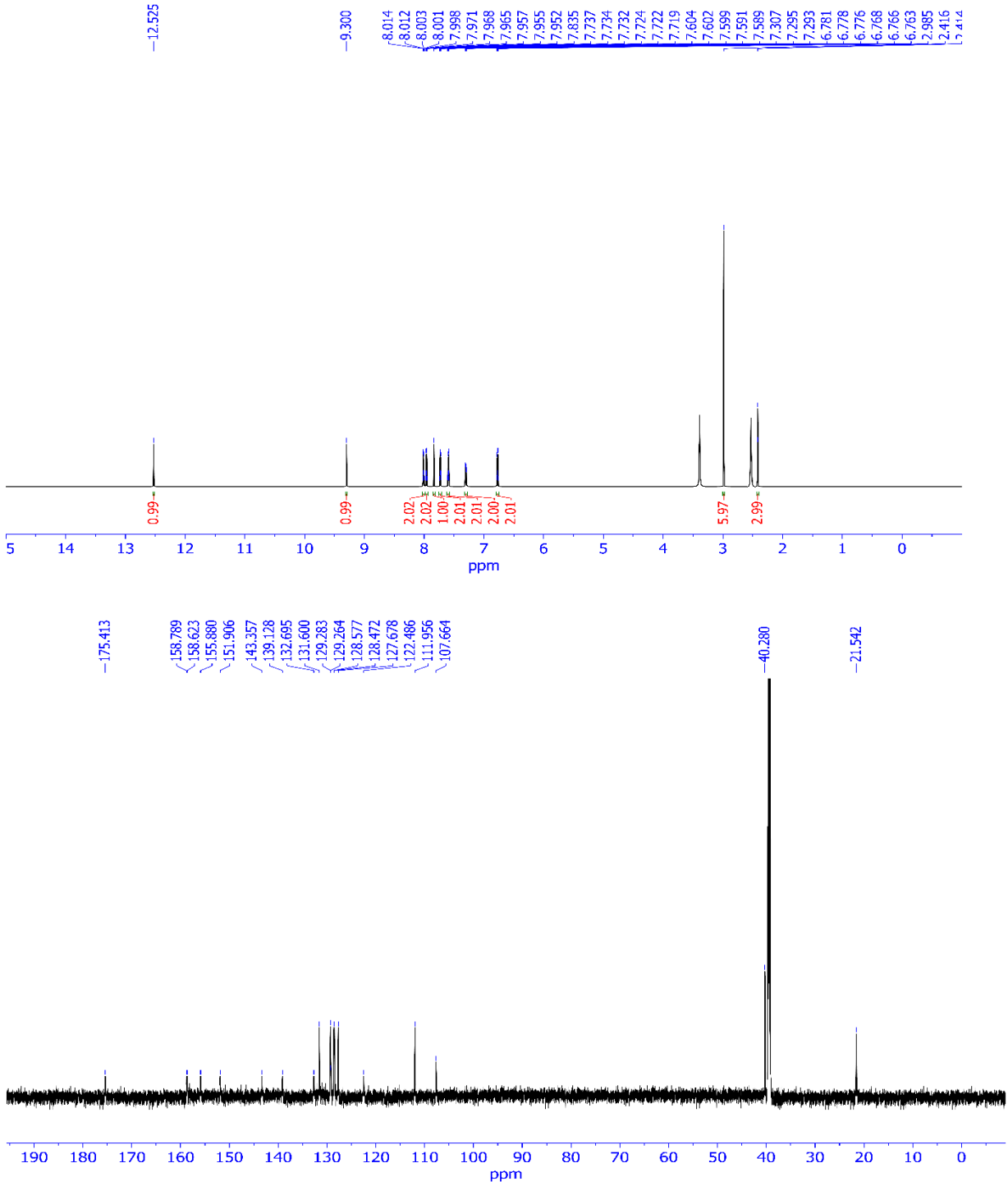
*N-((4-(4-Bromophenyl)-6-(4-hydroxyphenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7l**)*

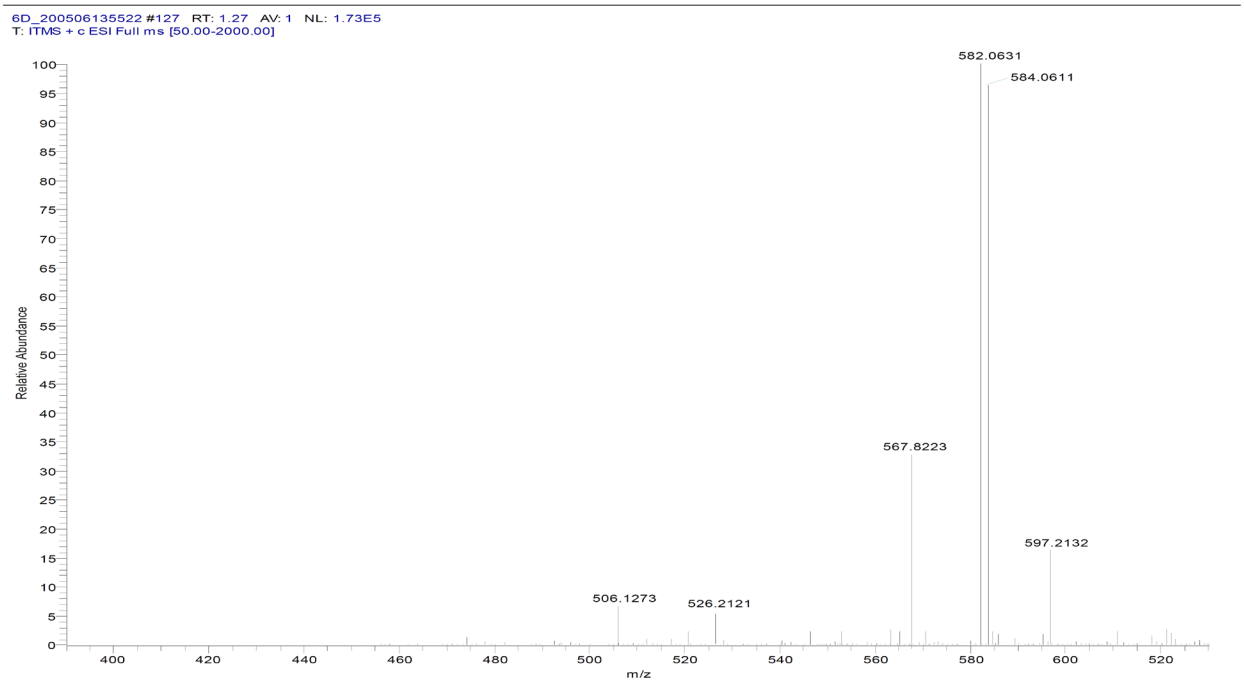



175.413
159.739
158.405
158.335
156.118
143.328
139.128
132.503
131.600
129.283
129.035
129.022
128.577
127.678
122.700
115.932
107.804
21.542
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
555.0158
557.0137
496.1223
531.2103
449.1272
469.2912

*N-((4-(4-Bromophenyl)-6-(4-(dimethylamino)phenyl)pyrimidin-2-yl)carbamothioyl)-4-methylbenzenesulphonamide (**7m**)*




6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
582.0631
584.0611
567.8223
597.2132
506.1273
526.2121
Relative Abundance
m/z