Aiding the versatility of simple ammonium ionic liquid by the synthesis of bioactive 1,2,3,4-tetrahydropyrimidine, 2-aminothiazole and quinazolinones derivatives.

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Experimental

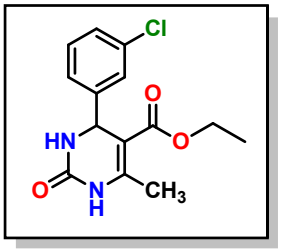
Single crystals of compound **4k and 6j** were operated. A suitable crystal was selected and was operated on a Xcalibur, Sapphire3 diffractometer. The crystal was kept at 298.8(6) K during data collection. Using Olex2 [1], the structure was solved with the olex 2.solve[2] structure solution program using Charge Flipping and refined with the olex 2. refine.[2] refinement package using Gauss-Newton minimisation.

Refinement model description

Number of restraints - 0

Number of constraints - 0

Table S1 Crystal data and structure refinement for compound **4k**



CCDC Number	**CCDC 1959600**
Molecular Formula	$C_{14}H_{15}ClN_2O_3$
Molecular weight	294.73
Temperature	298.8(6)
Radiation	Mo Kα (λ = 0.71073)
Crystal system	Triclinic
Space group	P-1

Unit cell dimensions	a/Å = 12.4372(5); α/ ^{o} = 90 b/Å = 7.2932(2); β/^{o} = 108.876(4) c/Å = 16.2417(6); ϒ/ ^{o} = 90
Volume /Å^3	1394.01(9)
Z	1
Density (ρcalcg/cm^3)	1.3322
Absorption coefficient (μ/mm^{-1})	0.280
F(000)	556.9
2θ range for data collection	6.66 to 59.2
Index ranges	-16 ≤ h ≤ 15, -9 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected	21213
Independent reflections	6822 [R_{int} = 0.0810, R_{sigma} = 0.0717]
Data/restraints/parameters	6822/0/161
Refinement method	Full-matrix least-squares on F2
Goodness-of-fit on F^2	2.607
Final R indexes [I>=2σ (I)]	R1 = 0.1831, wR2 = 0.4501
Final R indexes [all data]	R1 = 0.2272, wR2 = 0.4857
Largest diff. peak/hole / e Å^{-3}	3.02/-3.09

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound **4k**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U_{eq}
Cl01	10561(2)	-1519(3)	6071.8(17)	80.9(8)
Cl02	4435(2)	3481(3)	8931.3(17)	78.5(8)
O003	7707(4)	9481(6)	7595(3)	41.1(11)
O004	7293(4)	4484(6)	7399(3)	41.2(11)
O005	2997(4)	7635(6)	5123(3)	43.5(11)

O006	12007(4)	2633(6)	9876(3)	43.1(11)
O007	12145(4)	5592(7)	10173(3)	53.2(13)
O008	2854(4)	10591(7)	4828(3)	55.4(14)
N009	6134(4)	7857(7)	6888(3)	33.0(12)
N00A	8905(4)	6034(7)	8158(3)	33.8(12)
N00B	8871(4)	2866(7)	8119(3)	33.7(12)
N00C	6097(4)	11036(7)	6843(3)	36.5(12)
C00D	8317(5)	4426(8)	7866(4)	34.6(14)
C00E	4391(5)	7529(8)	7280(4)	31.2(13)
C00F	4873(5)	7786(8)	6539(4)	32.3(13)
C00G	4446(5)	9465(7)	5985(4)	29.7(13)
C00H	6684(5)	9428(8)	7138(4)	34.1(14)
C00I	10553(5)	4490(8)	9008(4)	30.5(13)
C00J	10607(5)	2526(8)	7727(4)	32.3(13)
C00K	5057(5)	11057(8)	6183(4)	32.3(13)
C00L	9948(5)	6049(8)	8823(4)	33.3(14)
C00M	10126(5)	2790(8)	8468(4)	33.4(14)
C00N	11629(5)	4355(8)	9735(4)	35.2(14)
C00O	3381(5)	9354(8)	5266(4)	35.2(14)
C00P	10414(6)	844(9)	7286(4)	43.1(16)
C00Q	4586(6)	5862(9)	7700(4)	41.0(15)
C00R	4741(6)	12850(9)	5753(4)	45.4(17)
C00S	10262(6)	7857(10)	9254(5)	47.4(17)
C00T	3773(6)	8871(10)	7515(5)	47.5(17)
C00U	11228(6)	3872(10)	7484(5)	47.9(17)
C00V	10831(6)	583(10)	6608(5)	47.9(17)
C00W	13070(6)	2355(10)	10596(5)	47.3(17)
C00X	11445(7)	1909(10)	6357(5)	52.1(18)
C00Y	1936(6)	7368(9)	4409(5)	45.2(17)
C00z	4177(6)	5590(10)	8385(5)	47.3(17)
C010	3552(7)	6915(11)	8635(5)	56(2)
C011	3354(6)	8545(10)	8218(5)	50.0(18)

C012	11644(6)	3545(10)	6780(5)	49.6(18)
C013	1657(8)	5346(12)	4411(6)	70(2)
C014	13342(8)	338(13)	10587(6)	74(3)

Table S3 Bond Lengths for compound **4k.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl01	**C00V**	1.741(8)	**C00F**	**C00G**	1.510(8)
Cl02	**C00Z**	1.753(7)	**C00G**	**C00K**	1.368(8)
O003	**C00H**	1.250(7)	**C00G**	**C00O**	1.457(8)
O004	**C00D**	1.255(7)	**C00I**	**C00L**	1.343(8)
O005	**C00O**	1.335(7)	**C00I**	**C00M**	1.512(8)
O005	**C00Y**	1.461(8)	**C00I**	**C00N**	1.473(8)
O006	**C00N**	1.335(7)	**C00I**	**C00M**	1.520(9)
O006	**C00W**	1.469(8)	**C00J**	**C00P**	1.401(9)
O007	**C00N**	1.199(7)	**C00J**	**C00U**	1.383(9)
O008	**C00O**	1.203(7)	**C00K**	**C00R**	1.474(9)
N009	**C00F**	1.487(8)	**C00L**	**C00S**	1.484(9)
N009	**C00H**	1.328(7)	**C00P**	**C00V**	1.374(10)
N00A	**C00D**	1.382(8)	**C00Q**	**C00Z**	1.380(10)
N00A	**C00L**	1.394(7)	**C00T**	**C011**	1.422(10)
N00B	**C00D**	1.325(8)	**C00U**	**C012**	1.420(10)
N00B	**C00M**	1.480(8)	**C00V**	**C00X**	1.373(10)
N00C	**C00H**	1.383(8)	**C00W**	**C014**	1.511(12)
N00C	**C00K**	1.388(8)	**C00X**	**C012**	1.359(10)
C00E	**C00F**	1.520(9)	**C00Y**	**C013**	1.515(11)
C00E	**C00Q**	1.377(9)	**C00Z**	**C010**	1.381(11)
C00E	**C00T**	1.372(9)	**C010**	**C011**	1.351(10)

Table S4 Bond Angles for compound **4k.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00Y	O005	C00O	116.4(5)	C00R	C00K	C00G	126.8(5)
C00W	O006	C00N	116.3(5)	C00I	C00L	N00A	118.7(5)
C00H	N009	C00F	121.5(5)	C00S	C00L	N00A	114.2(5)
C00L	N00A	C00D	122.0(5)	C00S	C00L	C00I	127.1(6)
C00M	N00B	C00D	122.0(5)	C00I	C00M	N00B	108.7(5)
C00K	N00C	C00H	122.2(5)	C00J	C00M	N00B	109.7(5)
N00A	C00D	O004	120.0(5)	C00J	C00M	C00I	114.1(5)
N00B	C00D	O004	122.7(5)	O007	C00N	O006	121.0(6)
N00B	C00D	N00A	117.3(5)	C00I	C00N	O006	112.2(5)
C00Q	C00E	C00F	116.7(5)	C00I	C00N	O007	126.8(6)
C00T	C00E	C00F	122.1(6)	O008	C00O	O005	120.3(6)
C00T	C00E	C00Q	121.1(6)	C00G	C00O	O005	111.9(5)
C00E	C00F	N009	109.9(5)	C00G	C00O	O008	127.8(6)
C00G	C00F	N009	108.9(5)	C00V	C00P	C00J	118.9(6)
C00G	C00F	C00E	114.8(5)	C00Z	C00Q	C00E	118.4(6)
C00K	C00G	C00F	119.2(5)	C011	C00T	C00E	119.2(6)
C00O	C00G	C00F	119.1(5)	C012	C00U	C00J	119.5(6)
C00O	C00G	C00K	121.8(5)	C00P	C00V	C101	117.5(5)
N009	C00H	O003	122.2(5)	C00X	C00V	C101	120.5(6)
N00C	C00H	O003	120.1(5)	C00X	C00V	C00P	122.1(7)
N00C	C00H	N009	117.7(5)	C014	C00W	O006	105.9(6)
C00M	C00I	C00L	119.9(5)	C012	C00X	C00V	119.7(7)
C00N	C00I	C00L	122.3(5)	C013	C00Y	O005	106.1(6)
C00N	C00I	C00M	117.9(5)	C00Q	C00Z	C102	118.6(6)
C00P	C00J	C00M	118.0(5)	C010	C00Z	C102	119.6(6)
C00U	C00J	C00M	122.3(6)	C010	C00Z	C00Q	121.7(7)
C00U	C00J	C00K	119.7(6)	C011	C010	C00Z	119.8(7)
C00G	C00K	N00C	118.7(5)	C010	C011	C00T	119.7(7)
C00R	C00K	N00C	114.5(5)	C00X	C012	C00U	120.0(7)

Single crystal X-Ray Diffraction (XRD) Analysis of 4k

Wilson plot: In order to validate the formation of synthesized 1,2,3,4-tetrahydropyrimidine-2-thione/ones and to authenticate this approach, we chose to perform the single X-ray diffraction analysis of compound **4k**. Firstly, we had carefully observed the E-STATISTICS of compound **4k.** The program E-STATISTICS carries out a Wilson plot, which calculates the normalised structure factors (E's) and the statistics of the distributions of these E-values. A graphical display of the Wilson plot is given in Figure S1. It is clearly visible from the graph that crystal structure shows perfect distributions of atoms.

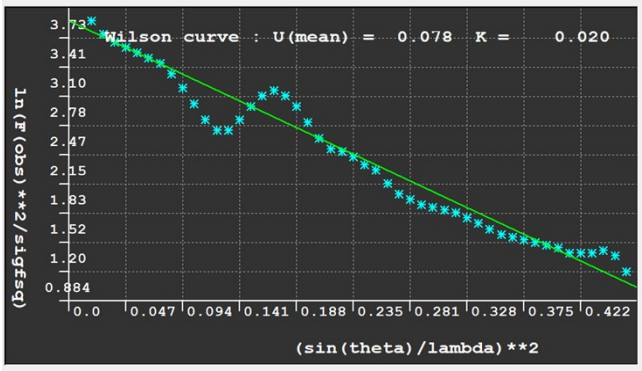


Figure S1. Wilson plot of compound **4k**

View Normal To (100), (010), (001): X-ray analysis revealed that the synthesized compounds are chemically as well as thermally stable. In the crystal structure, the molecules are linked by intermolecular interactions of different strengths. The compound **4k** was crystallized in triclinic cell with space group P-1. In order to check the stability of compound **4k** we had carefully observed their View Normal To (100), (010), (001) planes. These options provide views where the crystallographic bc, ac, ab planes respectively are placed in the plane of the illustration which eventually defines the stability of the compound. These sheets are connected in the (100), (010), (001) by the mixture of dipolar and vander wall forces for an extensively single crystal analysis as shown in Figure S2.

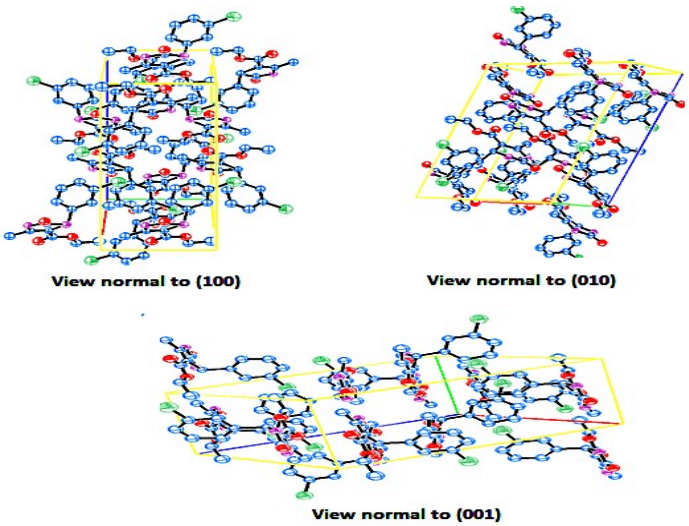
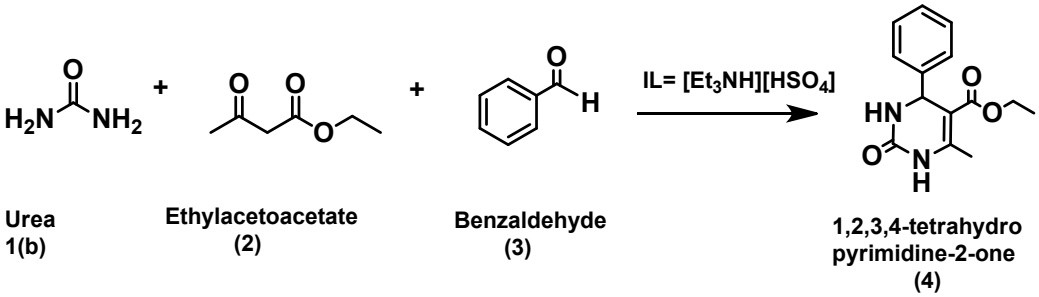


Figure S2. Illustration of compound **4k** along (100), (010), (001) planes.

Table S5 Calculation for green chemistry metrics for compound **4a**.



F.W.	60.05 g/mol	130.14 g/mol	106.12 g/mol	260.28 g/mol
mmol	1.0	1.0	1.0	0.8
amount	0.06 g	0.130 g	0.106 g	0.208 g

S. No.	Parameters	Formula	Characteristics	Ideal Value	Calculated value for compound 4a
1.	Environmental (E) factor	[Total mass of raw materials - the total mass of product]/ mass	E-factor signifies the total amount of waste generated in a	0	[(0.06 + 0.130 + 0.106)-0.208]/0.208 = 0.42

		of product	chemical reaction.		
2.	Process mass intensity (PMI)	∑ (mass of stoichiometric reactants)/[mass of stoichiometry product]	PMI takes into account reaction efficiency, stoichiometry, amount of solvent and all reagent used in the chemical reaction.	1	(0.06+0.130+0.106)/ 0.208 = 1.42
3.	Reaction mass efficiency (RME %)	[mass of product/∑ (mass of stoichiometric reactants)] × 100	RME accounts into atom economy, chemical yield and stoichiometry.	100%	[0.208/ (0.06 + 0.130 + 0.106)] × 100 = 70%
4.	Atom economy (AE %)	[MW of product] ÷ ∑(MW of stoichiometric reactants) × 100	Atom economy signifies the percentage of atoms wasted in chemical reaction. Higher the value of AE, greener is the reaction. Maximum value of atom economy is 100% which indicates that all the atoms	100%	[(260.28) / (60.05 + 130.14 + 106.12)] × 100 = 88%

			present in reactants lies in the product.		
5.	Carbon efficiency (CE %)	[Amount of carbon in product/ Total carbon present in reactants] x 100	CE signifies the percentage of carbons in the reactants that is left in the product.	100%	= [0.8 x 14 / (1.0 x 1+ 1.0 x 6 + 1.0 x 7)] x 100 = [11.2 / (1.0 + 6.0 + 7.0)] x 100 = 80%

Green chemistry parameters

Further, to explore the green chemistry aspect of the reaction, Environmental (E) factor, Process mass intensity (PMI), Reaction mass efficiency (RME%), Atom economy (AE %), and Carbon efficiency (CE%) for the reaction were calculated. Figure S3 clearly demonstrates that the calculated values are closer to the ideal values indicating an environment friendly process. All the calculations for the measurement of green chemistry parameters are provided in Table S5

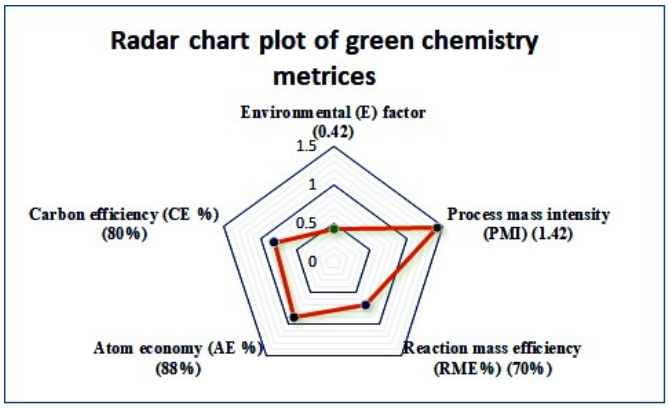
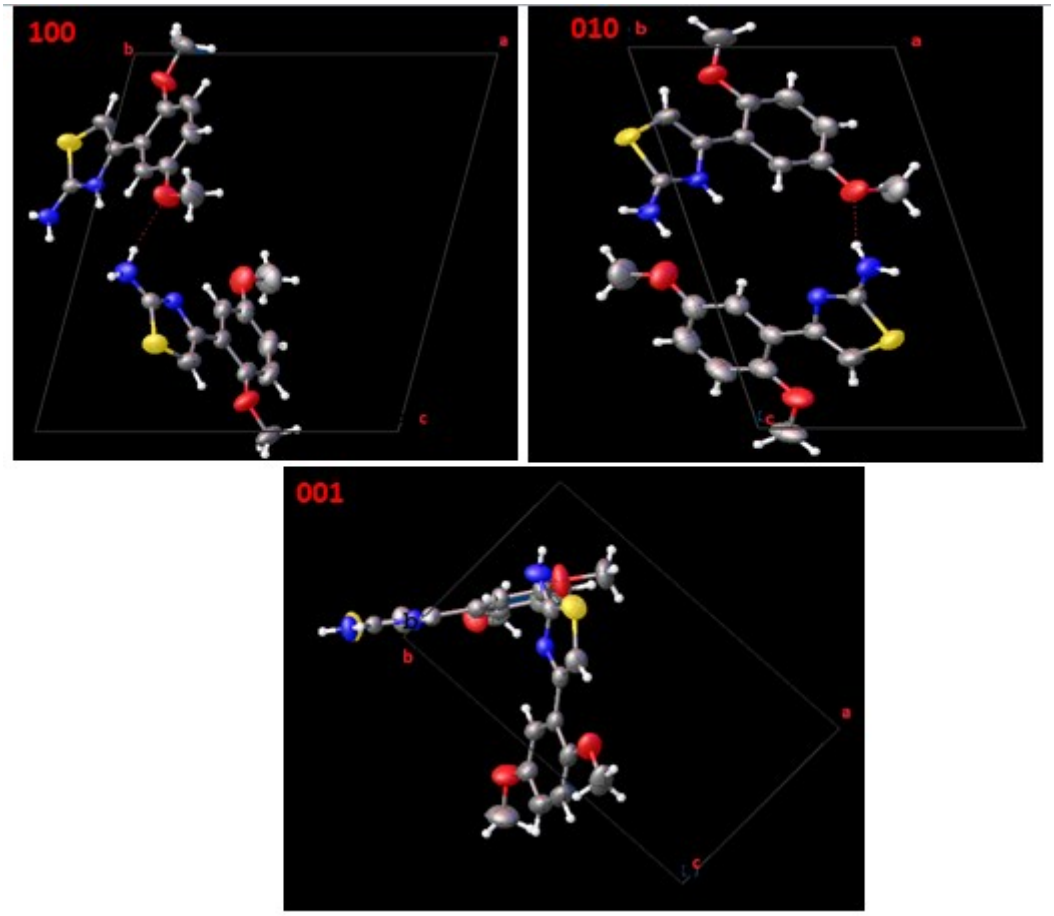
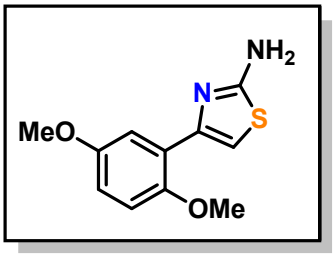


Figure S3. Radar chart for Green Chemistry Metrics for com-pound **4a**.



FigureS4: Illustration of compound **6j** along (100), (010), (110) directions.

Table S6 Crystal data and structure refinement for compound **6j**



CCDC Number	**CCDC 1963534**
Molecular Formula	$C_{11}H_{12}N_2O_2S$

Molecular weight	236.06
Temperature	293(2)
Radiation	Mo Kα (λ = 0.71073)
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a/Å = 7.2836(4); α/ ^{o} = 75.781(5) b/Å = 12.2470(7); β/^{o} = 74.928(5) c/Å = 13.7125(8); ϒ/ ^{o} = 89.897(5)
Volume /Å^3	1142.40(12)
Z	8
Density (ρcalcg/cm^3)	1.377
Absorption coefficient (μ/mm^{-1})	0.270
F(000)	498.0
2θ range for data collection	6.55 to 58.77
Index ranges	-9 ≤ h ≤ 10, -16 ≤ k ≤ 16, -18 ≤ l ≤ 18
Reflections collected	17516
Independent reflections	5494 [R_{int} = 0.0281, R_{sigma} = 0.0385]
Data/restraints/parameters	5494/0/298
Refinement method	Full-matrix least-squares on F2
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R1 = 0.0531, wR2 = 0.1175
Final R indexes [all data]	R1 = 0.0766, wR2 = 0.1329
Largest diff. peak/hole / e Å^{-3}	0.19/-0.57

Table S7 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound **6j**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	**y**	***z***	**U(eq)**

S001	-1161.5(9)	11158.1(6)	2344.7(4)	56.68(19)
S002	6139.2(9)	7338.6(6)	7672.3(5)	61.2(2)
N003	925(2)	10126.7(13)	3468.5(11)	34.9(3)
N004	3927(2)	7135.2(14)	6532.8(12)	40.2(4)
O005	2806(2)	9002.0(16)	718.0(12)	66.0(5)
N006	-1336(2)	11189.6(15)	4311.6(12)	46.3(4)
O007	6645(3)	8098.0(16)	3764.4(13)	71.6(5)
O008	1875(3)	4400.1(15)	9189.4(13)	73.6(5)
N009	6202(3)	8662.1(18)	5778.9(15)	57.0(5)
O00A	-1601(3)	5400.6(16)	5984.8(16)	81.9(6)
C00B	-468(3)	10791.2(15)	3493.9(13)	34.4(4)
C1	3170(3)	9156.8(16)	2347.0(14)	39.0(4)
C00D	1540(3)	9864.3(16)	2508.2(14)	37.5(4)
C2	4196(3)	8904.0(17)	3083.1(15)	43.9(5)
C00F	5369(3)	7752.8(18)	6549.3(15)	41.4(5)
C00G	3350(3)	6268.1(17)	7444.1(15)	42.5(5)
C00H	1686(3)	5521.5(17)	7549.0(16)	45.5(5)
C5	3799(3)	8738.0(19)	1454.4(16)	47.1(5)
C00J	5774(3)	8271.3(19)	2967.4(16)	49.1(5)
C00K	561(3)	10349(2)	1821.5(16)	53.5(6)
C00L	766(3)	5725.2(18)	6763.2(18)	50.1(5)
C00M	940(3)	4609.5(19)	8422.7(18)	56.4(6)
C4	5367(4)	8107(2)	1349.1(18)	58.9(6)
C00O	-837(3)	5087.3(19)	6816(2)	57.8(6)
C3	6365(3)	7868(2)	2094.5(19)	58.7(6)
C00Q	4378(4)	6269(2)	8135.8(18)	59.2(6)
C00R	-1562(4)	4213(2)	7677(2)	70.3(7)
C00S	-661(4)	3979(2)	8465(2)	72.1(8)
C00T	3557(4)	8731(3)	-250.6(18)	73.1(8)
C00U	8200(4)	7394(3)	3716(2)	77.7(8)

C00V	1073(5)	3527(2)	10113(2)	86.8(10)
C00W	-3107(5)	4686(3)	5950(3)	96.2(10)

Table S8 Anisotropic Displacement Parameters (Å2×103) for **6j**. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S001	61.6(4)	77.4(4)	39.0(3)	-15.2(3)	-27.0(3)	28.0(3)
S002	60.6(4)	78.5(5)	51.4(3)	-12.8(3)	-30.3(3)	4.6(3)
N003	37.4(8)	41.6(9)	27.9(7)	-7.0(6)	-14.1(6)	5.0(7)
N004	40.0(9)	42.1(9)	38.9(9)	-8.2(7)	-13.4(7)	6.0(7)
O005	73.0(11)	92.6(13)	48.1(9)	-38.5(9)	-24.1(8)	16.3(10)
N006	48.9(10)	57.5(11)	35.4(8)	-11.8(8)	-16.2(7)	22.5(8)
O007	73.5(11)	93.4(13)	61.5(10)	-30.2(9)	-32.0(9)	49.8(10)
O008	81.4(12)	65.6(11)	53.9(10)	13.0(8)	-10.0(9)	10.9(9)
N009	55.6(12)	64.2(13)	52.2(11)	-9.7(9)	-20.9(10)	-15.1(10)
O00A	79.0(13)	71.4(12)	101.0(15)	-13.1(11)	-41.9(12)	-18.4(10)
C00B	34.6(9)	37.3(10)	30.4(9)	-3.3(7)	-11.7(7)	2.0(8)
C1	41.8(11)	40.3(11)	33.0(9)	-8.9(8)	-6.9(8)	0.7(8)
C00D	41.1(10)	41.8(10)	29.7(9)	-7.9(8)	-10.9(8)	1.1(8)
C2	47.7(12)	49.0(12)	35.9(10)	-14.9(9)	-8.8(9)	12.9(10)
C00F	37.9(10)	49.8(12)	39.9(10)	-14.6(9)	-13.3(9)	9.1(9)
C00G	45.4(11)	41.4(11)	38.5(10)	-7.8(8)	-9.7(9)	12.6(9)
C00H	46.6(12)	36.6(11)	46.6(11)	-7.0(9)	-4.3(9)	10.4(9)
C5	52.0(12)	51.2(12)	39.5(11)	-16.8(9)	-9.7(9)	0.2(10)
C00J	51.2(13)	51.8(13)	45.3(11)	-13.9(10)	-12.9(10)	14.4(10)
C00K	61.8(14)	70.8(15)	34.4(10)	-17.8(10)	-20.2(10)	17.2(12)
C00L	52.3(13)	38.1(11)	55.3(13)	-6.2(9)	-11.5(10)	0.1(10)

C00M	61.1(15)	41.4(12)	53.4(13)	-1.2(10)	-2.7(11)	13.6(11)
C4	65.1(15)	65.1(15)	51.0(13)	-31.2(11)	-7.5(11)	9.7(12)
C00O	54.0(14)	43.1(13)	75.3(16)	-15.6(12)	-14.9(12)	2.6(11)
C3	56.6(14)	60.3(15)	61.6(14)	-26.7(12)	-9.4(11)	21.9(12)
C00Q	65.0(15)	66.2(15)	42.5(12)	-2.2(11)	-18.4(11)	9.5(12)
C00R	56.6(15)	49.3(15)	93(2)	-12.2(14)	-5.0(14)	-6.8(12)
C00S	67.8(17)	45.7(14)	76.5(18)	6.1(12)	6.1(14)	-2.7(13)
C00T	90(2)	90(2)	44.7(13)	-32.9(13)	-12.4(13)	-9.7(16)
C00U	72.1(18)	77.9(19)	93(2)	-24.8(16)	-36.7(16)	38.5(15)
C00V	106(2)	68.6(18)	53.5(15)	15.5(13)	5.8(15)	26.8(17)
C00W	79(2)	98(2)	120(3)	-37(2)	-34.0(19)	-22.8(18)

Table S9 Bond Lengths for **6j.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S001	**C00B**	1.7336(18)	**O00A**	**C00W**	1.422(3)
S001	**C00K**	1.717(2)	**C1**	**C00D**	1.471(3)
S002	**C00F**	1.7344(19)	**C1**	**C2**	1.382(3)
S002	**C00Q**	1.715(3)	**C1**	**C5**	1.410(3)
N003	**C00B**	1.298(2)	**C00D**	**C00K**	1.349(3)
N003	**C00D**	1.392(2)	**C2**	**C00J**	1.382(3)
N004	**C00F**	1.303(2)	**C00G**	**C00H**	1.475(3)
N004	**C00G**	1.394(2)	**C00G**	**C00Q**	1.352(3)
O005	**C5**	1.366(3)	**C00H**	**C00L**	1.384(3)
O005	**C00T**	1.418(3)	**C00H**	**C00M**	1.409(3)
N006	**C00B**	1.339(2)	**C5**	**C4**	1.374(3)
O007	**C00J**	1.374(3)	**C00J**	**C3**	1.372(3)
O007	**C00U**	1.420(3)	**C00L**	**C00O**	1.383(3)

O008	**C00M**	1.369(3)	**C00M**	**C00S**	1.381(4)
O008	**C00V**	1.429(3)	**C4**	**C3**	1.377(3)
N009	**C00F**	1.347(3)	**C00O**	**C00R**	1.370(3)
O00A	**C00O**	1.367(3)	**C00R**	**C00S**	1.376(4)

Table S 10 Bond Angles for **6j.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00K	**S001**	**C00B**	88.80(9)	**C00Q**	**C00G**	**C00H**	129.05(19)
C00Q	**S002**	**C00F**	88.60(10)	**C00L**	**C00H**	**C00G**	119.18(18)
C00B	**N003**	**C00D**	111.95(15)	**C00L**	**C00H**	**C00M**	117.2(2)
C00F	**N004**	**C00G**	111.10(16)	**C00M**	**C00H**	**C00G**	123.6(2)
C5	**O005**	**C00T**	118.4(2)	**O005**	**C5**	**C1**	117.19(19)
C00J	**O007**	**C00U**	117.79(19)	**O005**	**C5**	**C4**	122.95(19)
C00M	**O008**	**C00V**	117.9(2)	**C4**	**C5**	**C1**	119.9(2)
C00O	**O00A**	**C00W**	117.6(2)	**O007**	**C00J**	**C2**	115.57(18)
N003	**C00B**	**S001**	114.17(14)	**C3**	**C00J**	**O007**	124.8(2)
N003	**C00B**	**N006**	125.19(16)	**C3**	**C00J**	**C2**	119.6(2)
N006	**C00B**	**S001**	120.64(14)	**C00D**	**C00K**	**S001**	111.65(15)
C2	**C1**	**C00D**	119.50(17)	**C00O**	**C00L**	**C00H**	122.8(2)
C2	**C1**	**C5**	117.08(19)	**O008**	**C00M**	**C00H**	117.0(2)
C5	**C1**	**C00D**	123.40(18)	**O008**	**C00M**	**C00S**	123.7(2)
N003	**C00D**	**C1**	118.15(16)	**C00S**	**C00M**	**C00H**	119.4(2)
C00K	**C00D**	**N003**	113.42(18)	**C5**	**C4**	**C3**	121.9(2)
C00K	**C00D**	**C1**	128.38(18)	**O00A**	**C00O**	**C00L**	116.0(2)
C00J	**C2**	**C1**	122.56(19)	**O00A**	**C00O**	**C00R**	124.7(2)
N004	**C00F**	**S002**	114.77(15)	**C00R**	**C00O**	**C00L**	119.3(2)
N004	**C00F**	**N009**	124.07(18)	**C00J**	**C3**	**C4**	119.0(2)
N009	**C00F**	**S002**	121.14(16)	**C00G**	**C00Q**	**S002**	111.70(17)
N004	**C00G**	**C00H**	117.07(17)	**C00O**	**C00R**	**C00S**	119.2(2)
C00Q	**C00G**	**N004**	113.81(19)	**C00R**	**C00S**	**C00M**	122.0(2)

Table S 11 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **6j.**

Atom	*x*	*y*	*z*	U(eq)
H003	1409.41	9878.31	3983.44	42
H00A	-976.45	11007.32	4876.94	56
H00B	-2251.95	11627.68	4271.29	56
H00I	6011.06	8607.99	5197.19	68
H2	3809.14	9170.21	3679.33	53
H00K	791.58	10256.76	1147.93	64
H00L	1247.32	6316.3	6174.73	60
H4	5766.32	7833.39	757.76	71
H3	7424.27	7440.68	2007.32	70
H00Q	4156.17	5751.77	8783.4	71
H00R	-2650.56	3782.45	7729.46	84
H00S	-1145.17	3376.68	9042.88	87
H00C	2797.45	9036.67	-717.23	110
H00D	3536.78	7925.51	-140.39	110
H00E	4845.33	9046.98	-549.63	110
H00F	9217.49	7726.76	3109.45	117
H00G	7795.54	6664.55	3674.37	117
H00H	8636.53	7313.16	4331.21	117
H00M	1078.37	2814.19	9938.36	130
H00N	-212.48	3678.52	10419.99	130
H00O	1816.18	3500.86	10602.45	130
H00P	-3446.57	4964.82	5306.19	144
H00T	-4192.96	4676.88	6526.48	144
H00U	-2698.04	3934.15	5992.78	144
H00J	7100(40)	9020(20)	5887(18)	60(7)

Table S12. Comparing excellence of $[Et_3NH][HSO_4]$ with previously reported catalysts for the synthesis of 2-aminothiazoles.

Catalyst	**Solvent**	**Temperature**	**Time**	**Yield (%)**	**Ref.**
Fe_3O_4 nanoparticle-N-halo reagent	CH_3OH	65 ºC	2 hrs	85	3
palladium(II) acetate	$CH_3CH_2CH_2OH$	80 ºC	4 hrs	70	4
CuI	Toluene	105 ºC	12 hrs	80	5
Nanochitosan, I_2	Ethanol	80 ºC	3 hrs	80	6
Catalyst free	Water	R.T.	1-2 hrs	87	7
MW	EtOH	-	5 mins	98	8
NBS	PEG-400	R.T.	7 hrs	90	9
SiO_2-Cl	CH_3CN	80 °C	1 hr	82	10
TCCA, *p*-TSA	-	R.T.	6 hrs	90	11
$[Et_3NH][HSO_4]$	**SF[#]**	40 ℃	**30 min**	**92**	**PW[$]**
[$] Present Work. [#] Solvent Free.					

Table S13. Comparing excellence of $[Et_3NH][HSO_4]$ with previously reported catalysts for the synthesis of quinalinones.

Catalyst	**Solvent**	**Temperature**	**Time**	**Yield (%)**	**Ref.**
-	SF[#]	120℃	6 hrs	85	12
H-Y-zeolite (MW)	SF[#]	-	4 mins	85	13
Alum (MW)	SF[#]	-	5 mins	92	14
Nafion-H (MW)	SF#	-	2-6 mins	82	15
I_2	IL	80 °C	45 mins	90	16
$[Et_3NH][HSO_4]$	**SF[#]**	**R.T.**	**15-20 min**	**95**	**PW[$]**
[$] Present Work. [#] Solvent Free.					

Recyclability of IL $[Et_3NH][HSO_4]$

To investigate the potential of this procedure in a practical synthetic context and from the viewpoint of green and sustainable chemistry, the reuse of the catalytic system under study were then examined. Thus, the recyclability and the reusability of ionic liquid $[Et_3NH][HSO_4]$ was scrutinized under optimised conditions. After the end of each reaction cycle, the product

undergoes extraction for the determination of yield by ^{1}HNMR. Only the reactants were added freshly for the next run. The process was able to be repeated for six times without any conspicuous influence in the reaction outcome (Figure S5).

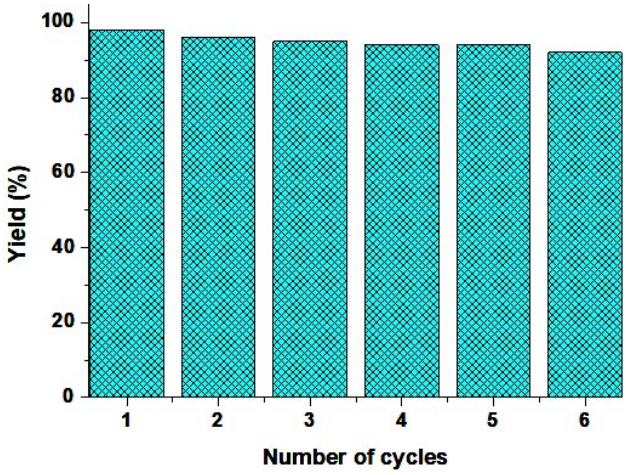


Figure S5. Recycle studies. Conditions: urea (1 mmol), ethyl aceoacetate (1 mmol), benzaldehyde (1 mmol), IL (15 mol%). To the recycled [IL], 1 mmol of urea, 1 mmol of ethyl acetoacetate and 1 mmol of benzaldehyde were added and the next cycle was carried out under the same reaction conditions. Same procedure was followed in the synthesis of 2-aminothiazoles and quinazolinones by taking suitable reactants.

[1]H NMR, [13]C NMR and MS spectra of all compounds.

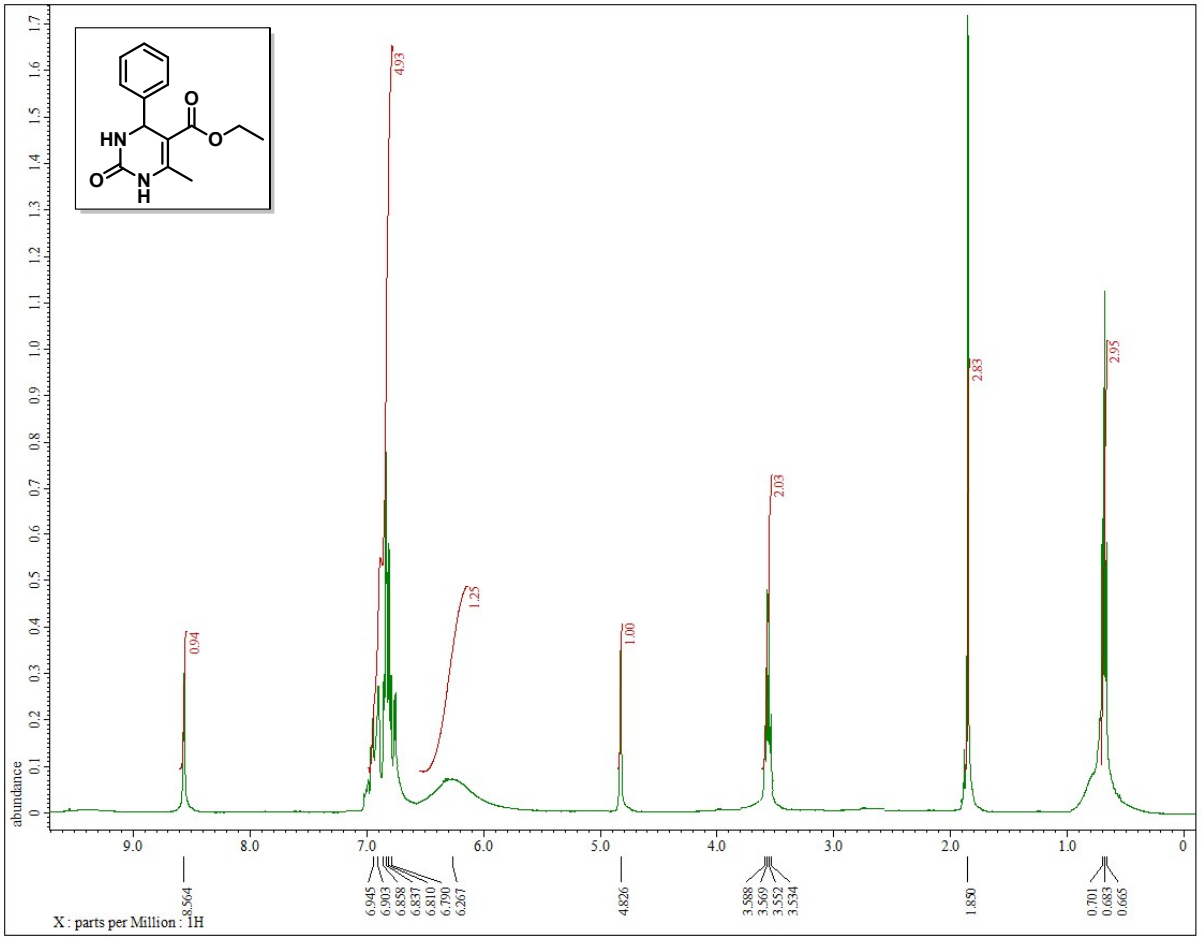


Figure S6 [1]H NMR spectra of ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4a).**

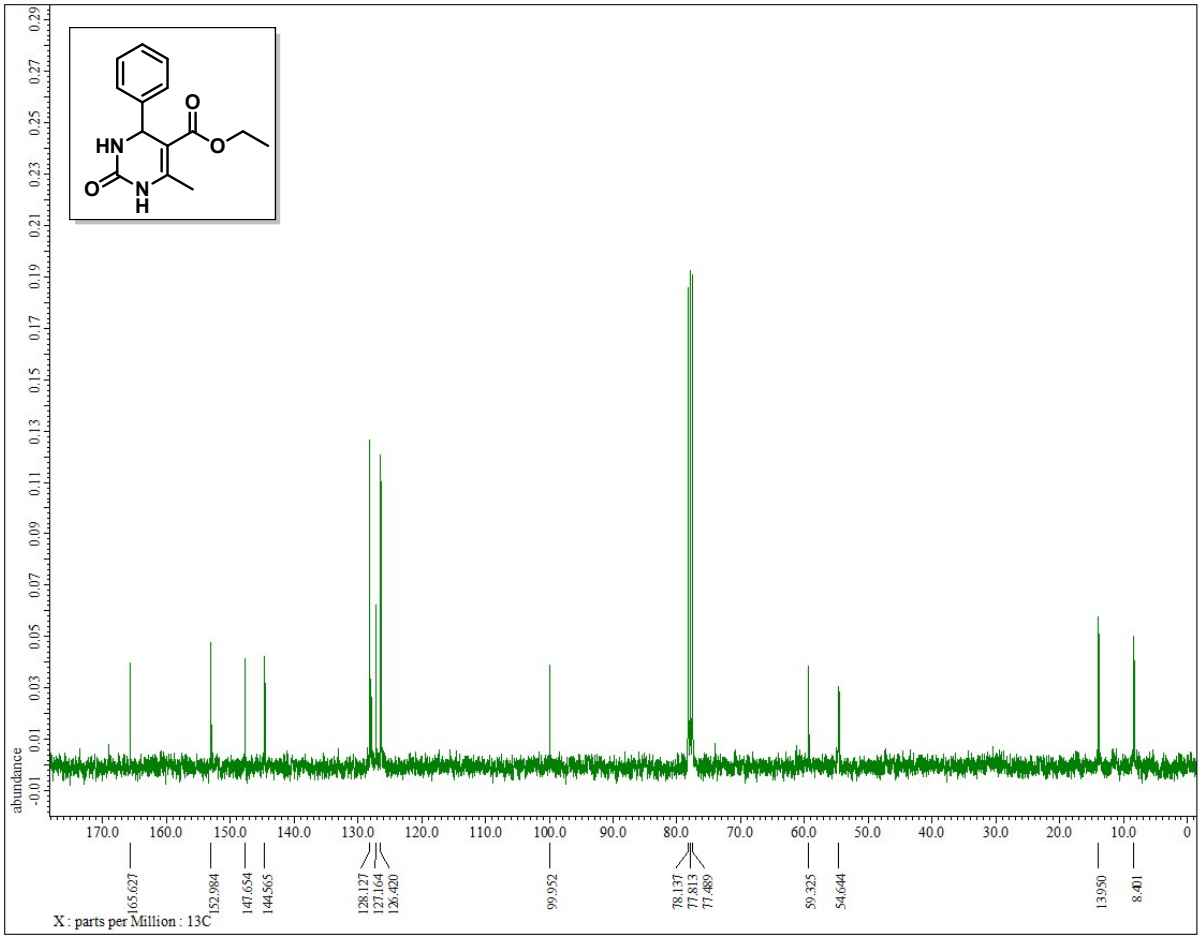
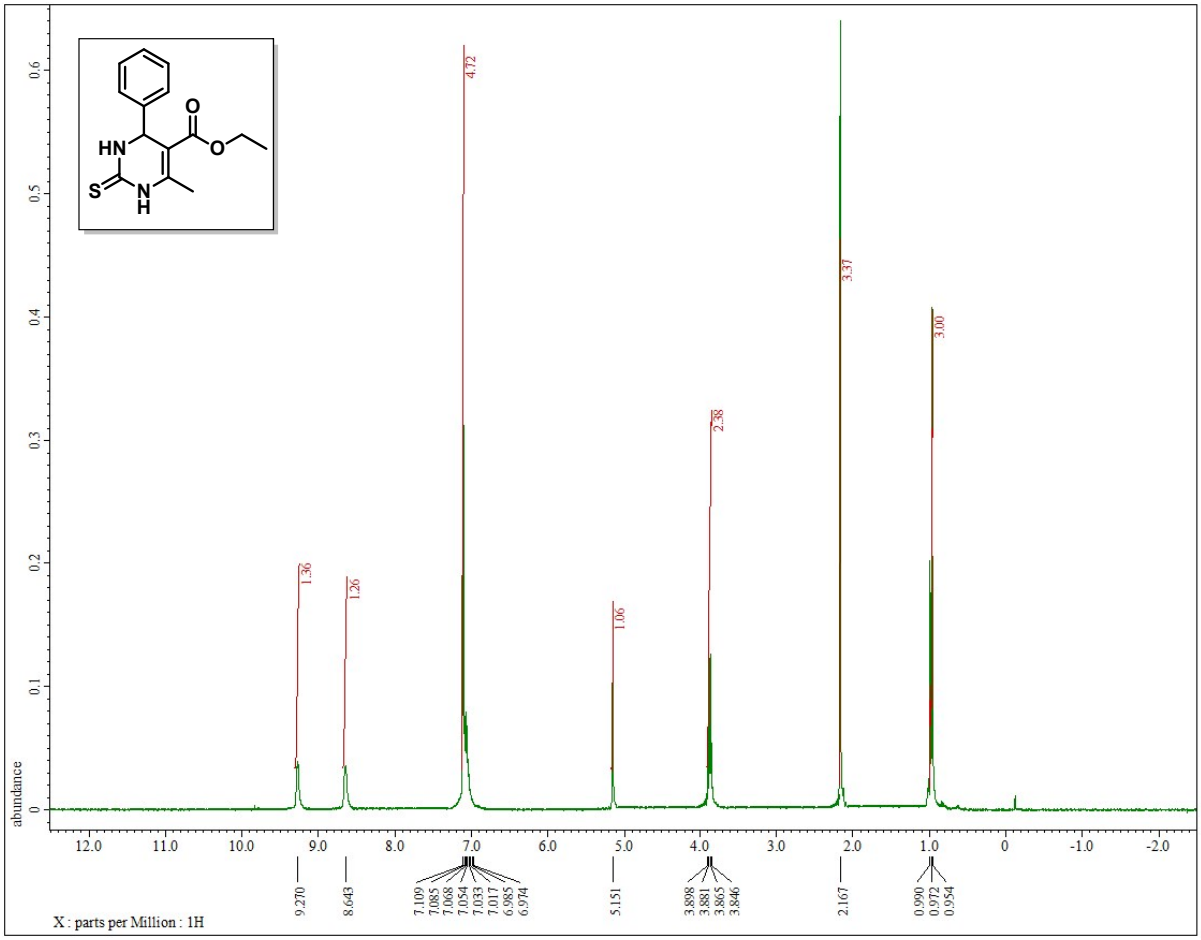
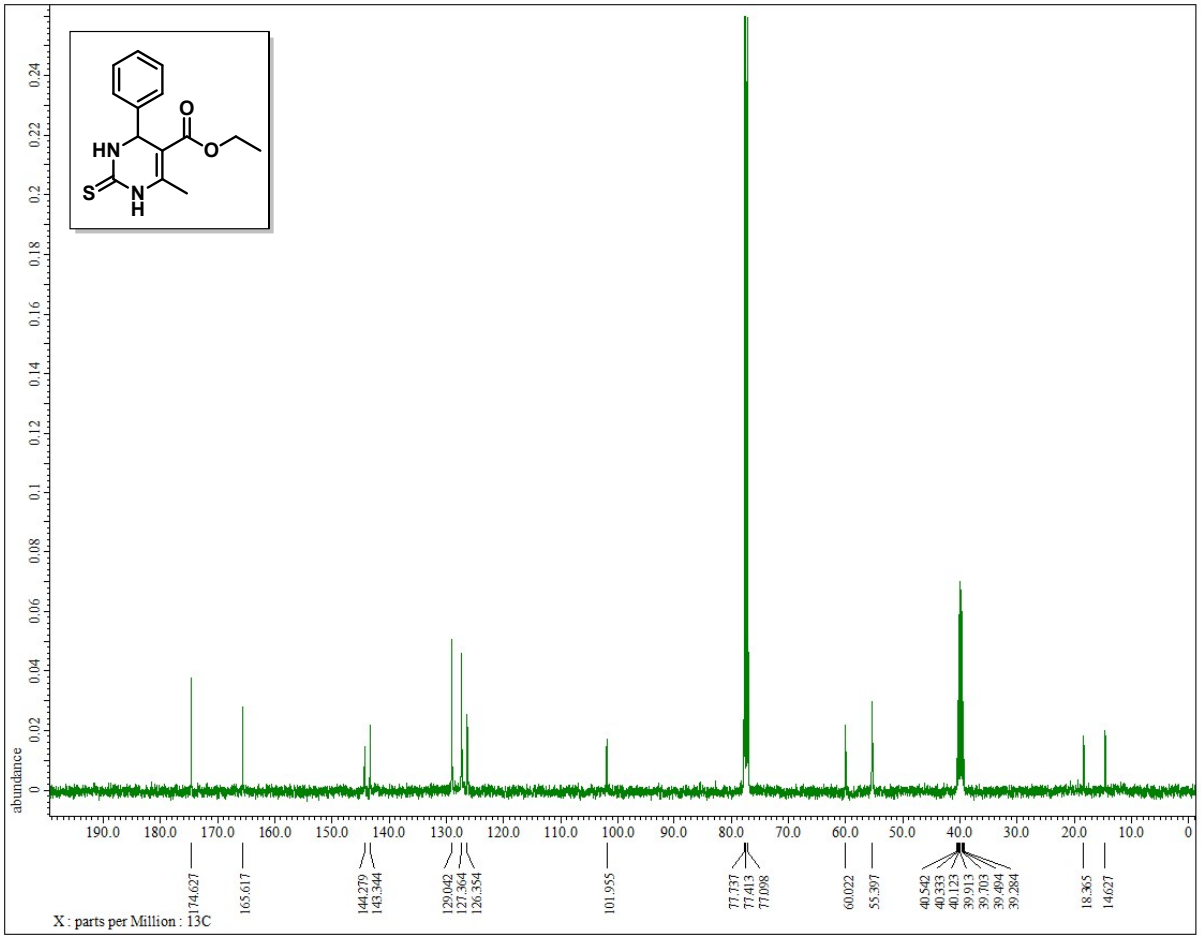


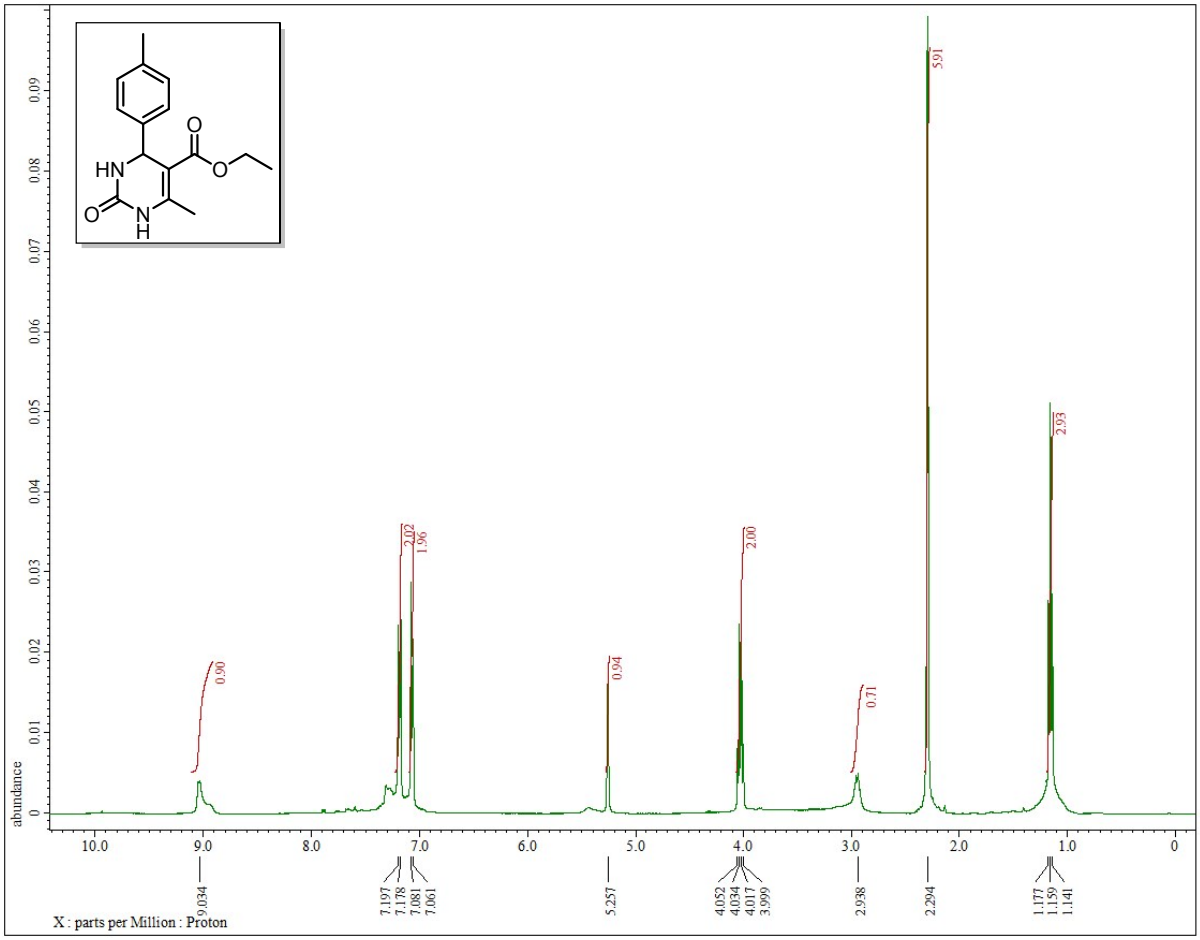
Figure S7 ^{13}C NMR spectra of ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4a).**



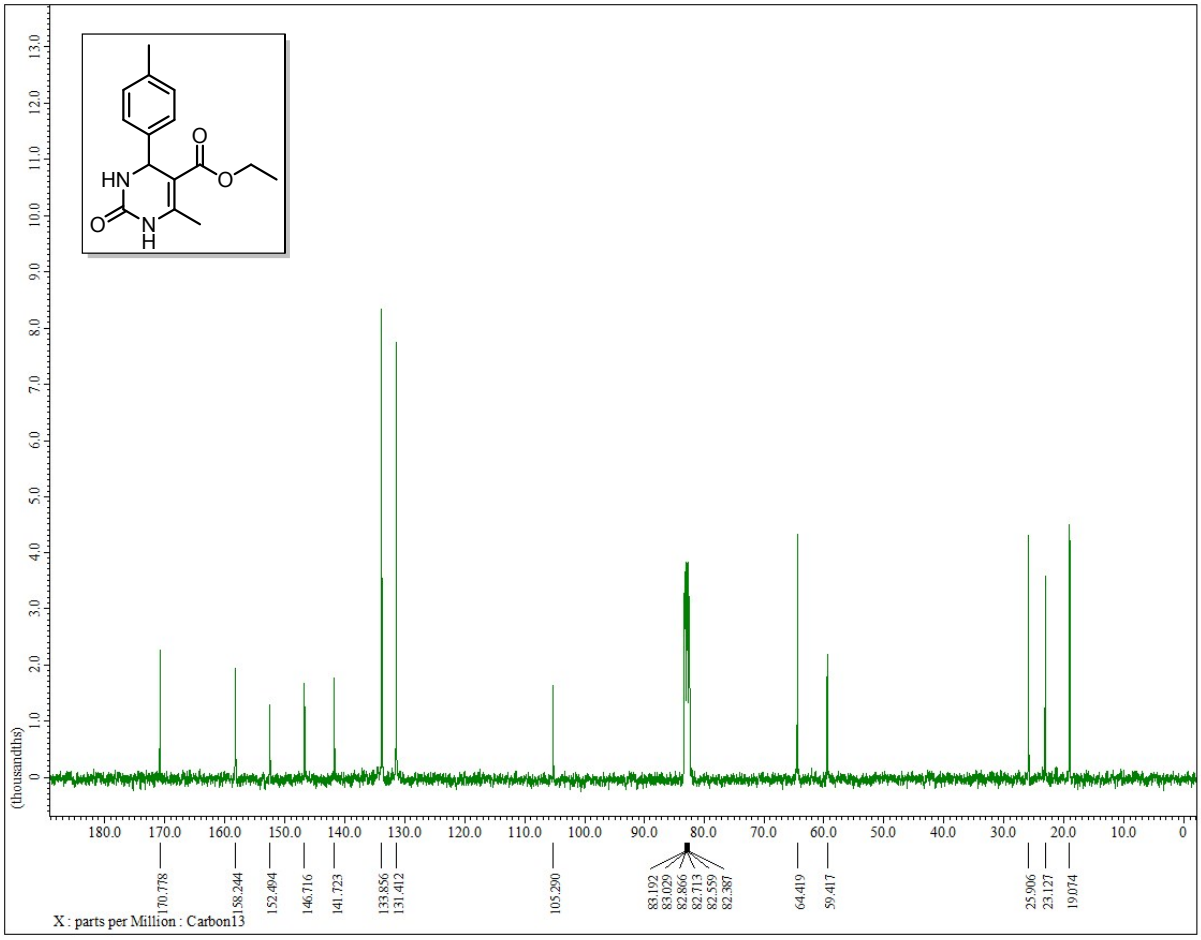
FigureS8 ^{1}H NMR spectra of ethyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4b).**



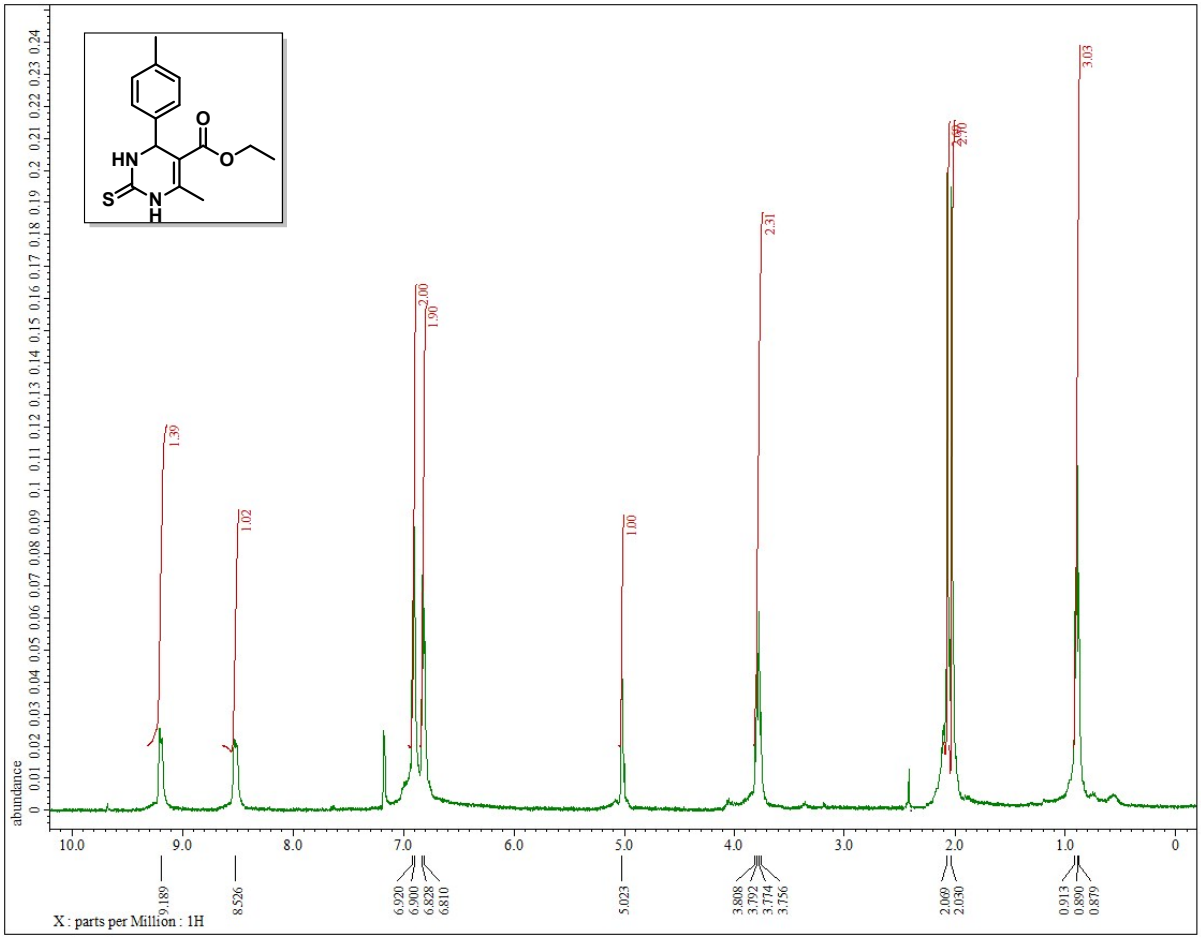
FigureS9 ^{13}C NMR spectra of ethyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4b).**



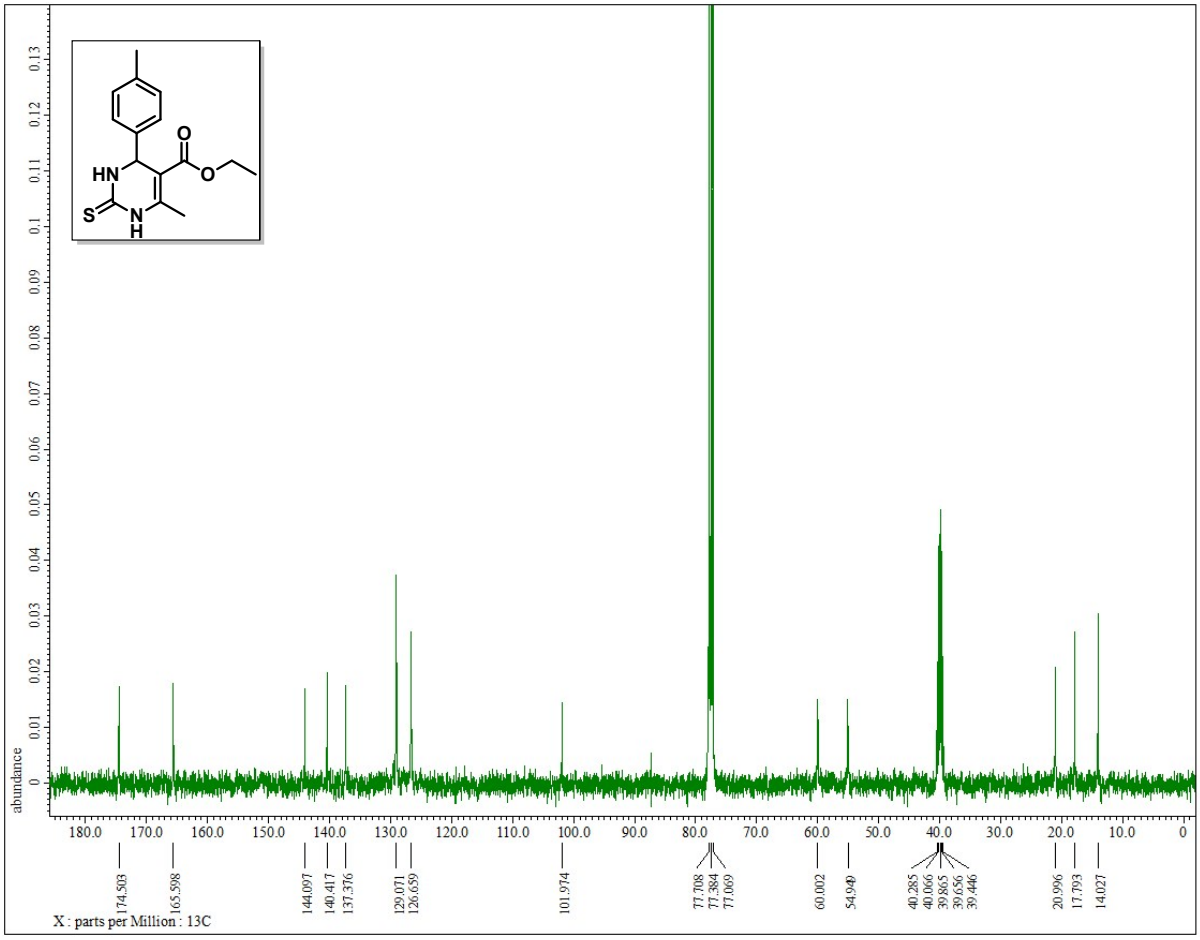
FigureS10 ^{1}H NMR spectra of ethyl-6-methyl-2-oxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4c).**



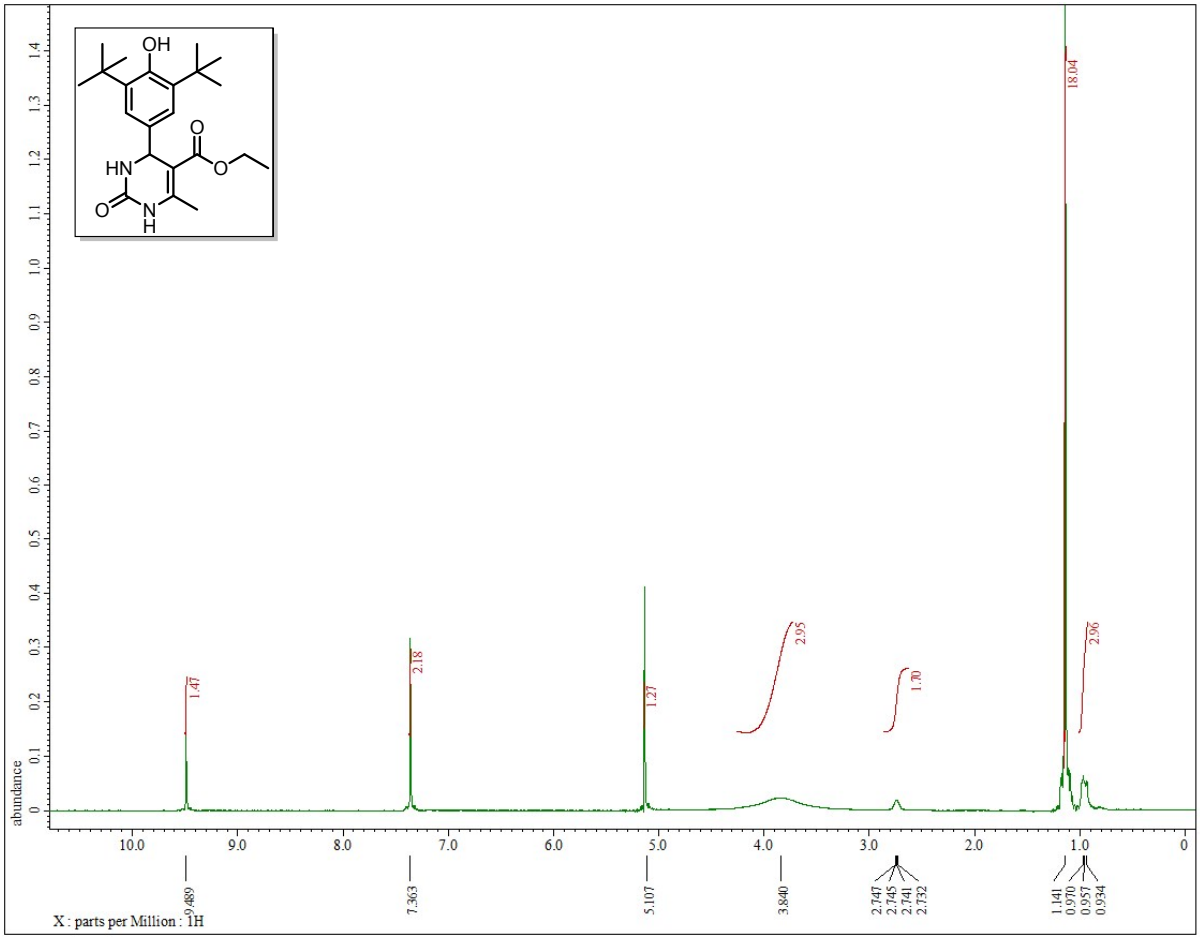
FigureS11 ^{13}C NMR spectra of ethyl-6-methyl-2-oxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4c).**



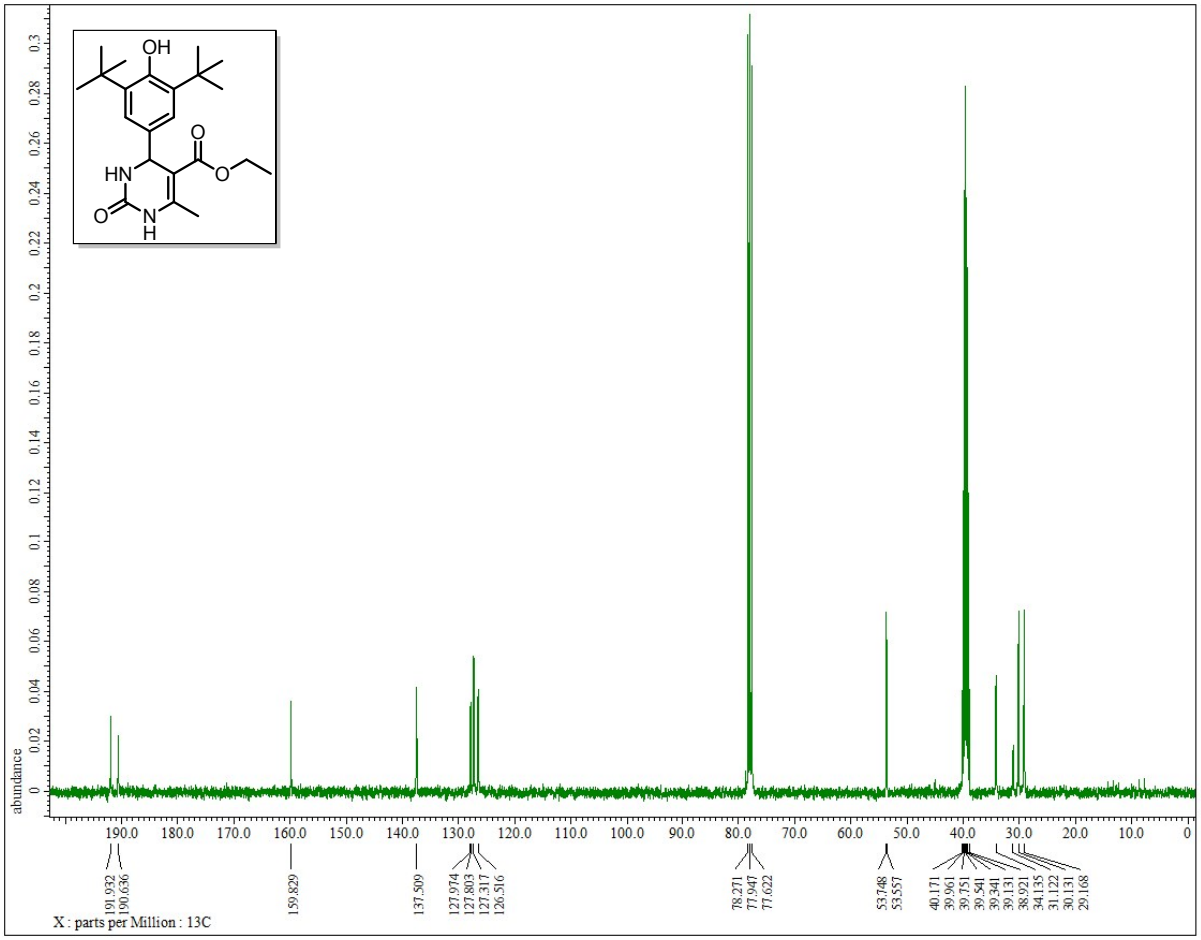
FigureS12 ^{1}H NMR spectra of ethyl-6-methyl-2-thioxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4d).**



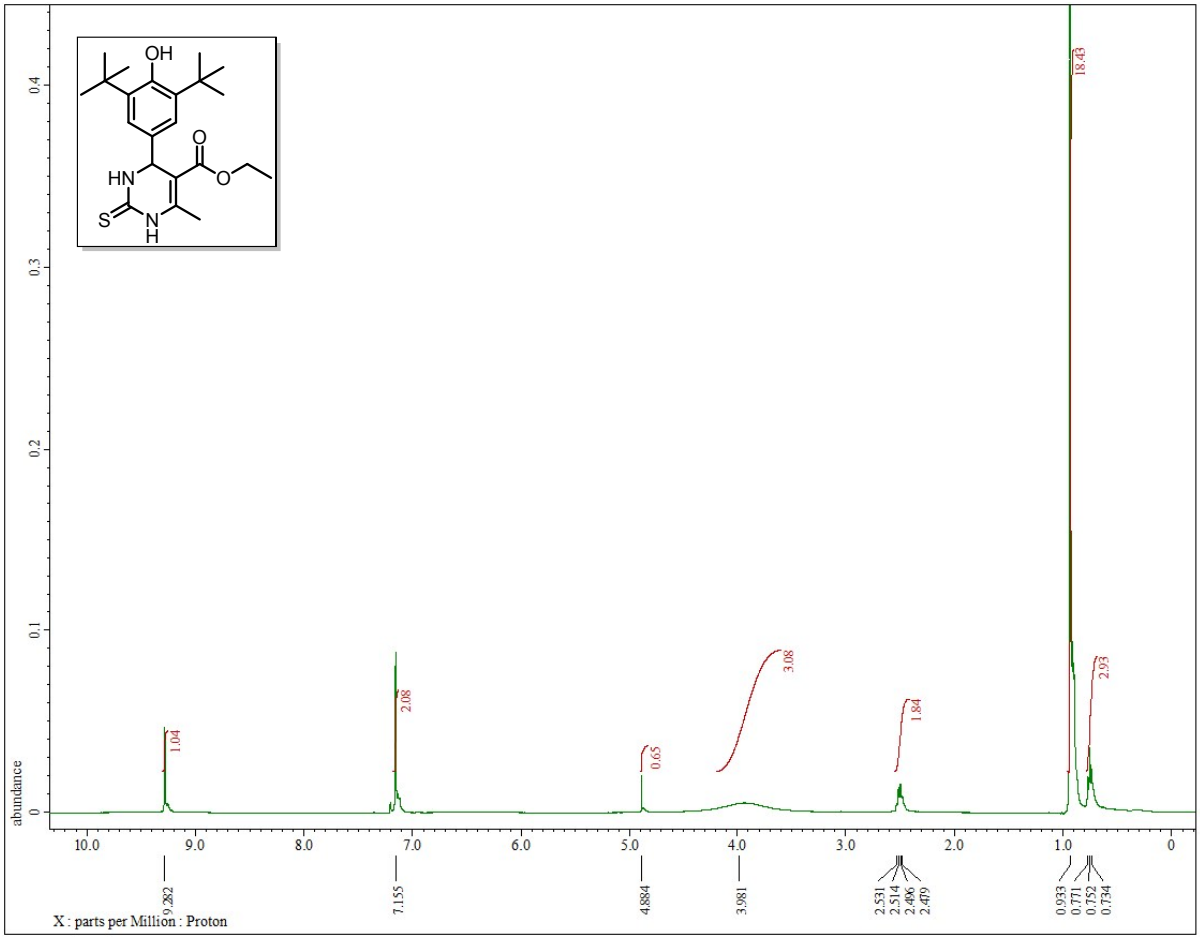
FigureS13 ^{13}C NMR spectra of ethyl-6-methyl-2-thioxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4d).**



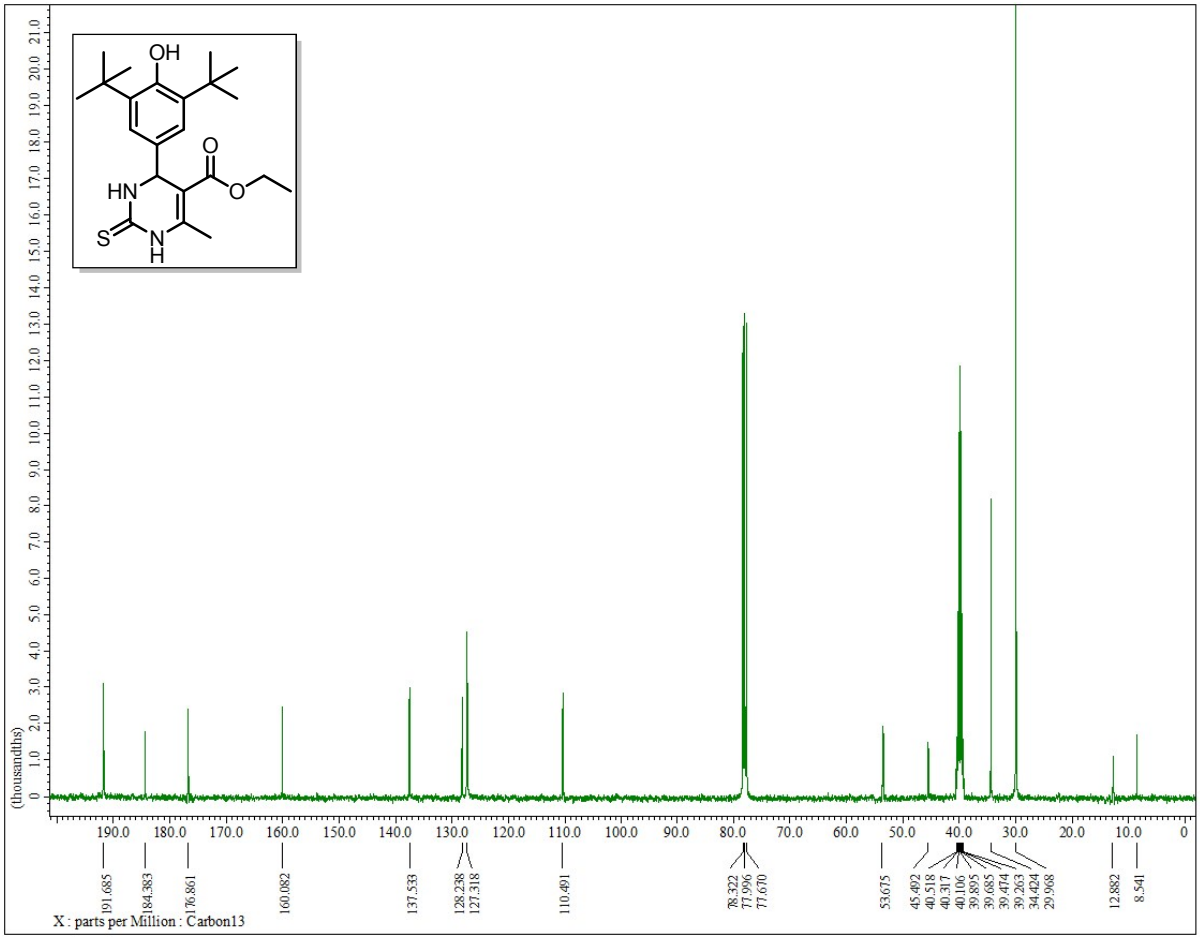
FigureS14 ^{1}H NMR spectra of ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4e).**



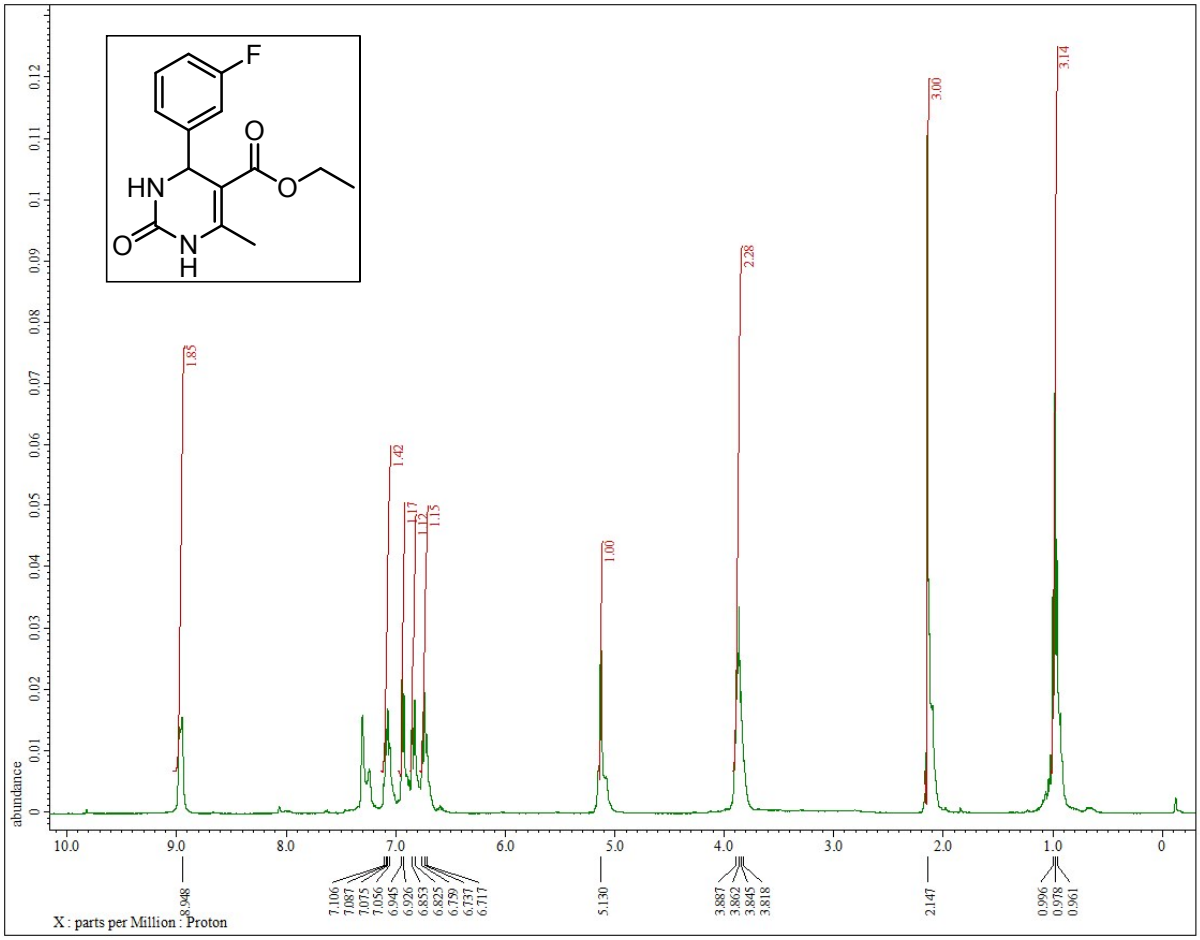
FigureS15 ^{13}C NMR spectra of ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4e).**



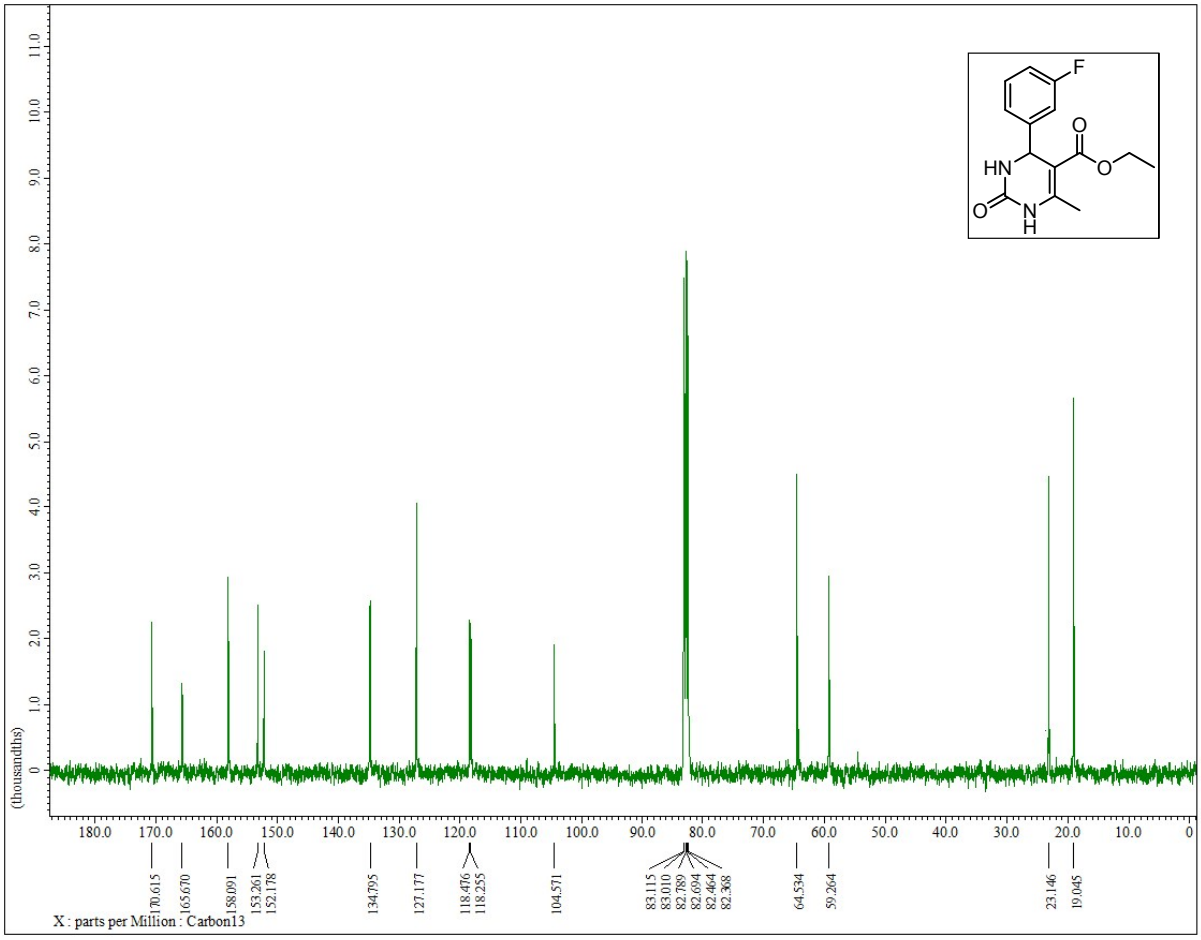
FigureS16 [1]H NMR spectra of ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4f).**



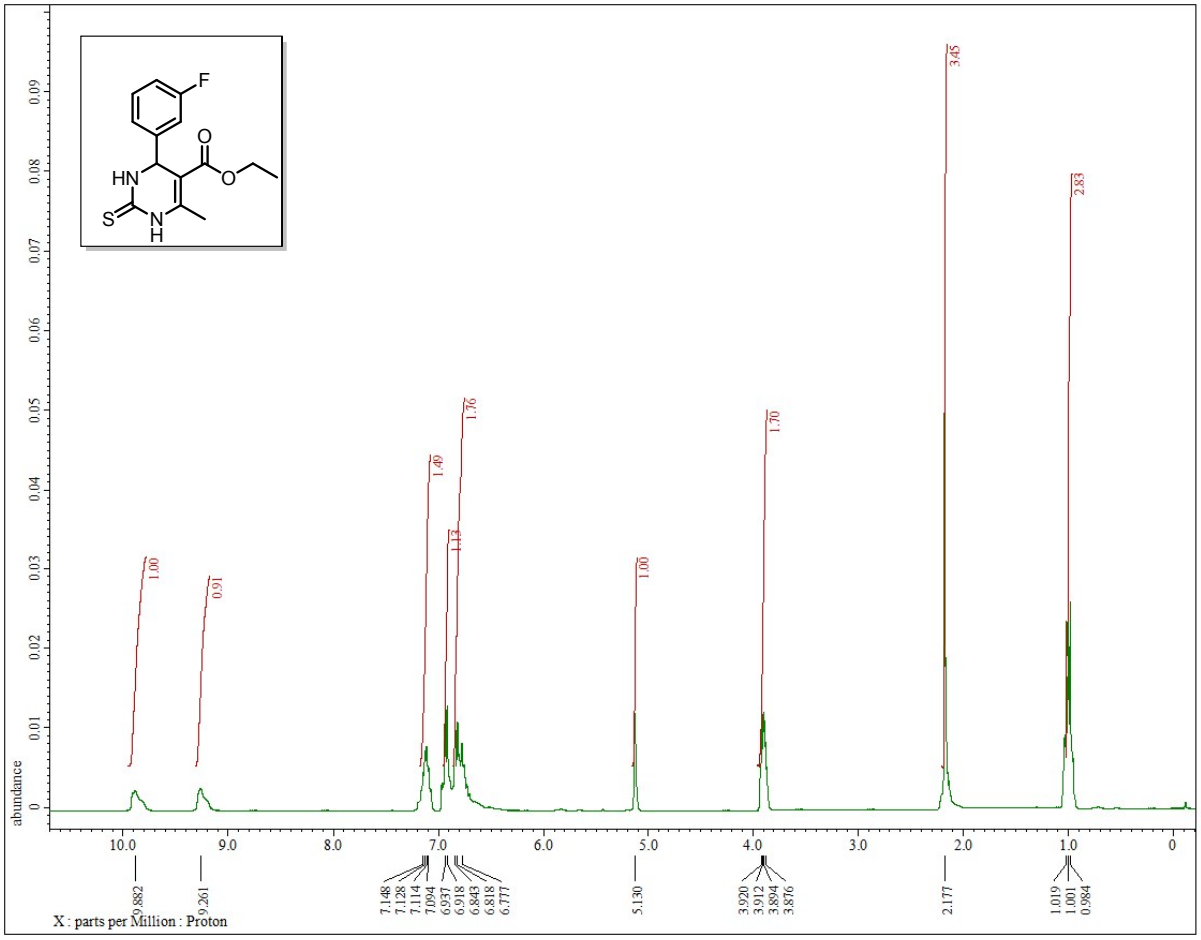
FigureS17 ^{13}C NMR spectra of ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4f).**



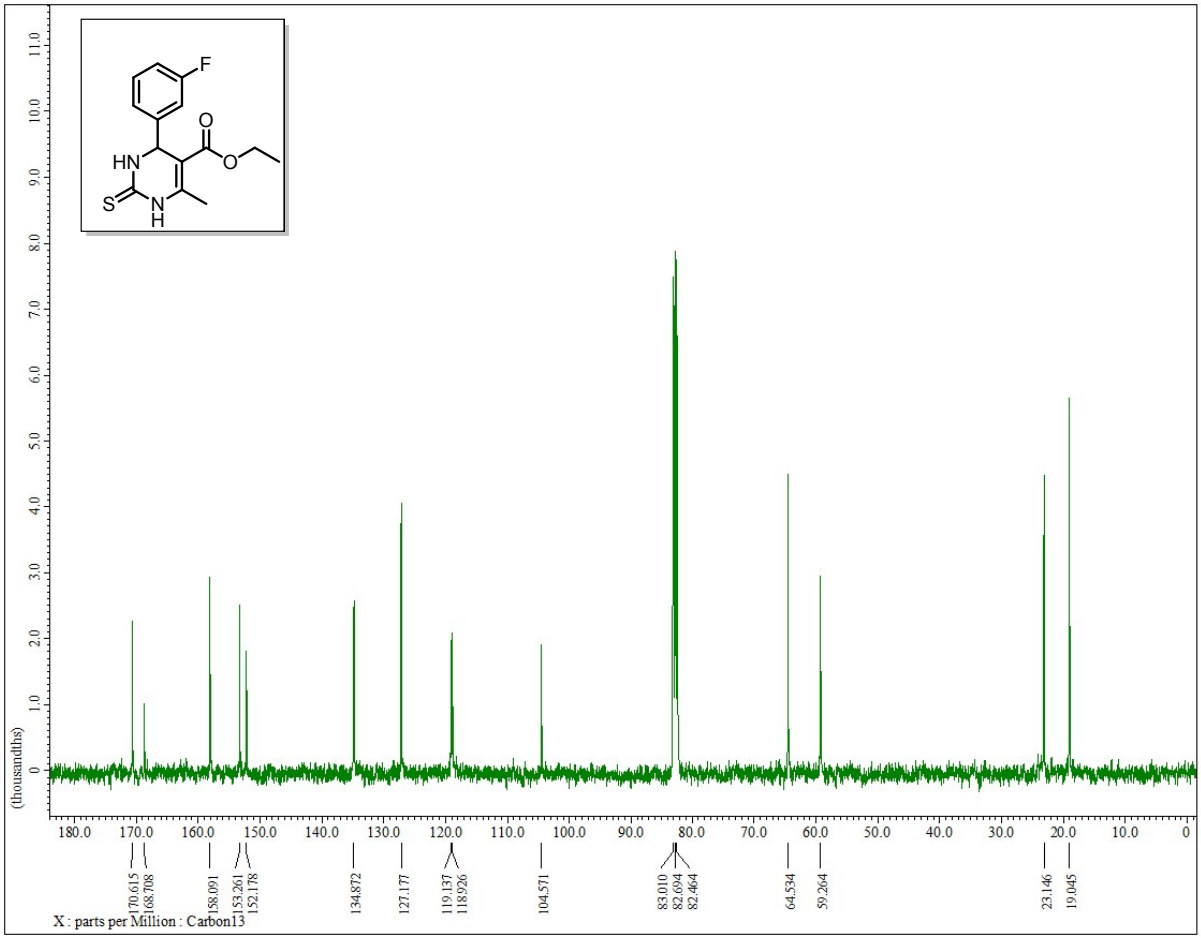
FigureS18 ^{1}H NMR spectra of ethyl-4-(3-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4g).**



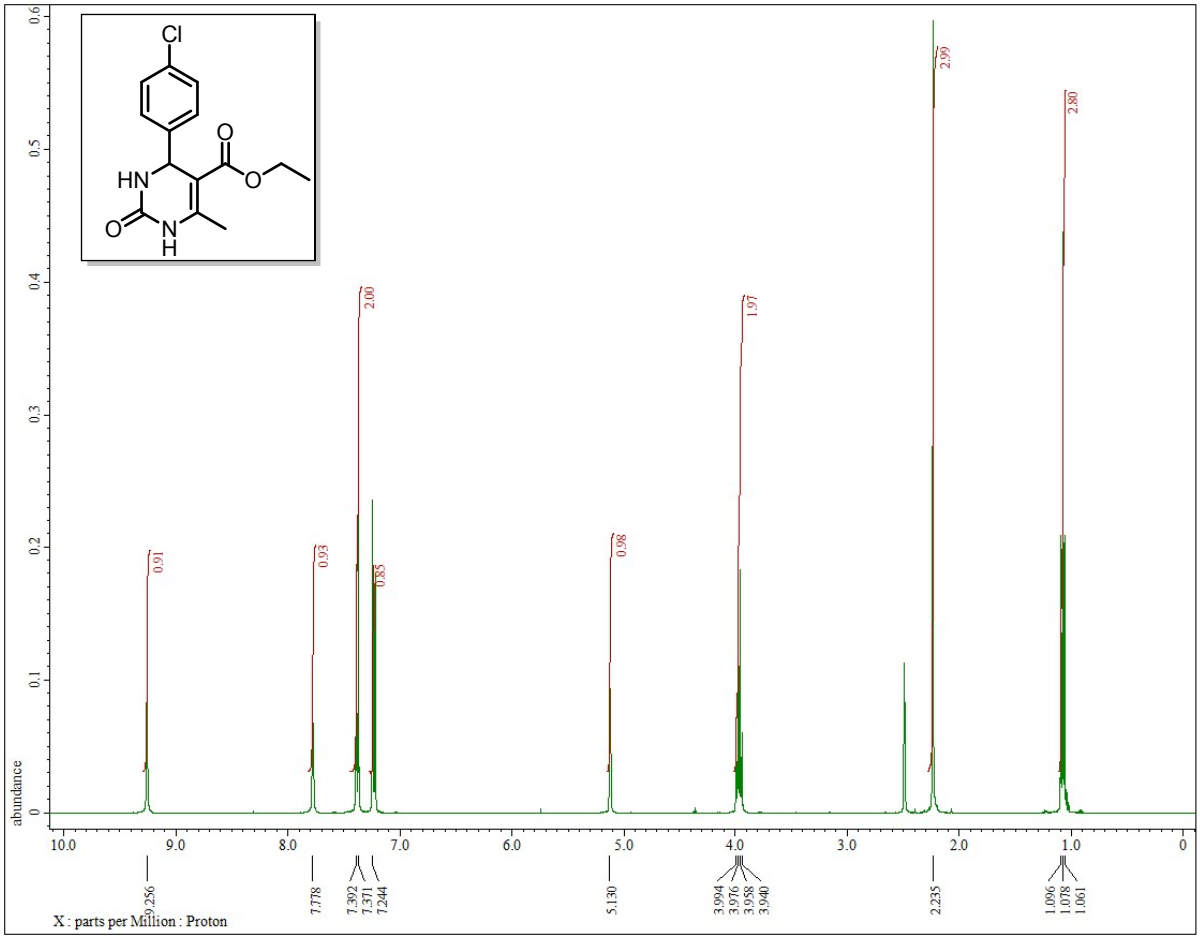
FigureS19 ^{13}C NMR spectra of ethyl-4-(3-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4g).**



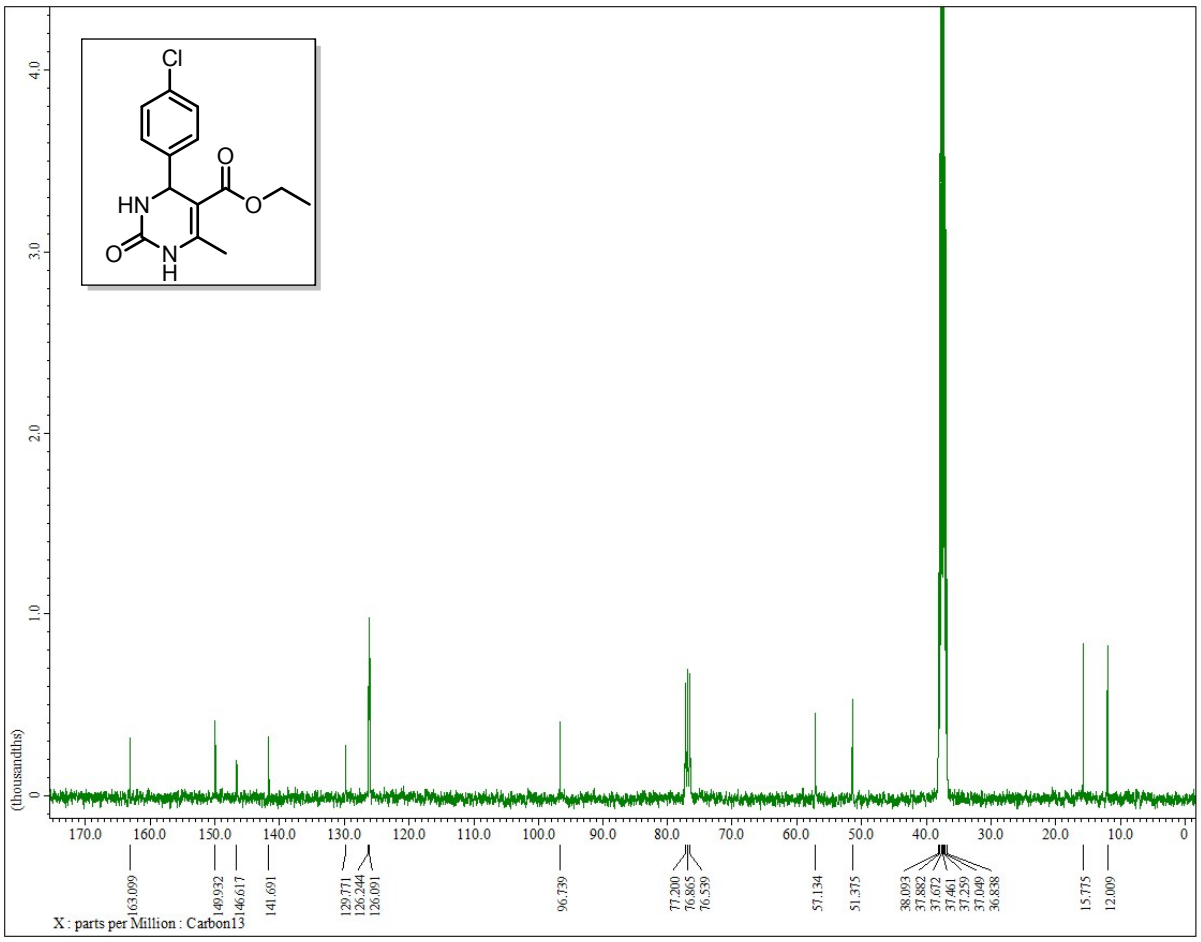
FigureS20 ^{1}H NMR spectra of ethyl-4-(3-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4h).**



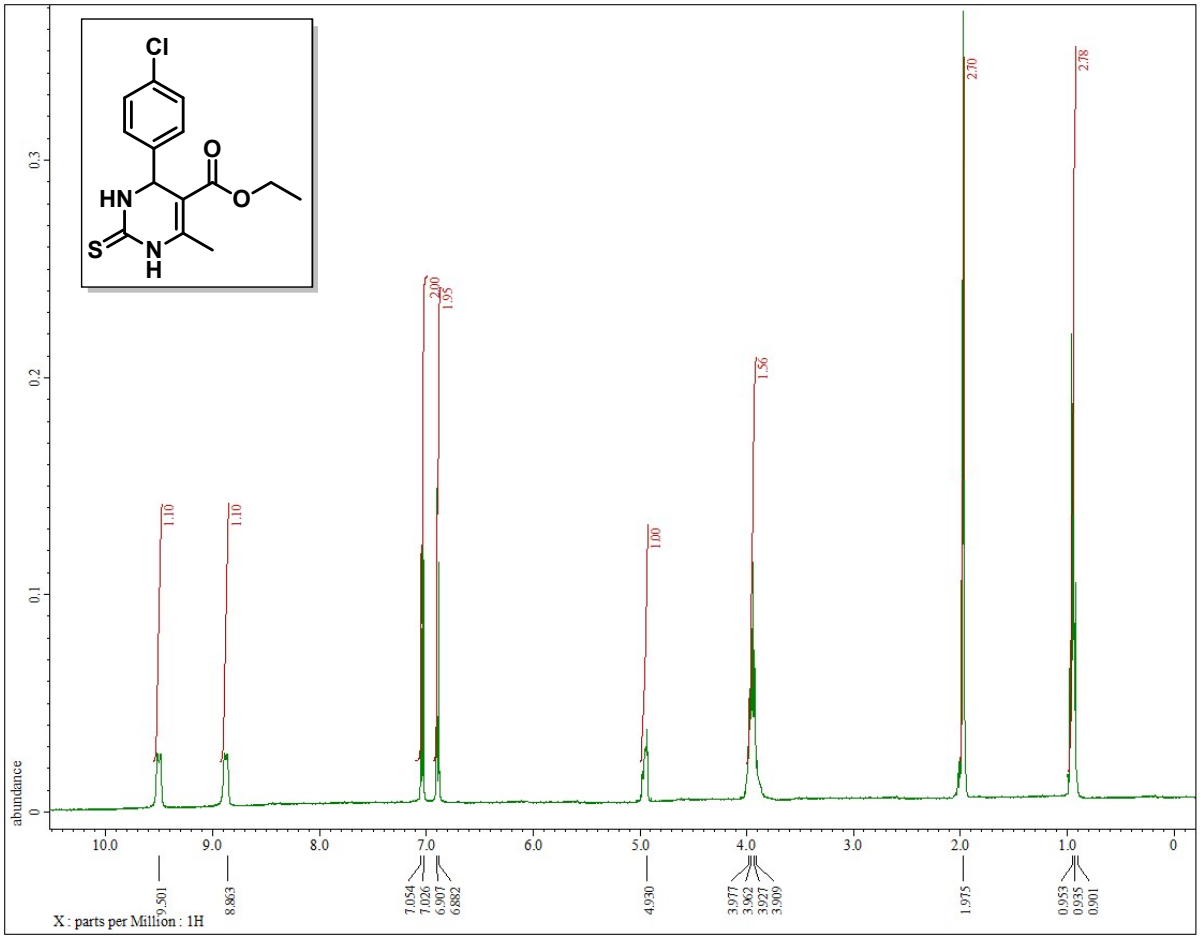
FigureS21 ^{13}C NMR spectra of ethyl-4-(3-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4h).**



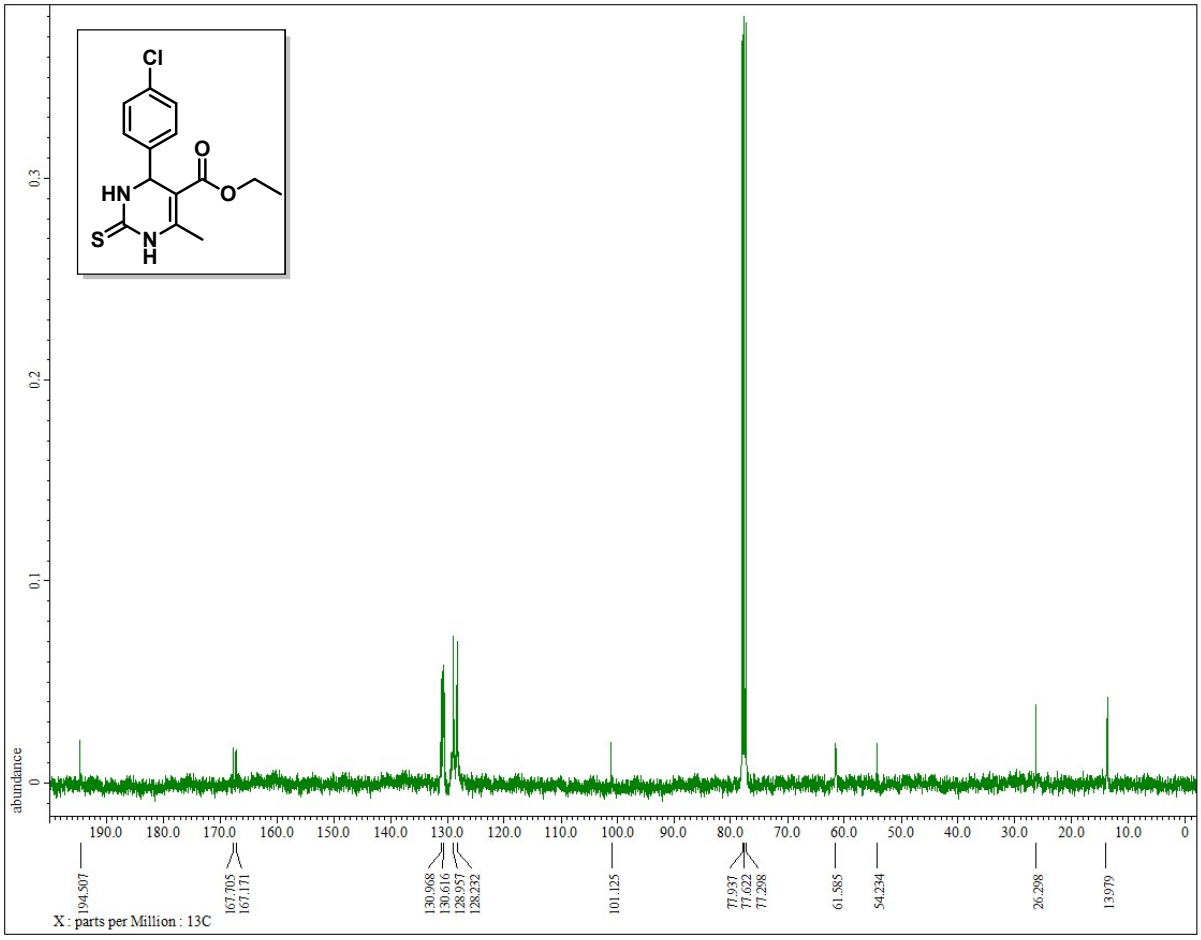
FigureS22 ^{1}H NMR spectra of ethyl-4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4i).**



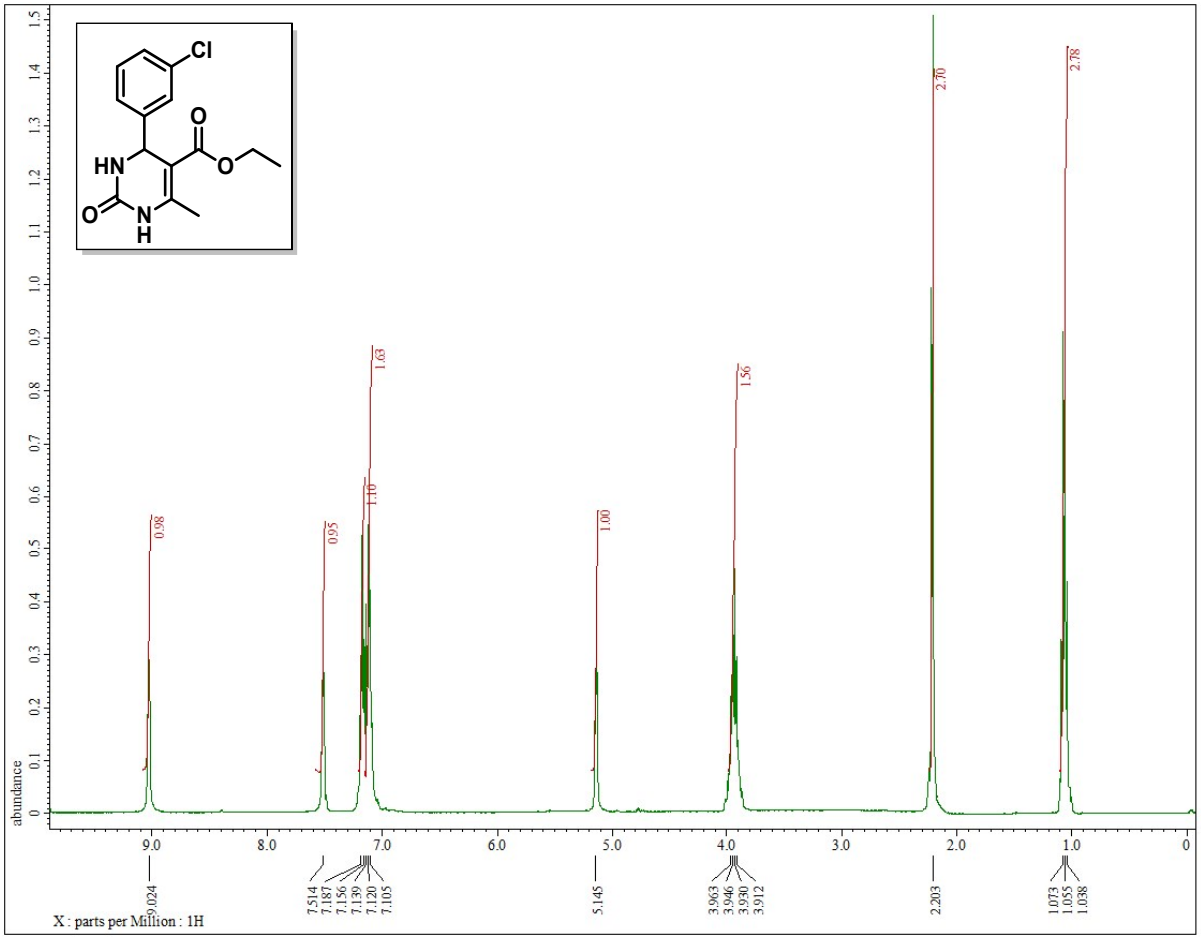
FigureS23 ^{13}C NMR spectra of ethyl-4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4i).**



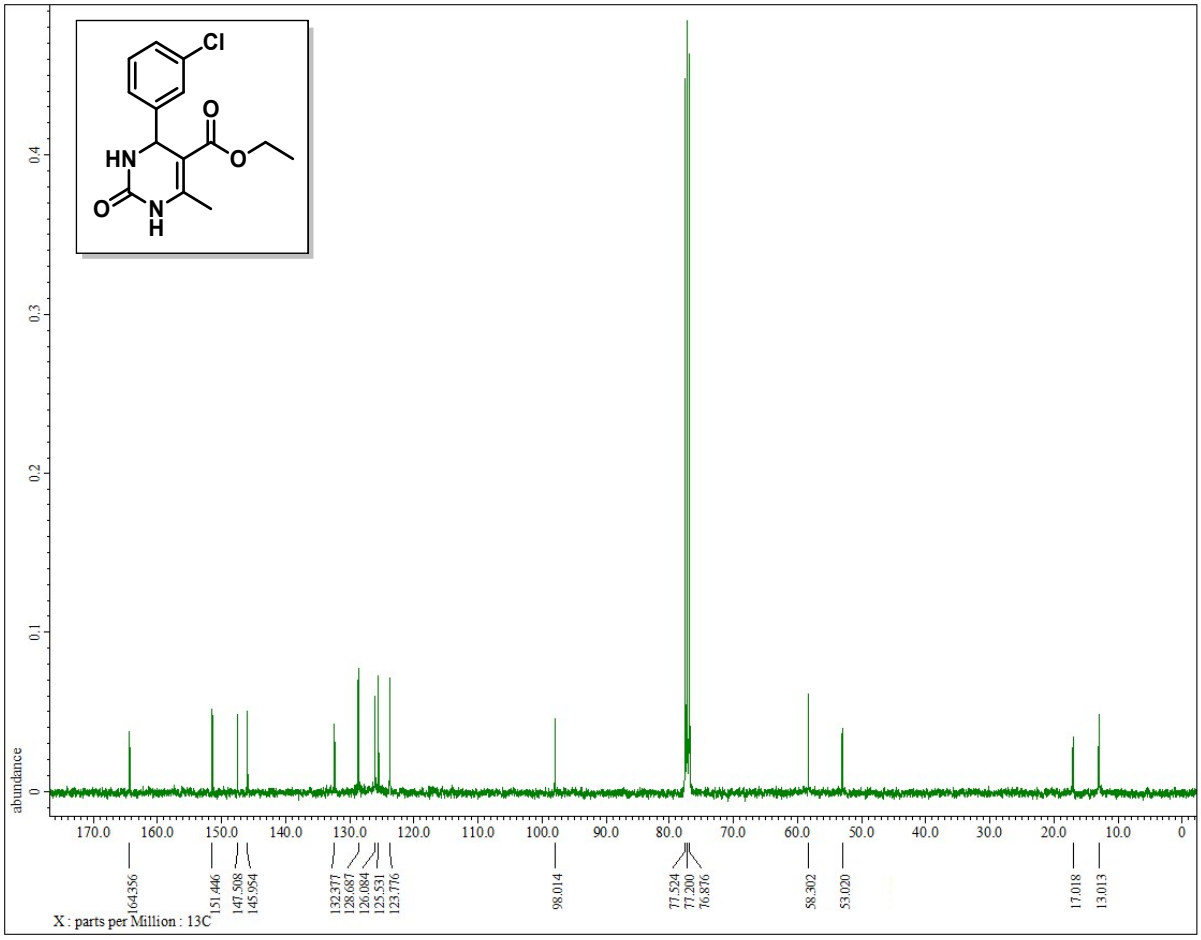
FigureS24 ^{1}H NMR spectra of ethyl-4-(4-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4j).**



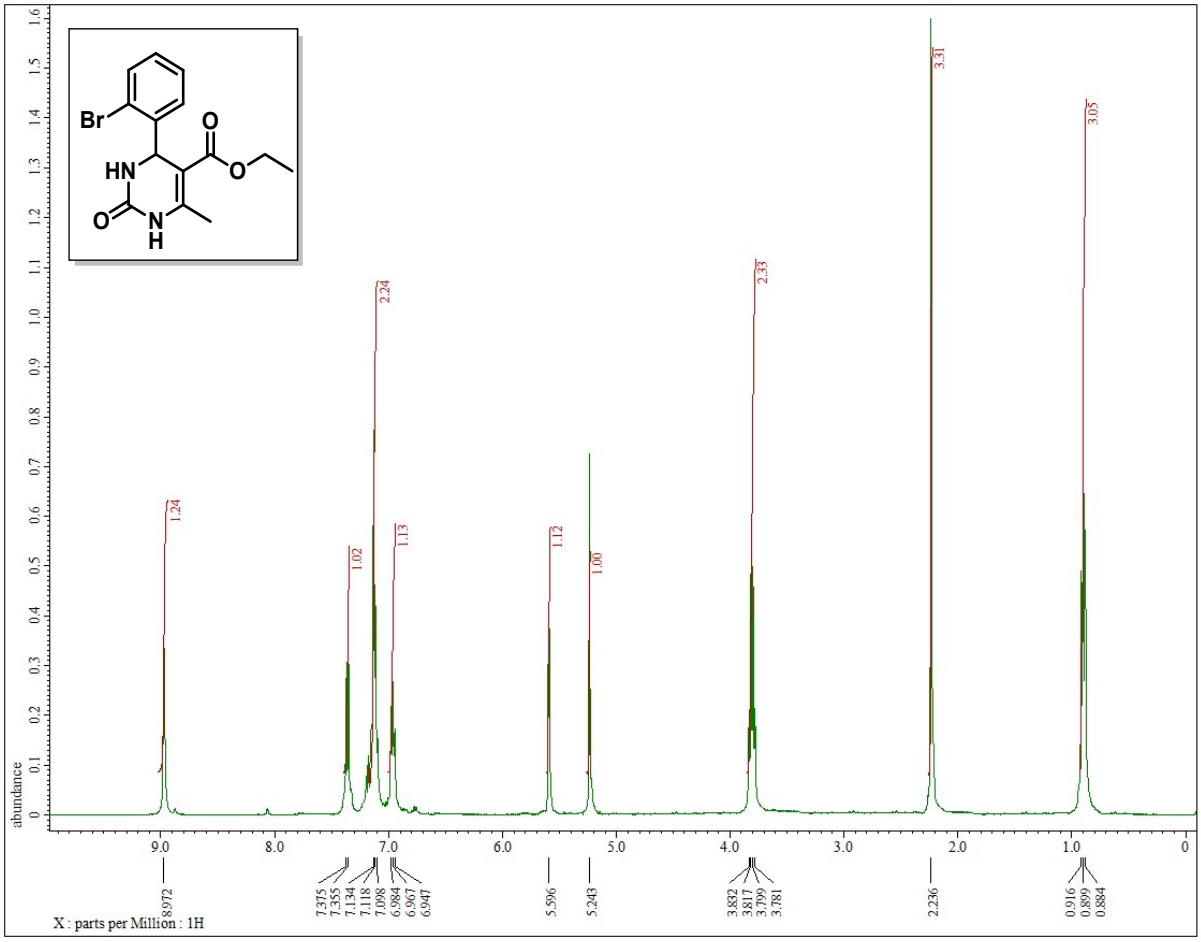
FigureS25 ^{13}C NMR spectra of ethyl-4-(4-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4j).**



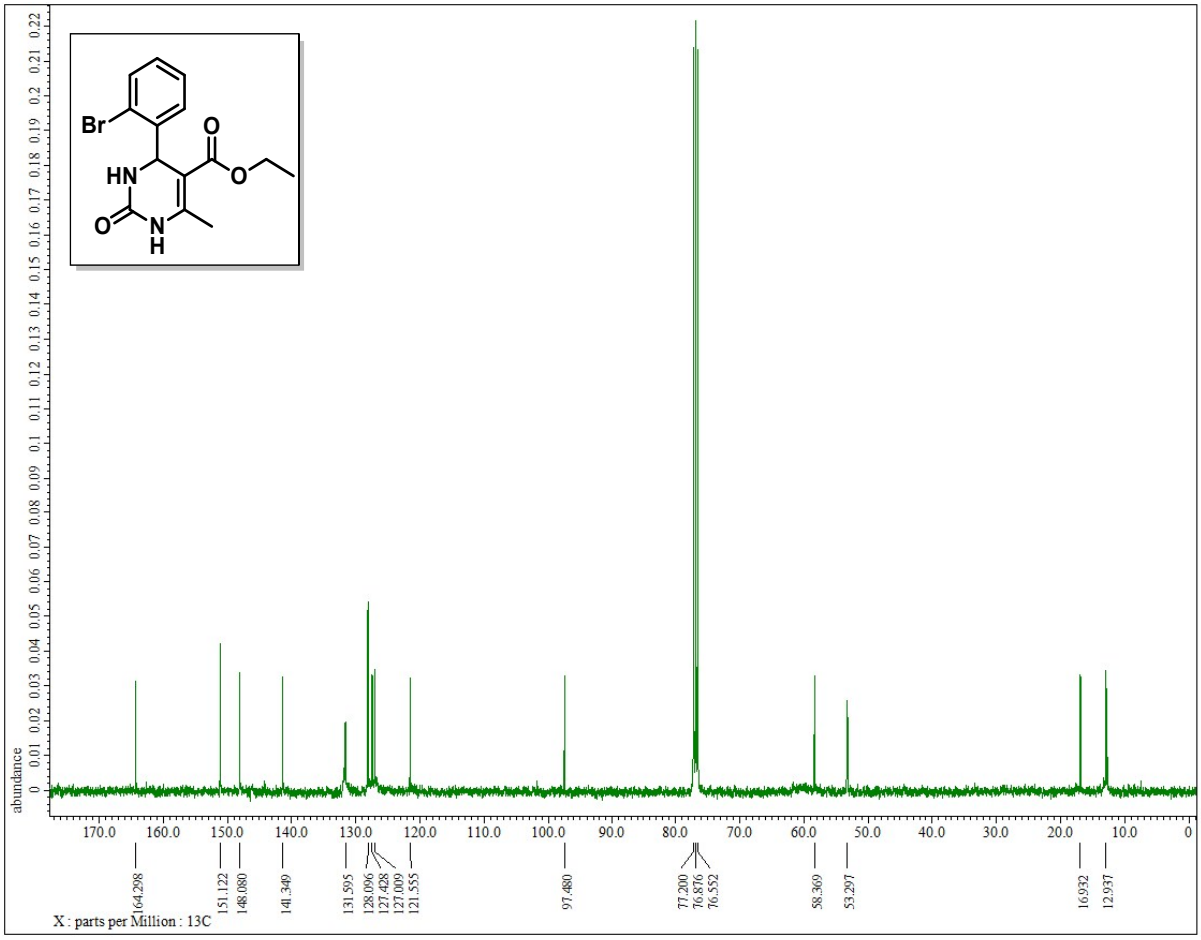
FigureS26 ^{1}H NMR spectra of ethyl-4-(3-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4k).**



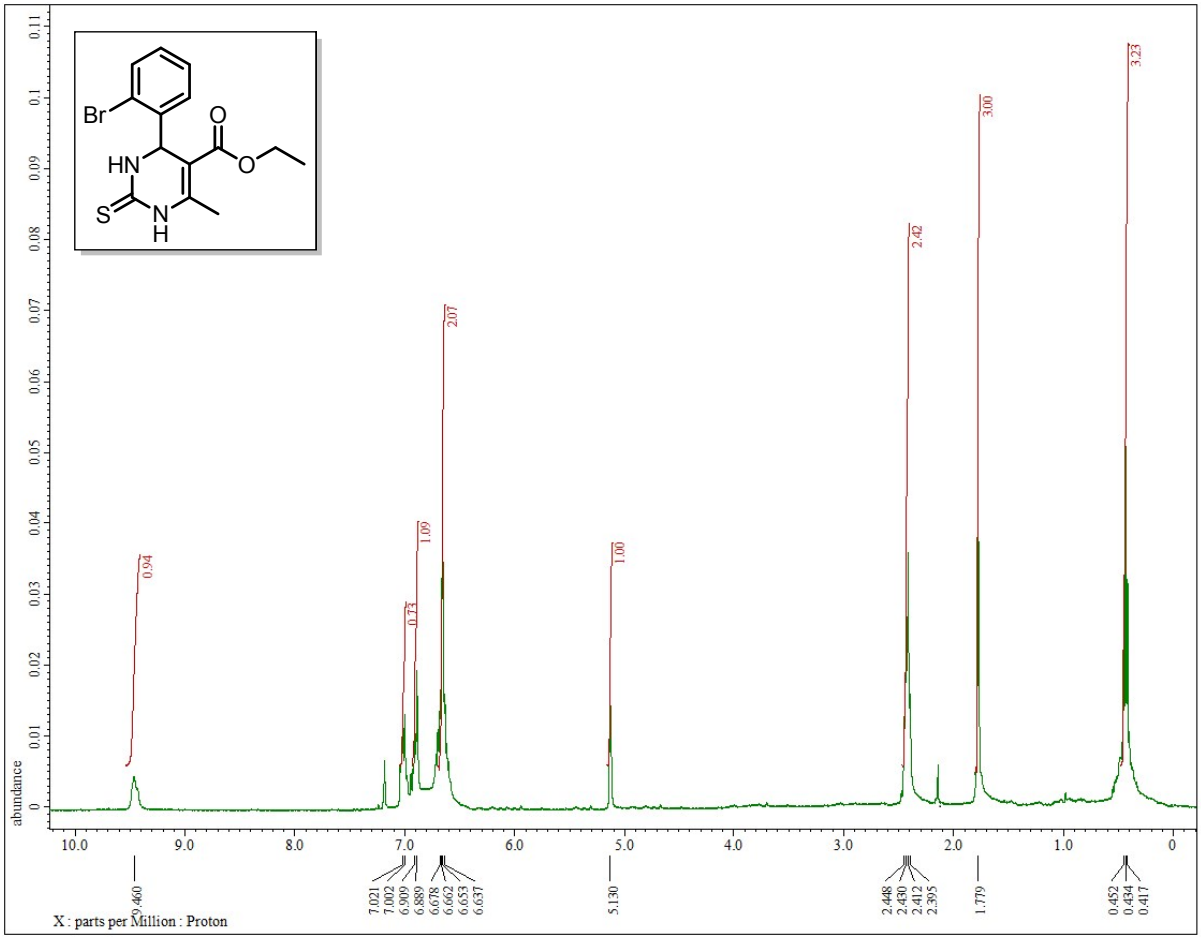
FigureS27 ^{13}C NMR spectra of ethyl-4-(3-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4k).**



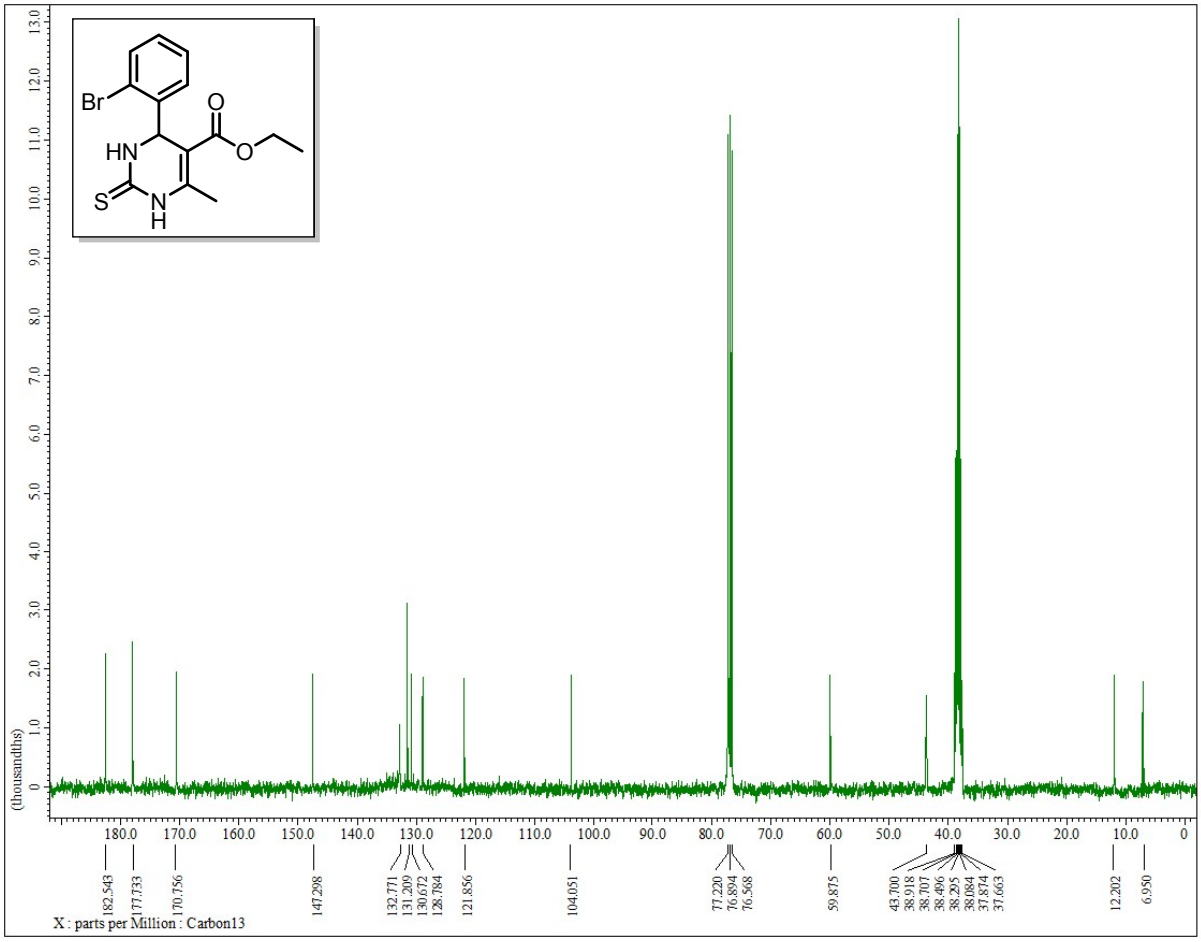
FigureS28 ^{1}H NMR spectra of ethyl-4-(2-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4l).**



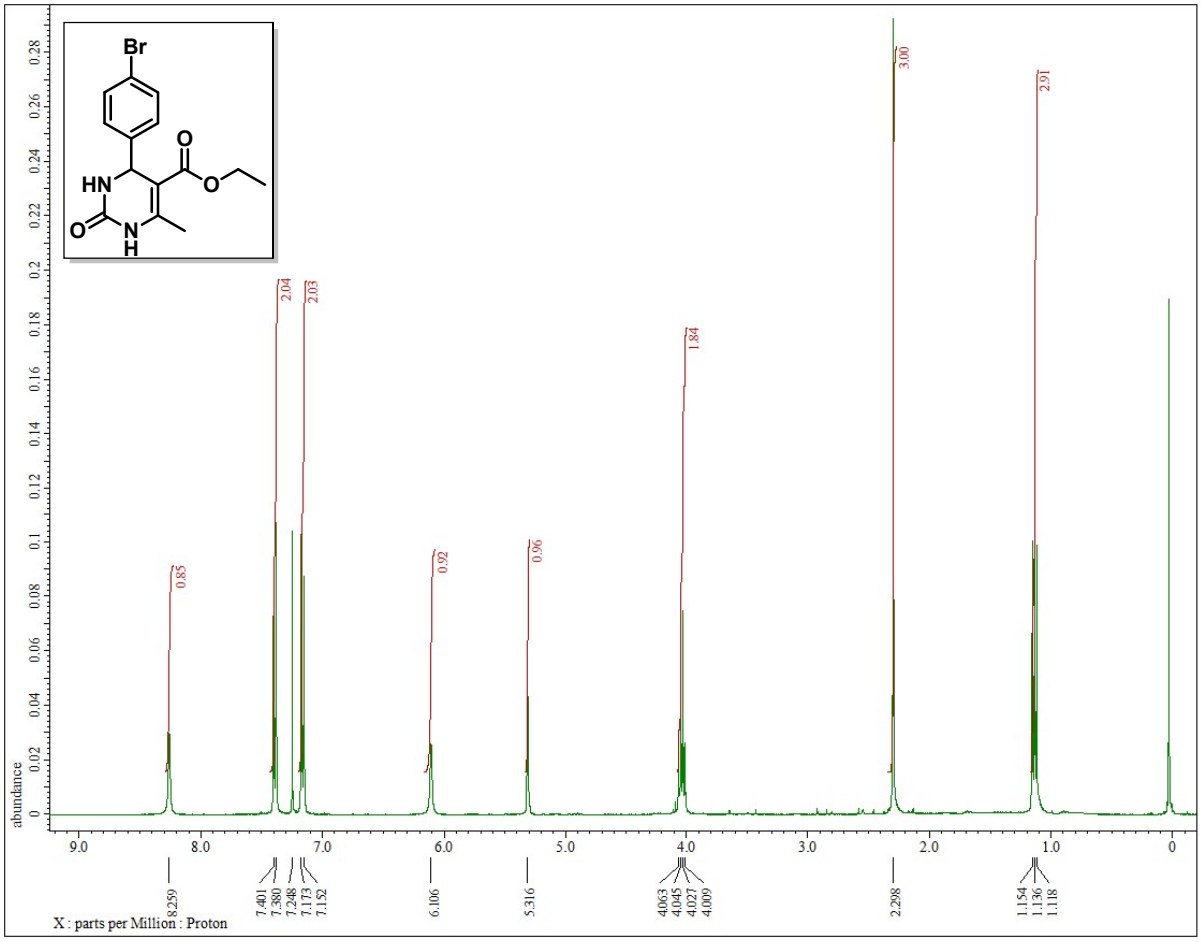
FigureS29 ^{13}C NMR spectra of ethyl-4-(2-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4l).**



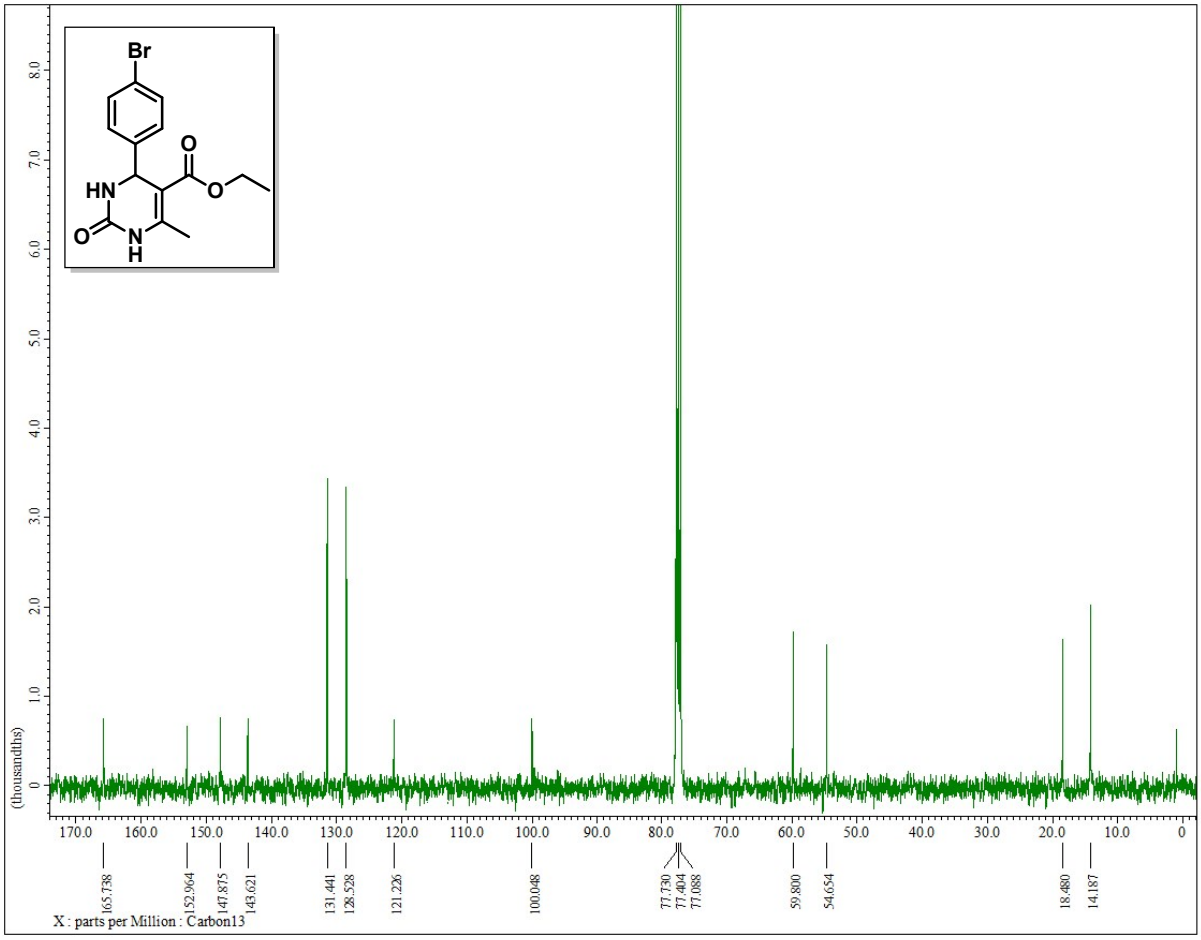
FigureS30 ^{1}H NMR spectra of ethyl-4-(2-bromophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4m).**



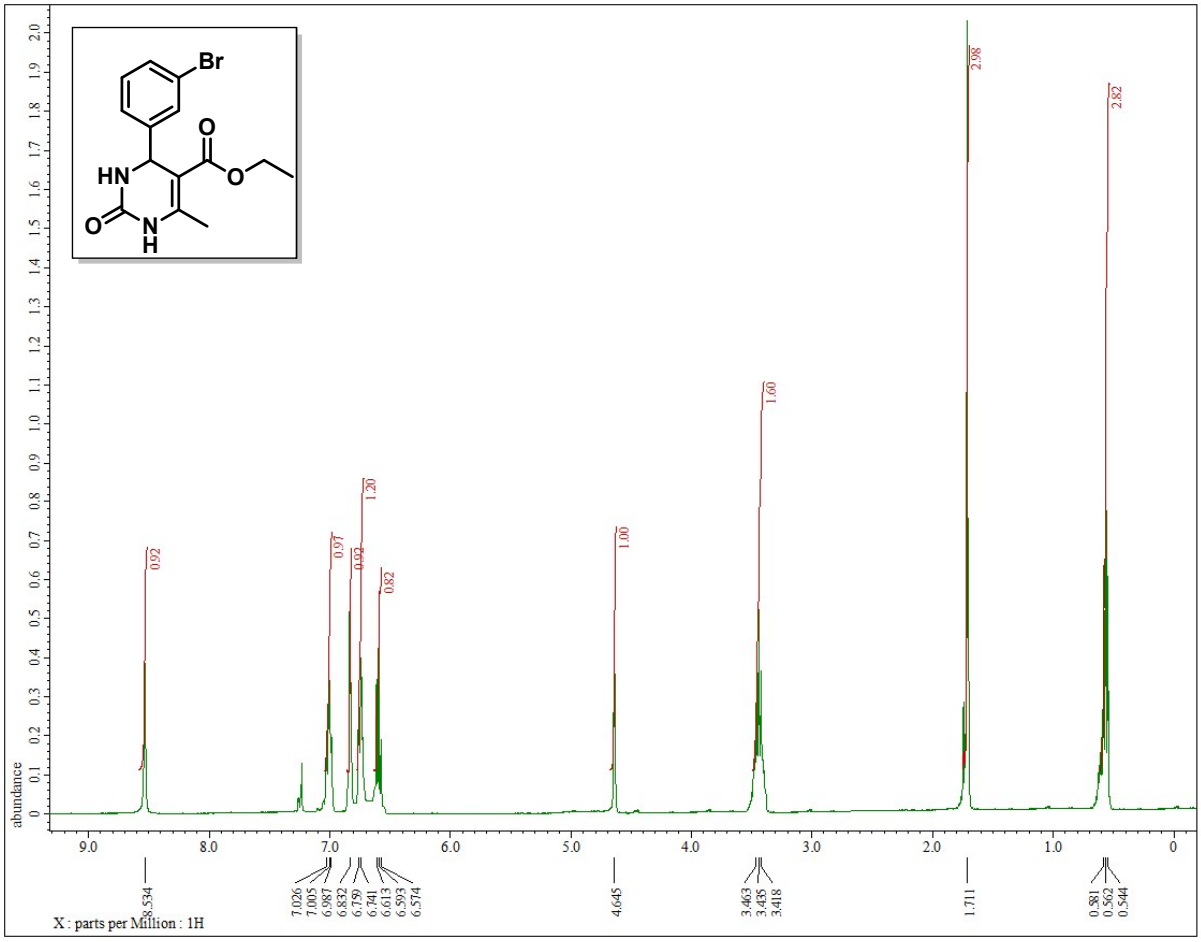
FigureS31 ^{13}C NMR spectra of ethyl-4-(2-bromophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4m).**



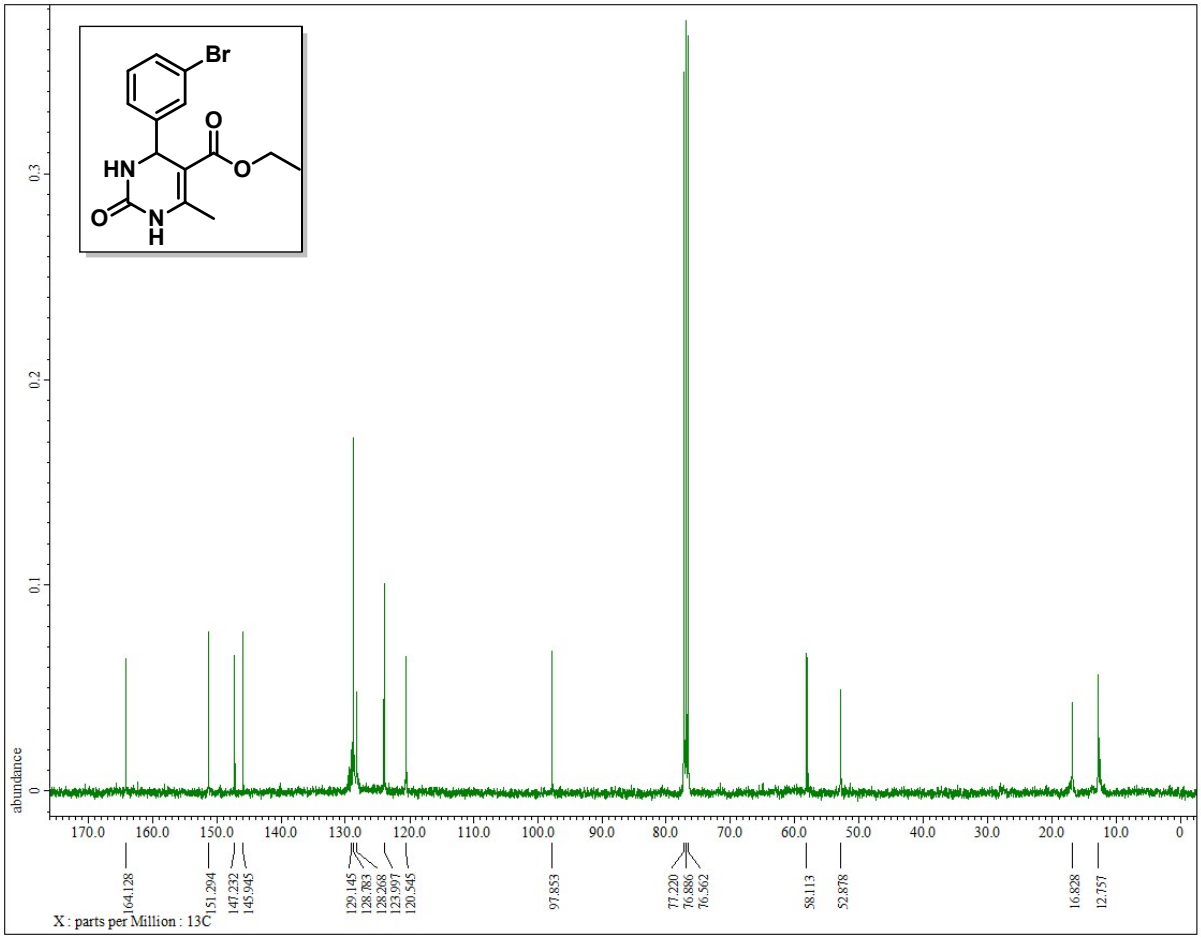
FigureS32 ^{1}H NMR spectra of ethyl-4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4n).**



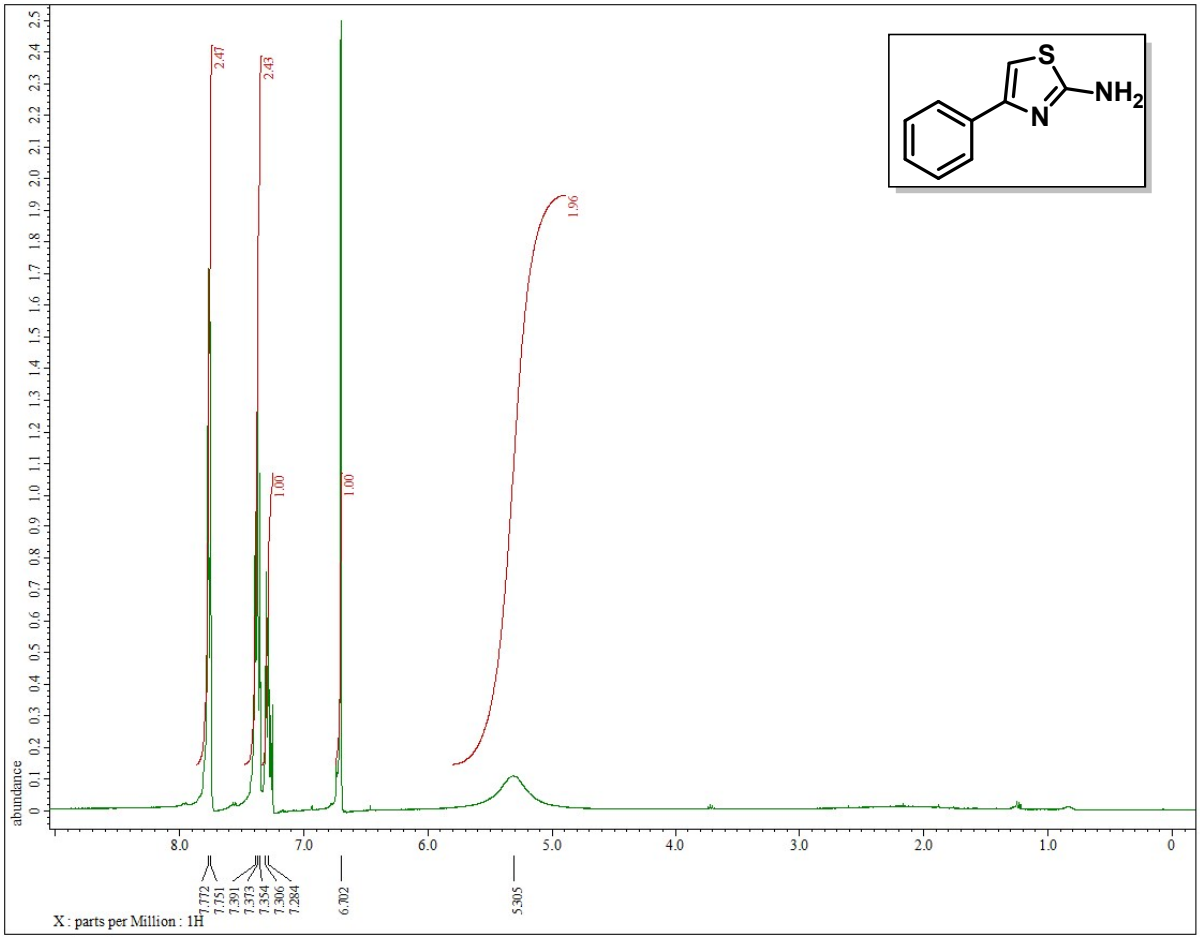
FigureS33 ^{13}C NMR spectra of ethyl-4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4n).**



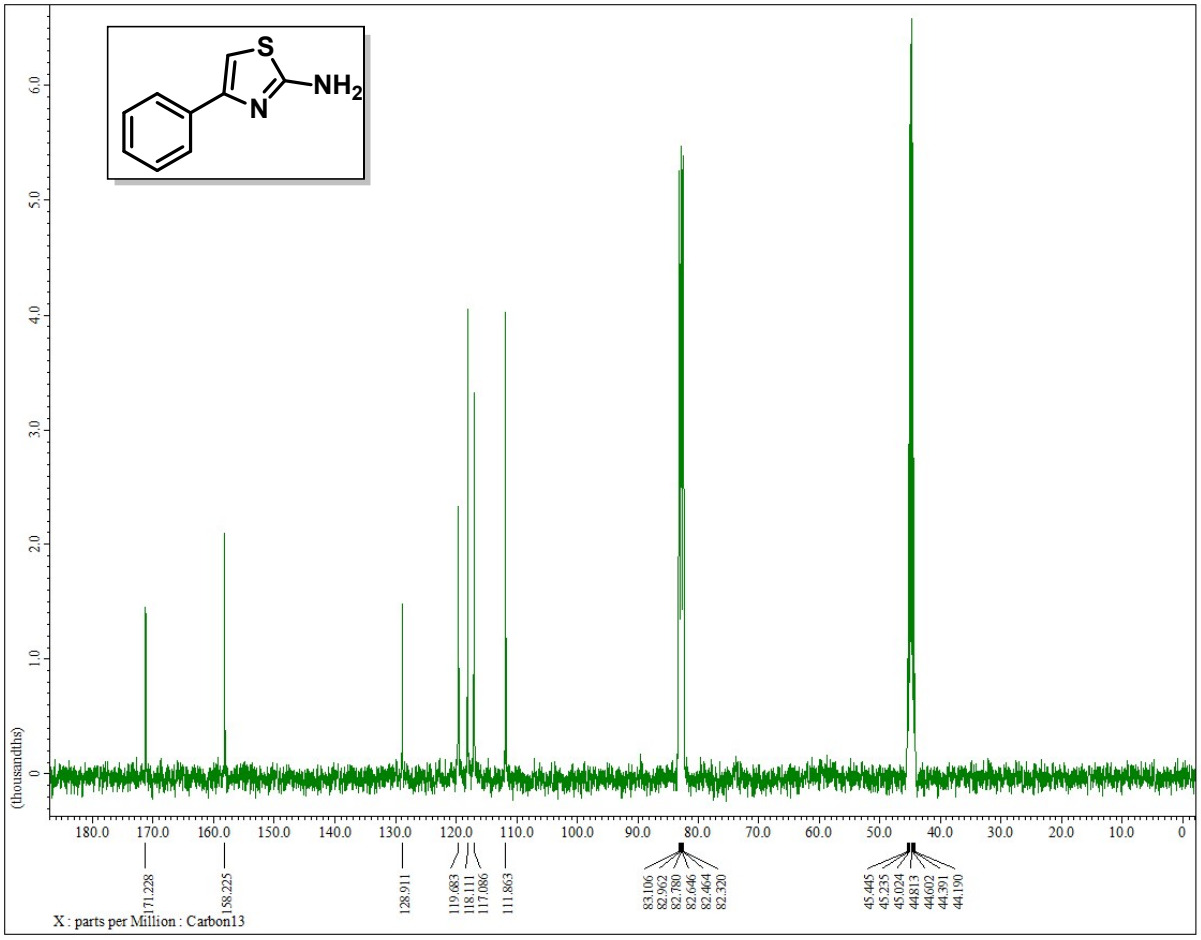
FigureS34 ^{1}H NMR spectra of ethyl-4-(3-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4o).**



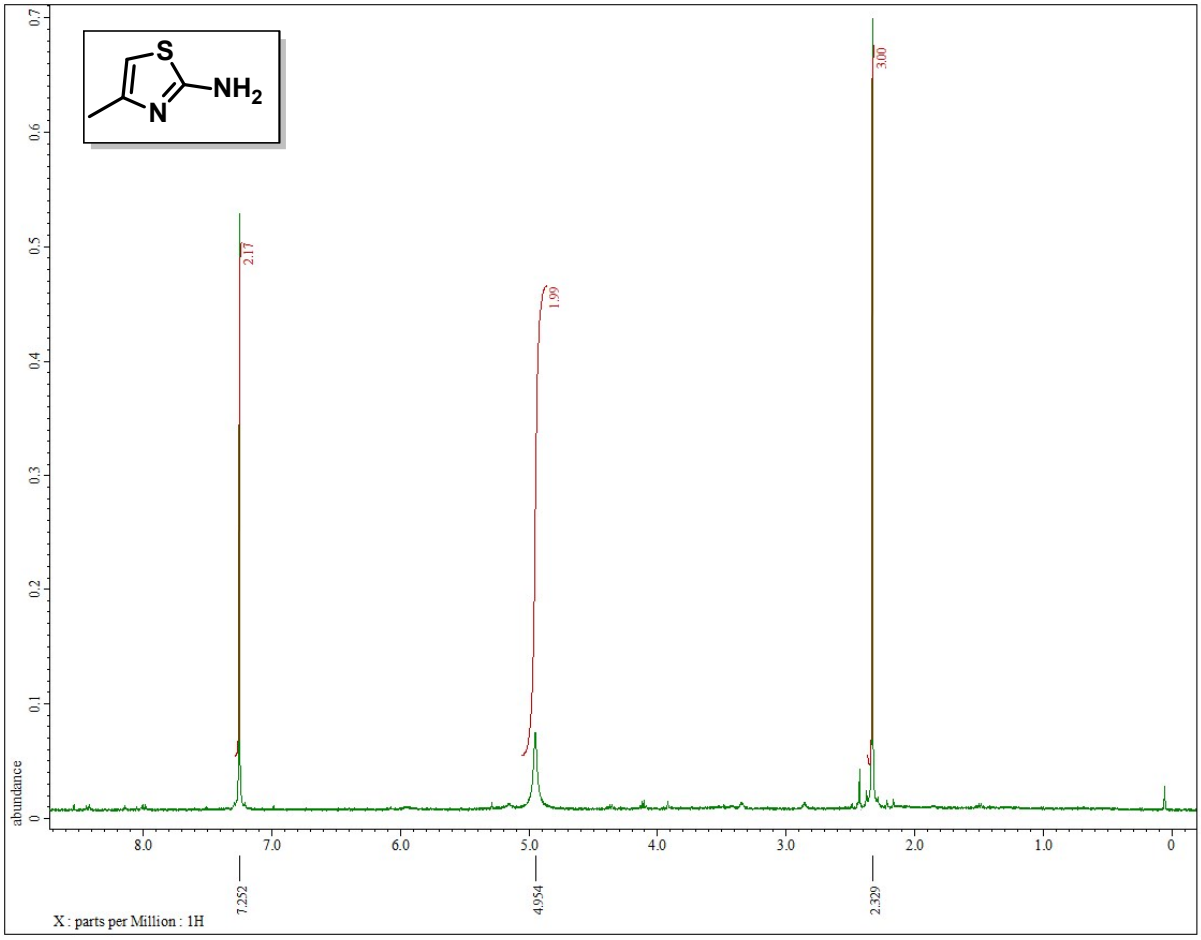
FigureS35 ^{13}C NMR spectra of ethyl-4-(3-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4o).**



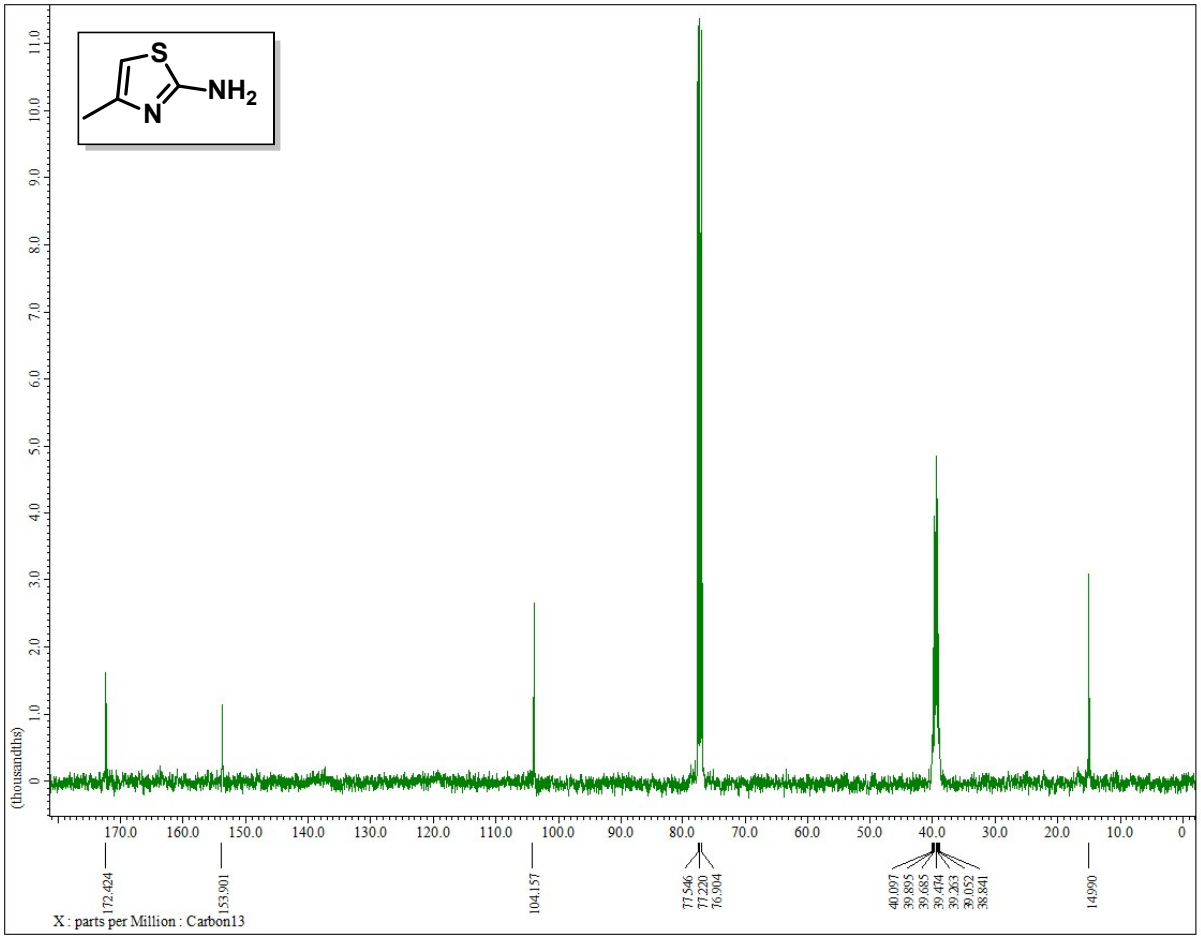
FigureS36 ^{1}H NMR spectra of 4-phenylthiazol-2-amine **(6a).**



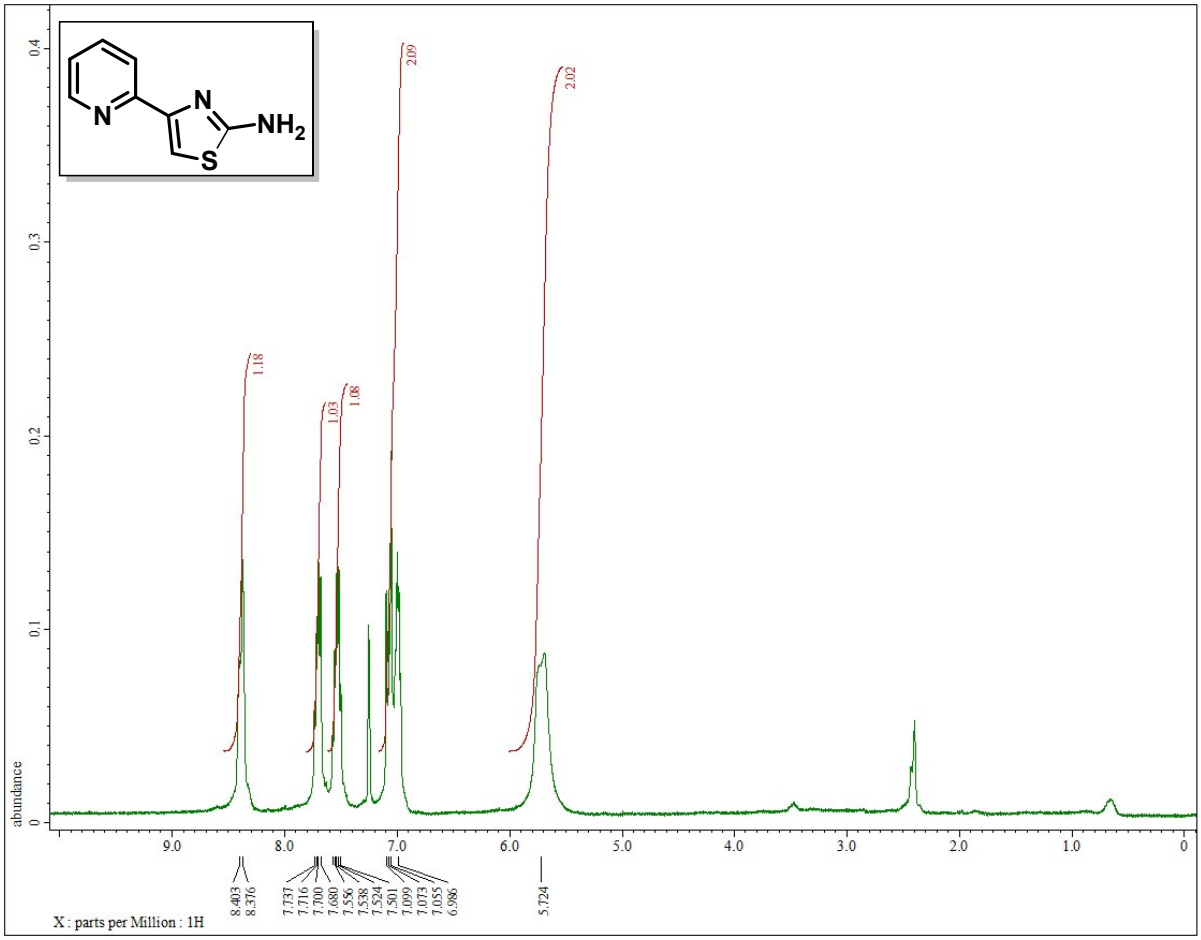
FigureS37 ^{13}C NMR spectra of 4-phenylthiazol-2-amine **(6a).**



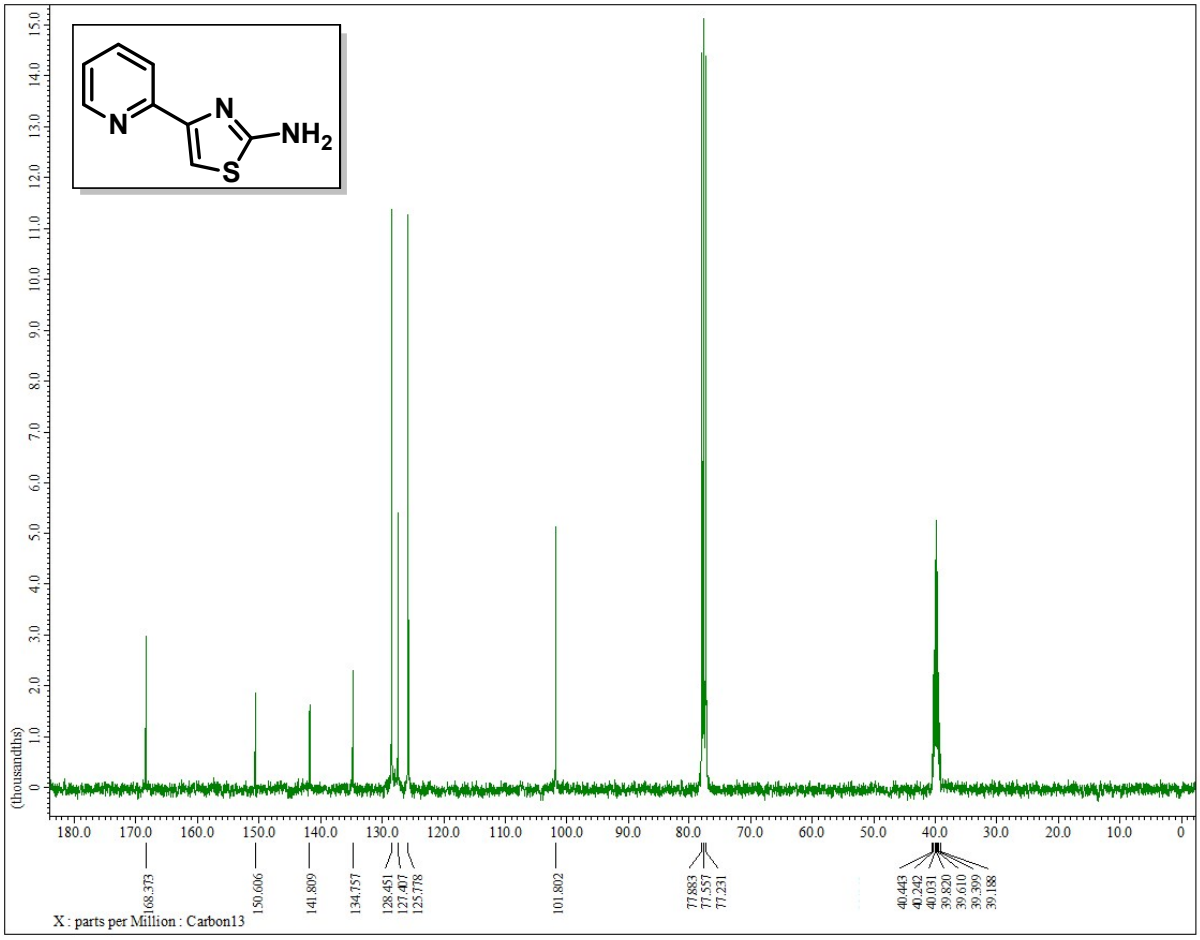
FigureS38 ^{1}H NMR spectra of 4-methylthiazol-2-amine **(6b).**



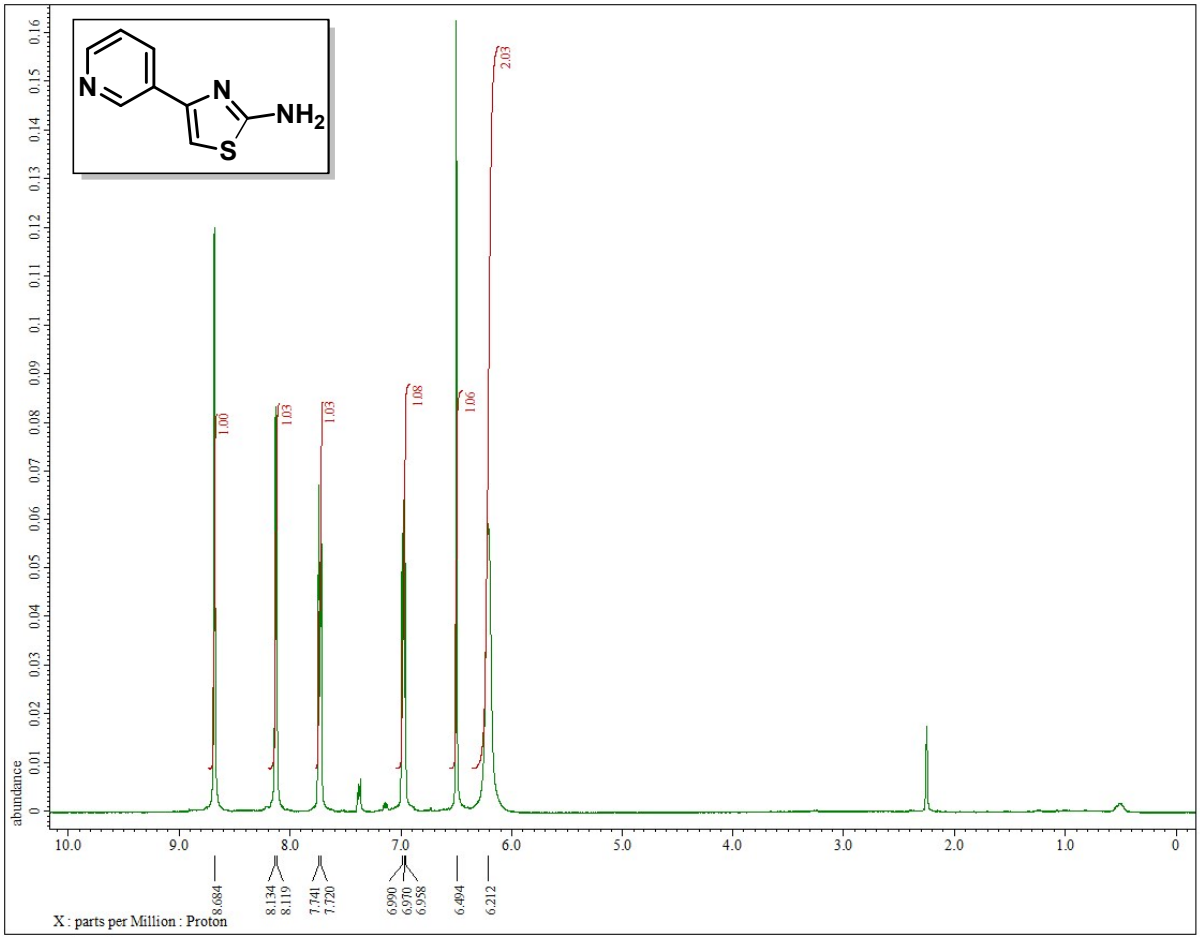
FigureS39 ^{13}CNMR spectra of 4-methylthiazol-2-amine **(6b).**



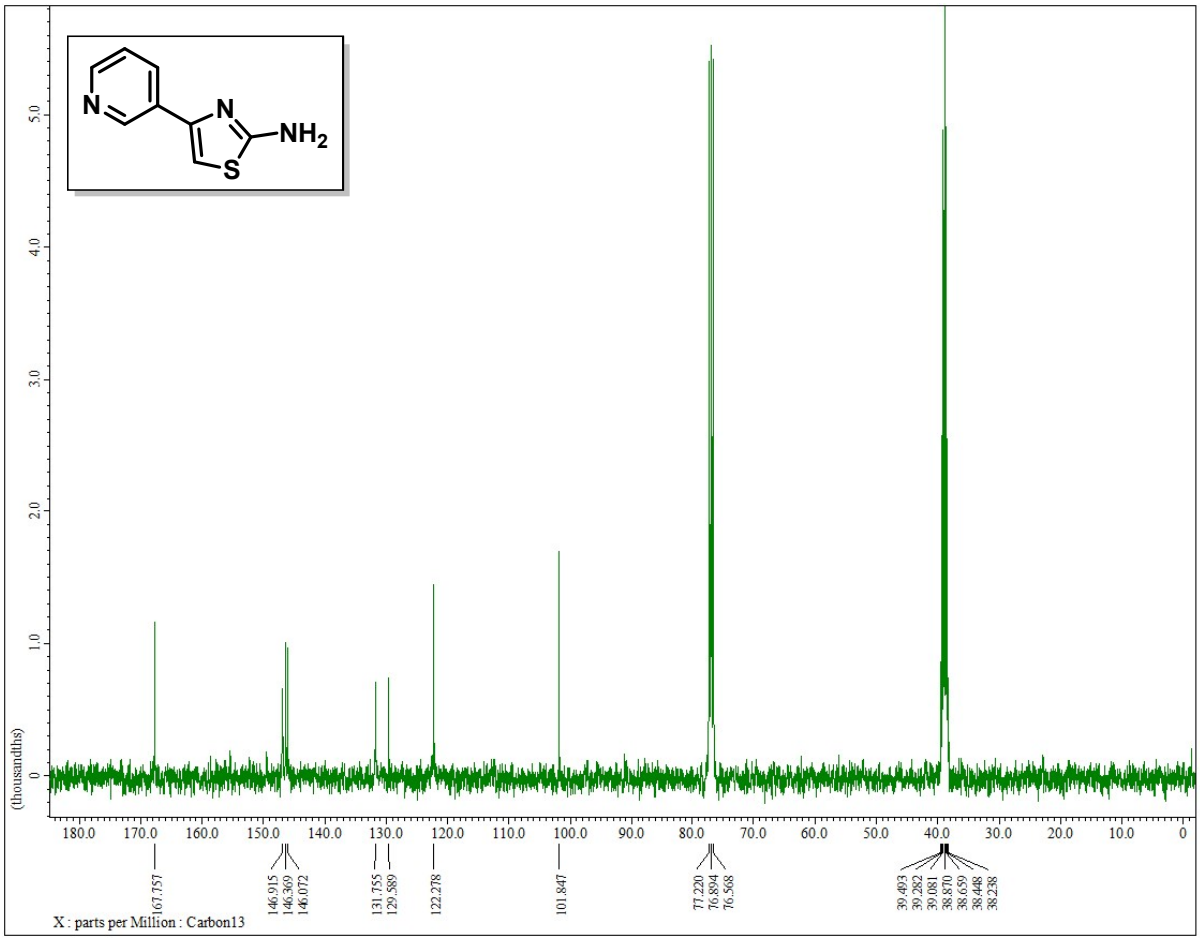
FigureS40 ^{1}H NMR spectra of 4-(pyridin-2-yl)thiazol-2-amine **(6c).**



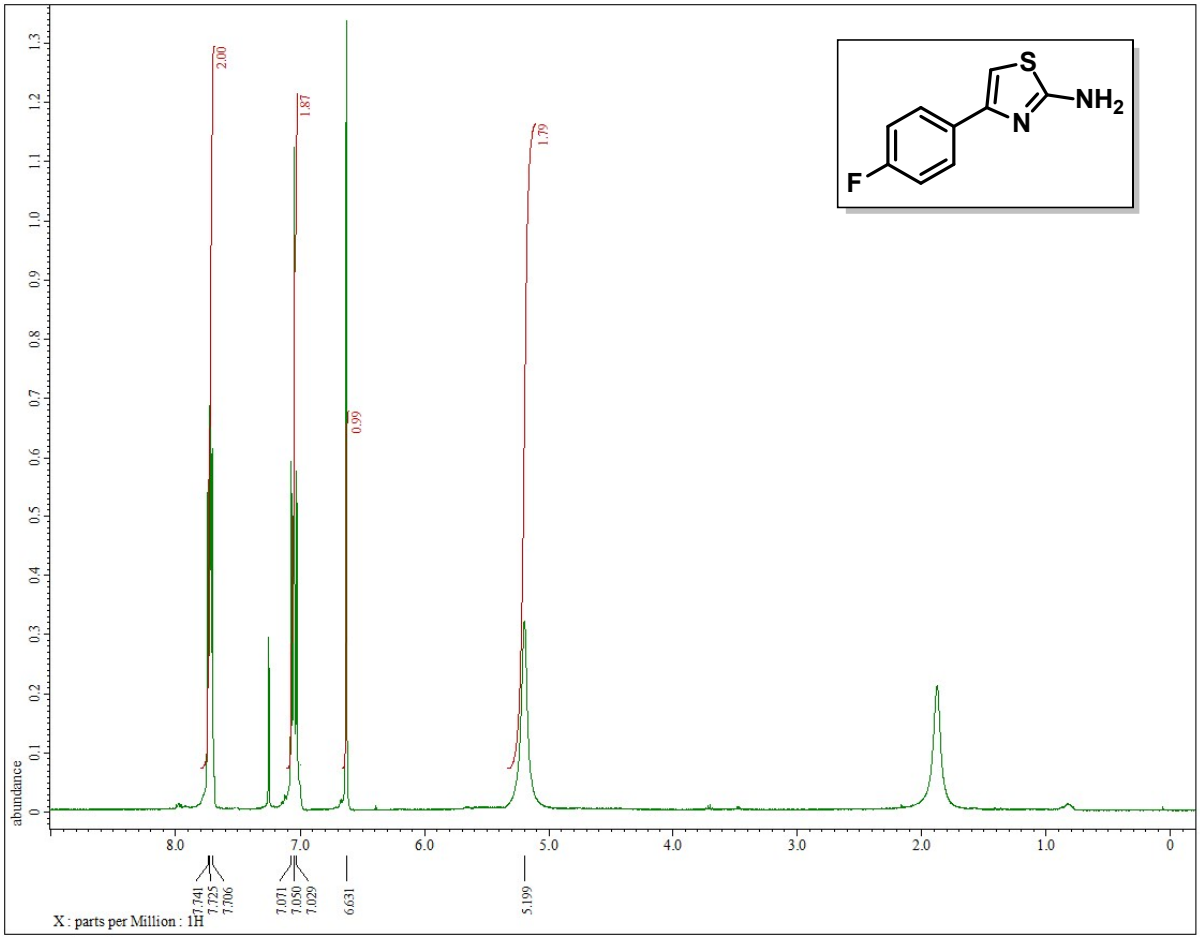
FigureS41 ^{13}C NMR spectra of 4-(pyridin-2-yl)thiazol-2-amine **(6c).**



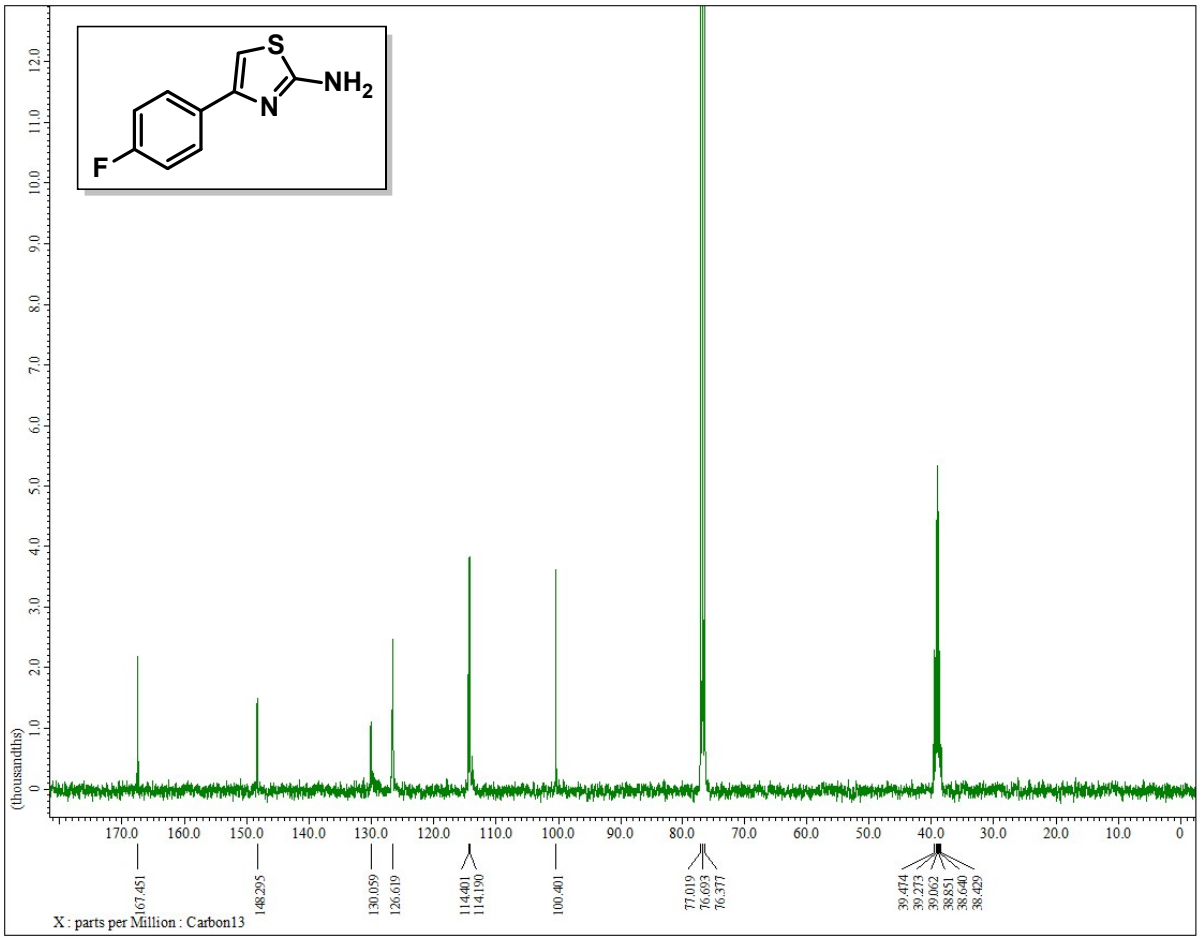
FigureS42 ^{1}H NMR spectra of 4-(pyridin-3-yl)thiazol-2-amine **(6d).**



FigureS43 ^{13}C NMR spectra of 4-(pyridin-3-yl)thiazol-2-amine **(6d).**



FigureS44 ^{1}H NMR spectra of 4-(4-fluorophenyl)thiazol-2-amine **(6e).**



FigureS45 ^{13}C NMR spectra of 4-(4-fluorophenyl)thiazol-2-amine **(6e).**

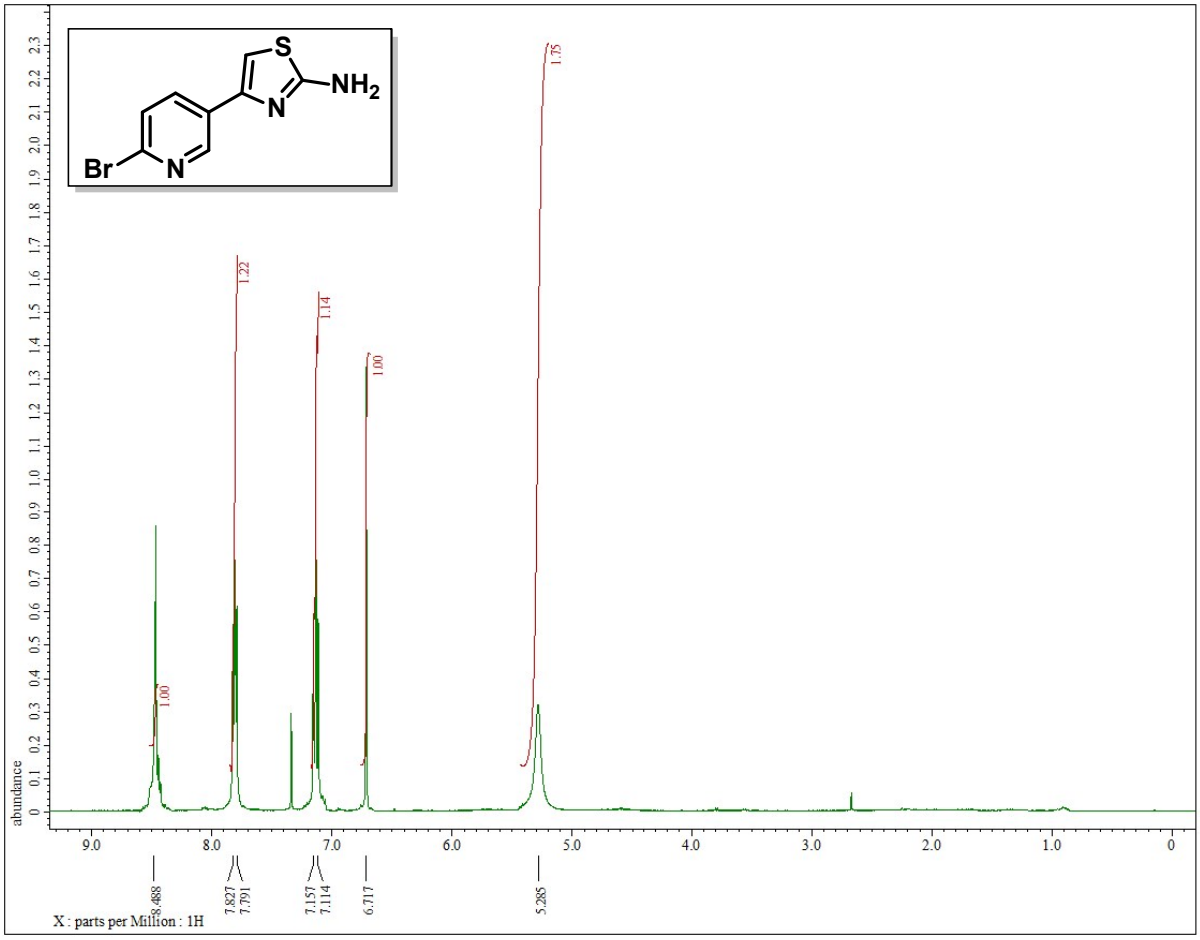


Figure S46 ^{1}H NMR spectra of 4-(6-bromopyridin-2-yl)thiazol-2-amine **(6f).**

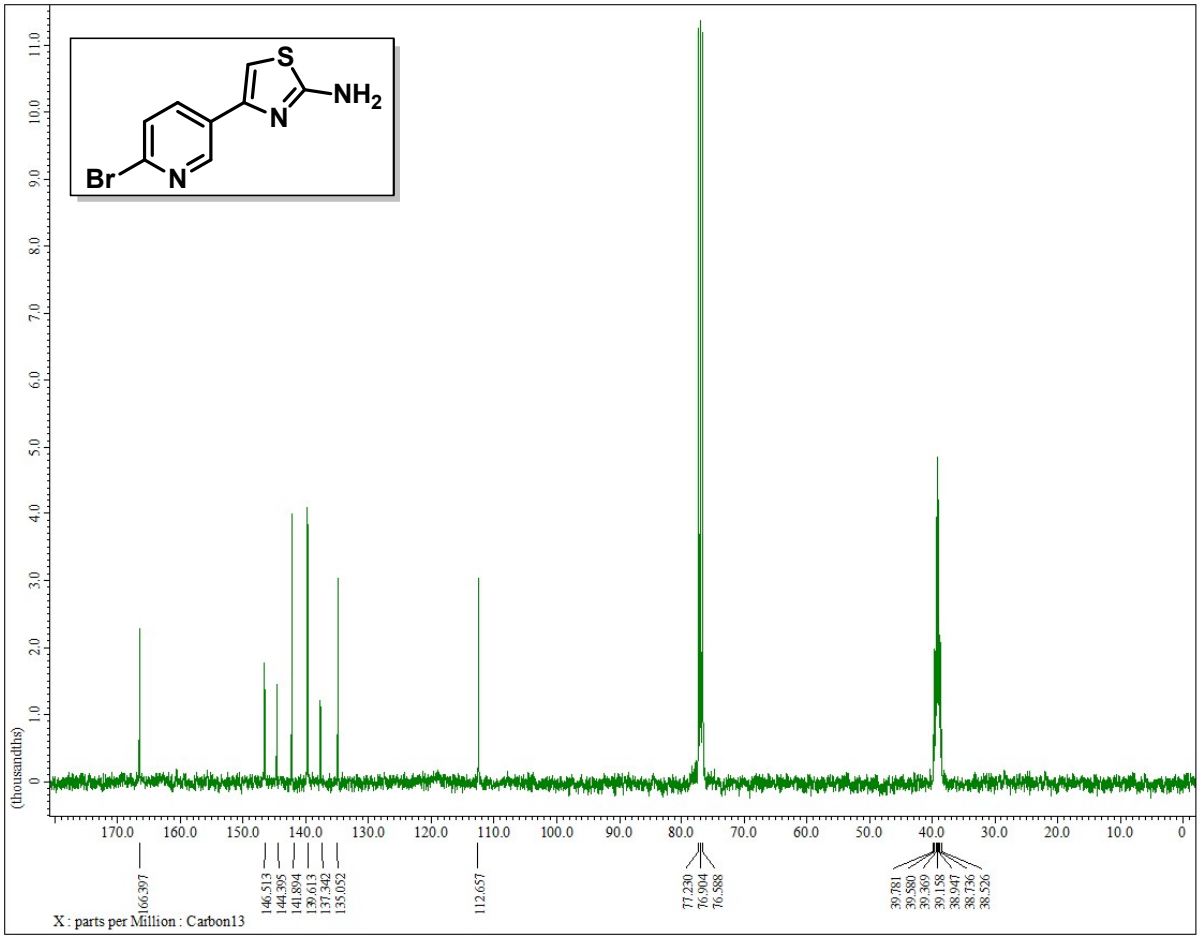
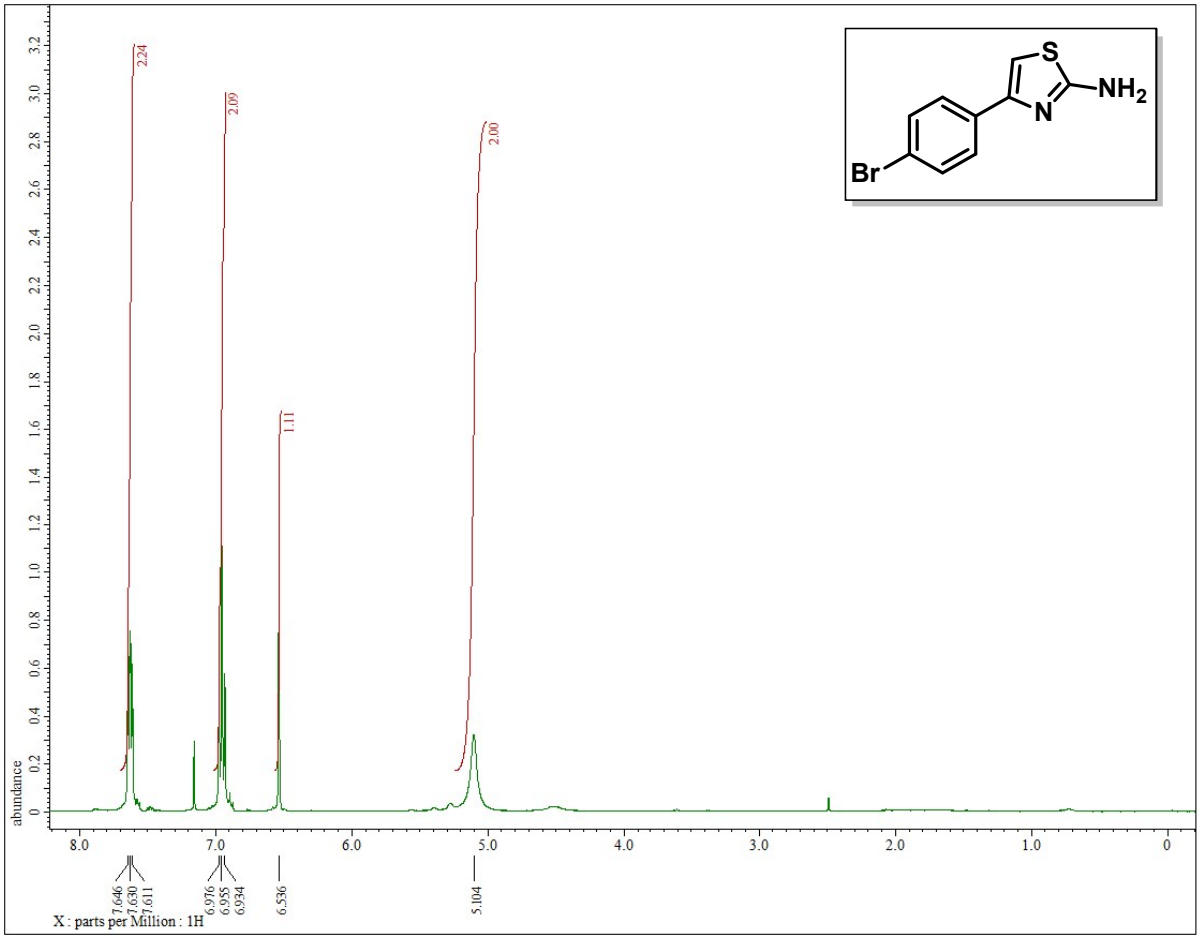
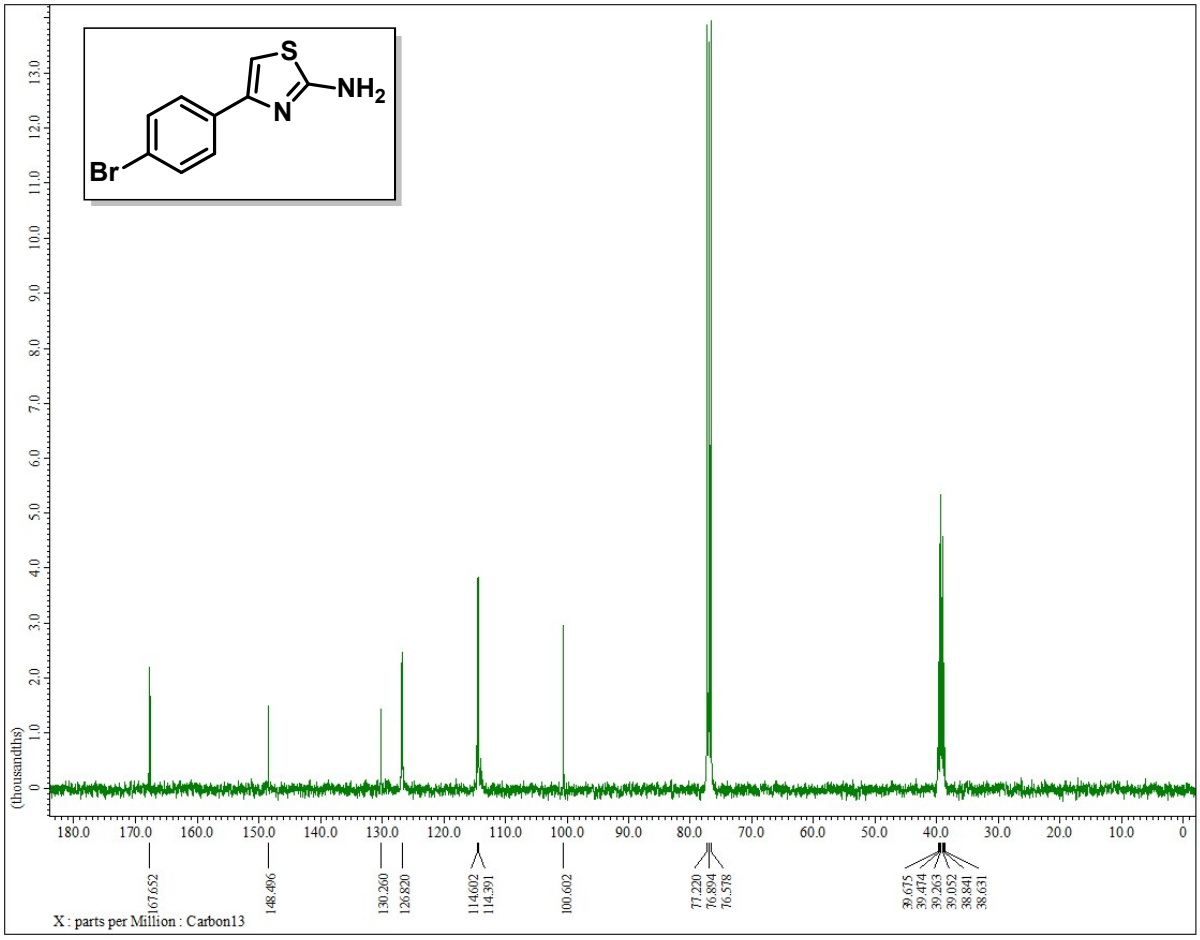


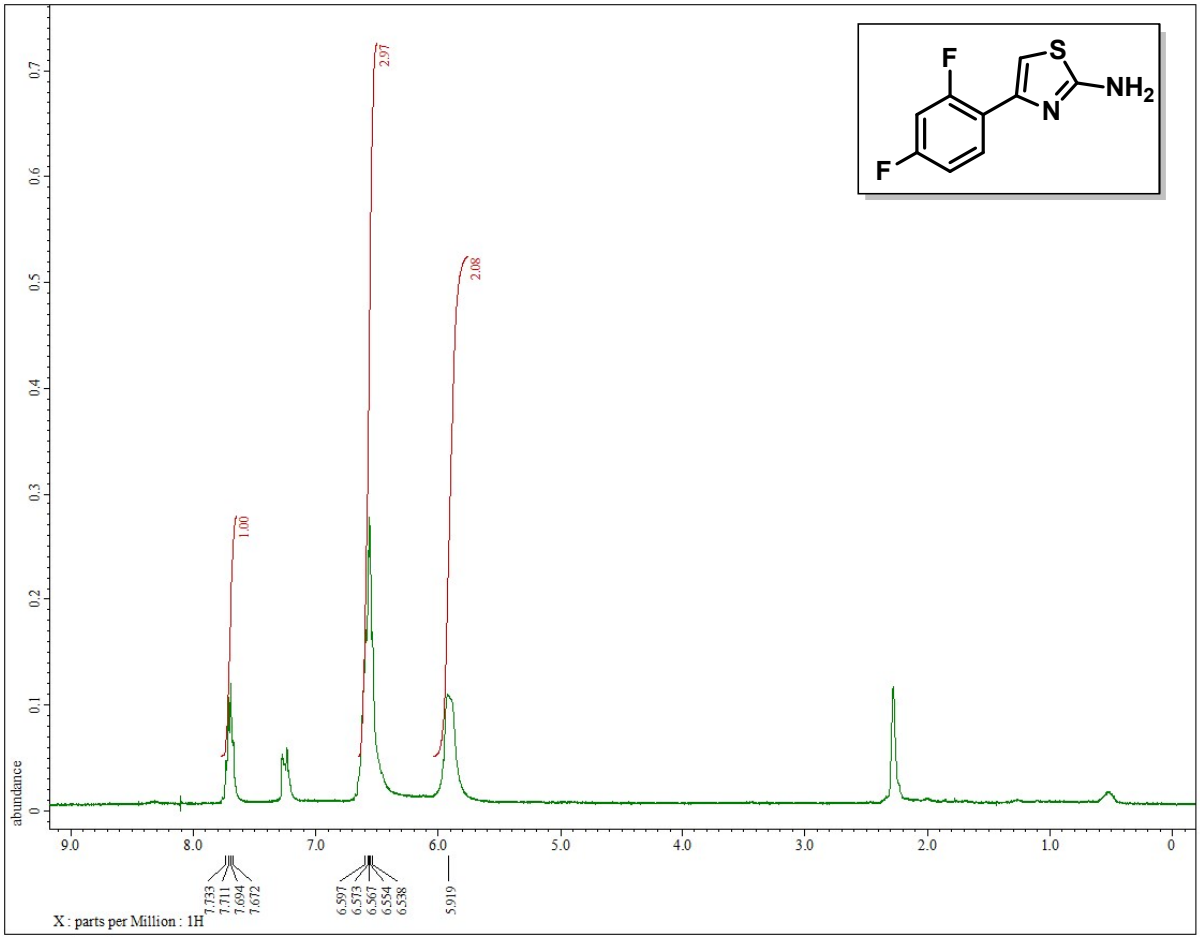
Figure S47 ^{13}C NMR spectra of 4-(6-bromopyridin-2-yl)thiazol-2-amine **(6f).**



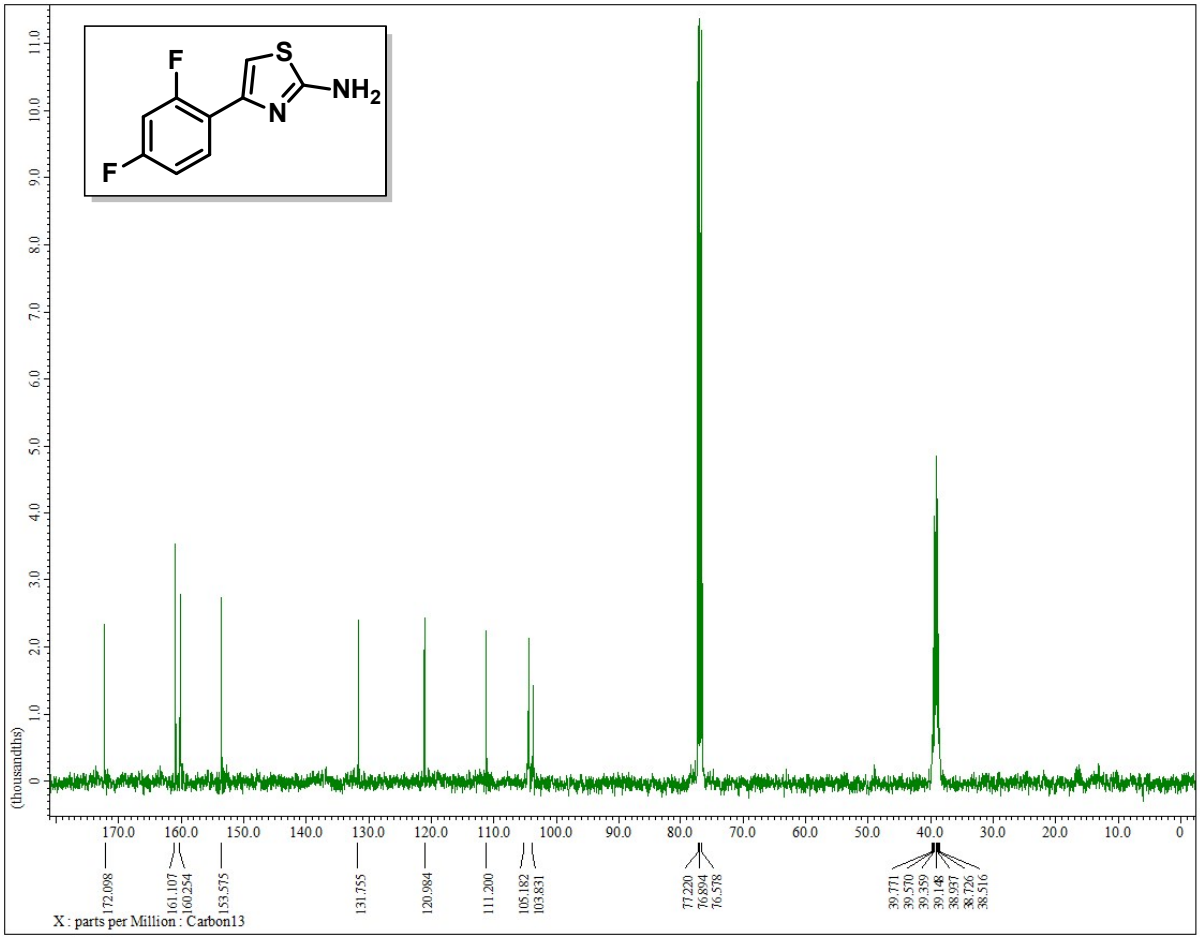
FigureS48 ^{1}H NMR spectra of 4-(4-bromophenyl)thiazol-2-amine **(6g).**



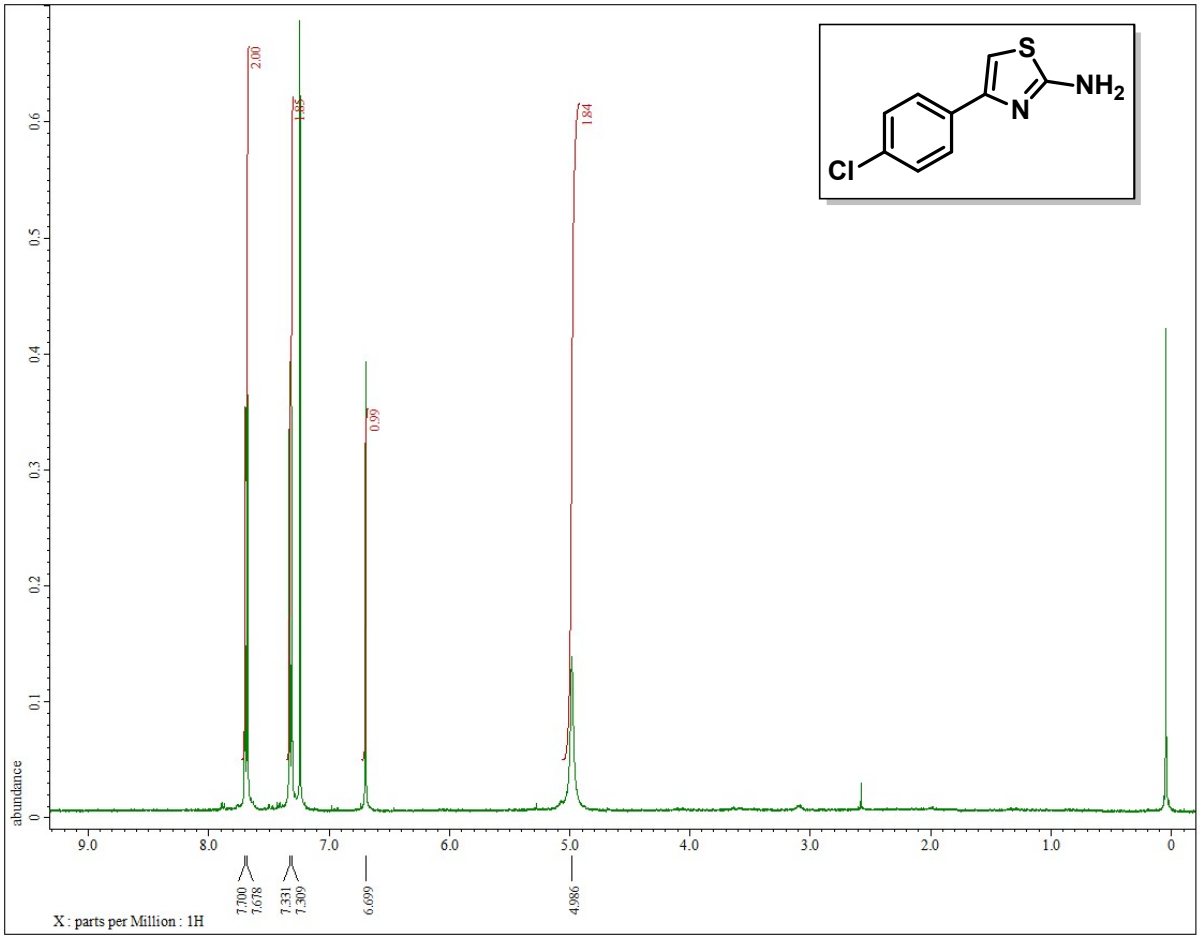
FigureS49 ^{13}C NMR spectra of 4-(4-bromophenyl)thiazol-2-amine **(6g).**



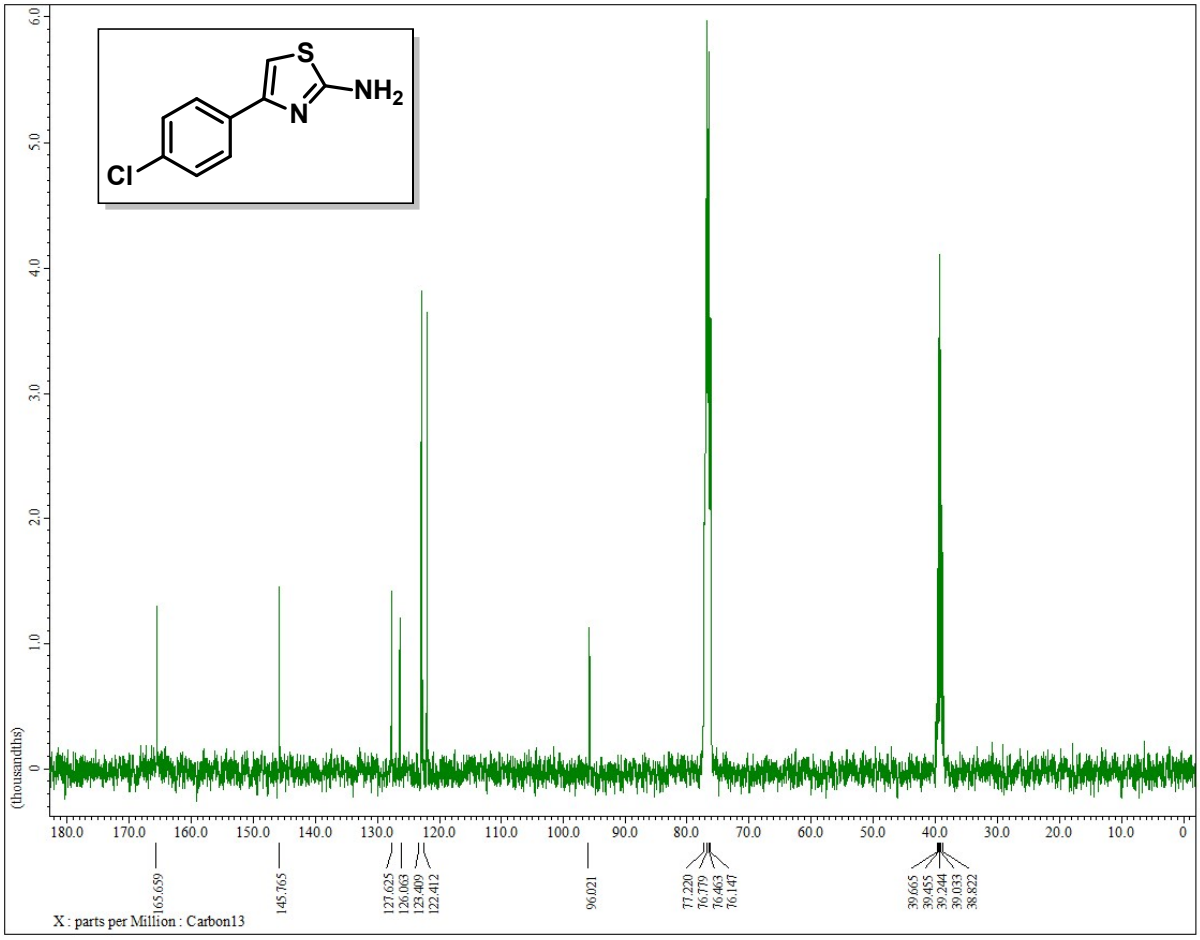
FigureS50 ^{1}H NMR spectra of 4-(2,4-difluorophenyl)thiazol-2-amine **(6h).**



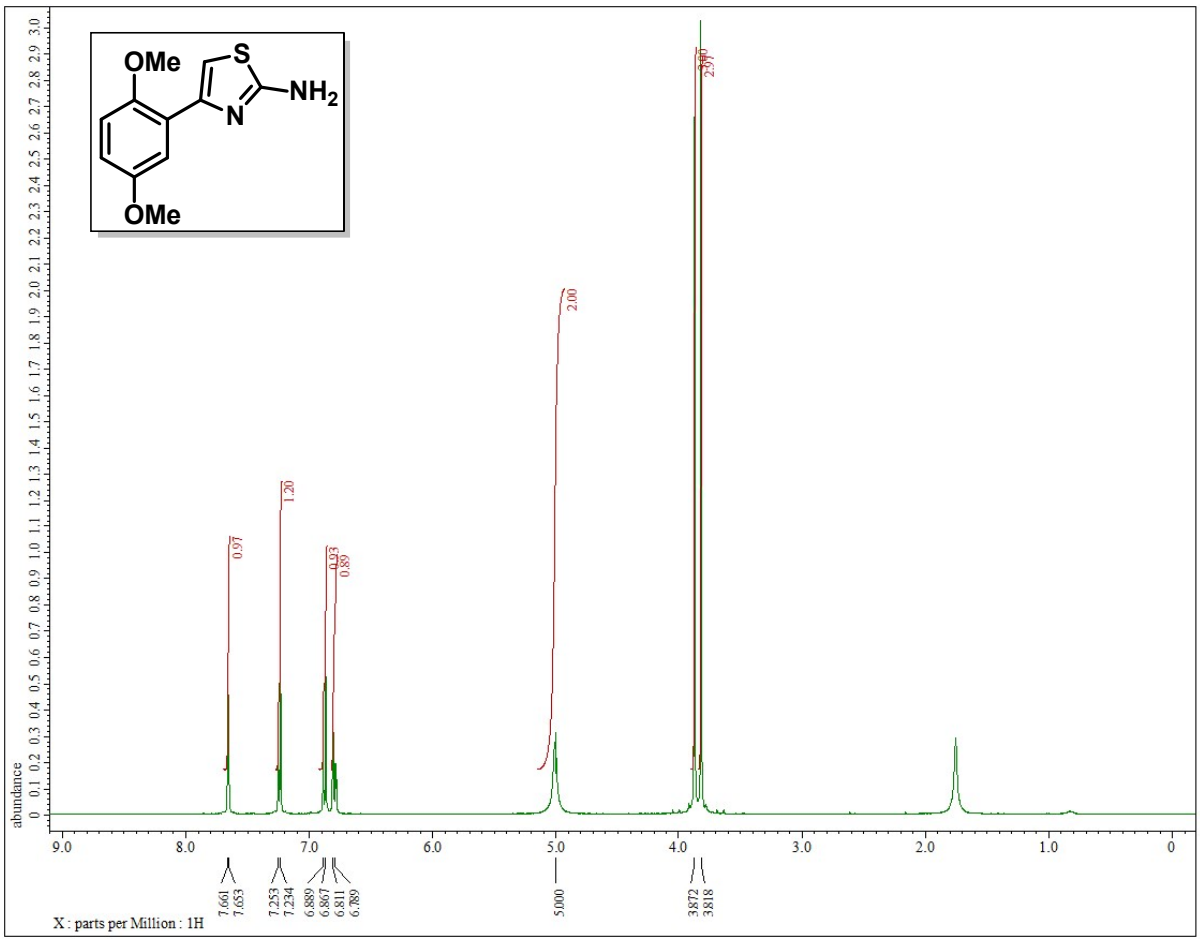
FigureS51 ^{13}C NMR spectra of 4-(2,4-difluorophenyl)thiazol-2-amine **(6h).**



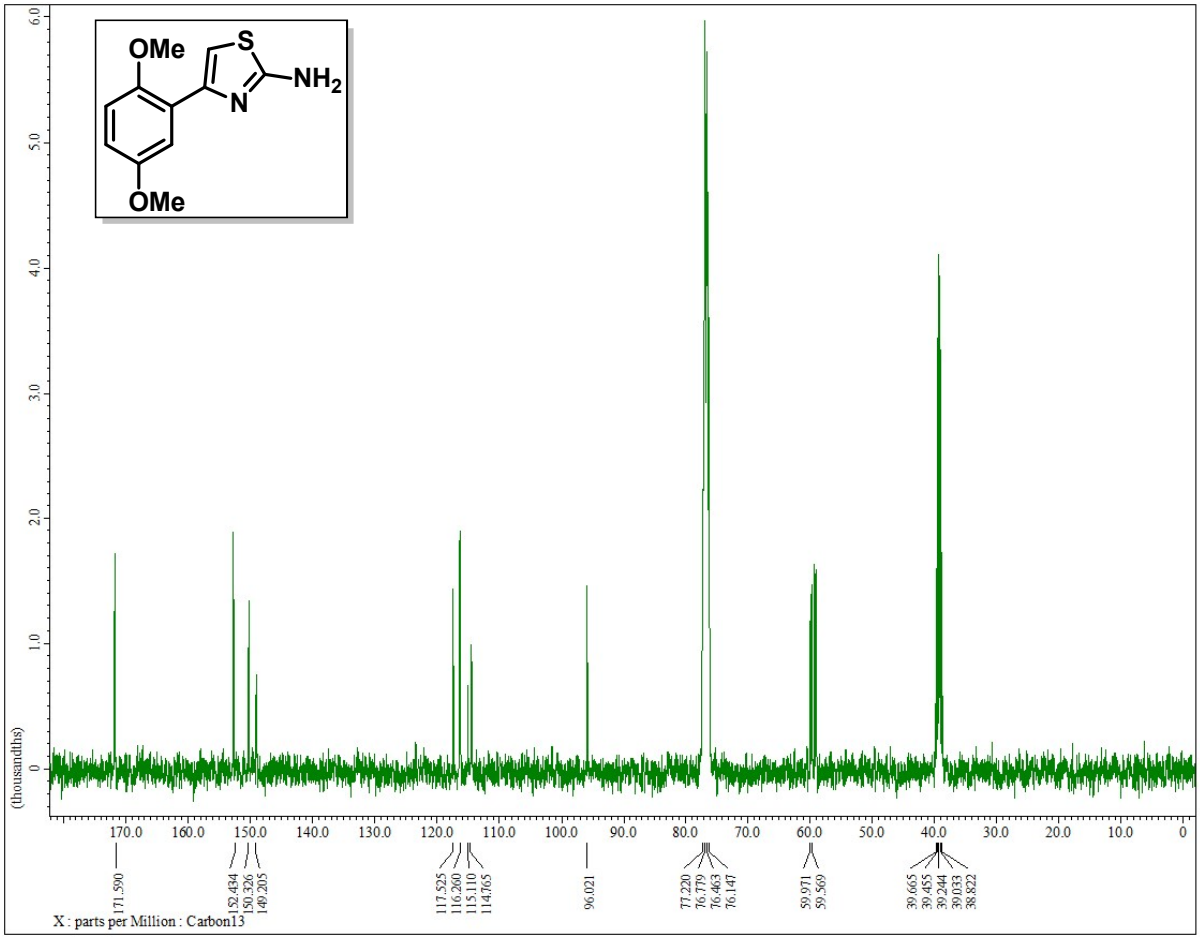
FigureS52 ^{1}H NMR spectra of 4-(4-chlorophenyl)thiazol-2-amine **(6i).**



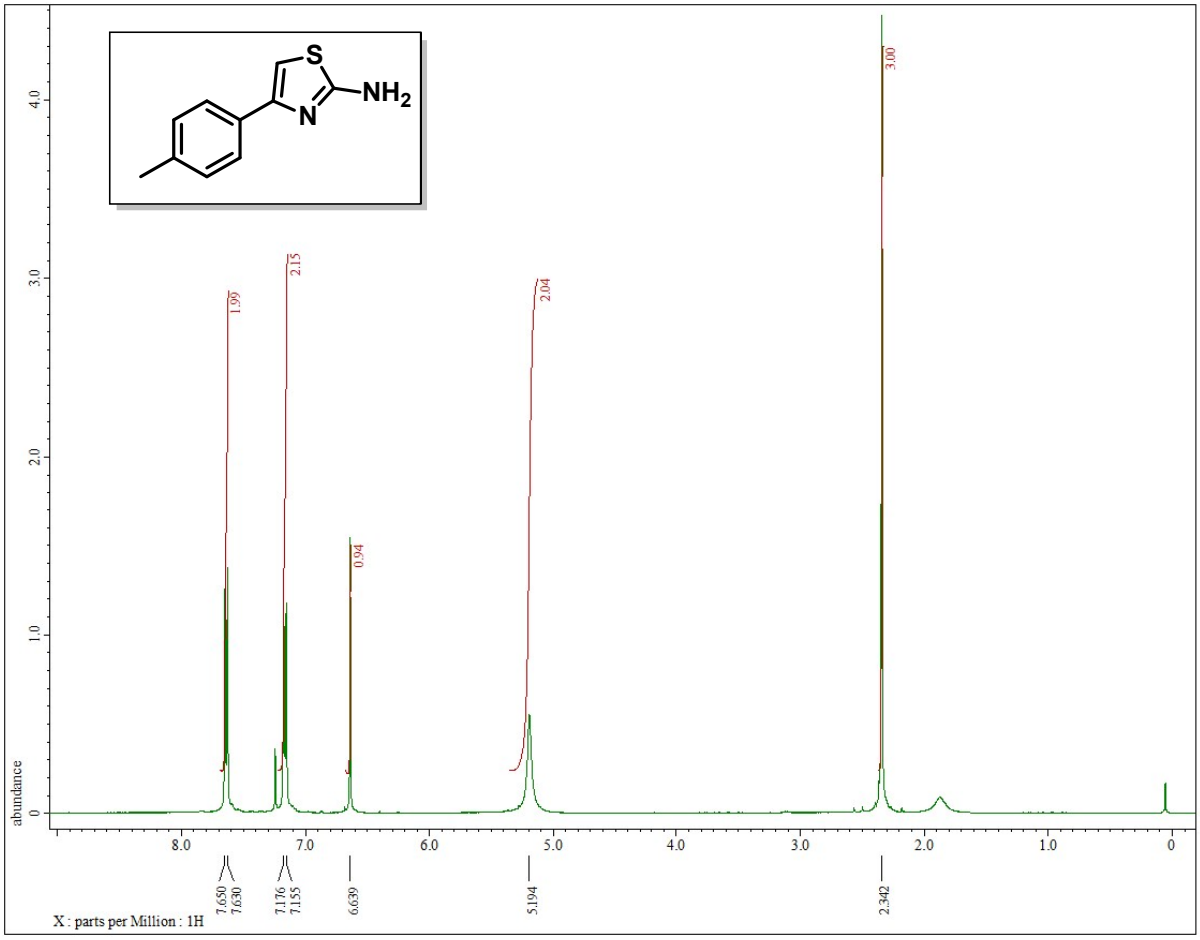
FigureS53 ^{13}C NMR spectra of 4-(4-chlorophenyl)thiazol-2-amine **(6i).**



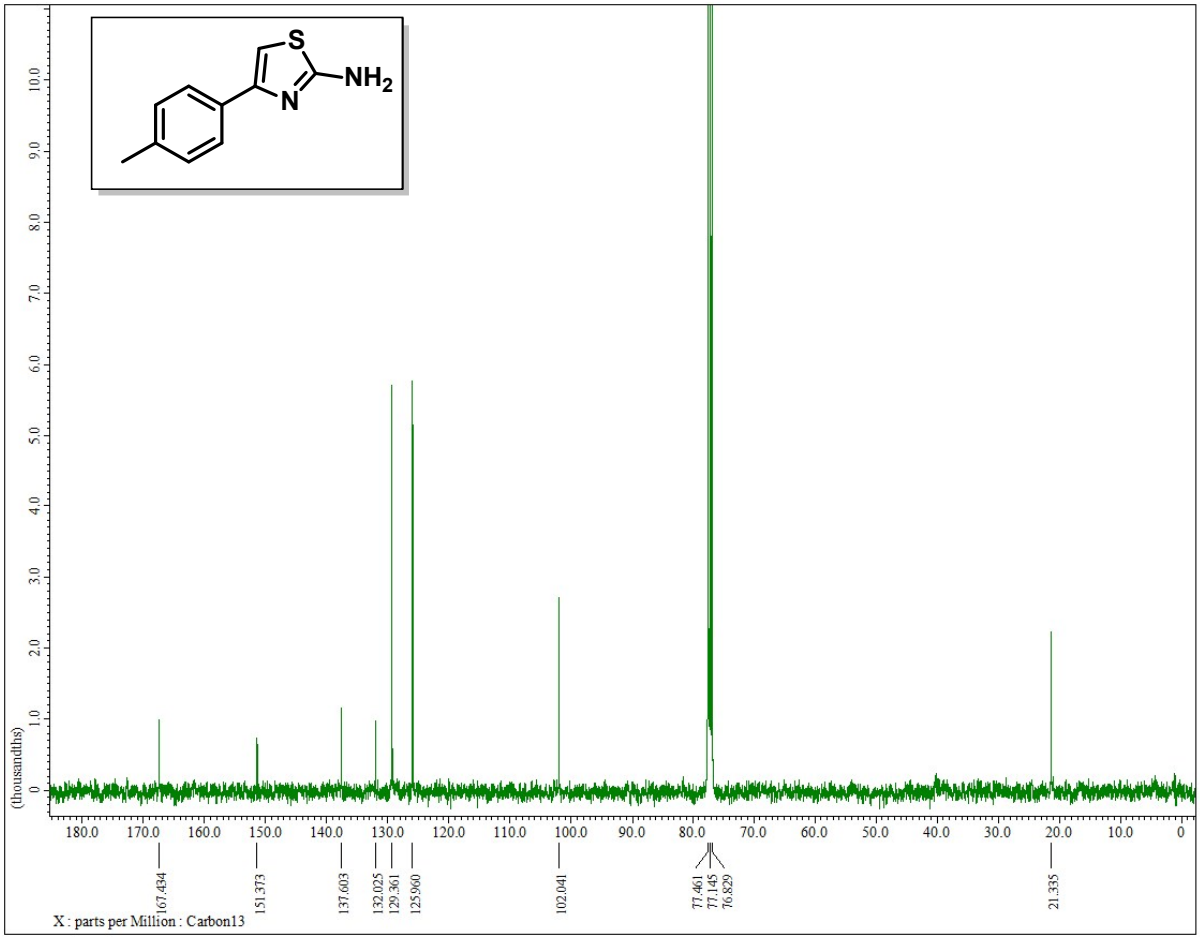
FigureS54 ^{1}H NMR spectra of 4-(2,5-dimethoxyphenyl)thiazol-2-amine **(6j).**



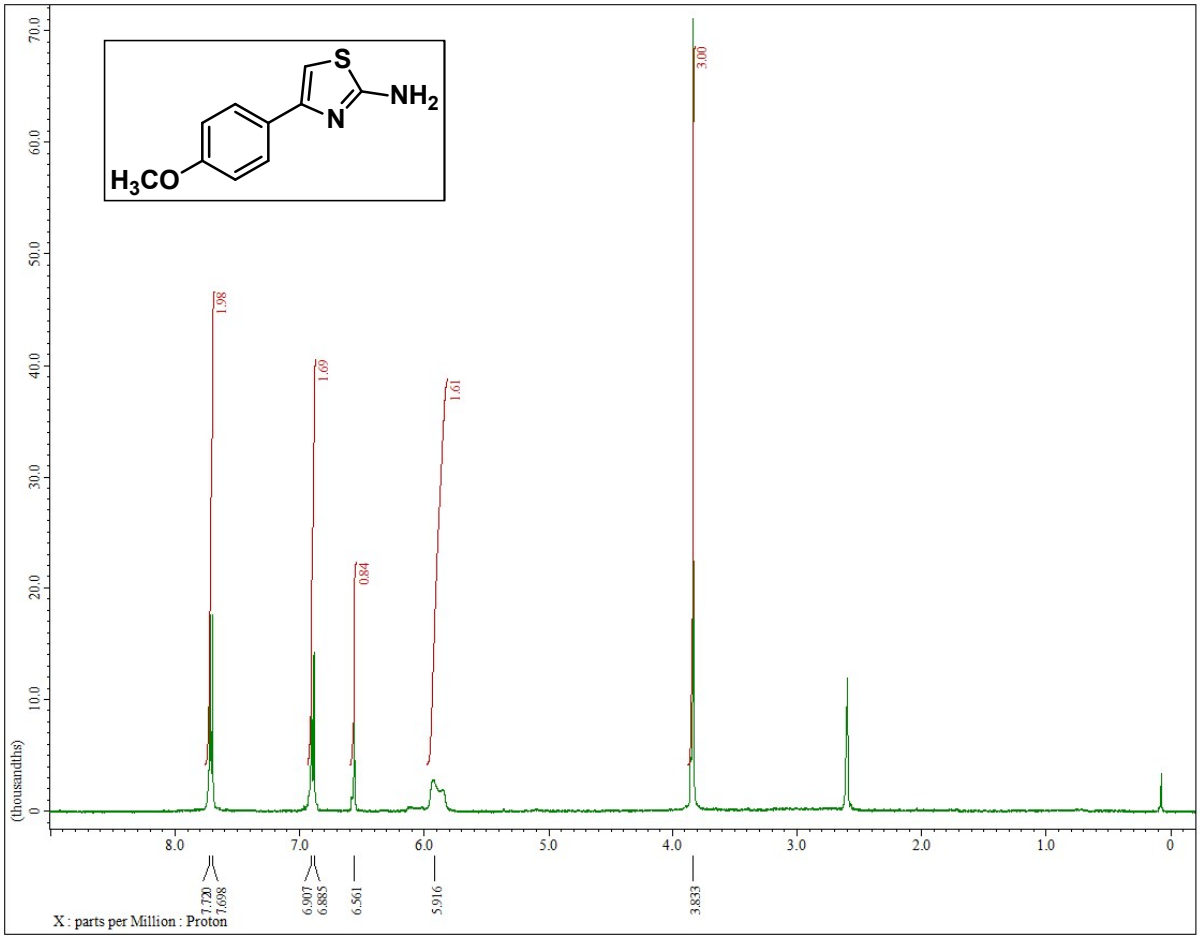
FigureS55 ^{13}C NMR spectra of 4-(2,5-dimethoxyphenyl)thiazol-2-amine **(6j).**



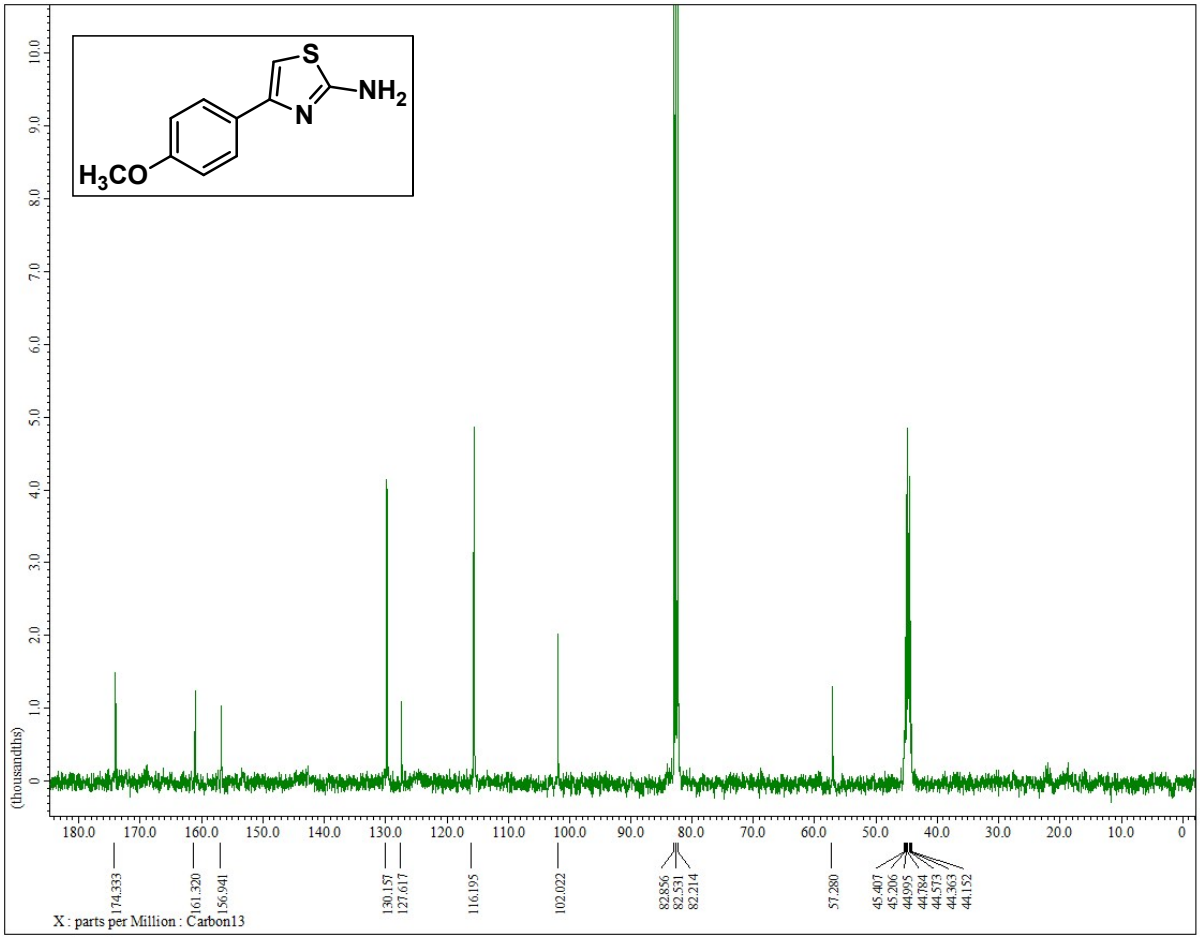
FigureS56 ^{1}H NMR spectra of 4-(p-tolyl)thiazol-2-amine **(6k).**



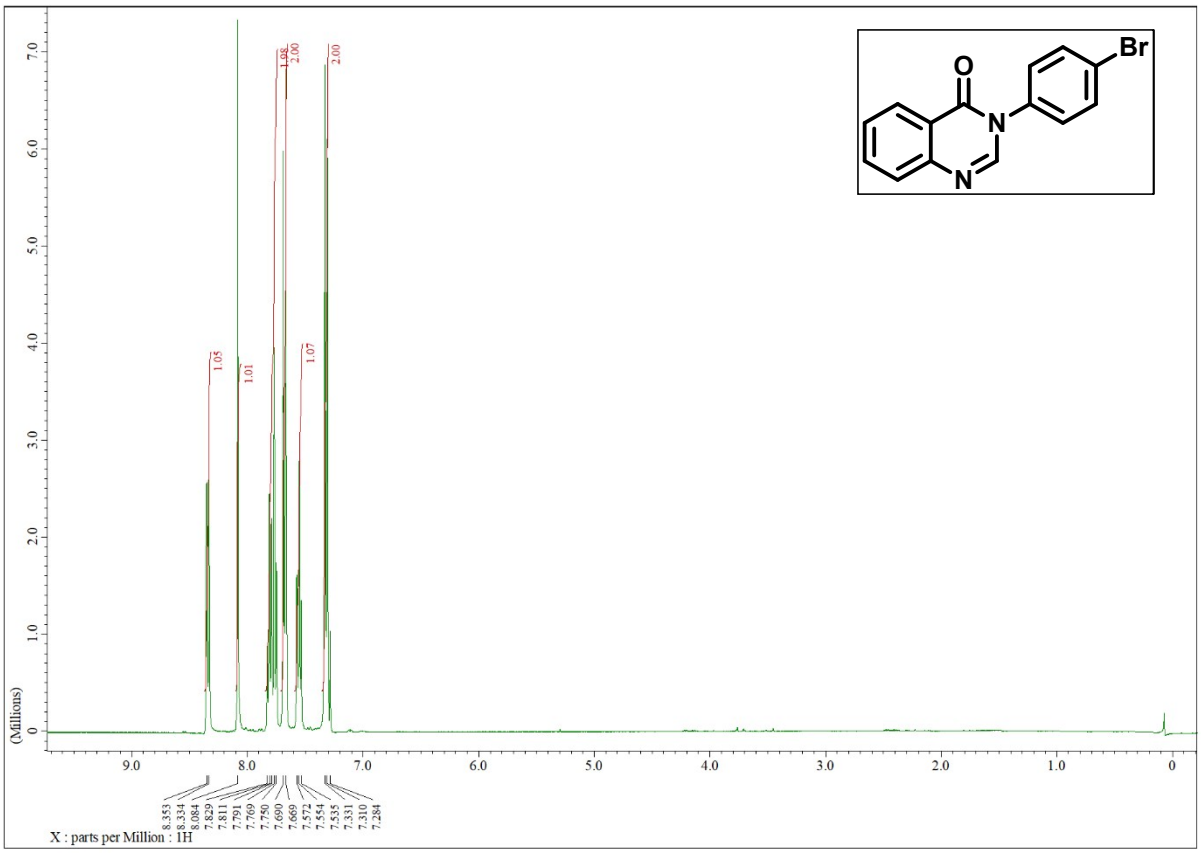
FigureS57 ^{13}C NMR spectra of 4-(p-tolyl)thiazol-2-amine **(6k).**



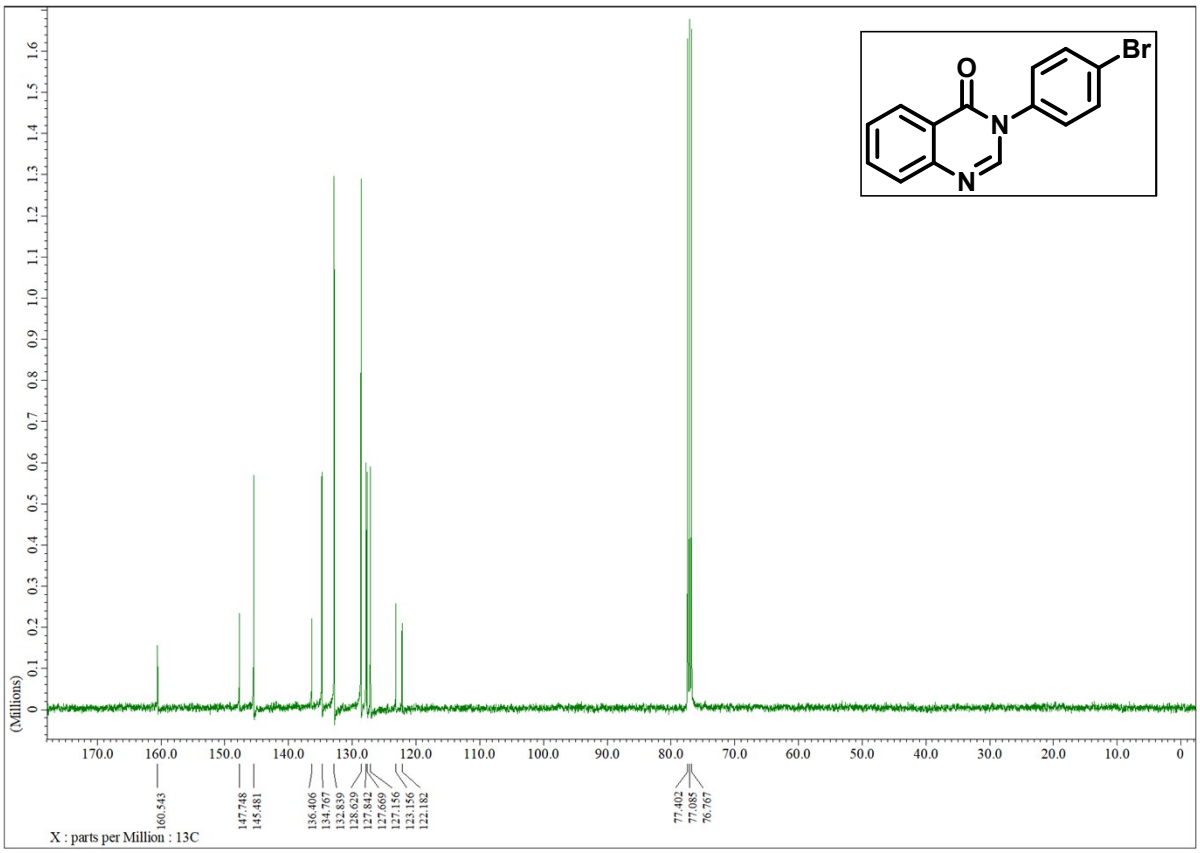
FigureS58 ^{1}H NMR spectra of 4-(4-methoxyphenyl)thiazol-2-amine **(6l).**



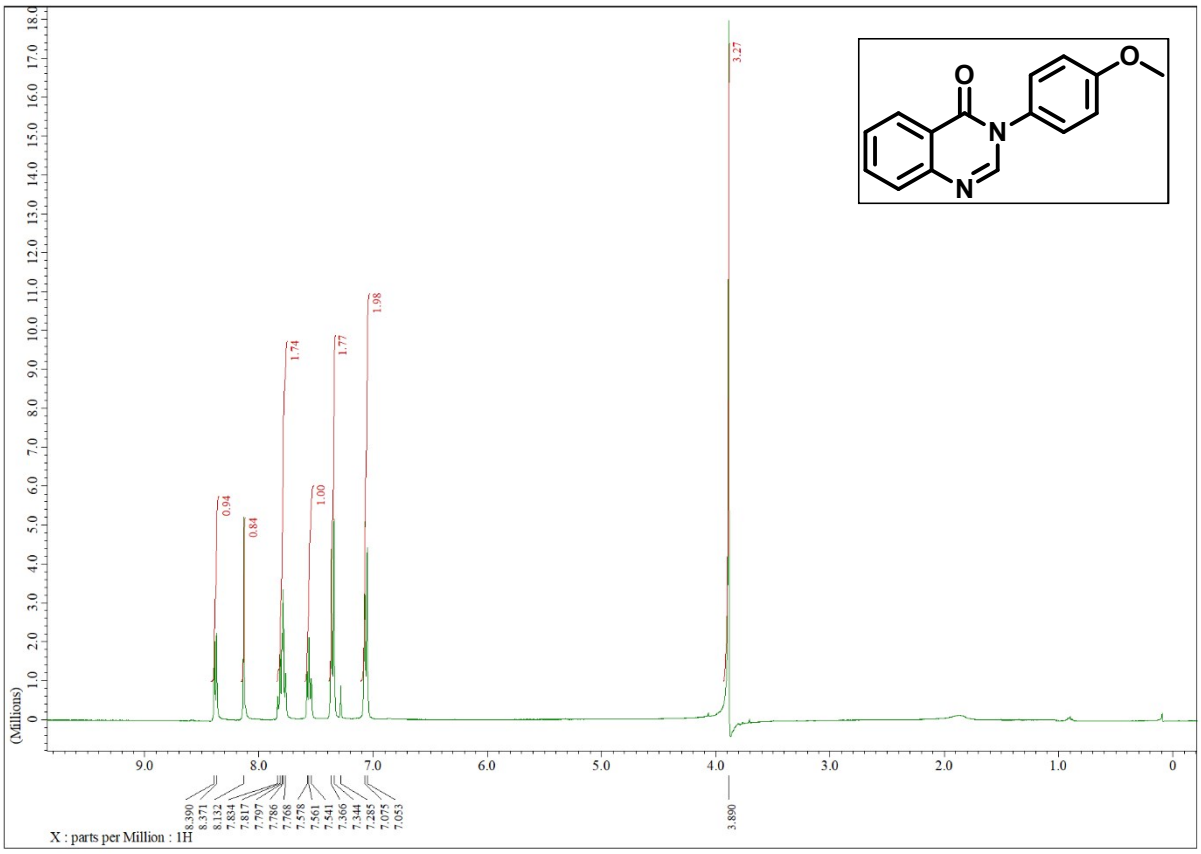
FigureS59 ^{13}C NMR spectra of 4-(4-methoxyphenyl)thiazol-2-amine **(6l).**



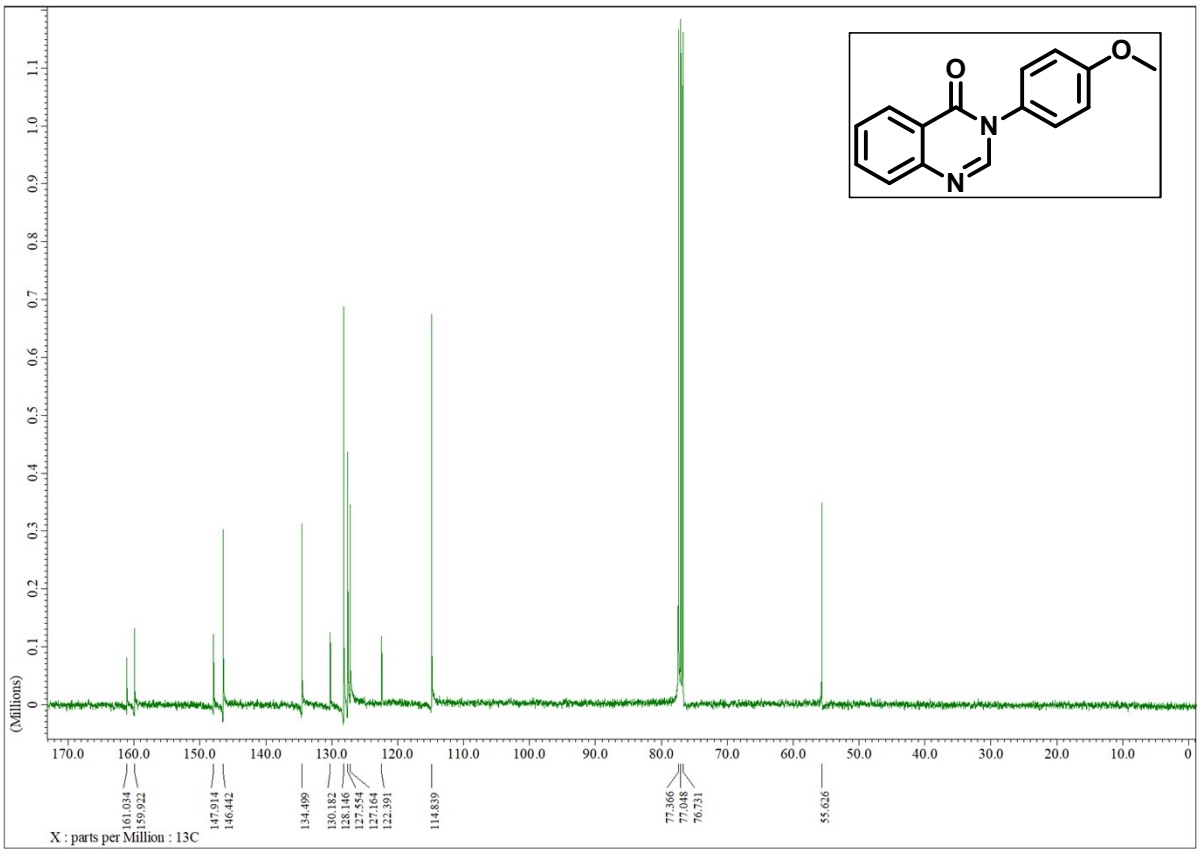
FigureS60 ^{1}H NMR spectra of 3-(4-bromophenyl)quinazolin-4(3H)-one **(10a).**



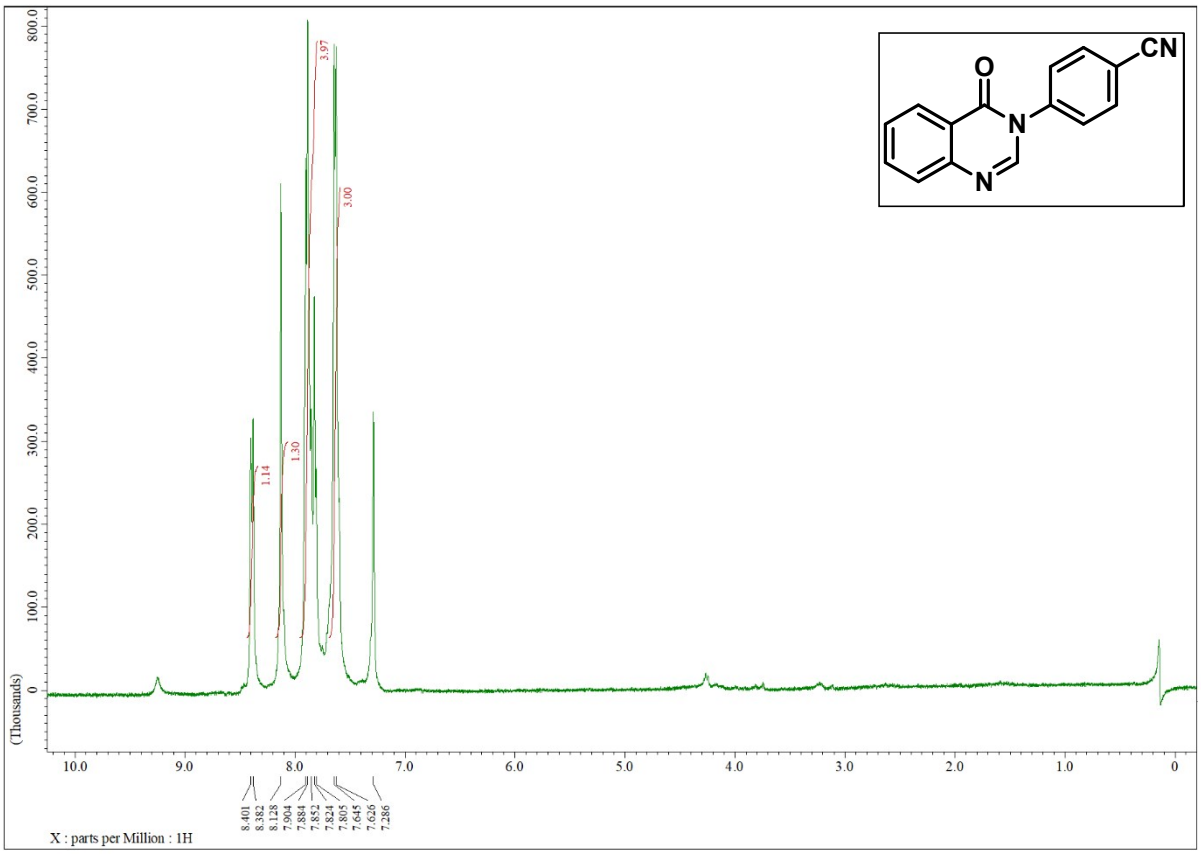
FigureS61 ^{13}C NMR spectra of 3-(4-bromophenyl)quinazolin-4(3H)-one **(10a).**



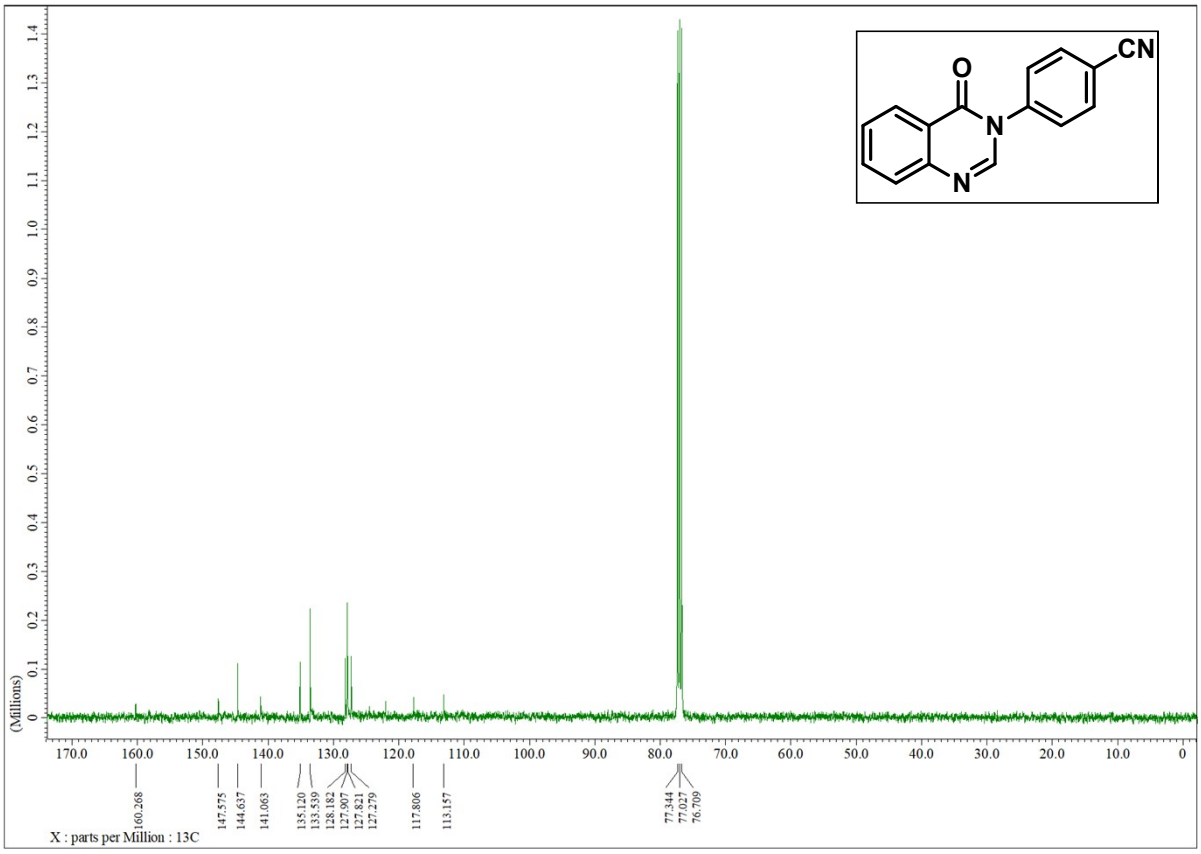
FigureS62 ^{1}H NMR spectra of 3-(4-methoxyphenyl)quinazolin-4(3H)-one **(10b).**



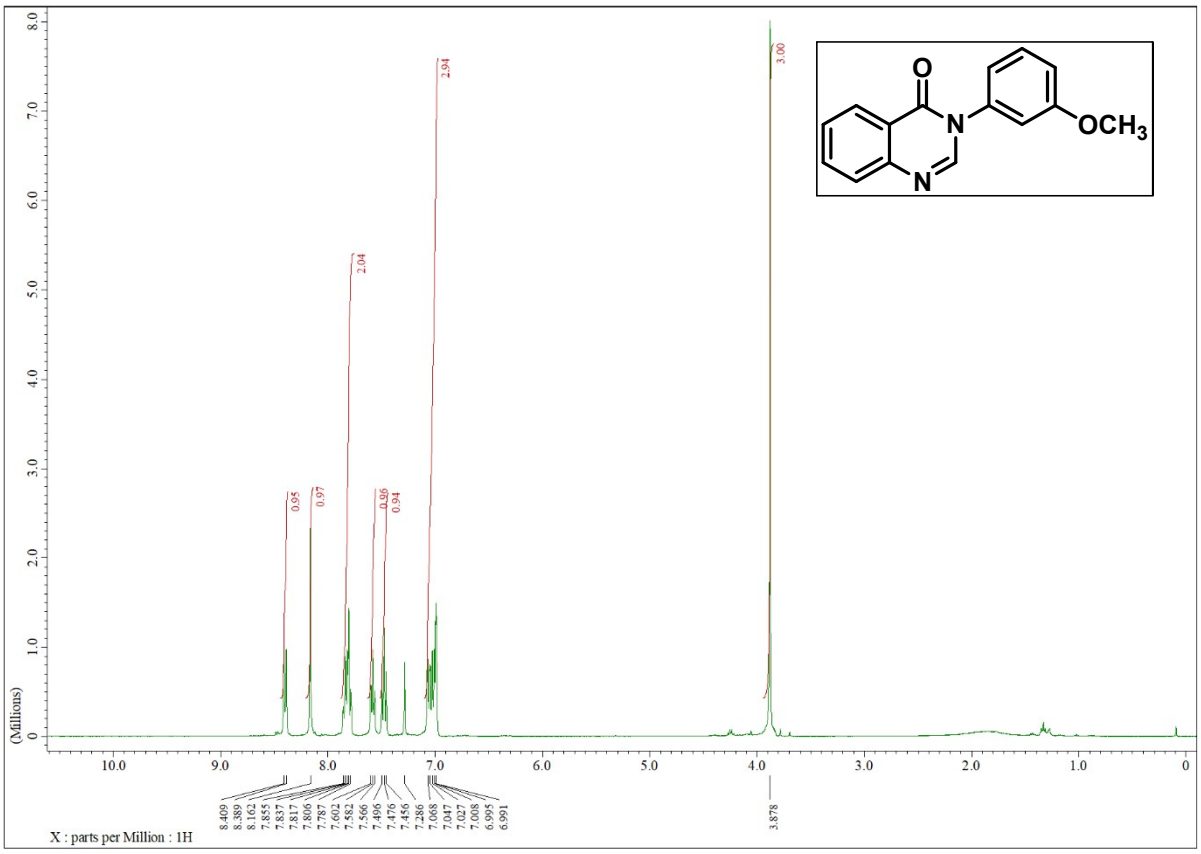
FigureS63 ^{13}C NMR spectra of 3-(4-methoxyphenyl)quinazolin-4(3H)-one **(10b).**



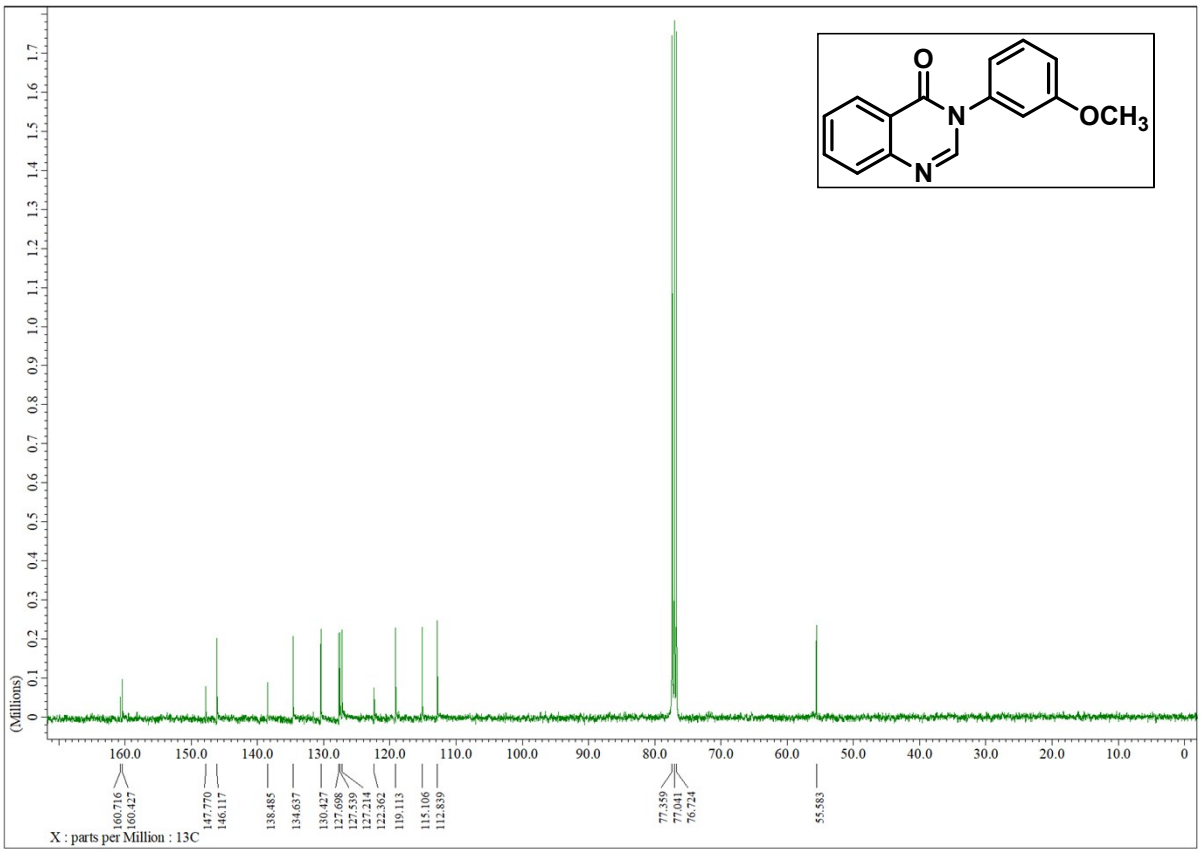
FigureS64 ^{1}H NMR spectra of 4-(4-oxoquinazolin-3(4H)-yl)benzonitrile **(10c).**



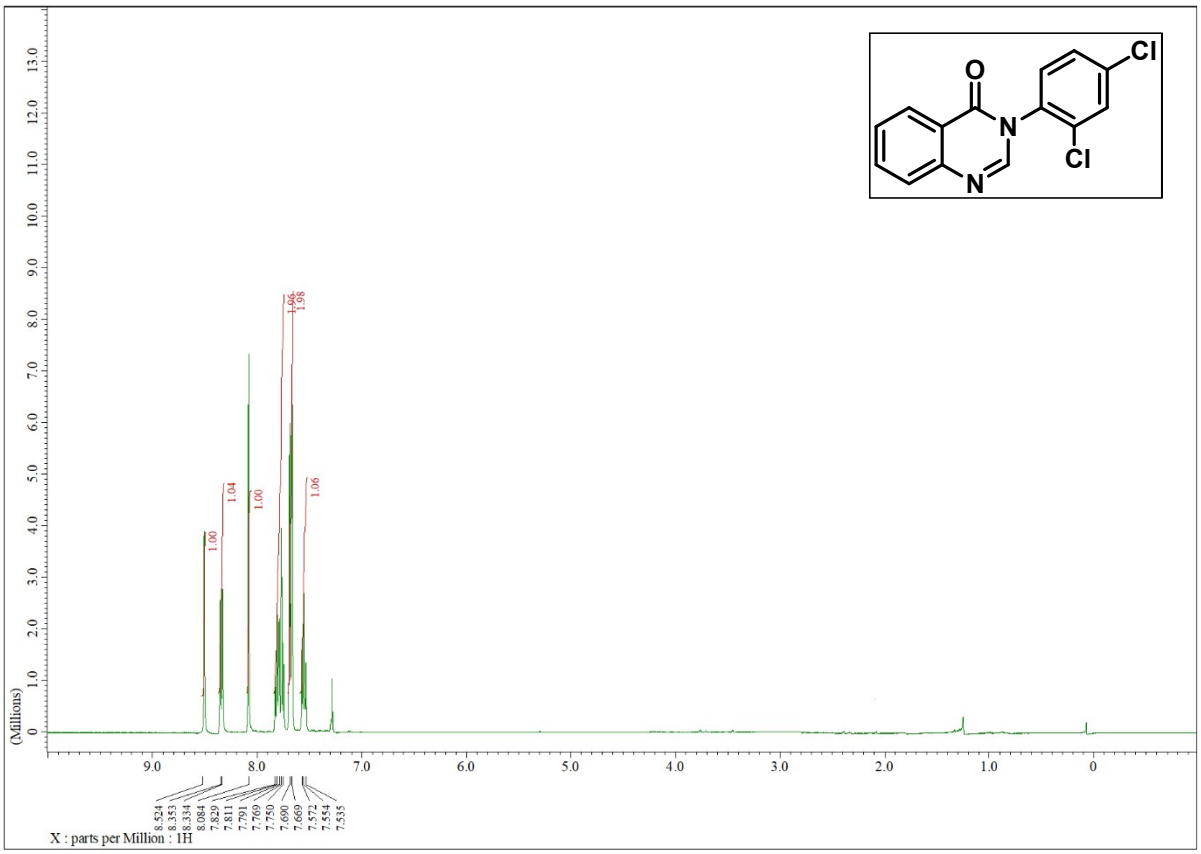
FigureS65 ^{13}C NMR spectra of 4-(4-oxoquinazolin-3(4H)-yl)benzonitrile **(10c).**



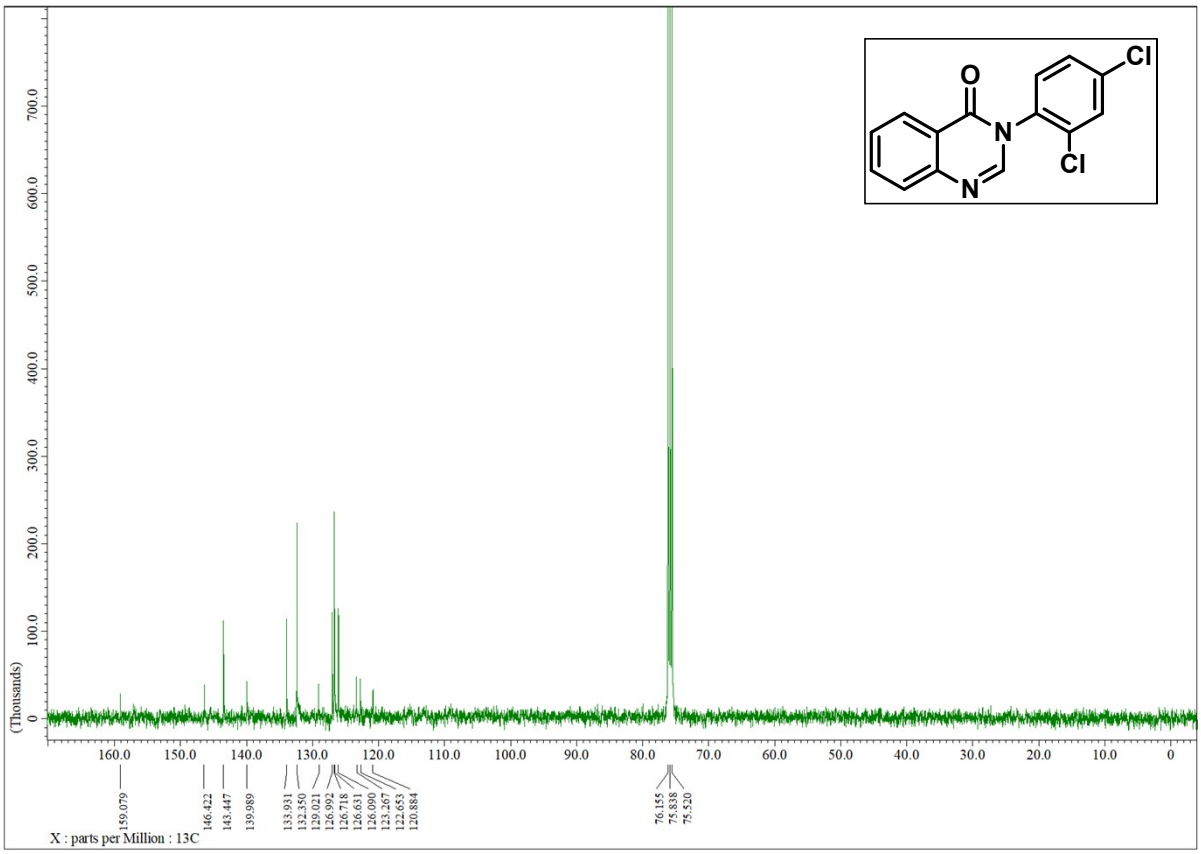
FigureS66 ^{1}H NMR spectra of 3-(3-methoxyphenyl)quinazolin-4(3H)-one **(10d).**



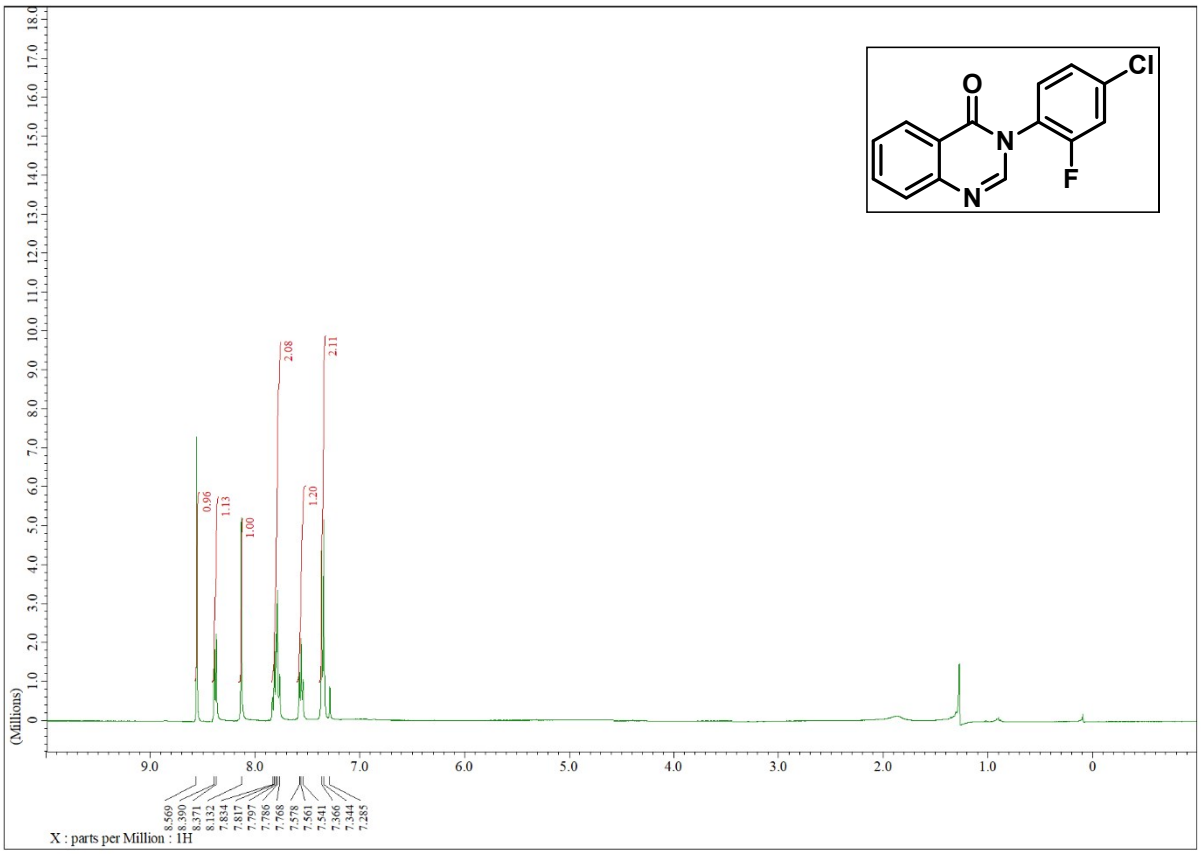
FigureS67 ^{13}C NMR spectra of 3-(3-methoxyphenyl)quinazolin-4(3H)-one **(10d).**



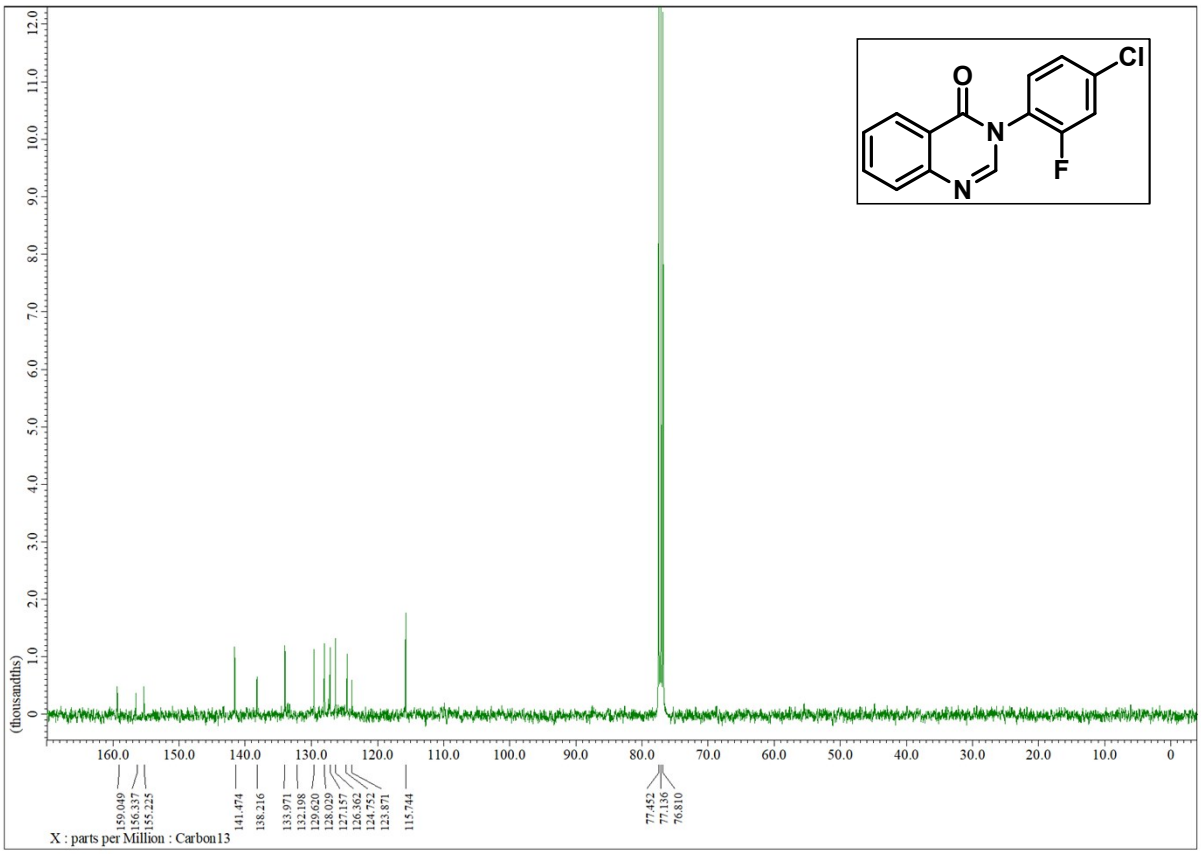
FigureS68 ^{1}H NMR spectra of 3-(2,4-dichlorophenyl)quinazolin-4(3H)-one **(10e).**



FigureS69 ^{13}C NMR spectra of 3-(2,4-dichlorophenyl)quinazolin-4(3H)-one **(10e).**



FigureS70 ^{1}H NMR spectra of 3-(4-chloro-2-fluorophenyl)quinazolin-4(3H)-one **(10f).**



FigureS71 ^{13}C NMR spectra of 3-(4-chloro-2-fluorophenyl)quinazolin-4(3H)-one **(10f).**

Qualitative Compound Report

Data File	IL-7.d	**Sample Name**	IL-7
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Comment			

Sample Group	**Info.**
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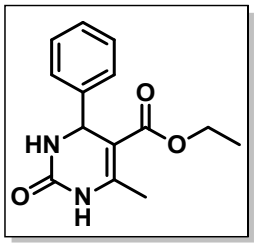
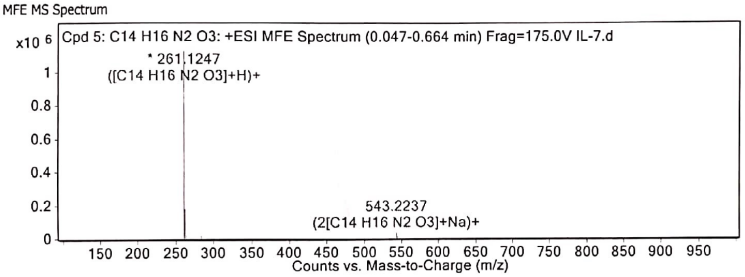


Compound Table

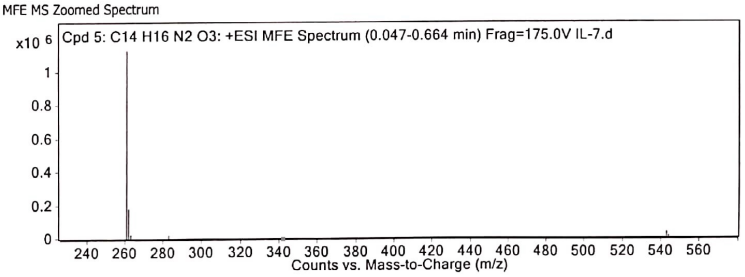
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C14 H16 N2 O3	0.098	260.1177	C14 H16 N2 O3	C14 H16 N2 O3	-6.15	C14 H16 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C14 H16 N2 O3	261.1247	0.098	Find by Molecular Feature	260.1177

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
261.1247	1	1127058.25	C14 H16 N2 O3	(M+H)+
262.1291	1	182069.44	C14 H16 N2 O3	(M+H)+
263.1343	1	21009.6	C14 H16 N2 O3	(M+H)+
264.1334	1	1698.96	C14 H16 N2 O3	(M+H)+
283.1068	1	18783.09	C14 H16 N2 O3	(M+Na)+
543.2237	1	36864.63	C14 H16 N2 O3	(2M+Na)+
544.2235	1	12694.55	C14 H16 N2 O3	(2M+Na)+
545.2322	1	2760.24	C14 H16 N2 O3	(2M+Na)+

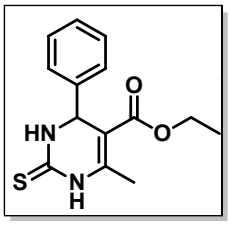
--- End Of Report ---

Figure S72 Mass spectra of Ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4a).**

Qualitative Compound Report

Data File	BS-11R.d	**Sample Name**	BS-11R
Sample Type	Sample	**Position**	P1-D8
Instrument Name	Instrument 1	**User Name**	
Acq Method	JKM2.m	**Acquired Time**	26-09-2019 14:55:29
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

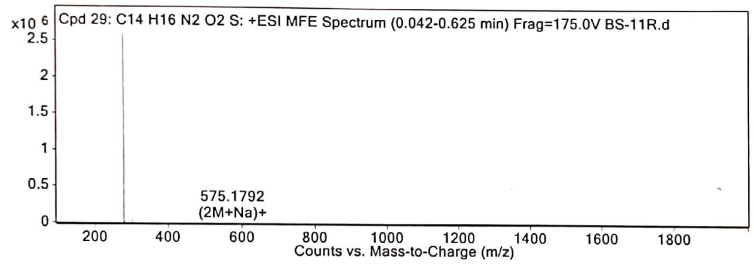


Compound Table

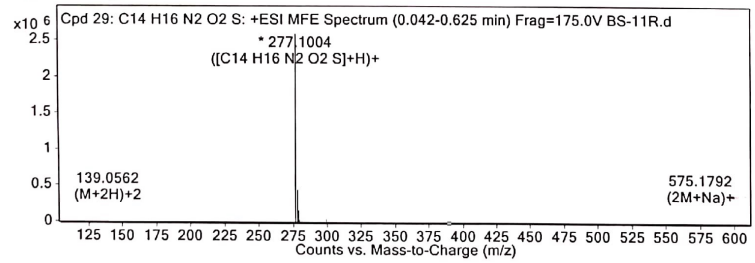
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C14 H16 N2 O2 S	0.092	276.0928	C14 H16 N2 O2 S	C14 H16 N2 O2 S	1.58	C14 H16 N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C14 H16 N2 O2 S	277.1004	0.092	Find by Molecular Feature	276.0928

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
139.0562	2	8479.56		(M+2H)+2
277.1004	1	2585286	C14 H16 N2 O2 S	(M+H)+
278.1007	1	432282.75	C14 H16 N2 O2 S	(M+H)+
279.0991	1	143728.7	C14 H16 N2 O2 S	(M+H)+
280.1014	1	31714.89	C14 H16 N2 O2 S	(M+H)+
281.1062	1	10327.09	C14 H16 N2 O2 S	(M+H)+
299.0799	1	34689.36		(M+Na)+
575.1792	1	8514.2		(2M+Na)+
576.1921	1	3674.48		(2M+Na)+

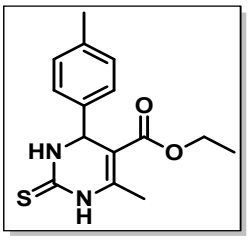
--- End Of Report ---

Figure S73 Mass spectra of Ethyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4b).**

Qualitative Compound Report

Data File	BS-12.d	**Sample Name**	BS-12
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	JKM2.m	**Acquired Time**	26-09-2019 12:07:04
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

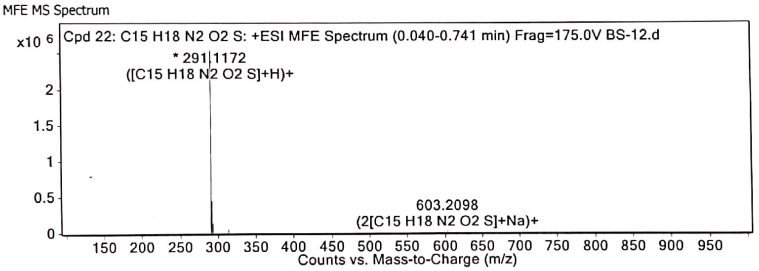


Compound Table

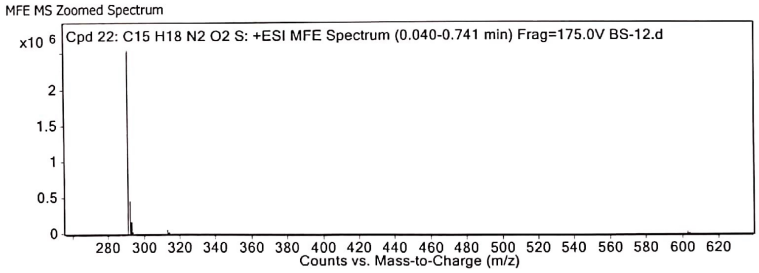
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C15 H18 N2 O2 S	0.093	290.1098	C15 H18 N2 O2 S	C15 H18 N2 O2 S	-3.03	C15 H18 N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C15 H18 N2 O2 S	291.1172	0.093	Find by Molecular Feature	290.1098

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
291.1172	1	2544948	C15 H18 N2 O2 S	(M+H)+
292.1201	1	447006	C15 H18 N2 O2 S	(M+H)+
293.1128	1	142780.94	C15 H18 N2 O2 S	(M+H)+
294.1162	1	28235.25	C15 H18 N2 O2 S	(M+H)+
295.1166	1	4465.9	C15 H18 N2 O2 S	(M+H)+
296.1208	1	332.11	C15 H18 N2 O2 S	(M+H)+
313.0994	1	50985.06	C15 H18 N2 O2 S	(M+Na)+
314.1069	1	10110.1	C15 H18 N2 O2 S	(M+Na)+
603.2098	1	20663.15	C15 H18 N2 O2 S	(2M+Na)+
604.2091	1	8452.32	C15 H18 N2 O2 S	(2M+Na)+

--- End Of Report ---

Figure S74 Mass spectra of Ethyl-6-methyl-2-thioxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4d).**

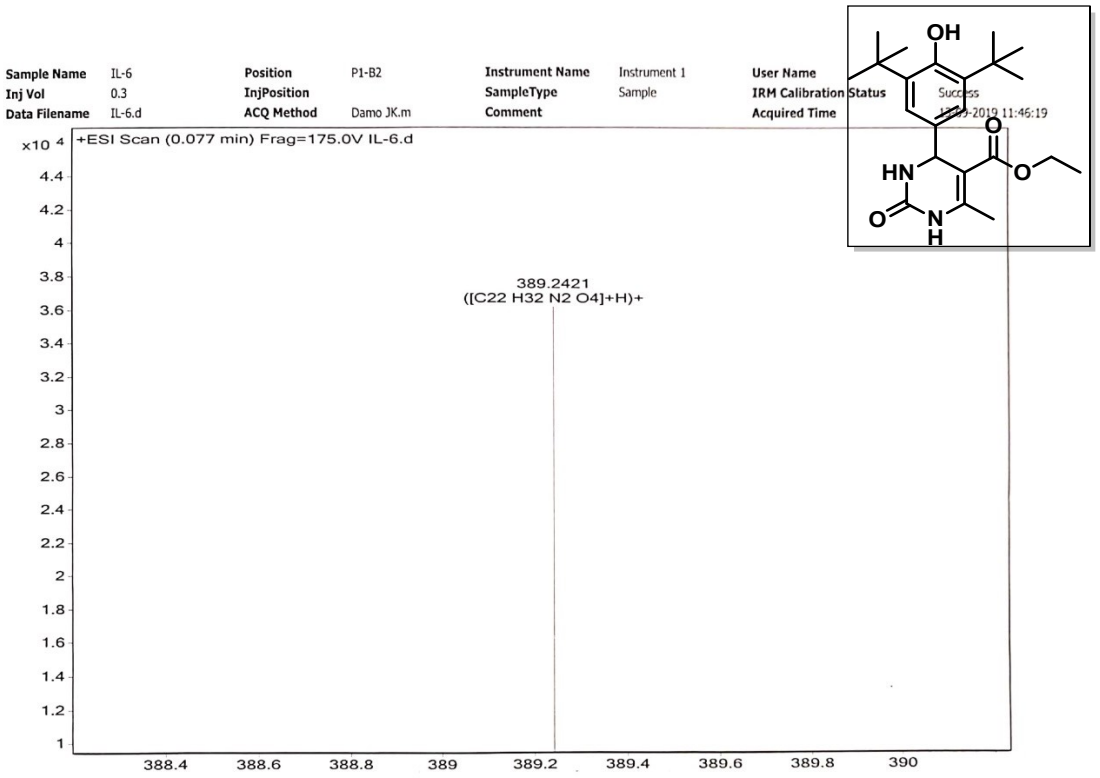


Figure S75 Mass spectra of Ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4e).**

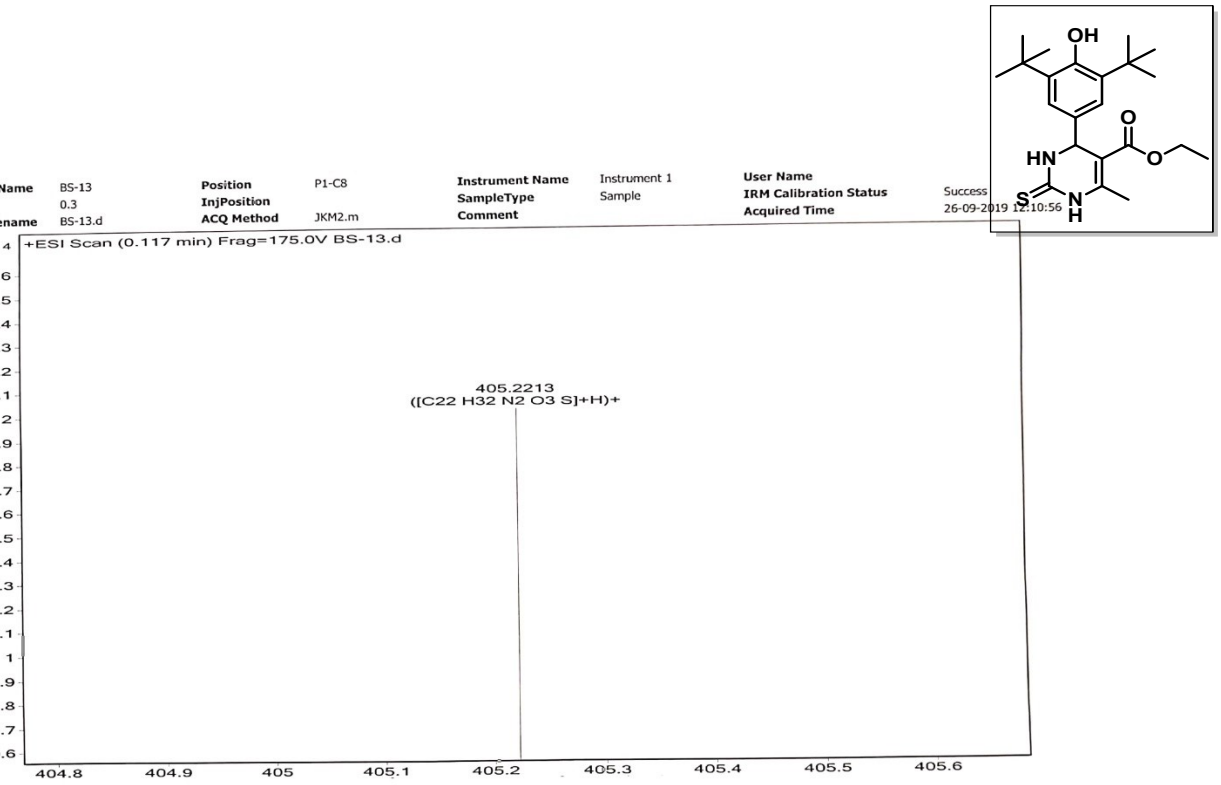


Figure S76 Mass spectra of Ethyl-4-(4-hydroxy-3,5-ditertbutylphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4f).**

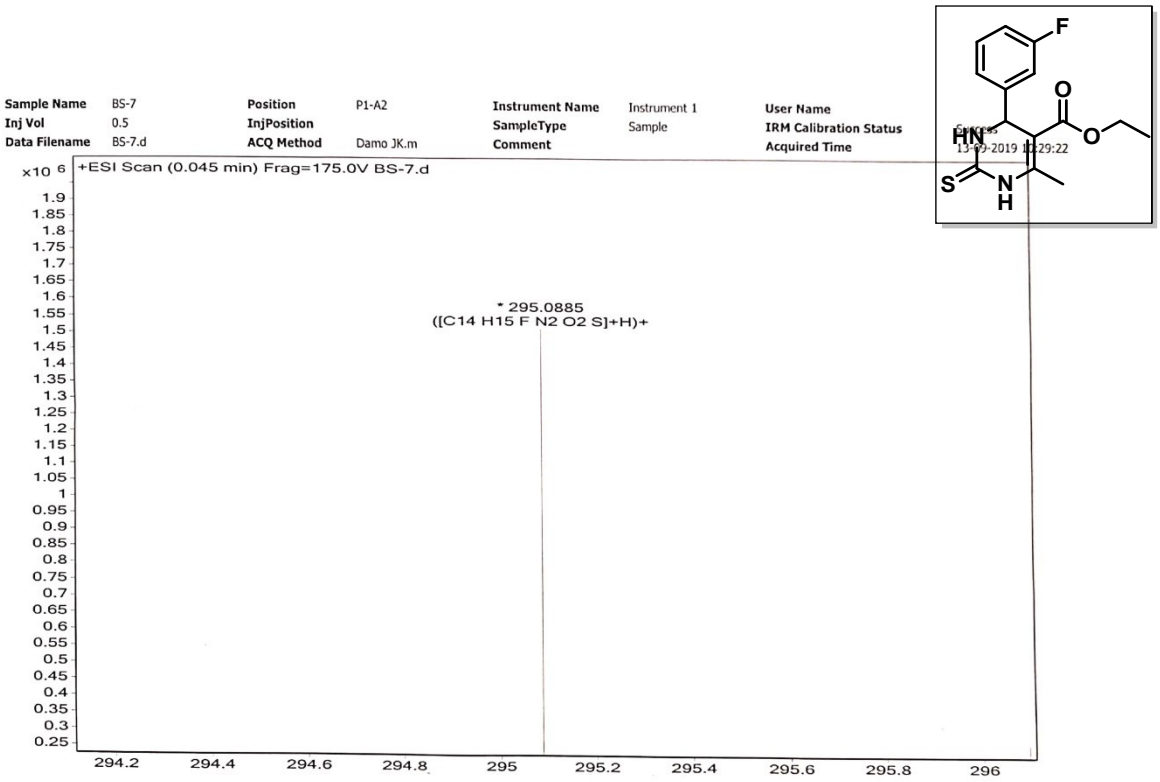


Figure S77 Mass spectra of Ethyl-4-(3-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4h).**

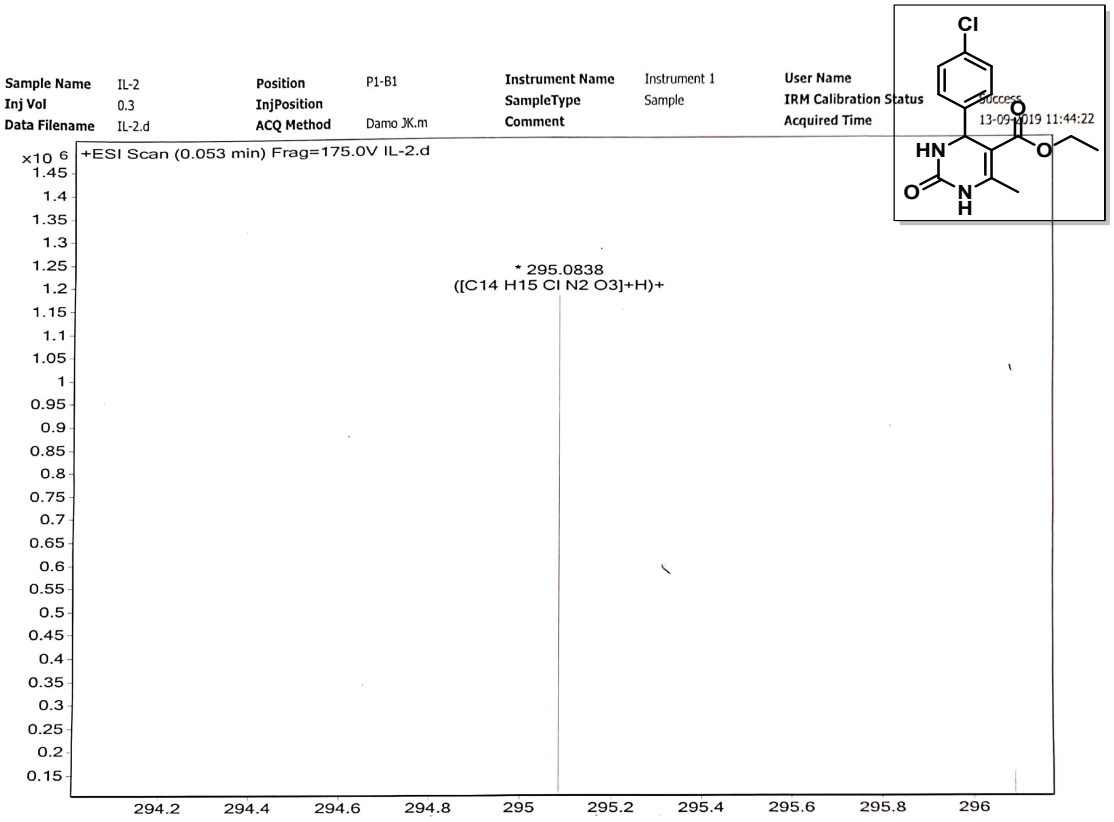
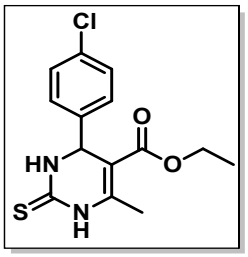


Figure S78 Mass spectra of Ethyl-4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4i).**

Qualitative Compound Report

Data File	BS-2.d	**Sample Name**	BS-2
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	03-09-2019 12:27:47
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

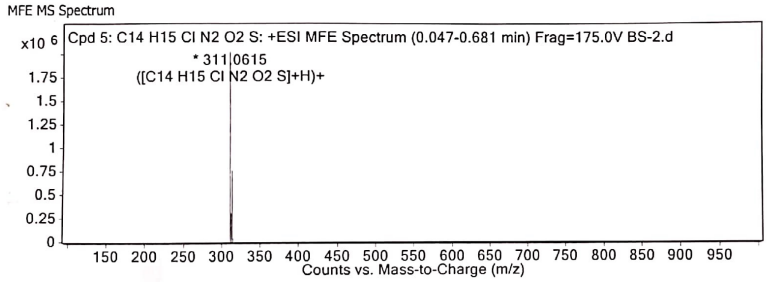


Compound Table

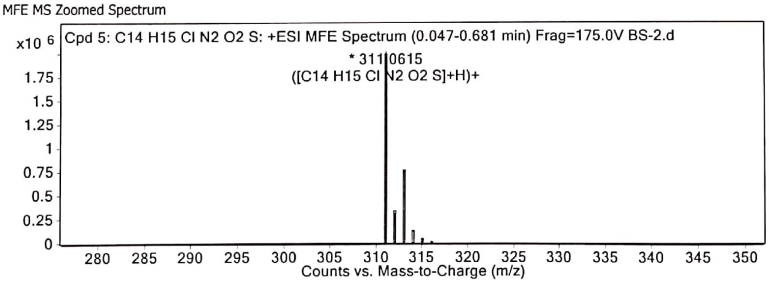
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C14 H15 Cl N2 O2 S	0.116	310.0535	C14 H15 Cl N2 O2 S	C14 H15 Cl N2 O2 S	2.66	C14 H15 Cl N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C14 H15 Cl N2 O2 S	311.0615	0.116	Find by Molecular Feature	310.0535

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
311.0615	1	2016023.38	C14 H15 Cl N2 O2 S	(M+H)+
312.0615	1	311147.08	C14 H15 Cl N2 O2 S	(M+H)+
313.0572	1	762642.82	C14 H15 Cl N2 O2 S	(M+H)+
314.0588	1	113888.83	C14 H15 Cl N2 O2 S	(M+H)+
315.0569	1	41609.68	C14 H15 Cl N2 O2 S	(M+H)+
316.0591	1	1346.15	C14 H15 Cl N2 O2 S	(M+H)+
317.0622	1	680.57	C14 H15 Cl N2 O2 S	(M+H)+

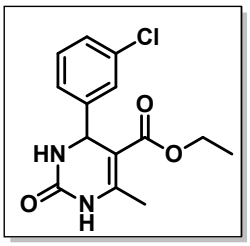
--- End Of Report ---

Figure S79 Mass spectra of Ethyl-4-(4-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4j).**

Qualitative Compound Report

Data File	IL-9.d	**Sample Name**	IL-9
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	JKM2.m	**Acquired Time**	26-09-2019 12:09:00
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

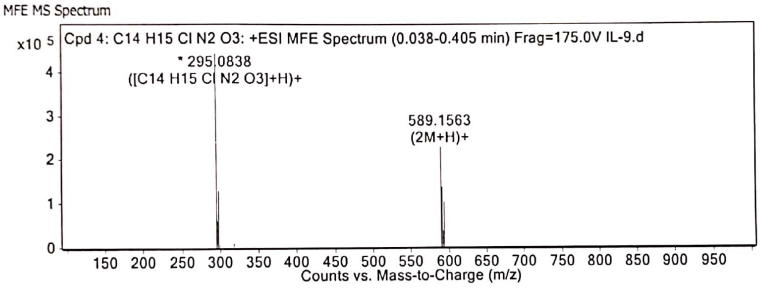


Compound Table

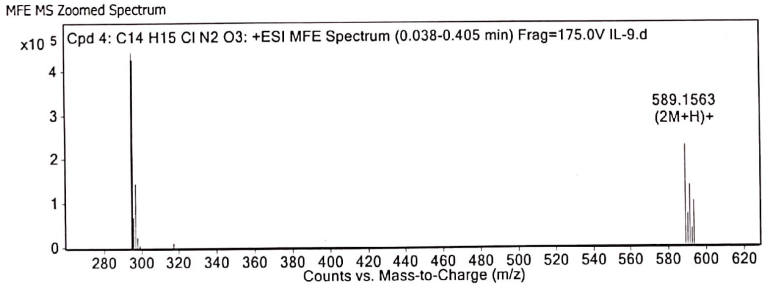
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C14 H15 Cl N2 O3	0.092	294.0769	C14 H15 Cl N2 O3	C14 H15 Cl N2 O3	0.72	C14 H15 Cl N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C14 H15 Cl N2 O3	295.0838	0.092	Find by Molecular Feature	294.0769

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
295.0838	1	442923.94	C14 H15 Cl N2 O3	(M+H)+
296.0871	1	60840.51	C14 H15 Cl N2 O3	(M+H)+
297.0828	1	129092.12	C14 H15 Cl N2 O3	(M+H)+
298.0822	1	21669.46	C14 H15 Cl N2 O3	(M+H)+
317.0673	1	9312.83	C14 H15 Cl N2 O3	(M+Na)+
589.1563	1	227651.31		(2M+H)+
590.1588	1	72353.38		(2M+H)+
591.1592	1	137207.96		(2M+H)+
592.1614	1	39199.82		(2M+H)+
593.1776	1	102539.73		(2M+H)+

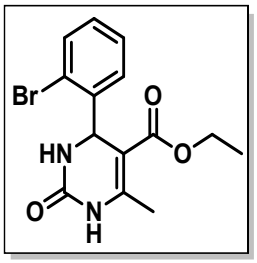
--- End Of Report ---

Figure S80 Mass spectra of Ethyl-4-(3-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4k).**

Qualitative Compound Report

Data File	IL-5.d	Sample Name	IL-5
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method	JKM2.m	Acquired Time	22-10-2019 12:09:03
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.1)

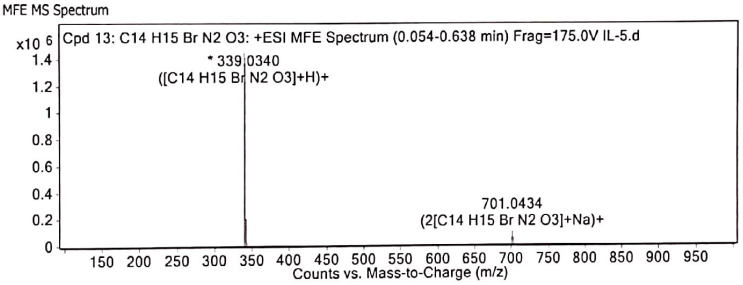


Compound Table

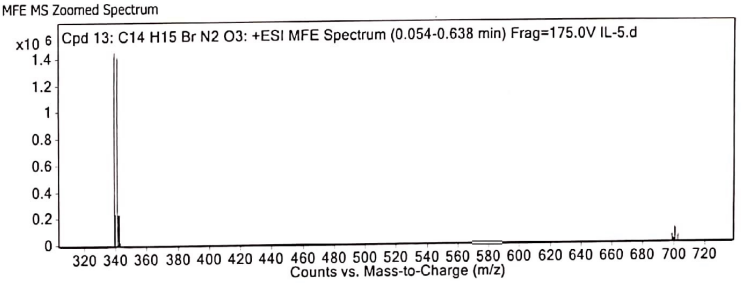
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C14 H15 Br N2 O3	0.098	338.0266	C14 H15 Br N2 O3	C14 H15 Br N2 O3	0.16	C14 H15 Br N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C14 H15 Br N2 O3	339.034	0.098	Find by Molecular Feature	338.0266

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
339.034	1	1451869.88	C14 H15 Br N2 O3	(M+H)+
340.0372	1	198951.81	C14 H15 Br N2 O3	(M+H)+
341.0317	1	1414947.25	C14 H15 Br N2 O3	(M+H)+
342.0348	1	199765.52	C14 H15 Br N2 O3	(M+H)+
343.0388	1	25349.52	C14 H15 Br N2 O3	(M+H)+
699.0421	1	50872.87	C14 H15 Br N2 O3	(2M+Na)+
700.0535	1	21453.63	C14 H15 Br N2 O3	(2M+Na)+
701.0434	1	100158.74	C14 H15 Br N2 O3	(2M+Na)+
702.052	1	40869.3	C14 H15 Br N2 O3	(2M+Na)+
703.0413	1	53491.82	C14 H15 Br N2 O3	(2M+Na)+

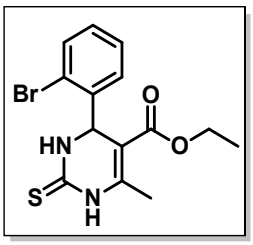
--- End Of Report ---

Figure S81 Mass spectra of Ethyl-4-(2-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4l).**

Qualitative Compound Report

BS-8

Data File	HA-F.d	**Sample Name**	HA-F
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	13-09-2019 12:14:16
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



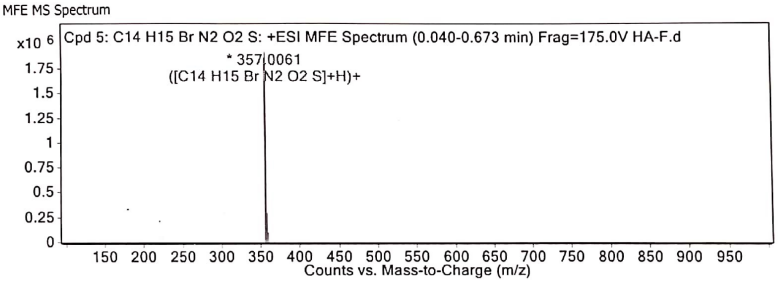
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

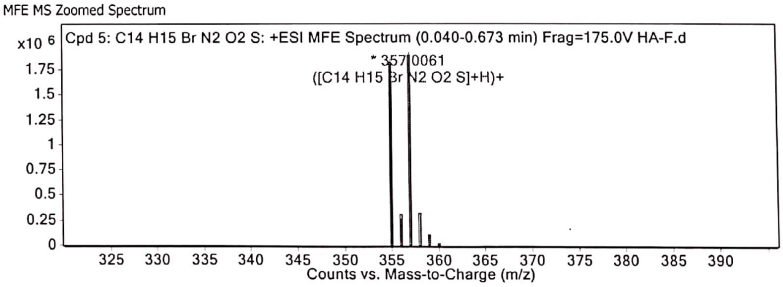
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C14 H15 Br N2 O2 S	0.072	354.0006	C14 H15 Br N2 O2 S	C14 H15 Br N2 O2 S	8.82	C14 H15 Br N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C14 H15 Br N2 O2 S	355.0074	0.072	Find by Molecular Feature	354.0006

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
355.0074	1	1858464.17	C14 H15 Br N2 O2 S	(M+H)+
356.0112	1	270790.21	C14 H15 Br N2 O2 S	(M+H)+
357.0061	1	1917009.5	C14 H15 Br N2 O2 S	(M+H)+
358.0089	1	299888.8	C14 H15 Br N2 O2 S	(M+H)+
359.0078	1	98233.78	C14 H15 Br N2 O2 S	(M+H)+
360.0099	1	12778.51	C14 H15 Br N2 O2 S	(M+H)+
361.0078	1	2057.8	C14 H15 Br N2 O2 S	(M+H)+

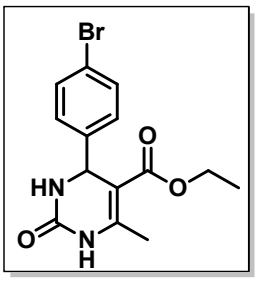
--- End Of Report ---

Figure S82 Mass spectra of Ethyl-4-(2-bromophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4m).**

Qualitative Compound Report

Data File	BS-3.d	**Sample Name**	BS-3
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	05-09-2019 13:58:44
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

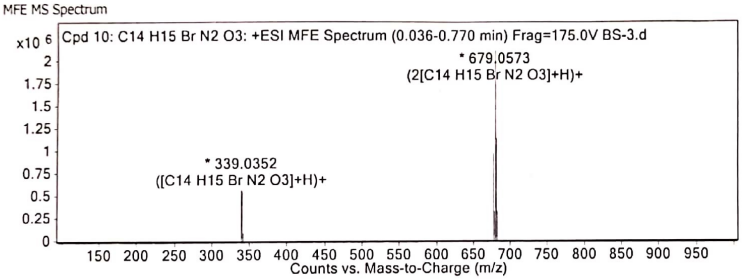


Compound Table

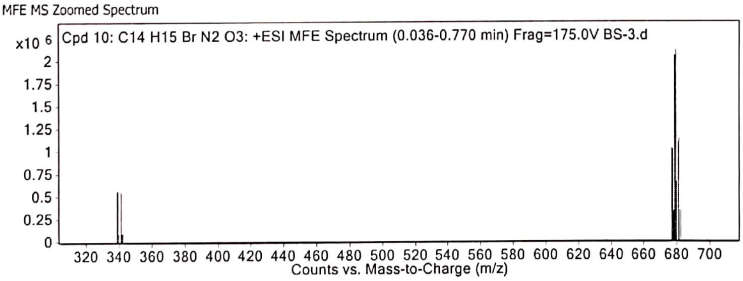
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C14 H15 Br N2 O3	0.092	338.0274	C14 H15 Br N2 O3	C14 H15 Br N2 O3	-2.27	C14 H15 Br N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C14 H15 Br N2 O3	677.061	0.092	Find by Molecular Feature	338.0274

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
339.0352	1	564586.75	C14 H15 Br N2 O3	(M+H)+
340.0367	1	94358.9	C14 H15 Br N2 O3	(M+H)+
341.0333	1	551163.88	C14 H15 Br N2 O3	(M+H)+
342.0358	1	83815.19	C14 H15 Br N2 O3	(M+H)+
677.061	1	967692.67	C14 H15 Br N2 O3	(2M+H)+
678.064	1	328649.09	C14 H15 Br N2 O3	(2M+H)+
679.0573	1	2108614	C14 H15 Br N2 O3	(2M+H)+
680.0639	1	584196.91	C14 H15 Br N2 O3	(2M+H)+
681.0615	1	1127792.02	C14 H15 Br N2 O3	(2M+H)+
682.0613	1	331890.76	C14 H15 Br N2 O3	(2M+H)+

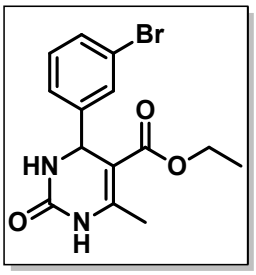
--- End Of Report ---

Figure S83 Mass spectra of Ethyl-4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4n).**

Qualitative Compound Report

Data File	IL-8.d	**Sample Name**	IL-8
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	JKM2.m	**Acquired Time**	22-10-2019 12:10:59
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

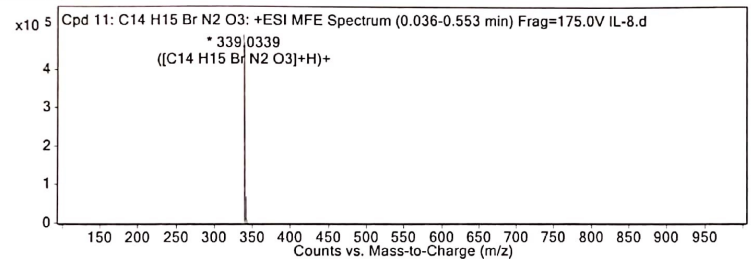


Compound Table

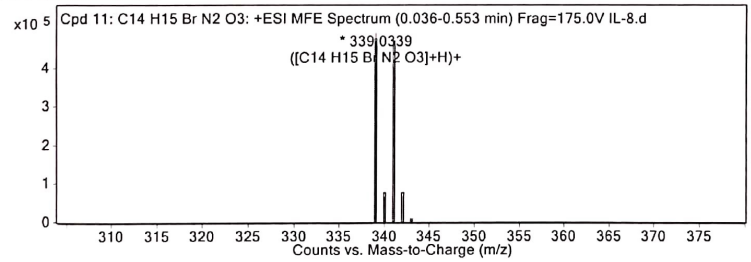
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C14 H15 Br N2 O3	0.1	338.0264	C14 H15 Br N2 O3	C14 H15 Br N2 O3	0.51	C14 H15 Br N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C14 H15 Br N2 O3	339.0339	0.1	Find by Molecular Feature	338.0264

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

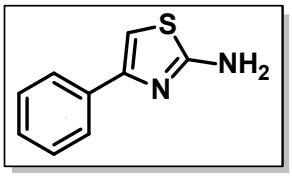
m/z	z	Abund	Formula	Ion
339.0339	1	489856.47	C14 H15 Br N2 O3	(M+H)+
340.0368	1	66210.09	C14 H15 Br N2 O3	(M+H)+
341.0316	1	469245.31	C14 H15 Br N2 O3	(M+H)+
342.0342	1	68016.78	C14 H15 Br N2 O3	(M+H)+
343.0395	1	8901.21	C14 H15 Br N2 O3	(M+H)+
344.0404	1	735.74	C14 H15 Br N2 O3	(M+H)+
345.0556	1	2376.24	C14 H15 Br N2 O3	(M+H)+

--- End Of Report ---

Figure S84 Mass spectra of Ethyl-4-(3-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **(4o).**

Qualitative Compound Report

Data File	THIA.d	Sample Name	THIA
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	07-06-2018 12:23:59
IRM Calibration Status	Success	DA Method	Default.m
Comment			



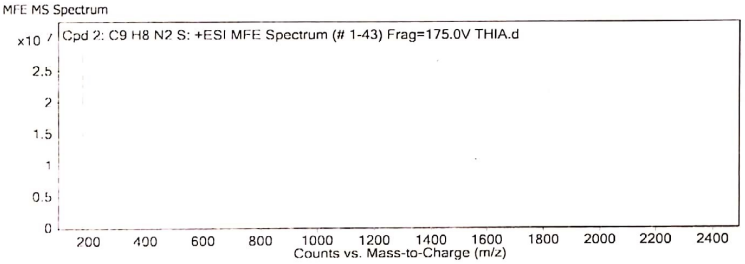
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

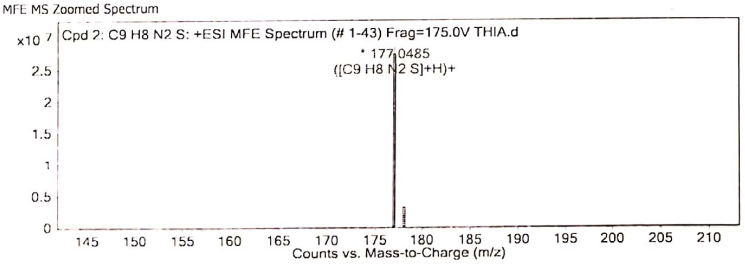
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C9 H8 N2 S	7	176.0412	C9 H8 N2 S	C9 H8 N2 S	-2.26	C9 H8 N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C9 H8 N2 S	177.0485	7	Find by Molecular Feature	176.0412

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
177.0485	1	28519820	C9 H8 N2 S	(M+H)+
178.0506	1	1860122.71	C9 H8 N2 S	(M+H)+

End Of Report

Figure S85 Mass spectra of 4-Phenylthiazol-2-amine **(6a).**

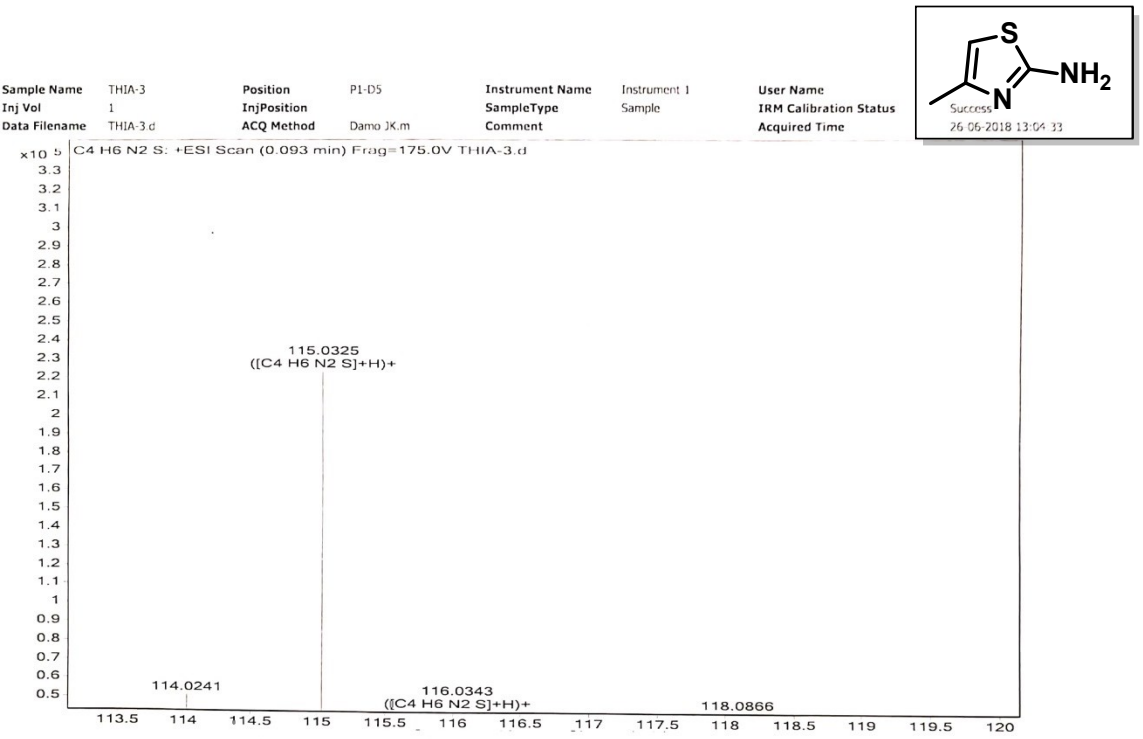


Figure S86 Mass spectra of 4-Methylthiazol-2-amine **(6b).**

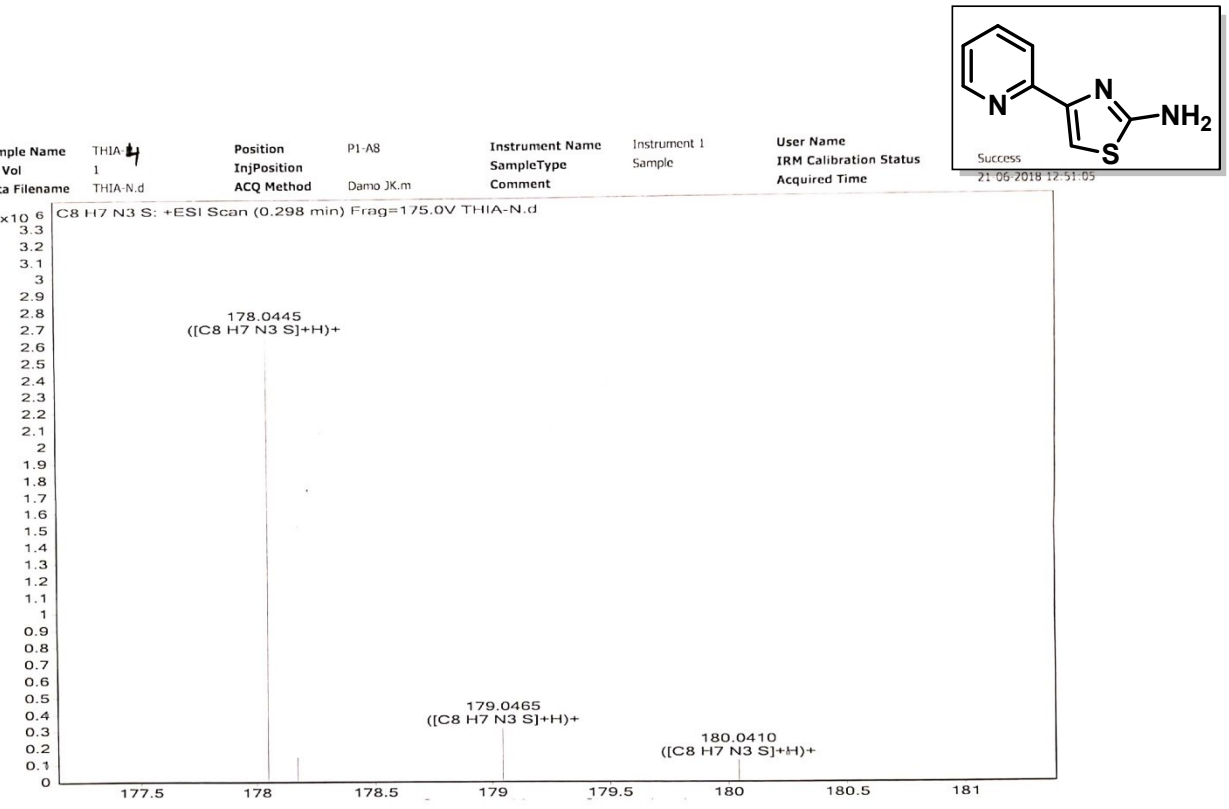


Figure S87 Mass spectra of 4-(Pyridin-2-yl)thiazol-2-amine **(6c).**

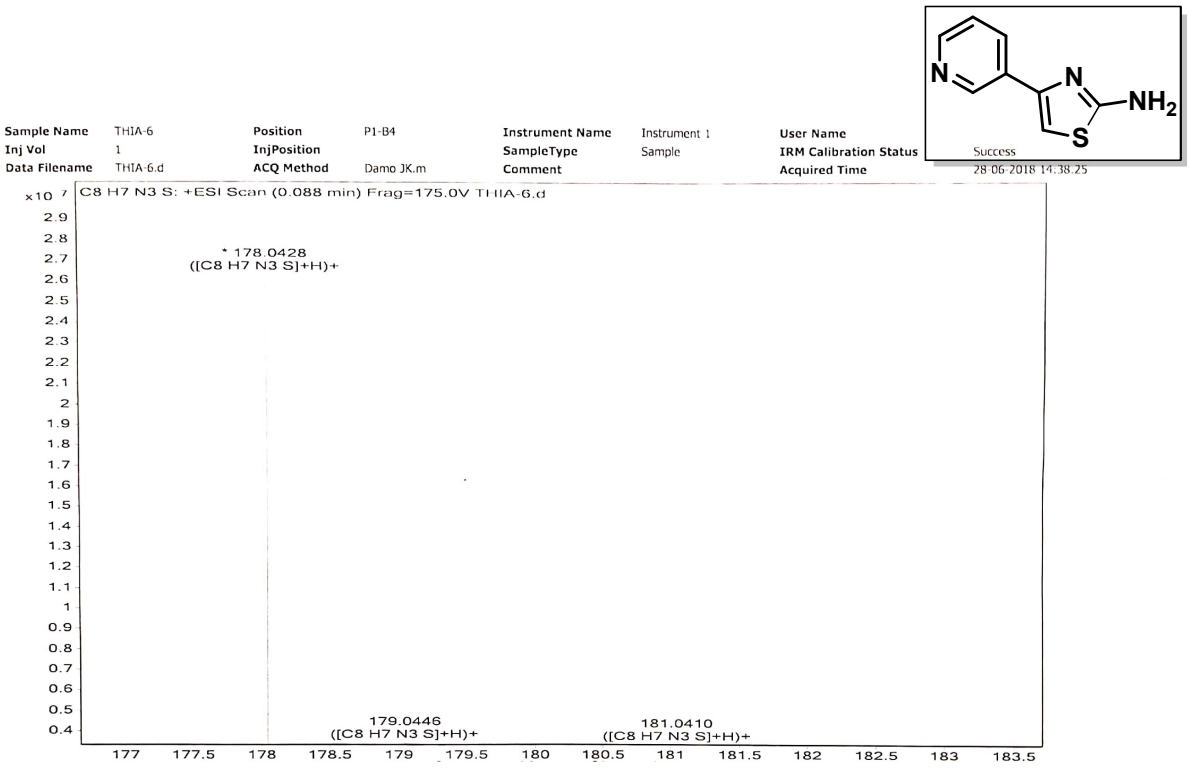
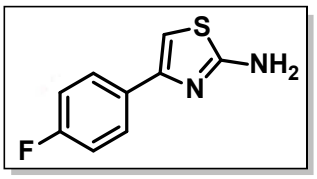


Figure S88 Mass spectra of 4-(pyridin-3-yl)thiazol-2-amine **(6d).**

Qualitative Compound Report

Data File	THIA-8.d	Sample Name	THIA-8
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	02-07-2018 15:47:41
IRM Calibration Status	Success	DA Method	Default.m
Comment			



Info.

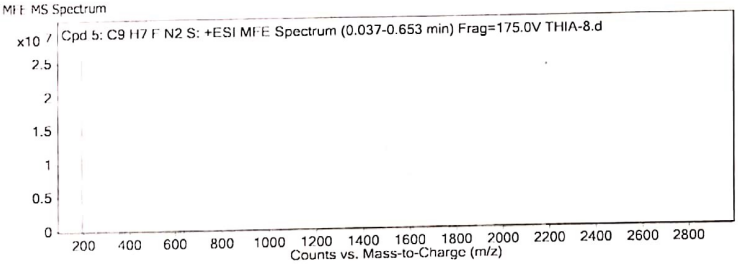
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

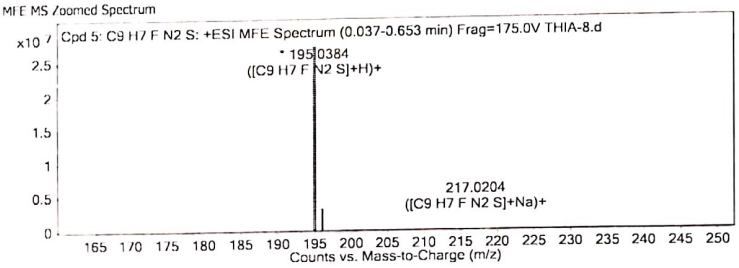
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C9 H7 F N2 S	0.117	194.0311	C9 H7 F N2 S	C9 H7 F N2 S	1.43	C9 H7 F N2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C9 H7 F N2 S	195.0384	0.117	Find by Molecular Feature	194.0311

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

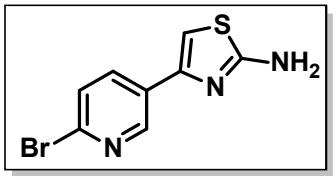
m/z	z	Abund	Formula	Ion
195.0384	1	2729017.6	C9 H7 F N2 S	(M+H)+
196.0413	1	325383.24	C9 H7 F N2 S	(M+H)+
217.0204	1	4987.02	C9 H7 F N2 S	(M+Na)+

--- End Of Report ---

Figure S89 Mass spectra of 4-(4-Fluorophenyl)thiazol-2-amine **(6e).**

Qualitative Compound Report

Data File	THIA-9.d	**Sample Name**	THIA-9
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	03-07-2018 12:27:25
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



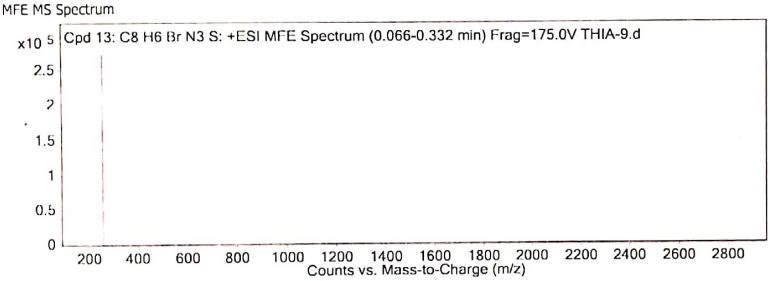
Sample Group Info.
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

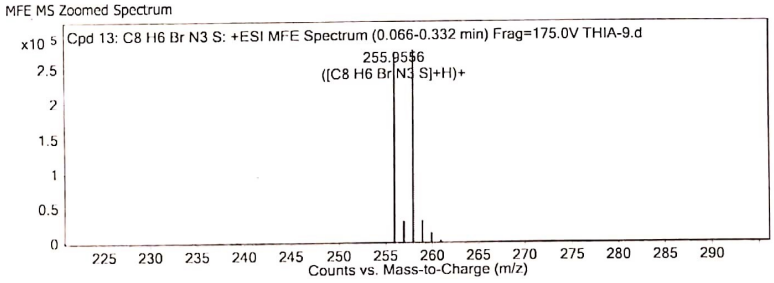
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C8 H6 Br N3 S	0.111	254.948	C8 H6 Br N3 S	C8 H6 Br N3 S	-5.65	C8 H6 Br N3 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C8 H6 Br N3 S	255.9556	0.111	Find by Molecular Feature	254.948

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

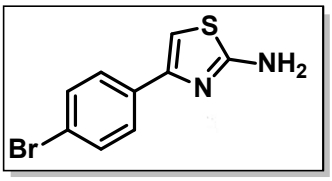
m/z	z	Abund	Formula	Ion
255.9556	1	275943.13	C8 H6 Br N3 S	(M+H)+
256.9585	1	31488.29	C8 H6 Br N3 S	(M+H)+
257.9528	1	272895.37	C8 H6 Br N3 S	(M+H)+
258.9552	1	26995.21	C8 H6 Br N3 S	(M+H)+
259.9494	1	12777.69	C8 H6 Br N3 S	(M+H)+
260.9519	1	489.71	C8 H6 Br N3 S	(M+H)+

--- End Of Report ---

Figure S90 Mass spectra of 4-(3-Bromopyridin-2-yl)thiazol-2-amine **(6f).**

Qualitative Compound Report

Data File	THIA-10.d	Sample Name	THIA-10
Sample Type	Sample	Position	P1-D2
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	03-07-2018 12:29:07
IRM Calibration Status	Success	DA Method	Default.m
Comment			



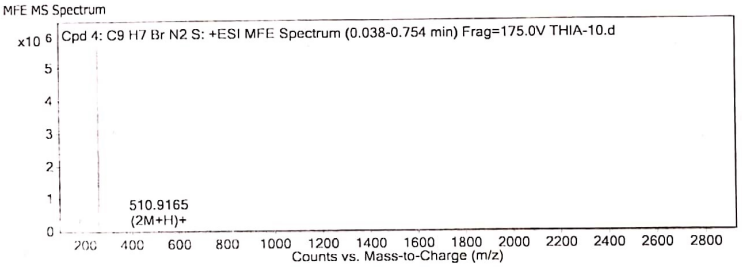
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

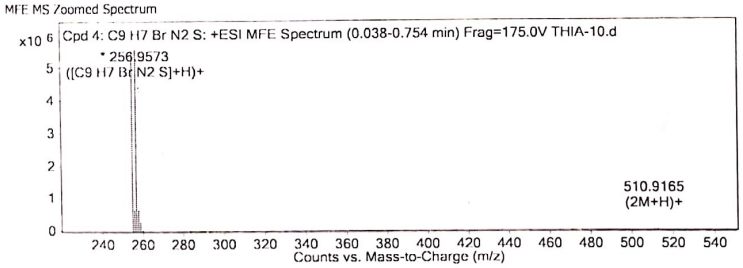
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C9 H7 Br N2 S	0.097	253.9521	C9 H7 Br N2 S	C9 H7 Br N2 S	-3.2	C9 H7 Br N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C9 H7 Br N2 S	254.9594	0.097	Find by Molecular Feature	253.9521

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

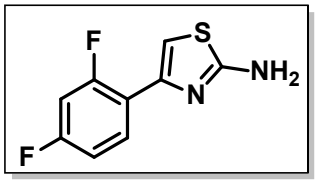
m/z	z	Abund	Formula	Ion
254.9594	1	5546305.32	C9 H7 Br N2 S	(M+H)+
255.9622	1	619003.75	C9 H7 Br N2 S	(M+H)+
256.9573	1	5588750.5	C9 H7 Br N2 S	(M+H)+
257.9602	1	647728.73	C9 H7 Br N2 S	(M+H)+
258.9543	1	259856.18	C9 H7 Br N2 S	(M+H)+
259.9567	1	25784.47	C9 H7 Br N2 S	(M+H)+
510.9165	1	59865.15		(2M+H)+
511.9193	1	13716.13		(2M+H)+
512.9158	1	59641.35		(2M+H)+
513.9186	1	13759.51		(2M+H)+

End Of Report

Figure S91 Mass spectra of 4-(4-Bromophenyl)thiazol-2-amine **(6g).**

Qualitative Compound Report

Data File	THIA-11.d	**Sample Name**	THIA-11
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	23-07-2018 12:58:19
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



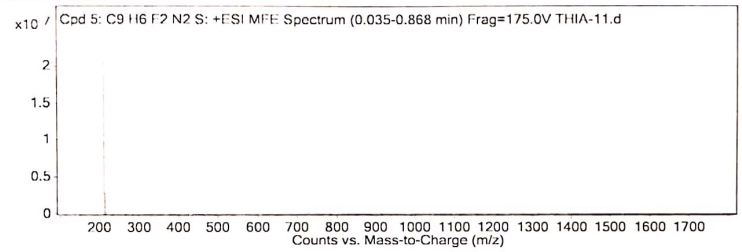
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

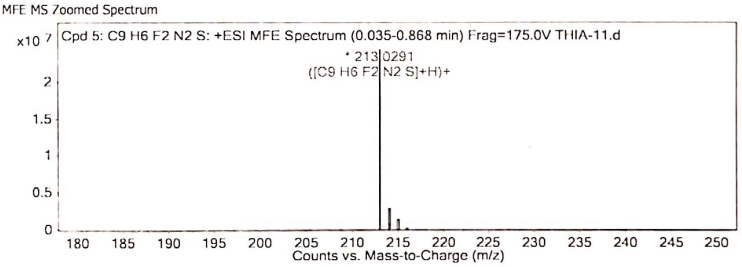
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C9 H6 F2 N2 S	0.157	212.0219	C9 H6 F2 N2 S	C9 H6 F2 N2 S	0.38	C9 H6 F2 N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C9 H6 F2 N2 S	213.0291	0.157	Find by Molecular Feature	212.0219

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

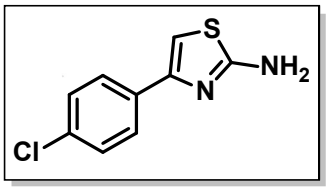
m/z	z	Abund	Formula	Ion
213.0291	1	2436268	C9 H6 F2 N2 S	(M+H)+
214.0322	1	286598.96	C9 H6 F2 N2 S	(M+H)+
215.0266	1	1263296.28	C9 H6 F2 N2 S	(M+H)+
216.0285	1	122876.38	C9 H6 F2 N2 S	(M+H)+
217.0298	1	114.36	C9 H6 F2 N2 S	(M+H)+

--- End Of Report ---

Figure S92 Mass spectra of 4-(2,4-Difluorophenyl)thiazol-2-amine **(6h).**

Qualitative Compound Report

Data File	THIA-16.d	**Sample Name**	THIA-16
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	10-07-2018 11:41:49
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



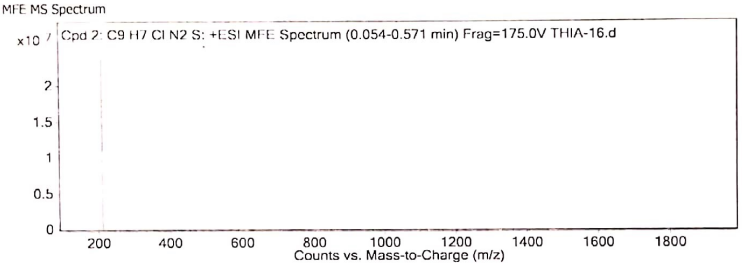
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q TOF B.05.01 (B5125.1)

Compound Table

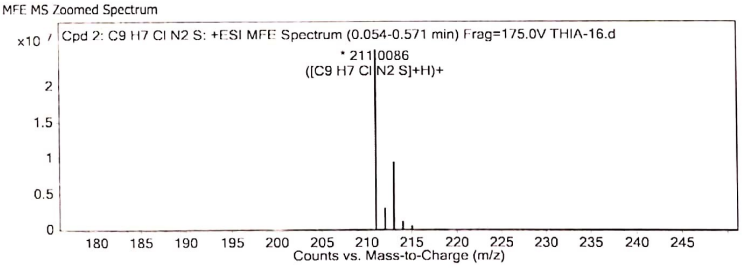
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C9 H7 Cl N2 S	0.107	210.0014	C9 H7 Cl N2 S	C9 H7 Cl N2 S	2.23	C9 H7 Cl N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C9 H7 Cl N2 S	211.0086	0.107	Find by Molecular Feature	210.0014

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
211.0086	1	25213890	C9 H7 Cl N2 S	(M+H)+
212.0115	1	2896608.91	C9 H7 Cl N2 S	(M+H)+
213.0058	1	9081259.58	C9 H7 Cl N2 S	(M+H)+
214.0086	1	902763.31	C9 H7 Cl N2 S	(M+H)+
215.0028	1	364487.99	C9 H7 Cl N2 S	(M+H)+
216.0049	1	41203.81	C9 H7 Cl N2 S	(M+H)+

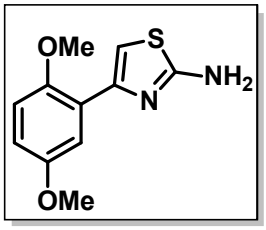
-- End Of Report --

Figure S93 Mass spectra of 4-(4-chlorophenyl)thiazol-2-amine **(6i).**

Qualitative Compound Report

Data File	THIA-18.d	Sample Name	THIA-18
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	16-07-2018 11:55:42
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

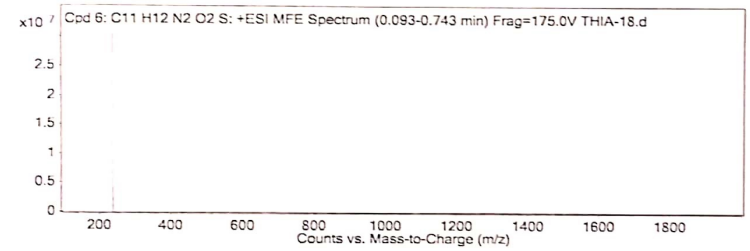


Compound Table

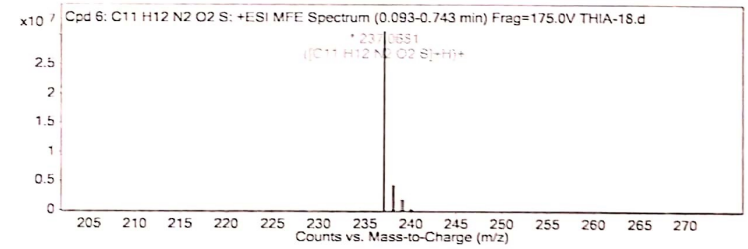
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C11 H12 N2 O2 S	0.162	236.0609	C11 H12 N2 O2 S	C11 H12 N2 O2 S	4.43	C11 H12 N2 O2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C11 H12 N2 O2 S	237.0681	0.162	Find by Molecular Feature	236.0609

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

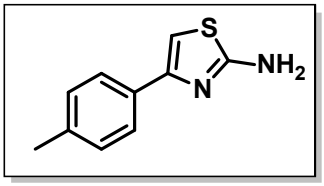
m/z	z	Abund	Formula	Ion
237.0681	1	30705320	C11 H12 N2 O2 S	(M+H)+
238.0712	1	4305851.98	C11 H12 N2 O2 S	(M+H)+
239.0661	1	1714986.93	C11 H12 N2 O2 S	(M+H)+
240.0683	1	192631.86	C11 H12 N2 O2 S	(M+H)+
241.0689	1	14464.28	C11 H12 N2 O2 S	(M+H)+

— End Of Report —

Figure S94 Mass spectra of 4-(2,5-Dimethoxyphenyl)thiazol-2-amine **(6j).**

Qualitative Compound Report

Data File	THIA-19.d	**Sample Name**	THIA-19
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	06-08-2018 11:33:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



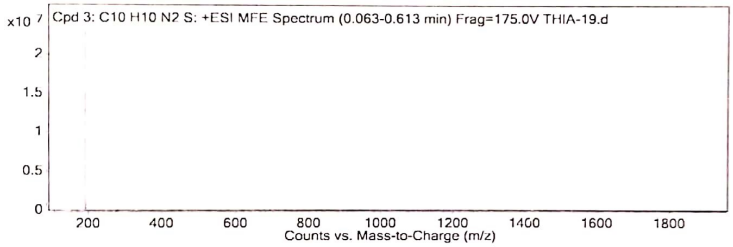
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

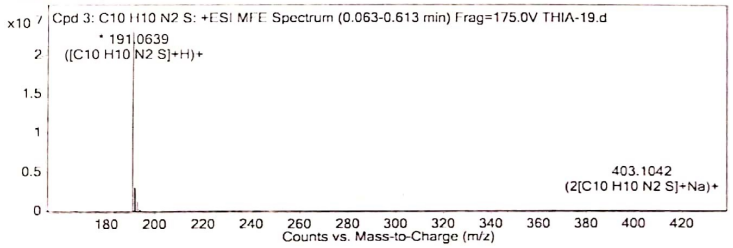
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C10 H10 N2 S	0.123	190.0566	C10 H10 N2 S	C10 H10 N2 S	-0.94	C10 H10 N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C10 H10 N2 S	191.0639	0.123	Find by Molecular Feature	190.0566

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

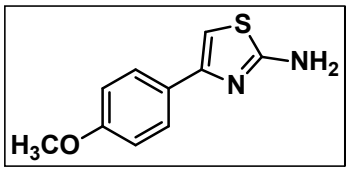
m/z	z	Abund	Formula	Ion
191.0639	1	22900734	C10 H10 N2 S	(M+H)+
192.0669	1	3201262.07	C10 H10 N2 S	(M+H)+
193.0614	1	1288089.79	C10 H10 N2 S	(M+H)+
194.0633	1	142448.06	C10 H10 N2 S	(M+H)+
403.1042	1	9006.84	C10 H10 N2 S	(2M+Na)+

End Of Report

Figure S95 Mass spectra of 4-(p-tolyl)thiazol-2-amine **(6k)**

Qualitative Compound Report

Data File	THIA-20.d	**Sample Name**	THIA-20
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	06-08-2018 11:35:06
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



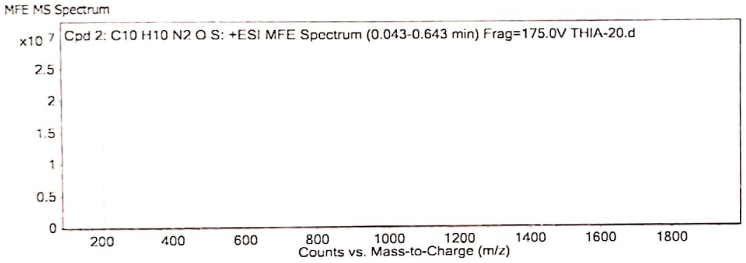
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

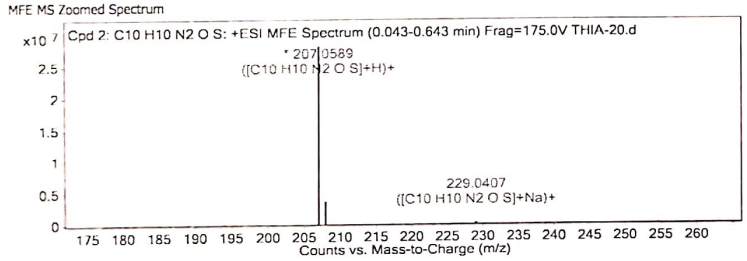
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C10 H10 N2 O S	0.097	206.0517	C10 H10 N2 O S	C10 H10 N2 O S	-1.69	C10 H10 N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C10 H10 N2 O S	207.0589	0.097	Find by Molecular Feature	206.0517

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
207.0589	1	28198302	C10 H10 N2 O S	(M+H)+
208.0617	1	3599029.43	C10 H10 N2 O S	(M+H)+
229.0407	1	74070.84	C10 H10 N2 O S	(M+Na)+
230.0438	1	8863.61	C10 H10 N2 O S	(M+Na)+
231.0432	1	4243.43	C10 H10 N2 O S	(M+Na)+

--- End Of Report ---

Figure S96 Mass spectra of 4-(4-methoxyphenyl)thiazol-2-amine **(6l)**

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