Supplementary Information

Effect of substitution on molecular conformation and packing features in a series of aryl substituted ethyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylates.

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Table S1: Melting points and relevant details about the synthesized compounds (PYR 1-8)

Compound code	Mol. Formulae	Mol. Weight	Yield (%)	M.P (^{0}C)
PYR1 (-*p*-F)	$C_{14}H_{15}FN_2O_2S$	294	48.00	252-254
PYR2 (-*o*-Cl)	$C_{14}H_{15}ClN_2O_2S$	310	52.00	212-214
PYR3 (-*m*-Cl)	$C_{14}H_{15}ClN_2O_2S$	310	64.80	180-182
PYR4 (-*p*-Me)	$C_{15}H_{18}N_2O_2S$	290	58.70	244-248
PYR5 (-*p*-NMe_2)	$C_{16}H_{21}N_3O_2S$	319	56.00	188-190
PYR6 (-*p*-OMe)	$C_{15}H_{18}N_2O_3S$	306	50.40	150-152
PYR7 (-*m*-OMe)	$C_{15}H_{18}N_2O_3S$	306	49.00	144-146
PYR8 (tris-$(OMe)_3$)	$C_{17}H_{22}N_2O_5S$	366	48.61	200-202

Table S2: Relevant Bond Lengths (Å) and Bond Angles (°).

Geometrical Parameter	PYR1	PYR2	PYR3	PYR4	PYR5	PYR6	PYR7	PYR8
C1-S1	1.684(3)	1.679(3), 1.678(3)	1.676(3)	1.680(2)	1.683(2)	1.682(2)	1.678(2)	1.684(2)
C1-N1	1.355(2)	1.355(3), 1.351(3)	1.363(4)	1.361(2)	1.363(2)	1.328(2)	1.354(3)	1.364(2)
C1-N2	1.329(3)	1.325(3), 1.325(3)	1.324(4)	1.327(2)	1.322(3)	1.361(2)	1.318(3)	1.321(2)
C5-O1	1.208(4)	1.204(3), 1.194(3)	1.208(4)	1.206(2)	1.206(2)	1.211(2)	1.206(3)	1.346(2)
O2-C6	1.451(3)	1.450(3), 1.454(3)	1.447(4)	1.451(2)	1.455(3)	1.455(2)	1.450(3)	1.450(2)
C3-C2	1.347(3)	1.344(3), 1.346(3)	1.348(4)	1.348(2)	1.351(3)	1.352(2)	1.341(3)	1.341(2)
C2-N1	1.395(2)	1.381(3), 1.395(3)	1.386(4)	1.392(2)	1.390(2)	1.397(2)	1.393(3)	1.394(2)
N2-C1-S1	123.4(3)	123.1(2), 122.7(2)	124.2(2)	123.7(2)	124.2(2)	120.2(1)	122.4(2)	124.0(1)
N1-C2-C8	112.95(2)	113.3(2), 113.6(2)	112.8(2)	112.9(1)	112.7(2)	112.8(1)	113.3(2)	113.0(2)
C4-C3-C5	114.6(2)	116.9(2), 117.5(2)	114.3(2)	114.1(1)	114.8(2)	114.7(1)	118.7(2)	116.9(1)

Table S3: Cremer and Pople ring puckering parameters for the six membered tetrahydropyrimidine ring [N1-N2/C1-C4]

Compound name	Q (Å)	Thetha (°)	Phi (°)
PYR1	0.293(2)	106.6(7)	347.7(2)
PYR2	-	-	-
PYR3	0.295(2)	108.7(2)	348.8(3)
PYR4	0.299(3)	107.1(2)	347.7(4)
PYR5	0.288(2)	72.1(4)	167.6(4)
PYR6	0.302(2)	110.3(4)	346.5(4)
PYR7	0.332(2)	105.3(3)	352.5(4)
PYR8	0.165(2)	114.1(6)	345.3(2)

Table S4: Dihedral Angles between the least squares plane passing through C9/C14 (Plane 1; aryl group), C1-C4/N1-N2 (Plane 2: tetrahydropyrimidine ring) and C5-O2-C6-C7 (ester group)

Compound name	Plane 1 and 2 (°)	Plane 1 and 3 (°)	Plane 2 and 3 (°)
PYR1	80.36(2)	86.05(2)	26.10(2)
PYR2			
Molecule A	84.44(1)	84.07(1)	12.52(2)
Molecule B	82.68(1)	88.00(1)	10.13(2)
PYR3	80.23(2)	89.67(2)	14.71(2)
PYR4	80.93(2)	89.30(2)	19.84(2)
PYR5	82.67(2)	85.93(2)	20.89(2)
PYR6	87.61(2)	85.39(2)	12.97(2)
PYR7	82.94(2)	89.96(2)	10.10(12)
PYR8	83.87(2)	49.32(7)	42.34(2)

Table S5: Deviation of N1 and C4 from the weighted least squares plane passing through N2/C1/C2/C3

Compound name	N1 (Å)	C4 (Å)
PYR1	-0.138(3)	-0.346(3)
PYR2		
Molecule A	+0.03479(3)	+0.0116(3)
Molecule B	+0.0890(3)	+0.0787(3)
PYR3	+0.1246(3)	+0.3600(3)
PYR4	-0.1311(3)	-0.3473(3)
PYR5	0.1232(2)	0.3557(2)
PYR6	-0.1051(2)	-0.3839(2)
PYR7	-0.1681(2)	-0.3937(2)
PYR8	0.0434(2)	0.2198(2)

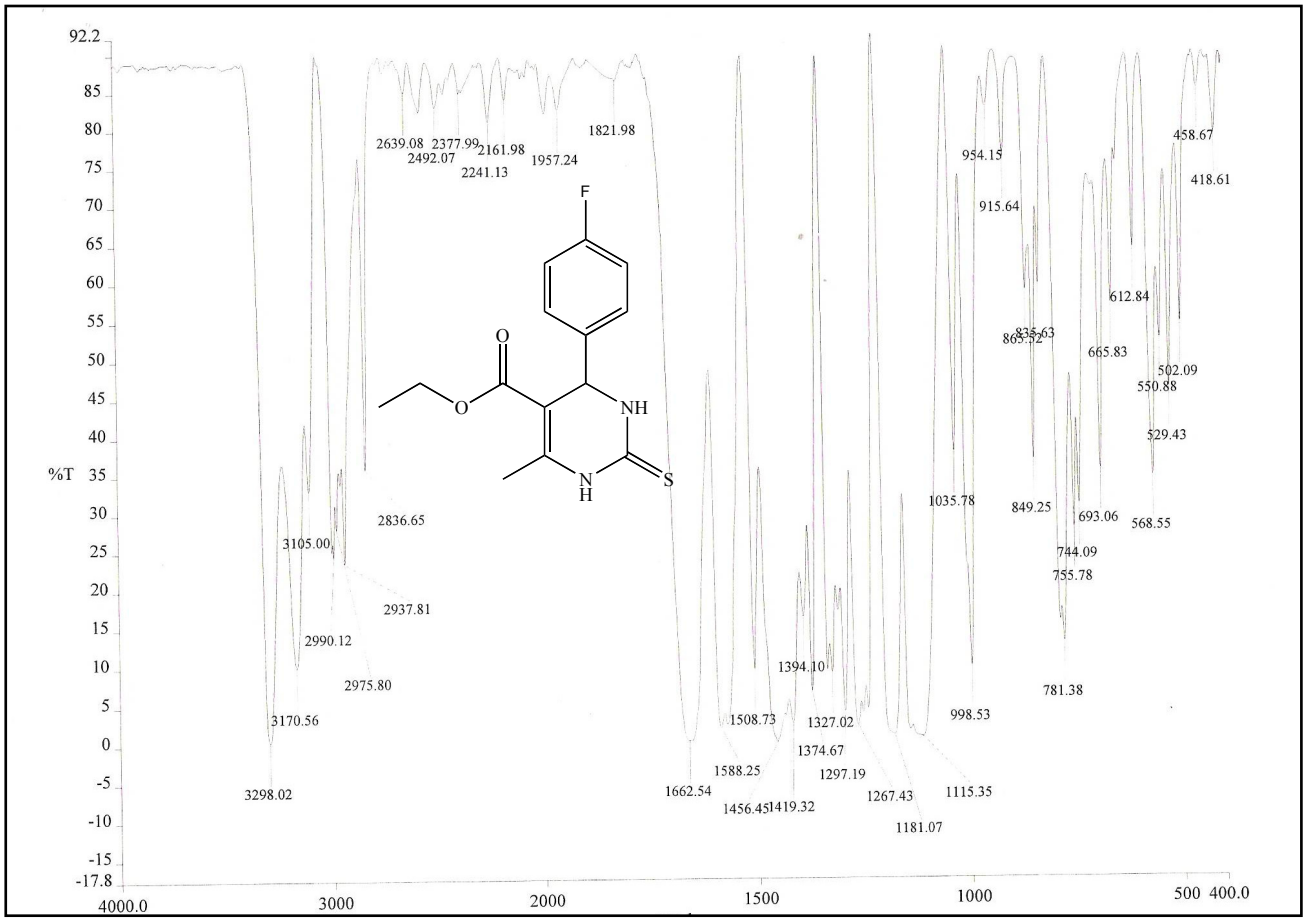
Table S6: Relevant Torsion angles (°): theoretical calculation at B3LYP-6-31G** for the optimized structure

Torsion	PYR1	PYR2	PYR3	PYR4	PYR5	PYR6	PYR7	PYR8
C9-C4-C3-C5	83.8	79.1*	87.0	83.7	87.0	82.4	74.3	80.2
C4-C3-C5-O2	-178.2	2.31	-178.8	-177.4	-158.2	-176.6	6.02	2.3
C9-C4-N2-C1	91.5	93.3	89.4	91.7	92.0	92.9	99.3	92.2
C14-C9-C4-C3	**92.5**	**21.3**	**97.9**	**91.3**	**22.0**	**89.3**	**48.2**	**12.3**
C4-N2-C1-N1	16.6	17.7	17.1	16.5	16.9	16.4	15.2	18.8

*: Starting from the orthogonal coordinates for either Molecule A or B, on optimization, the equilibrium geometry for the optimized conformation for either molecule A and B will be identical.

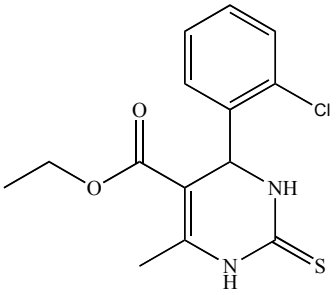
PYR1(-4F) :Ethyl-4-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

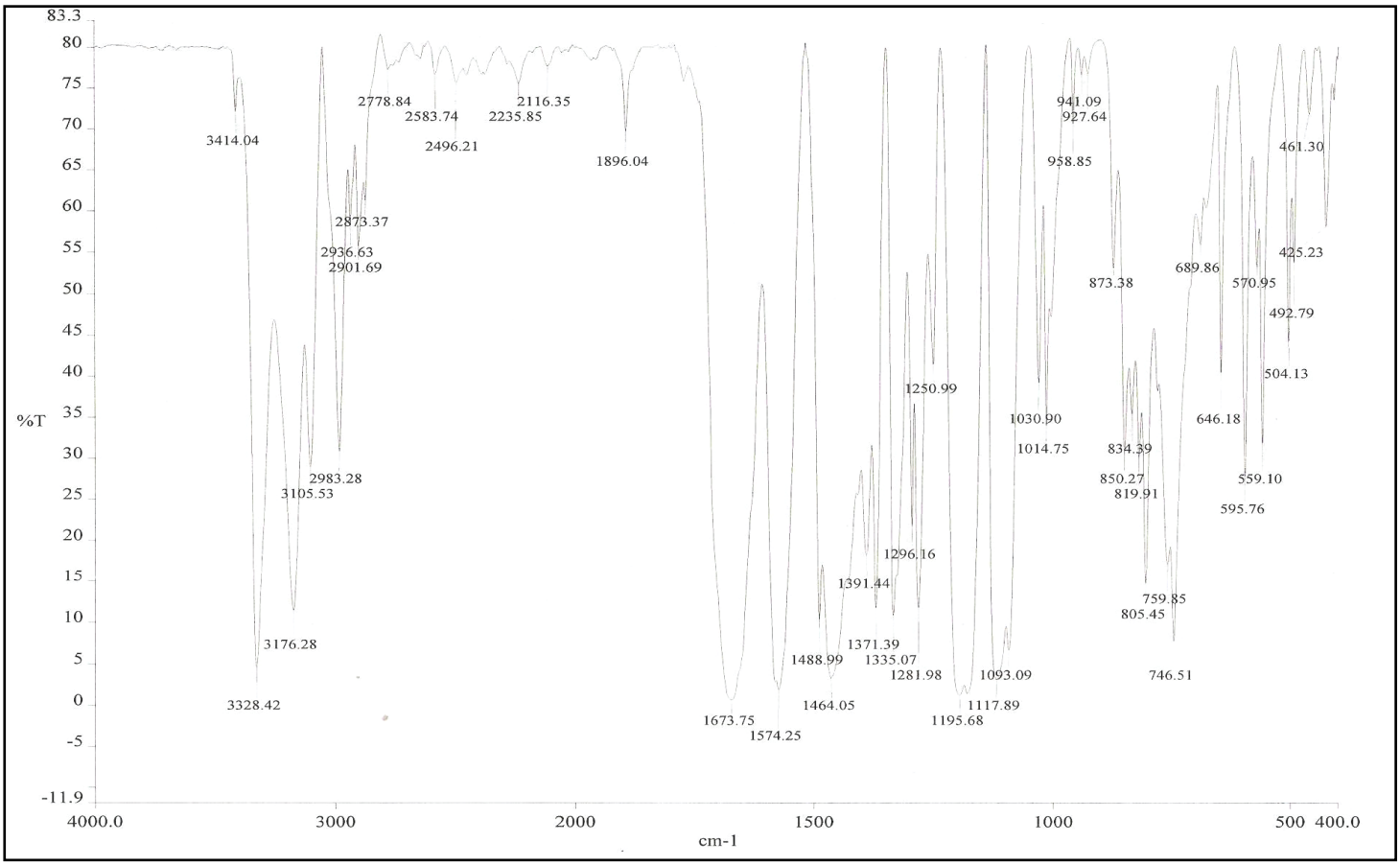
IR (KBr) cm^{-1}: 3298.02 (N-H str), 3105.00 (ArC-H str), 1662.54 ($C=O_{COOEt}$ str), 1588.25, 15.8.73, 1456.45 (C=C str), 1327.02 (C-N str), 1181.07 (Ar-F str).



PYR2(-*o*-Cl): Ethyl-4-(2-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

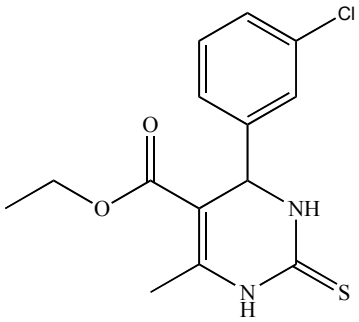
IR (KBr) cm^{-1}: 3328.42 (N-H str), 3105.53 (ArC-H str), 1673.75 (C=O_{COOEt} str), 1574.25, 1488.99, 1464.05 (C=C str), 1335.67, (C-N str), 746.51 (Ar-Cl str).

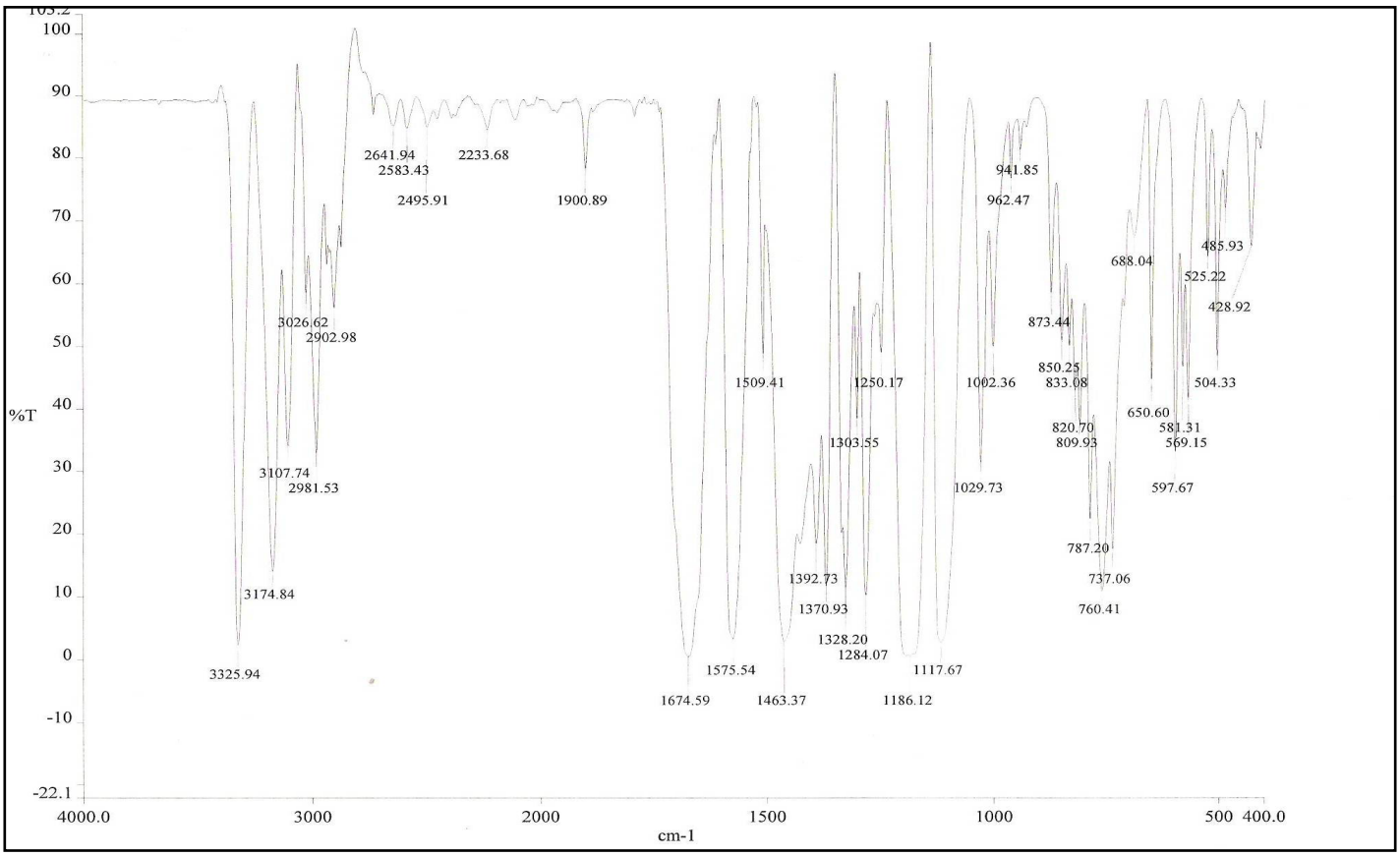




PYR3(-*m*-Cl):Ethyl-4-(3-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

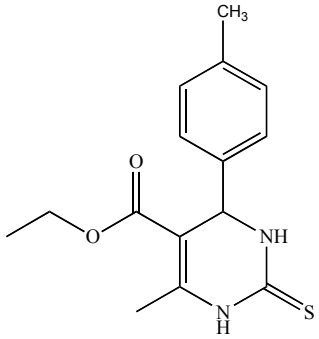
IR (KBr) cm^{-1}: 3325.94 (N-H str), 3107.74 (ArC-H str), 1674.59 (C=O$_{COOEt}$ str), 1575.54, 1509.41, 1463.37 (C=C str), 1328.20, (C-N str), 760.41 (Ar-Cl str).

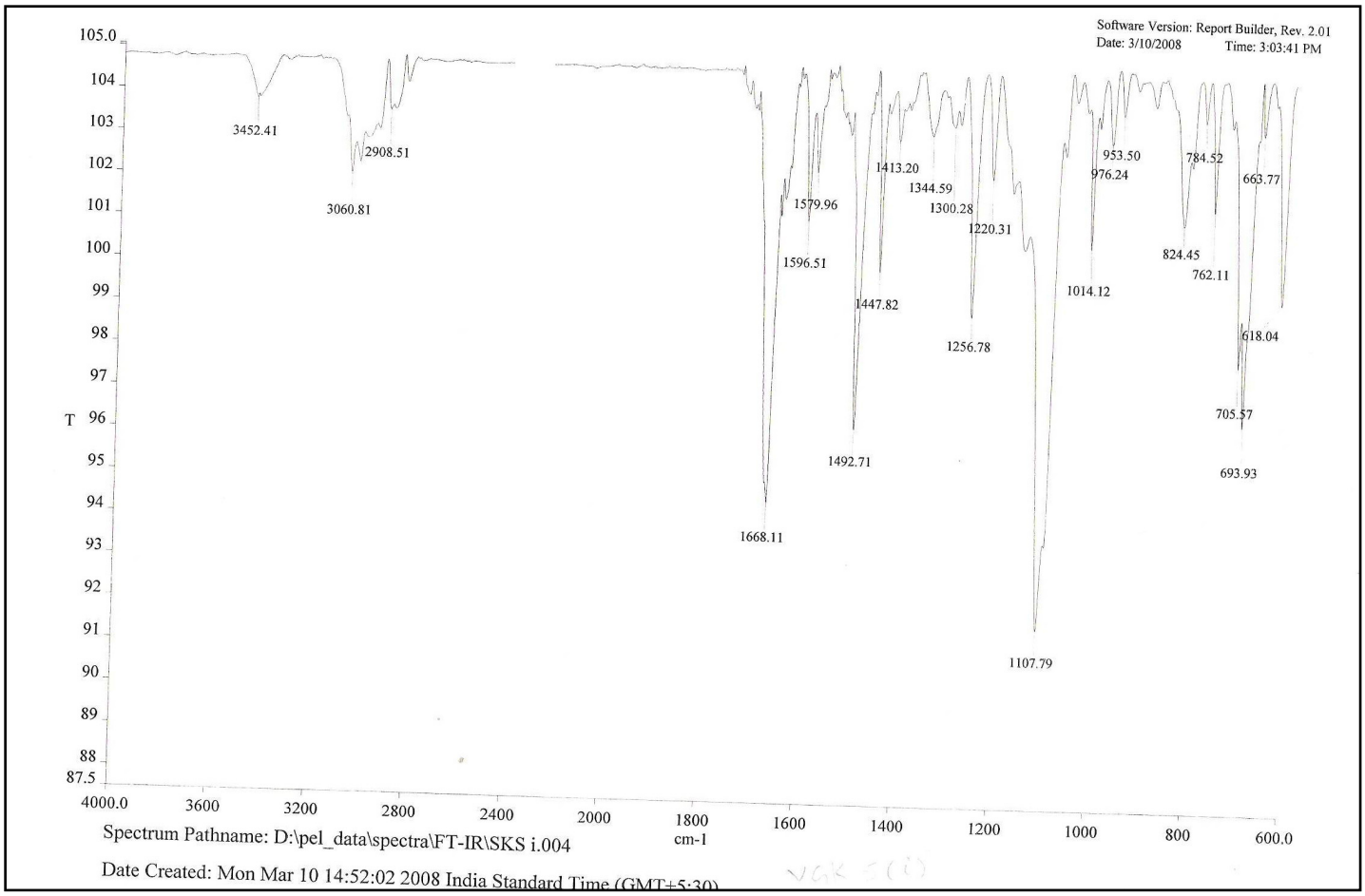




PYR4(-*p*-Me) : Ethyl-6-methyl-2-thioxo-4-*p*-tolyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate

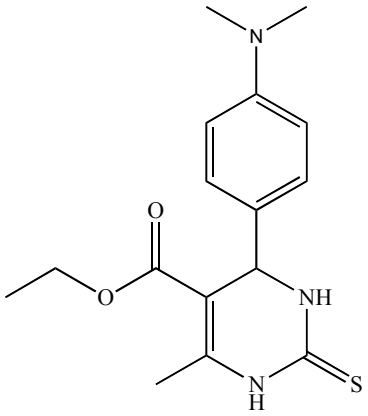
IR (KBr) cm^{-1}: 3452.41 (N-H str), 3060.81 (ArC-H), 2908.51 (AlpC-H str), 1668.11 (C=O$_{COOEt}$ str), 1596.51, 1492.71, 1447.82 (C=C str), 1344.59 (C-N str).

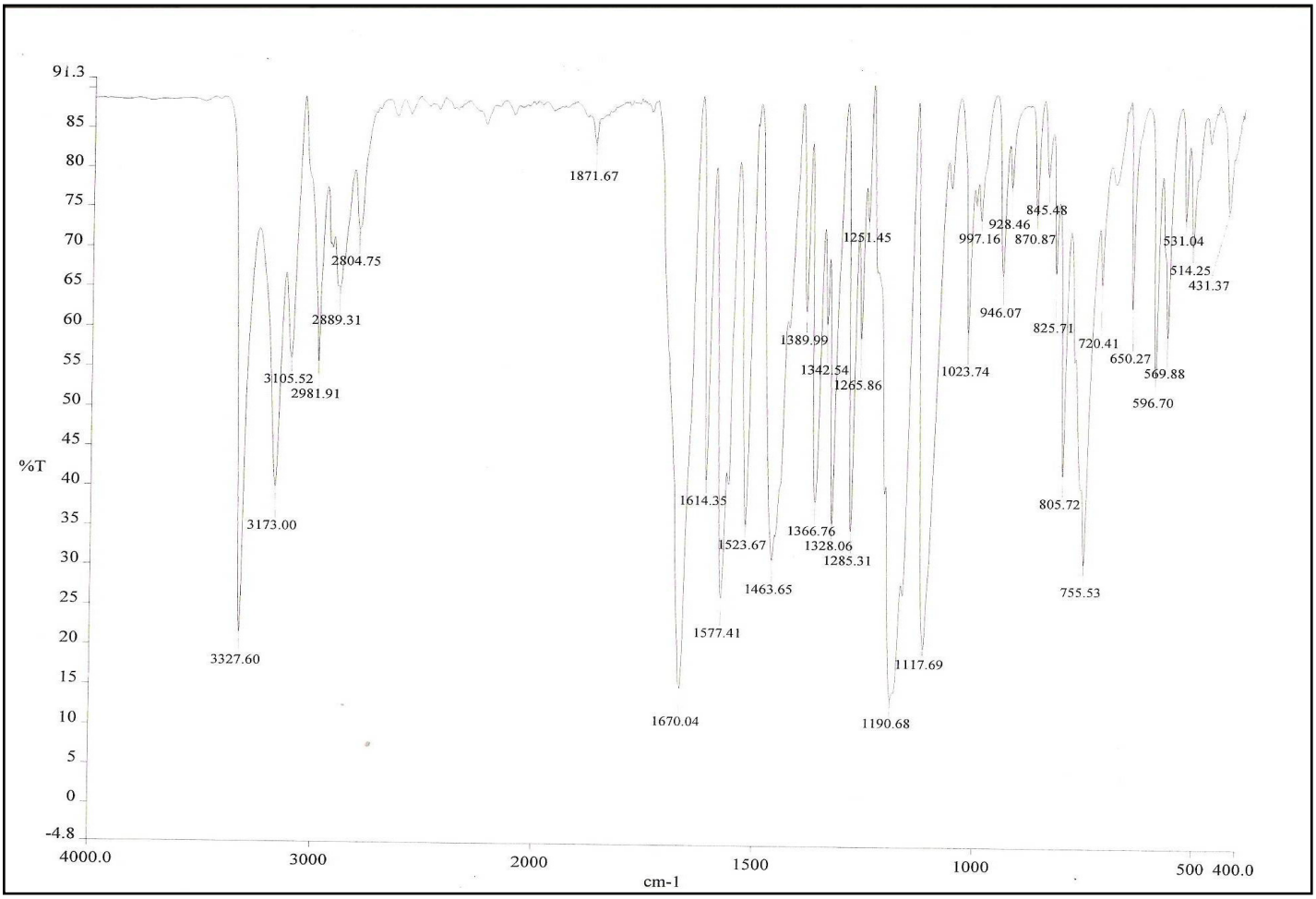




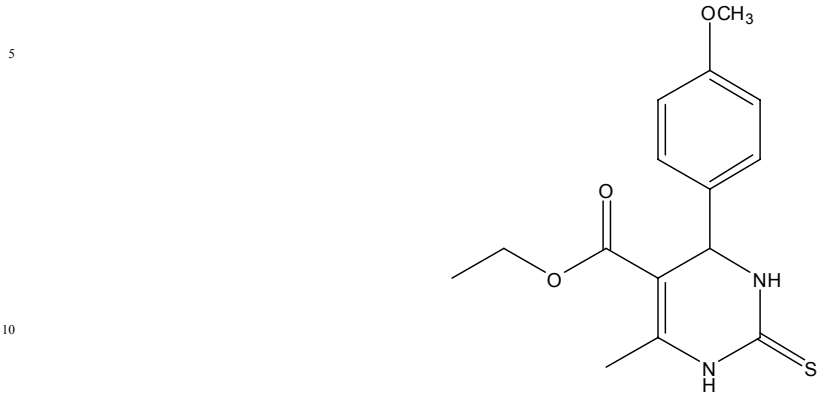
PYR5(-*p*-NMe_2):Ethyl-4-(4-(dimethylamino)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

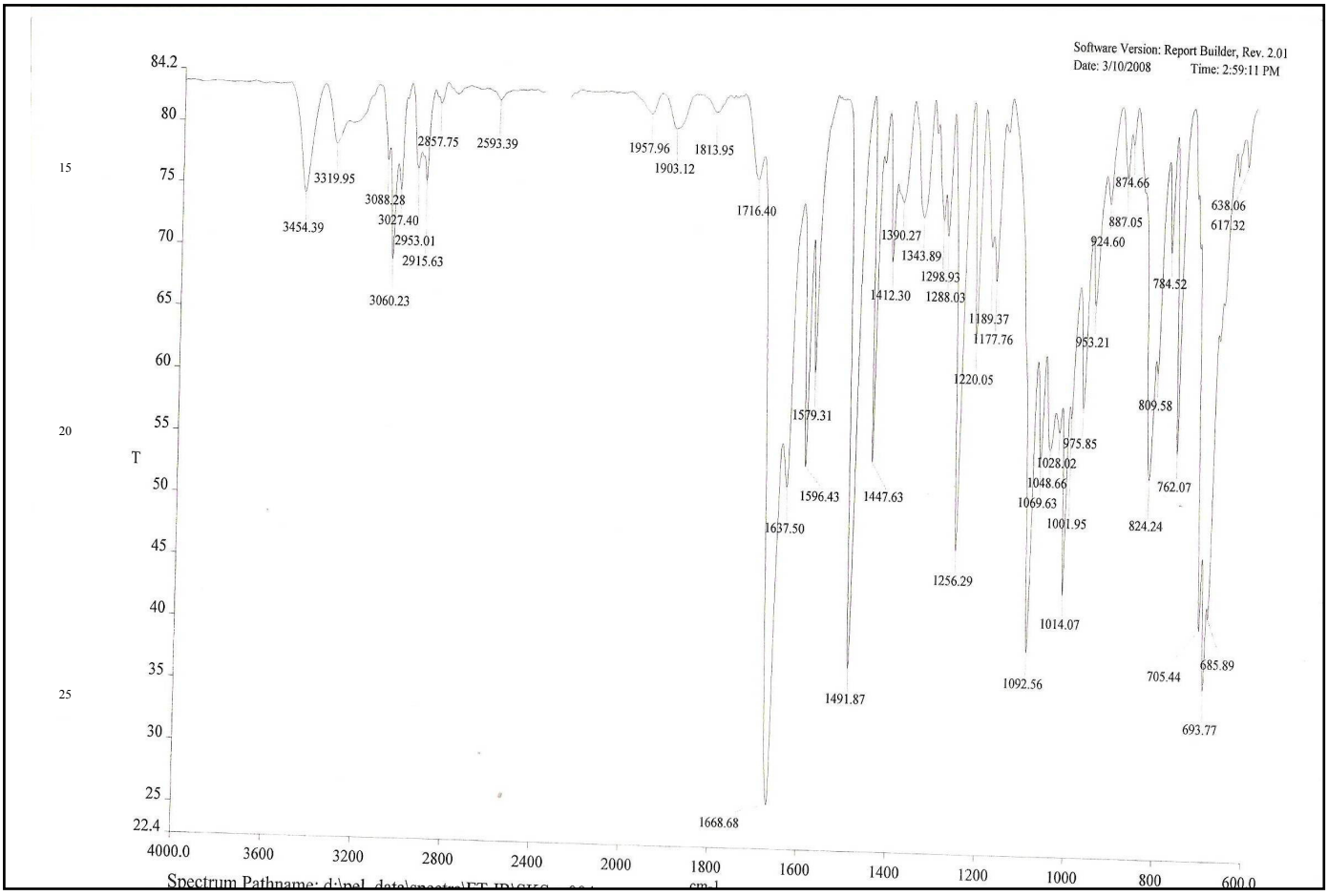
IR (KBr) cm^{-1}: 3327.60 (N-H str), 3105.52 (ArC-H str), 2889.31 (AlpC-H str), 1670.04 ($C=O_{COOEt}$ str), 1577.41, 1523.67, 1463.65 (C=C str), 1328.06, (C-N str).





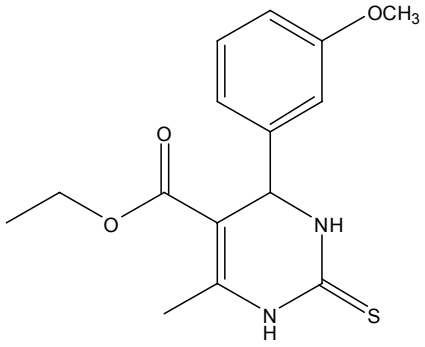
PYR6 (-*p*-OMe): Ethyl-4-(4-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate IR (KBr) cm^{-1}: 3454.39 (N-H str), 3088.28, (ArC-H), 2915.63 (AlpC-H str), 1668.68 ($C{=}O_{COOEt}$ str), 1596.43, 1491.87, 1447.63 (C=C str), 1343.89 (C-N str).

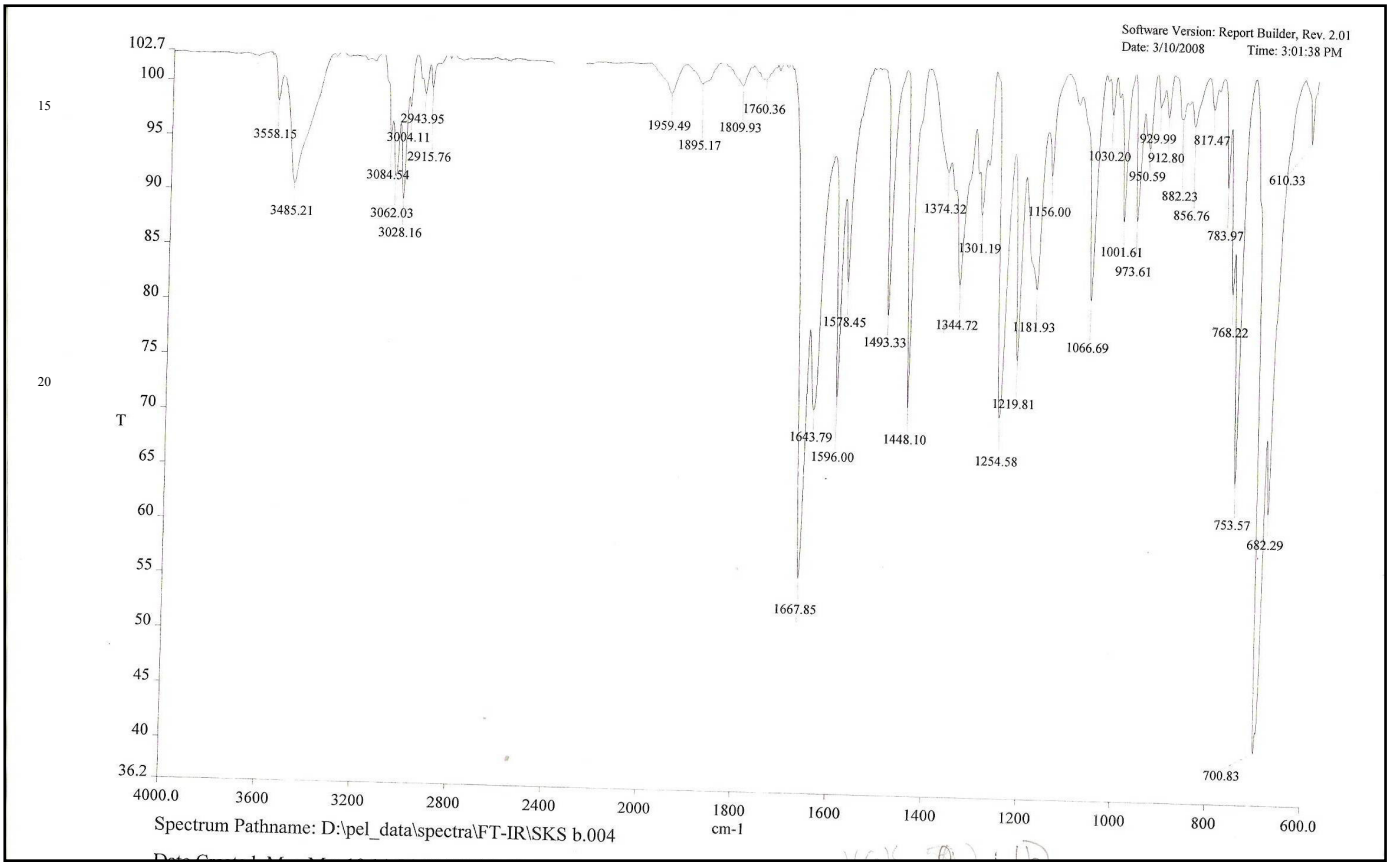




PYR7 (-*m*-OMe): Ethyl-4-(3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

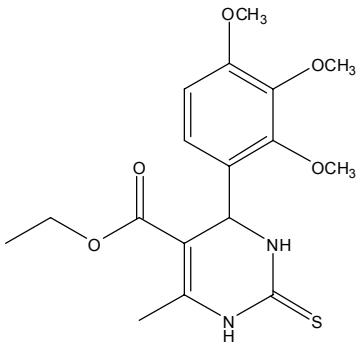
IR (KBr) cm^{-1}: 3485.21 (N-H str), 3084.54 (ArCH str), 2915.76 (AlpC-H str), 1667.85 (C=O$_{COOEt}$ str), 1596.00, 1493.33, 1448.10 (C=C str), 1344.72 (C-N str).

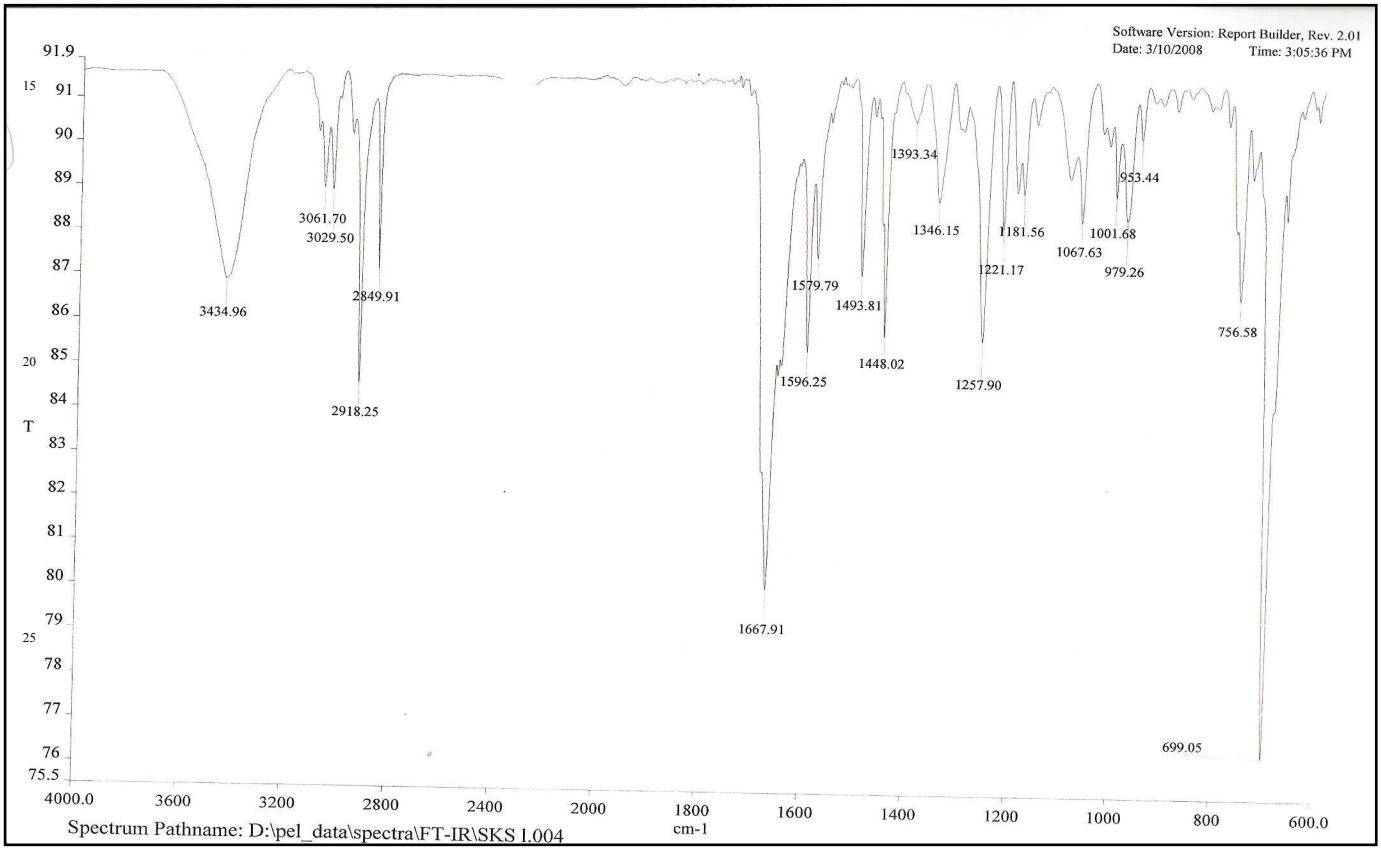




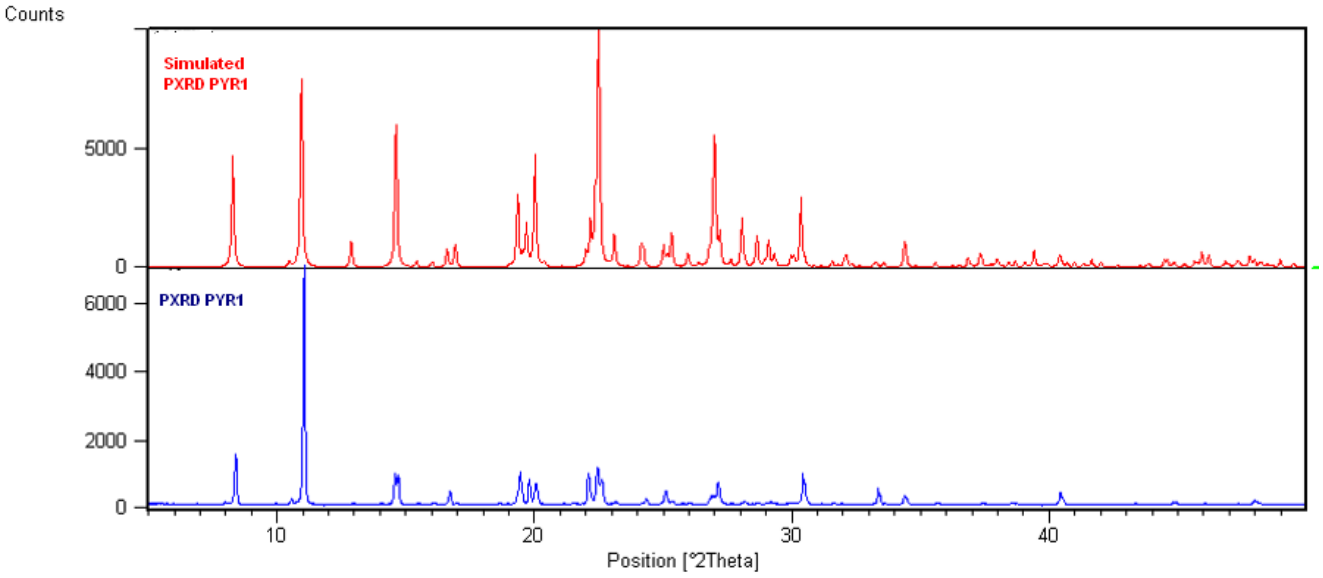
PYR8(tris-(OMe)$_3$): Ethyl-6-methyl-2-thioxo-4-(2,3,4-trimethoxyphenyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate

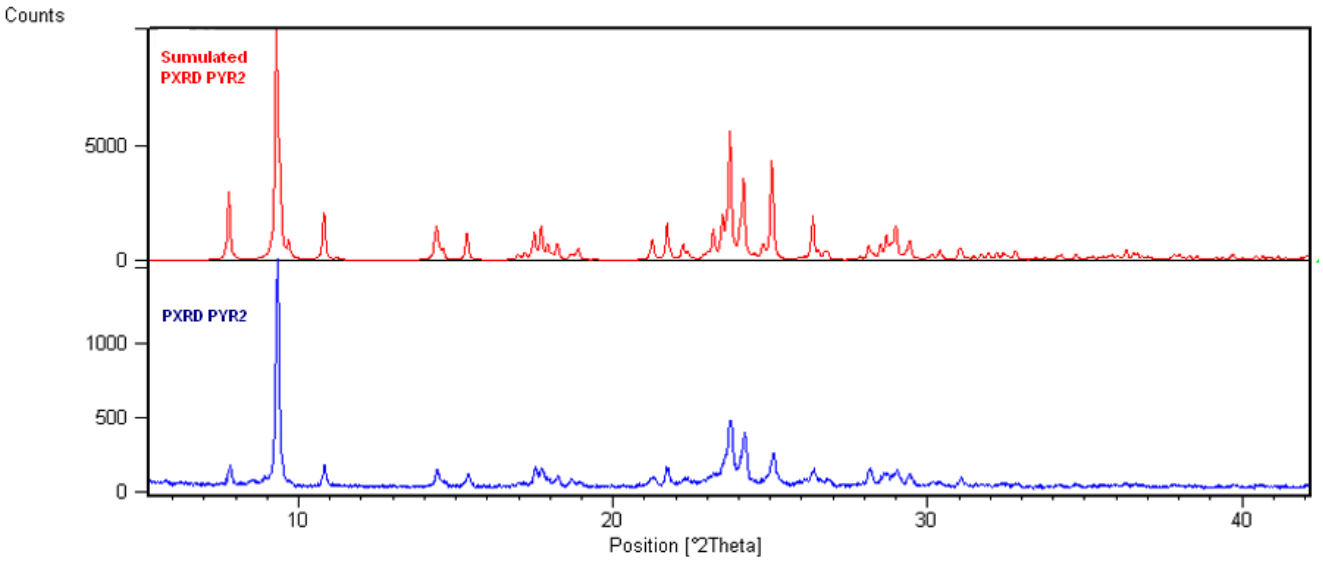
IR (KBr) cm^{-1}: 3434.96 (N-H str), 3061.70, (ArC-H str), 2918.25 (AlpC-H str), 1667.91 (C=O$_{COOEt}$ str), 1596.25, 1493.81, 1448.02 (C=C str), 1346.15 (C-N).

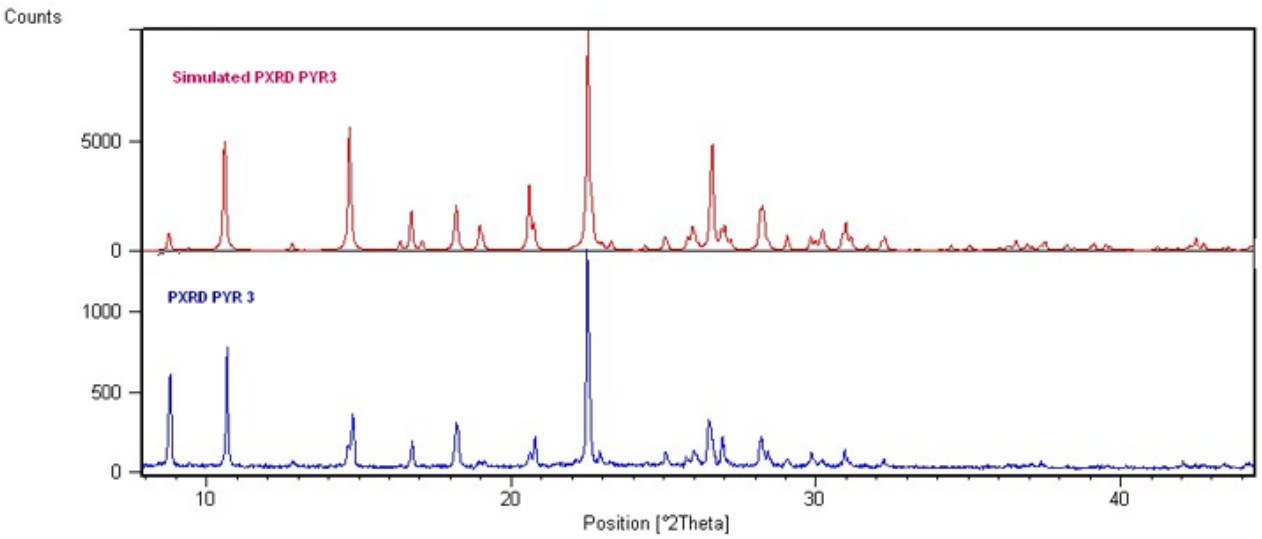




Comparison of the Simulated Powder X-Ray Data (obtained from Single Crystal) with the Experimental data for the same polycrystalline sample.



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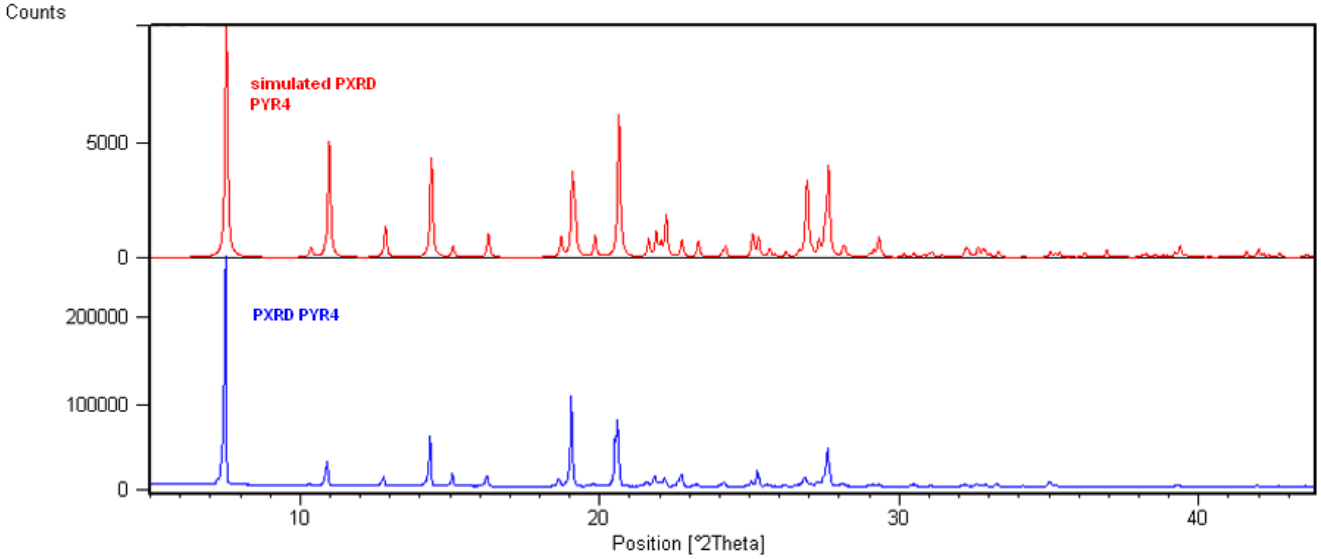
0
PXRD PYR 3
1000
500
0
10
20
30
40
Position [°2Theta]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simulated PXRD
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0
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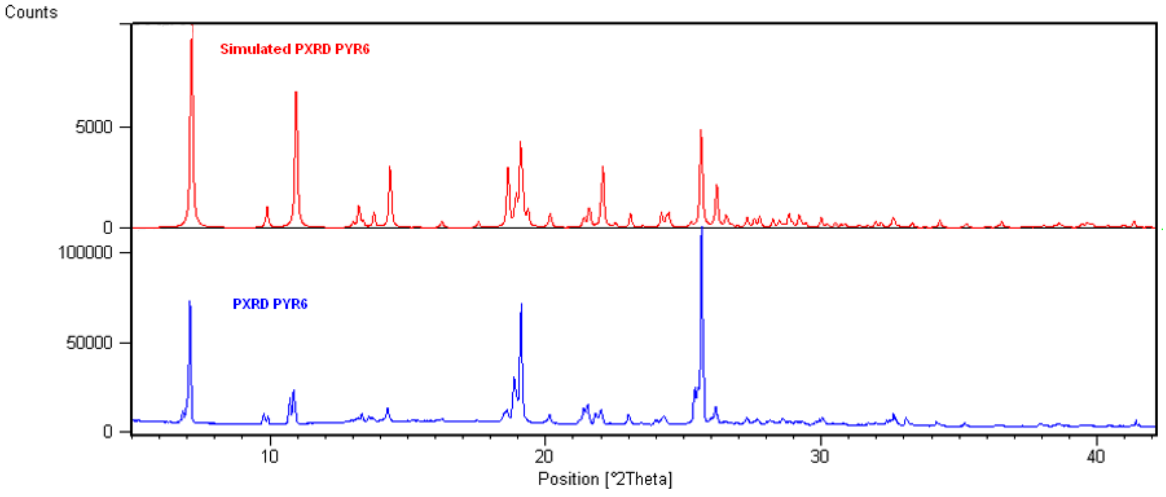
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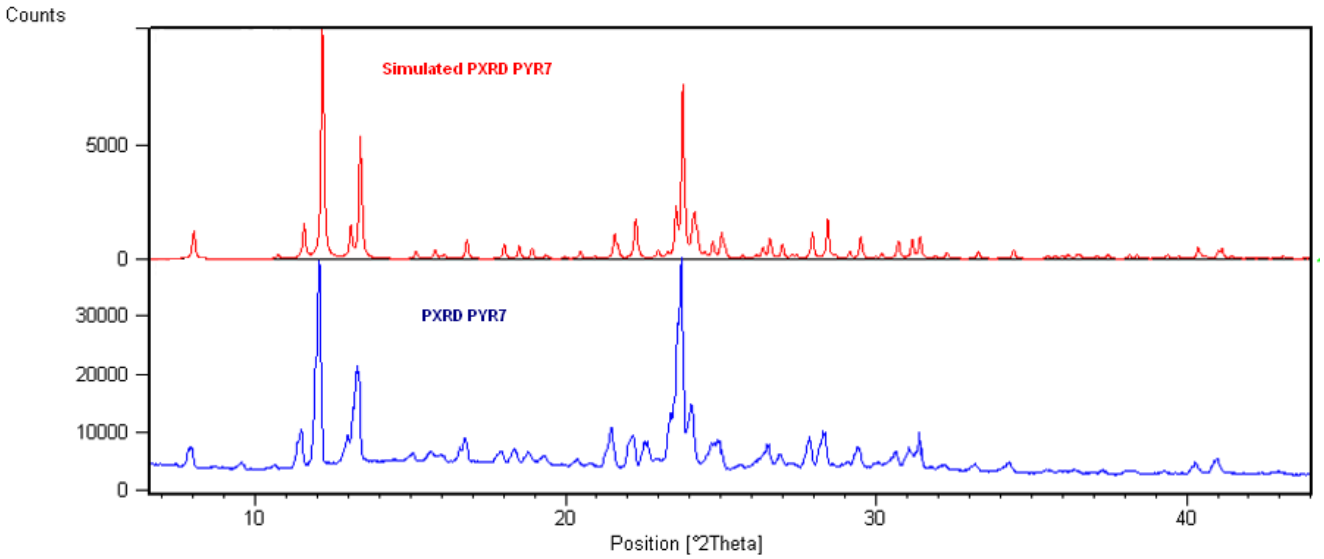
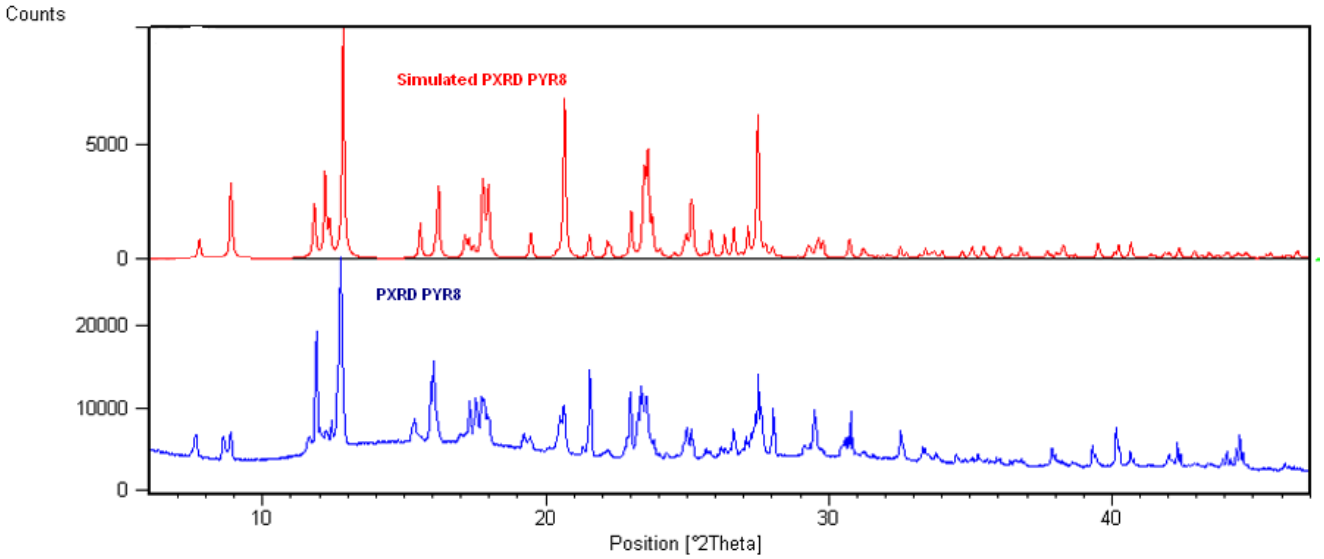
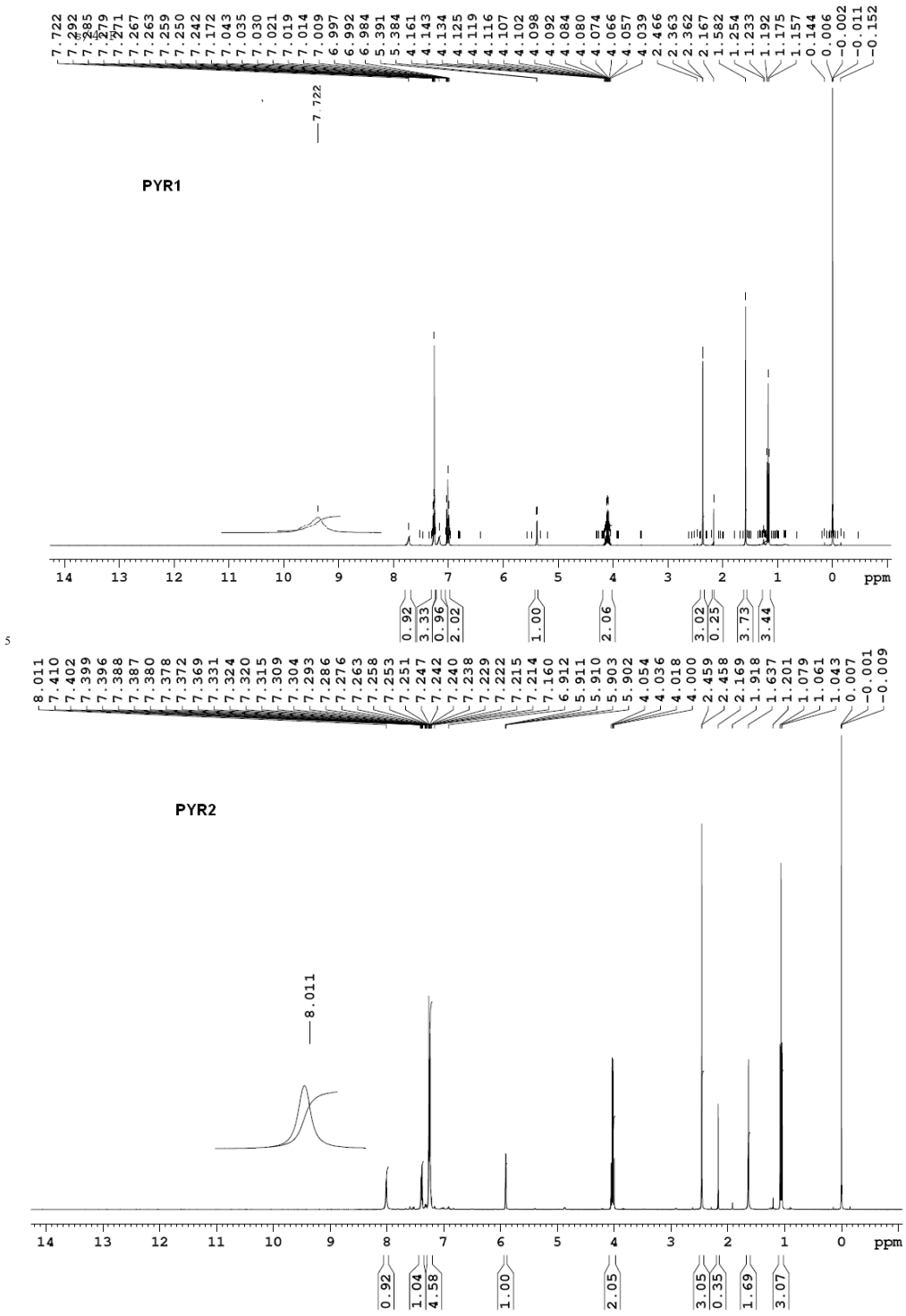
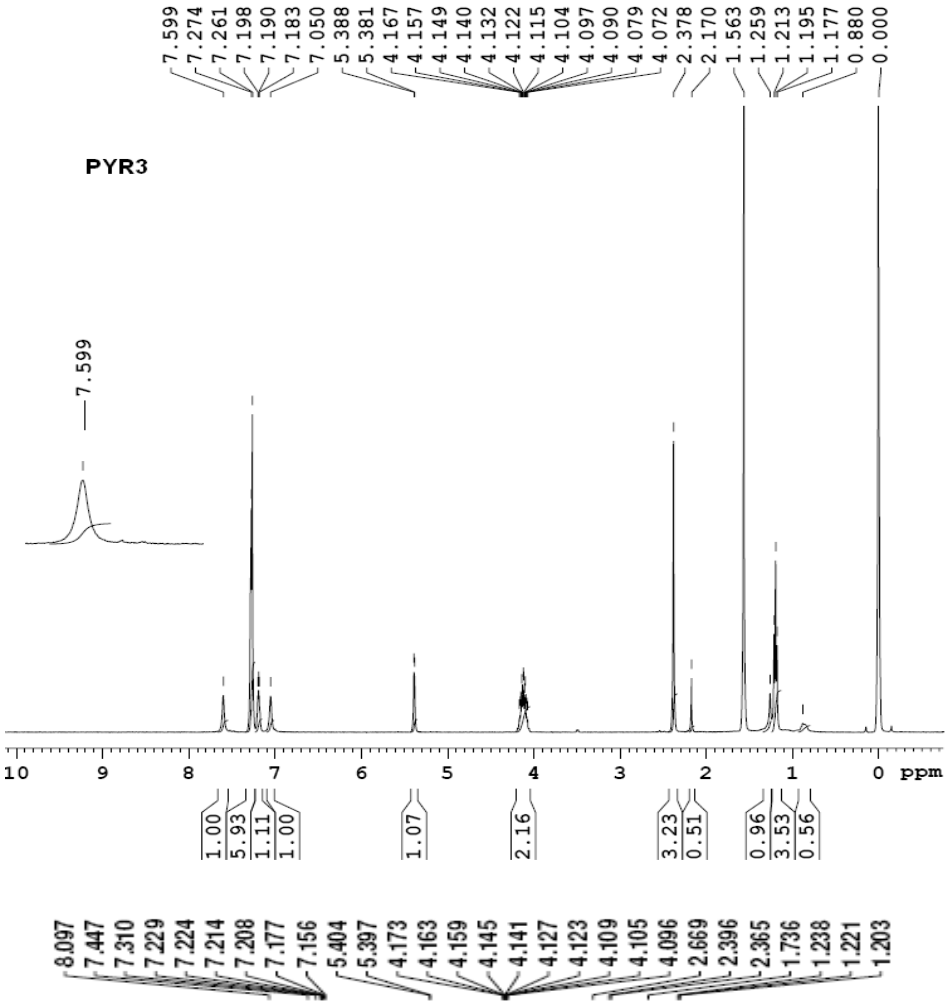




Experimental 1H-NMR spectrum for the studied compounds (Spectra recorded in $CDCl_3$ + DMSO)

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4.140
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4.122
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4.090
4.079
4.072
2.378
2.170
1.563
1.259
1.213
1.195
1.177
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0.000
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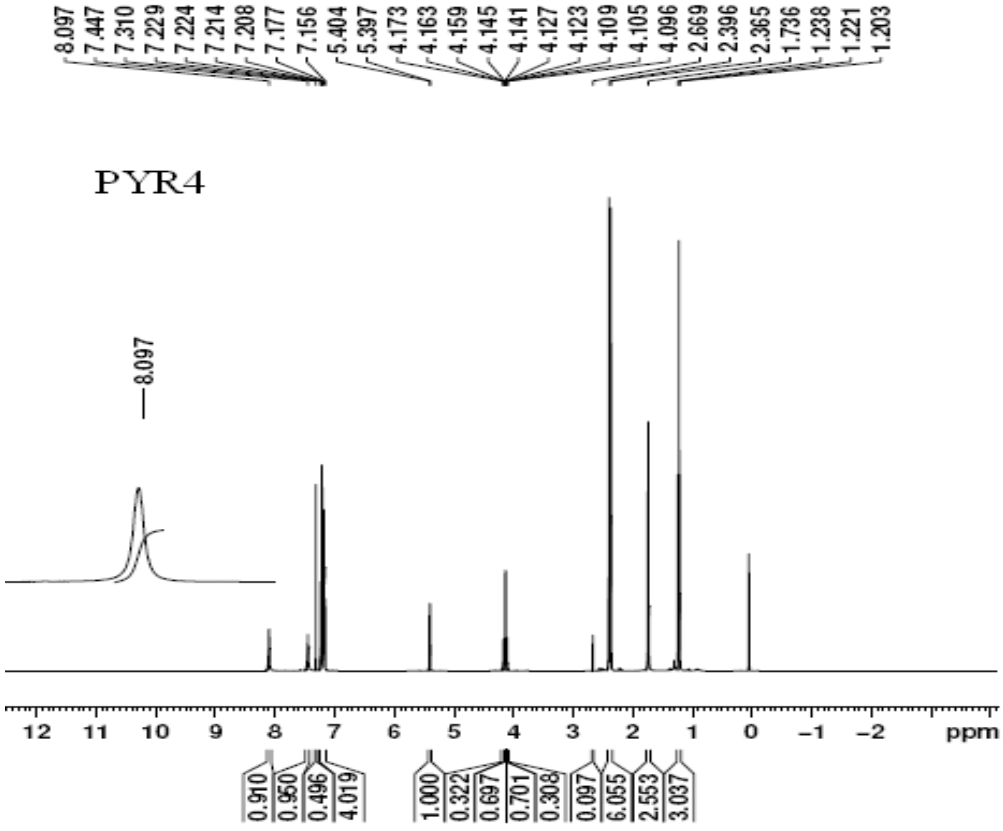
0.56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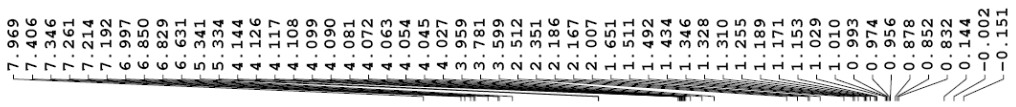
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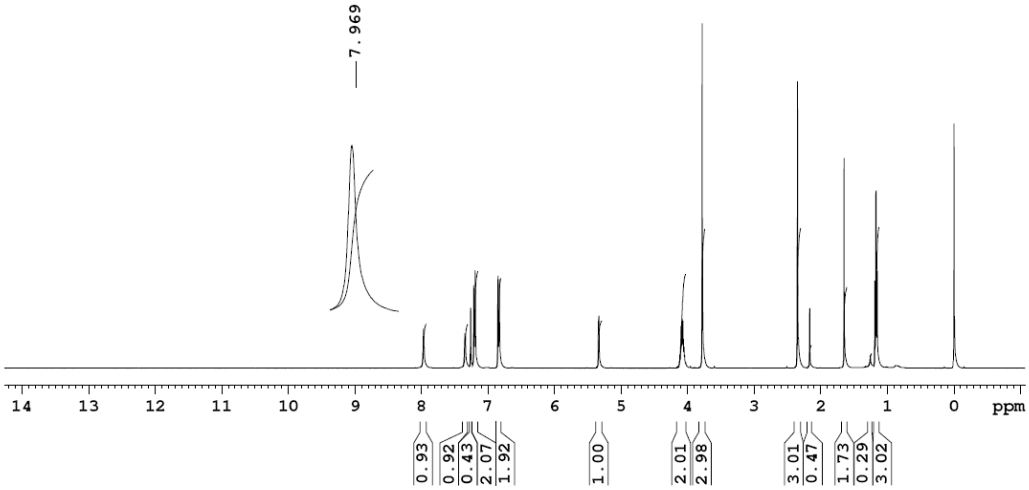
PYR6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2.07
1.92
1.00
2.01
2.98
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3.02


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3.821
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2.361
2.360
2.304
2.253
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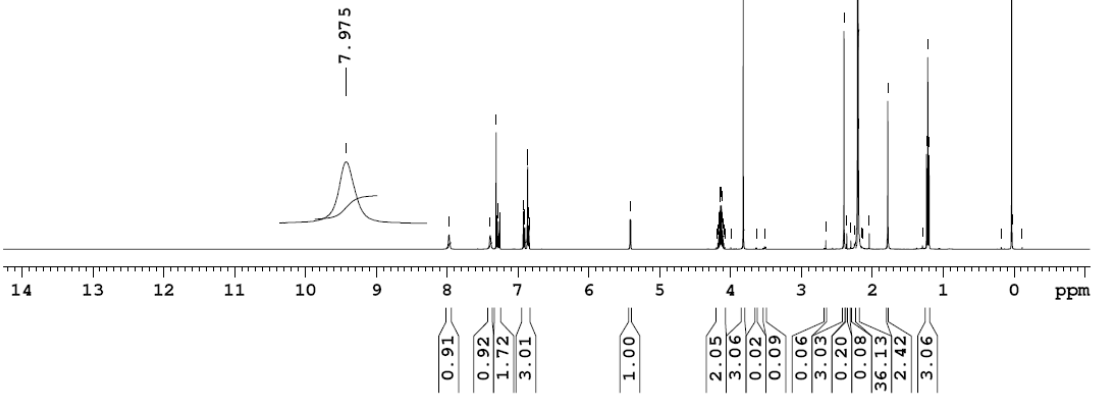
-0.115

PYR7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