

Supplementary Information

Insights into conformational and packing features in a series of aryl substituted ethyl-6-methyl-4-phenyl-2-oxo-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 (°C)
PYRO1 (-o-F)	C ₁₄ H ₁₅ FN ₂ O ₃	278	58	258-260
PYRO2 (-p-F)	C ₁₄ H ₁₅ FN ₂ O ₃	278	57	178-182
PYRO3 (-p-Cl)	C ₁₄ H ₁₅ ClN ₂ O ₃	294	68	210-212
PYRO4 (-p-Br)	C ₁₄ H ₁₅ BrN ₂ O ₃	338	62	231-233
PYRO5 (-p-Me)	C ₁₅ H ₁₈ N ₂ O ₃	274	60	214-216
PYRO6 (-p-OMe)	C ₁₅ H ₁₈ N ₂ O ₄	290	59	202-204
PYRO7 (-m-OMe)	C ₁₅ H ₁₈ N ₂ O ₄	290	60	222-224
PYRO8 (m-(OMe) p-OH)	C ₁₅ H ₁₈ N ₂ O ₅	306	54	186-188

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

Geometrical Parameter	PYRO1	PYRO2A	PYRO2B A/B	PYRO3 A/B	PYRO4	PYRO5 A/B	PYRO6 A/B	PYRO7	PYRO8
C1-O1	1.230(3)	1.244(2)	1.237(3)/1.236(3)	1.232(2)/1.234(2)	1.232(4)	1.243(2)/1.241(2)	1.243(2)/1.245(2)	1.243(2)	1.240(2)
C1-N1	1.367(2)	1.379(3)	1.375(3)/1.382(4)	1.340(2)/1.337(2)	1.363(6)	1.374(2)/1.370(3)	1.370(2)/1.376(2)	1.373(1)	1.374(3)
C1-N2	1.339(2)	1.330(3)	1.333(5)/1.340(4)	1.370(2)/1.373(2)	1.340(4)	1.337(2)/1.334(3)	1.339(2)/1.325(2)	1.326(2)	1.335(3)
C5-O2	1.211(2)	1.206(3)	1.220(4)/1.207(4)	1.215(1)/1.208(1)	1.198(6)	1.213(2)/1.207(3)	1.206(2)/1.209(3)	1.203(2)	1.204(2)
O3-C6	1.447(2)	1.455(3)	1.511(2)/1.449(2)	1.457(1)/1.456(3)	1.448(5)	1.4621(2)/1.451(3)	1.455(3)/1.475(3)	1.453(2)	1.462(2)
C3-C2	1.345(2)	1.346(3)	1.342(2)/1.344(2)	1.345(2)/1.347(3)	1.3404(7)	1.348(2)/1.351(3)	1.346(2)/1.345(2)	1.342(2)	1.338(3)
C2-N1	1.380(2)	1.390(2)	1.390(3)/1.393(3)	1.395(2)/1.391(2)	1.391(6)	1.395(2)/1.309(2)	1.393(2)/1.401(2)	1.391(2)	1.398(2)
N2-C1-O1	123.5(1)	124.1(2)	123.7(2)/124.4(3)	123.2(1)/123.9(1)	123.8(3)	123.3(2)/124.2(3)	124.0(2)/123.4(2)	123.4(1)	123.2(3)
N1-C2-C8	112.8(1)	114.4(2)	112.0(2)/112.8(2)	112.9(2)/112.9(1)	113.05(5)	112.5(2)/113.3(2)	113.2(2)/113.5(2)	113.7(2)	113.7(2)
C4-C3-C5	117.9(1)	119.9(1)	119.0(2)/119.69(2)	118.8(2)/119.5(2)	117.8(5)	118.9(2)/119.7(3)	119.4(2)/119.6(2)	118.9(1)	118.9(2)

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

Compound name	Q (Å)	Theta (°)	Phi (°)
PYRO1	0.430(2)	74.0(3)	171.2(3)
PYRO2A	0.430(2)	74.0(3)	171.2(3)
PYRO2B (Molecule A/B)	0.355(2)/0.364(3)	72.7(5)/71.2(5)	169.1(5)/169.5(4)
PYRO3 (Molecule A/B)	0.343(2)/0.380(2)	108.4(3)/110.0(3)	131.4(3)/132.3(3)
PYRO4	0.213(5)	71.0(13)	155.2(14)
PYRO5 (Molecule A/B)	0.349(2)/0.380(2)	71.4(3)/70.2(3)	167.5(4)/166.8(4)
PYRO6 (Molecule A/B)	0.364(2)/0.359(2)	70.6(3)/72.8(3)	162.1(3)/175.6(4)

PYRO7	0.354(2)	105.9(3)	353.3(3)
PYRO8	0.377(2)	72.1(3)	172.7(4)

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-O3 (ester group)

Compound name	Plane 1 and 2 (°)	Plane 1 and 3 (°)	Plane 2 and 3 (°)
PYRO1	89.3(1)	89.9(1)	5.1(1)
PYRO2A	81.7(1)	86.7(1)	18.5(2)
PYRO2B (Molecule A/B)	76.3(1)/76.7(1)	81.9(2)/78.1(2)	12.3(3)/13.1(3)
PYRO3 (Molecule A/B)	73.8(1)/79.8(1)	79.2(1)/80.0(1)	11.4(2)/15.7(2)
PYRO4	86.4(2)	88.4(4)	6.2(4)
PYRO5 (Molecule A/B)	75.0(1)/79.9(1)	81.0(2)/83.3(1)	11.8(3)/12.7(3)
PYRO6 (Molecule A/B)	79.9(1)/88.7(1)	82.2(2)/81.7(1)	9.2(2)/14.4(2)
PYRO7	83.2(1)	89.0(1)	7.99(1)
PYRO8	84.1(1)	85.6(2)	10.7(2)

5 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)
PYRO1	-0.061(2)	-0.242(2)
PYRO2A	-0.210(2)	-0.510(2)
PYRO2B (Molecule A/B)	0.155(2)/0.156(2)	0.438(3)/0.456(3)
PYRO3 (Molecule A/B)	+0.043(2)/-0.065(2)	-0.445(2)/0.482(2)
PYRO4	-0.074(4)	-0.258(4)
PYRO5 (Molecule A/B)	-0.142(2)/+0.143(2)	-0.432(2)/+0.477(2)
PYRO6 (Molecule A/B)	+0.132(2)/+0.166(2)	+0.450(2)/+0.438(2)
PYRO7	-0.174(2)	-0.424(2)
PYRO8	+0.166(2)	+0.462(2)

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

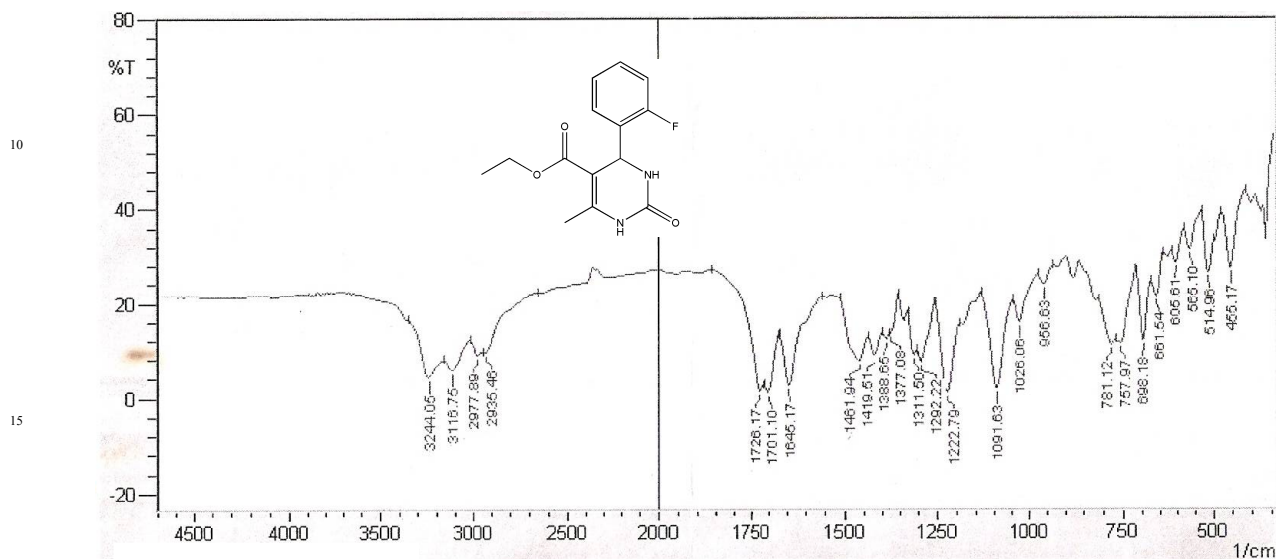
Torsion	PYRO1	PYRO2A	PYRO2B*	PYRO3*	PYRO 4	PYRO 5*	PYR O6*	PYRO 7	PYRO 8
C9-C4-C3-C5	71.52	-118.50	75.09	74.87	-74.43	74.71	73.67	74.24	74.13
C4-C3-C5-O2	-171.24	176.08	-174.90	-174.93	176.46	-174.45	-174.77	-178.07	-178.07
C9-C4-N2-C1	99.22	-97.14	95.83	96.44	-97.38	95.88	97.62	97.22	97.22
C14-C9-C4-C3	62.32	-60.66	55.83	58.31	-55.55	52.23	56.24	51.24	51.24
C4-N2-C1-N1	18.04	-16.61	17.49	16.77	-16.90	18.09	17.43	18.04	18.04
C5-O3-C6-C7#	-172.87	85.28	-177.58	-85.54	-178.74	177.72	85.68	178.75	-178.87

10 *: 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.

#: In cases where the ethyl group (or one of the carbon atom) of the ester moiety is disordered, the torsion angle with respect to the major conformer is taken.

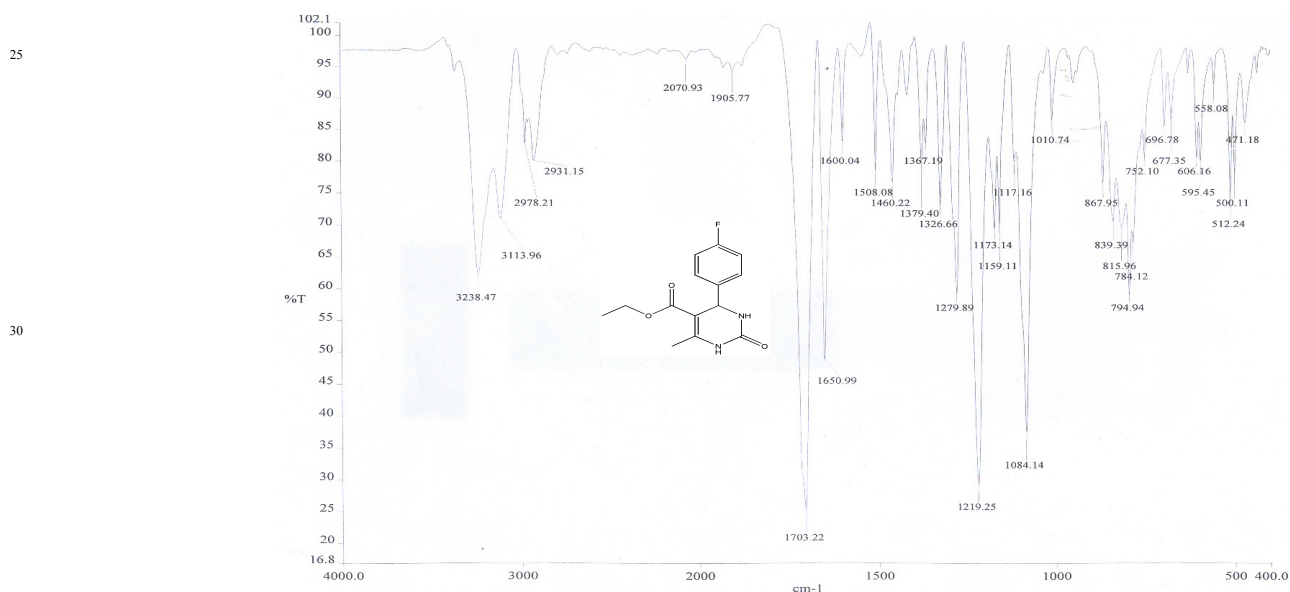
[PYRO1]:4-(2-fluoro-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3244.05 (N-H str), 3116.75, (ArC-H str), 2977.89 (Alp C-H), 1726.17 (C=O str), 1701.10 (C=O_{COOEt} str), 1645.17, 1461.94 (C=C str), 1388.65 (C-N str).



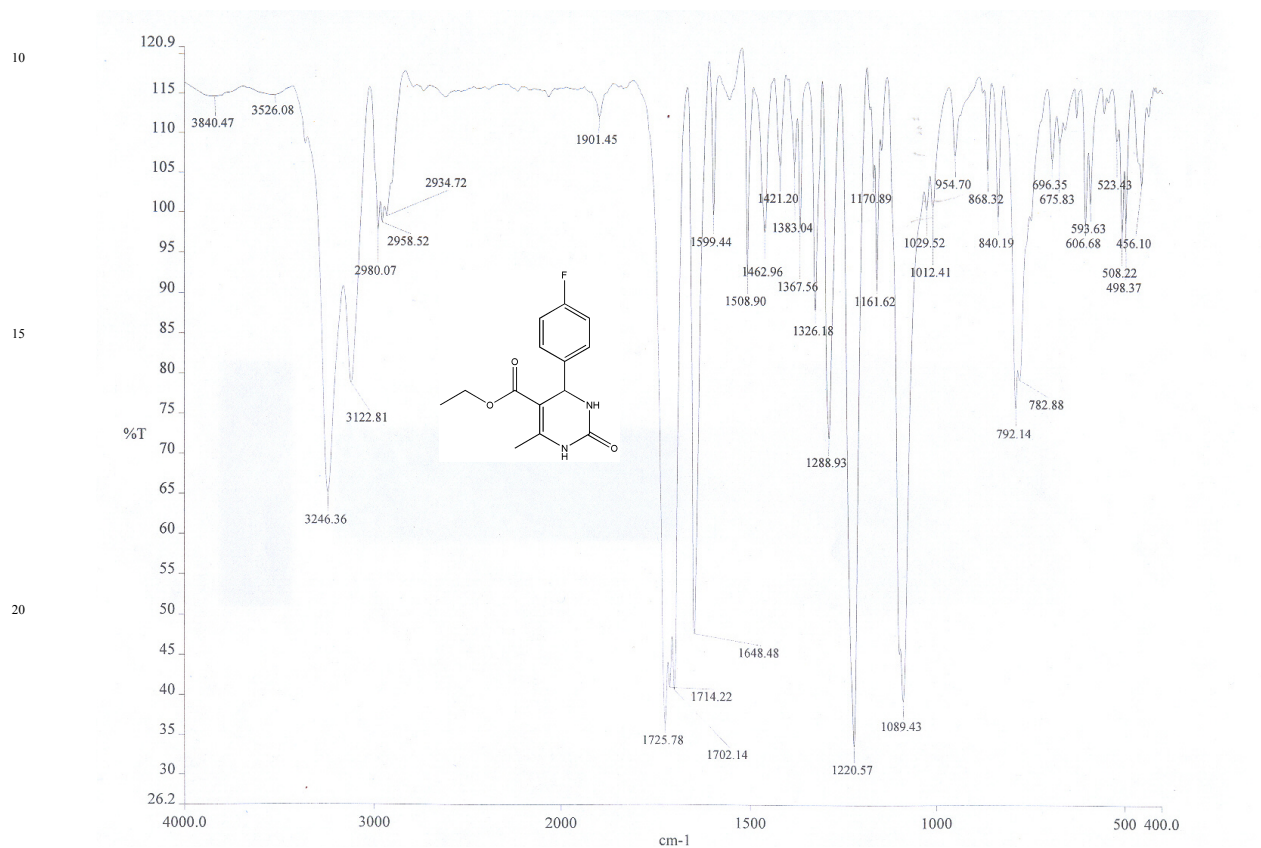
[PYRO2A]:4-(4-fluoro-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3238.47 (N-H str), 3113.96, (ArC-H str), 2978.21, (AlpC-H str), 1703.22 (C=O str), (C=O_{COOEt} str), 1650.99, 1450.99, 1460.22 (C=C str), 1379.40 (C-N str).



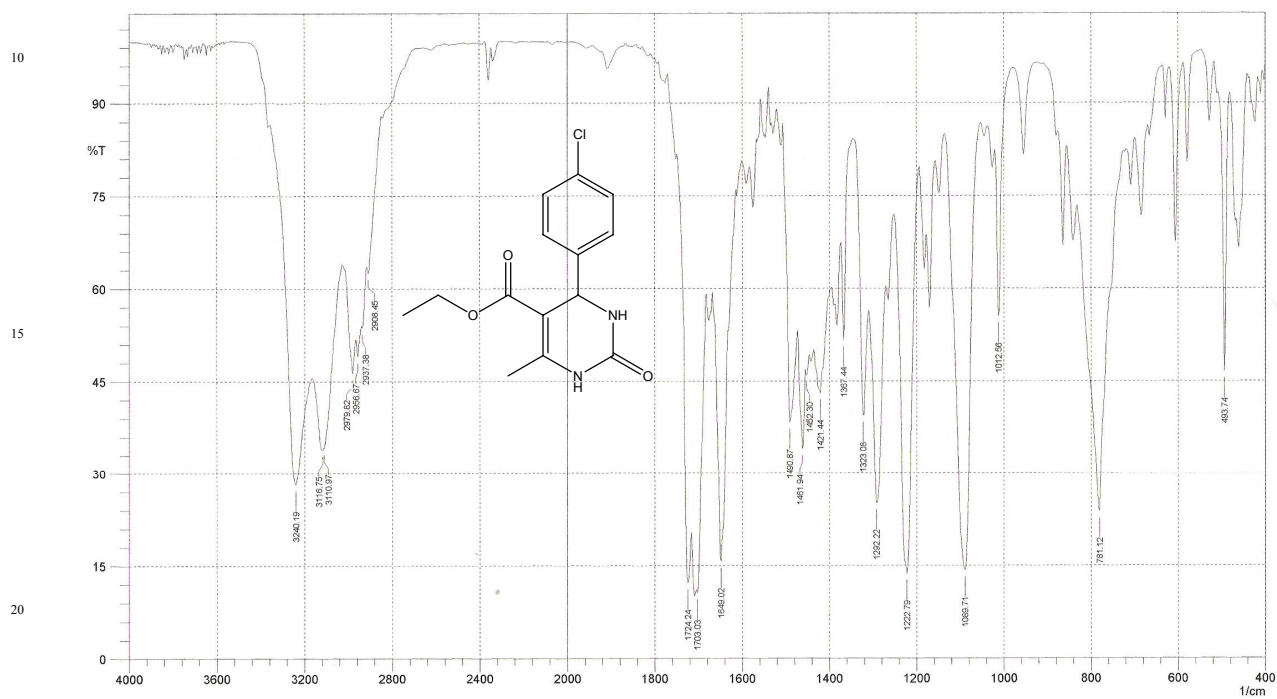
[PYRO2B]:4-(4-fluoro-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3246.36 (N-H str), 3122.81, (ArC-H str), 2980.07, (AlpC-H str), 1725.78 (C=O str), 1702.14 (C=O_{COOEt} str), 1648.48, 1450.99, 1462.96 (C=C str), 1367.56 (C-N str).



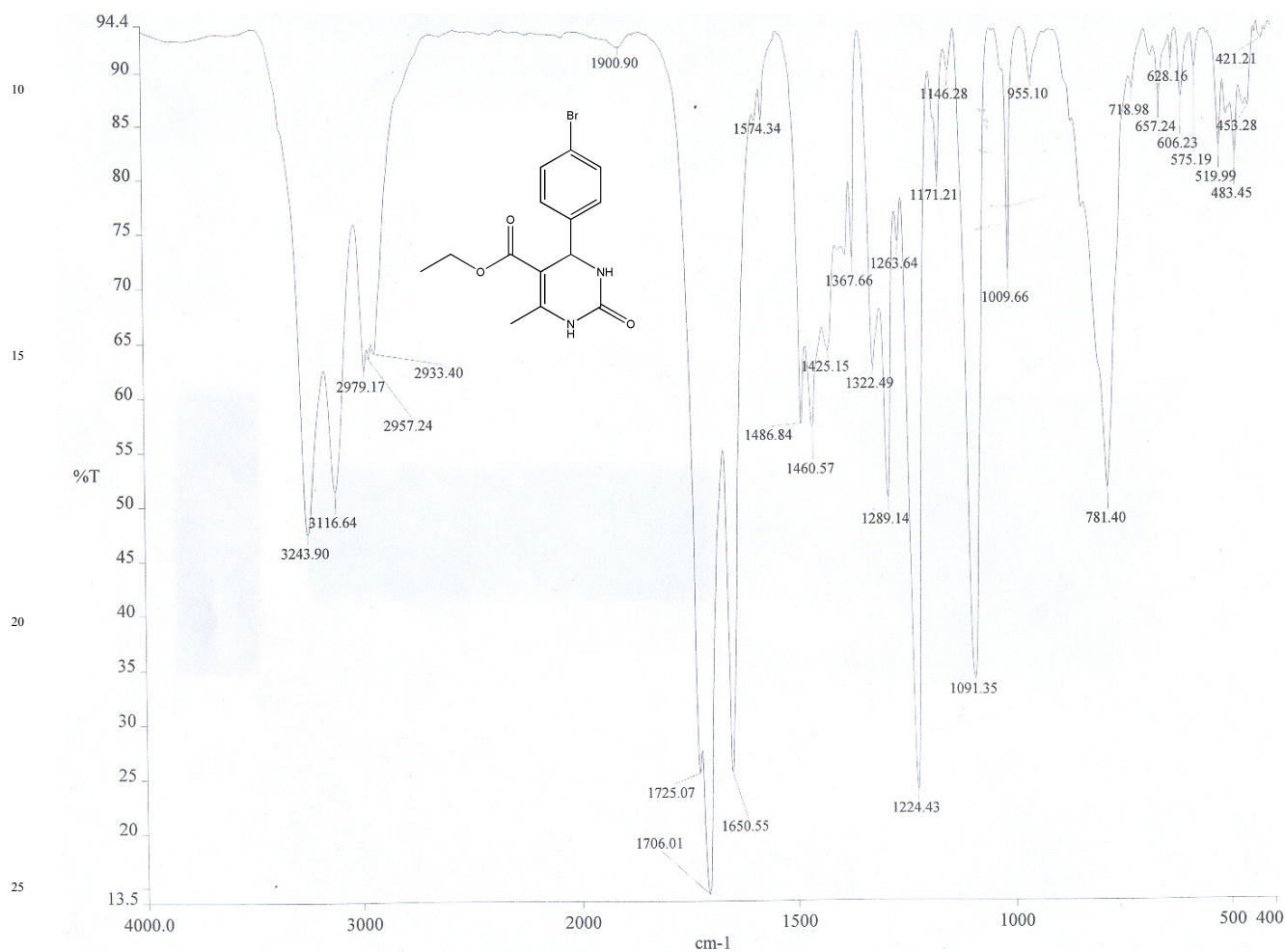
[PYRO3] 4-(4-chloro-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3240.19 (N-H str), 3116.75, (ArC-H str), 2979.82, (AlpC-H str), 1724.24 (C=O str), 1703.03 (C=O_{COOEt} str), 1649.02, 1490.87, 1461.94 (C=C str), 1323.08 (C-N str), 781.12 (ArC-Cl).



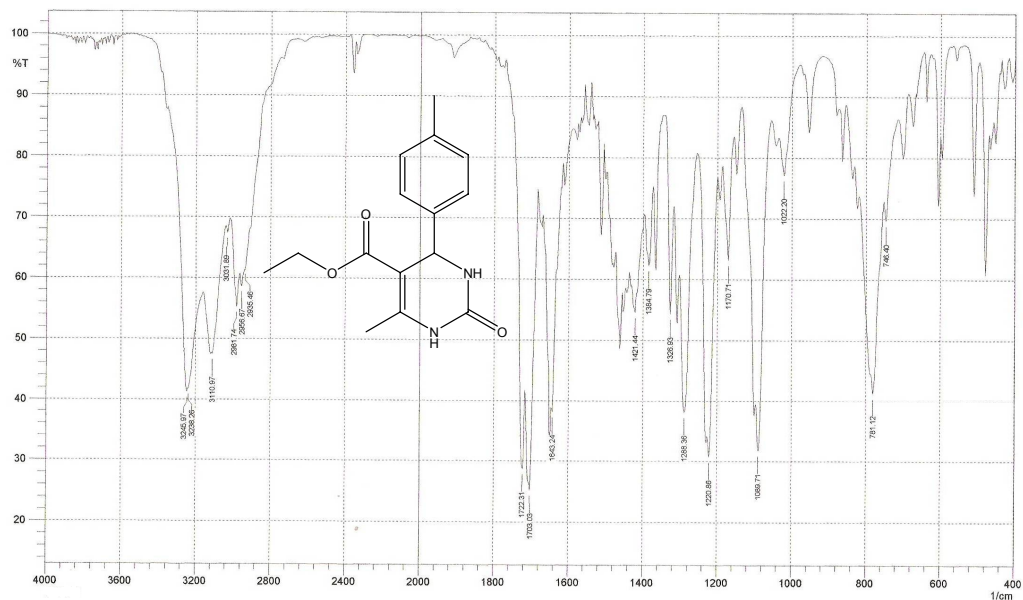
[PYRO4] R = *p*-Br; 4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3243.90, (N-H str), 3116.64 (ArC-H str), 2979.17, (AlpC-H str), 1725.07 (C=O str), 1706.01 (C=O_{COOEt} str), 1650.55, 1486.84 (C=C str), 1322.49 (C-N str).



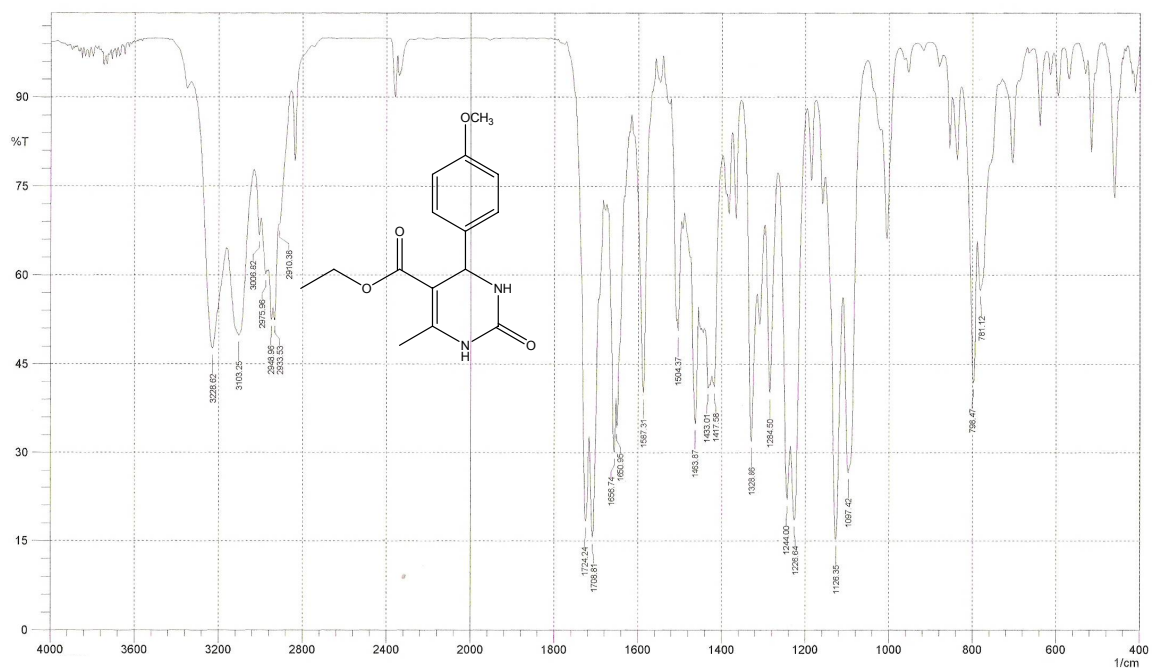
[PYRO5] R = *p*-Me: 4-(4-methylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester

IR (KBr) cm^{-1} : 3245.97, (N-H str), 3110.97 (ArC-H str), 2981.74, (AlpC-H str), 1722.31 (C=O str), 1703.03 (C=O_{COOEt} str), 1643.24, 1421.44 (C=C str), 1326.93 (C-N str).



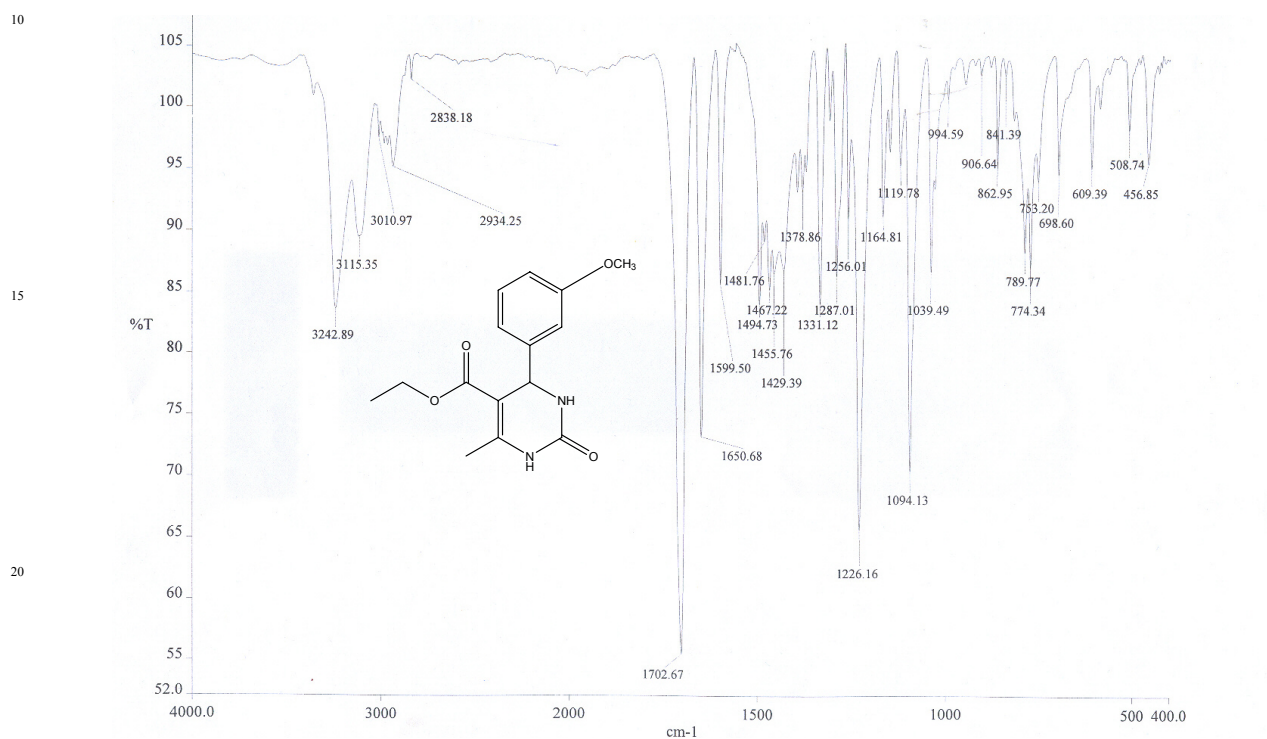
PYRO6: 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester.

IR (KBr) cm^{-1} : 3228.62 (N-H str), 3103.25 (ArC-H str), 2948.96, (AlpC-H str), 1724.24 (C=O str),
s 1708.81 (C=O_{COOEt} str), 1656.74, 1587.31, 1463.87 (C=C str), 1328.86 (C-N str).



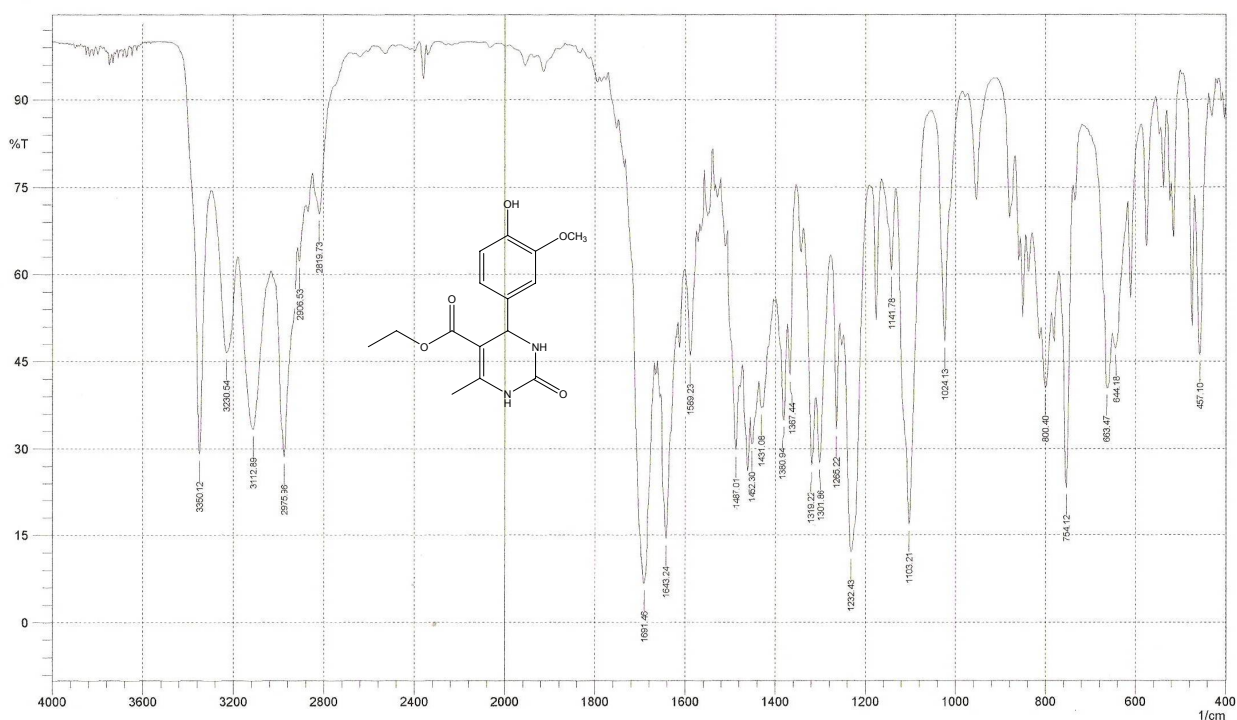
PYRO7: 4-[3-methoxyphenyl]-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester

IR (KBr) cm^{-1} : 3242.12 (N-H str), 3115.35 (ArC-H str), 2934.25 (Alp C-H), 1702.67 ($\text{C}=\text{O}_{\text{COOEt}}$ str), (C=O str), 1650.24, 1599.68, 1455.76 (C=C str), 1331.12 (C-N str).



PYRO8:4-(3-methoxy-4-hydroxy-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ethyl ester .

IR (KBr) cm^{-1} : 3350.12 (OH), 3230.54 (N-H str), 3112.89 (ArC-H str), 2975.96 (Alp C-H), 1691.46 (C=O_{COOEt} str), (C=O str), 1643.24, 1589.23, 1452.30 (C=C str), 1319.22 (C-N str).

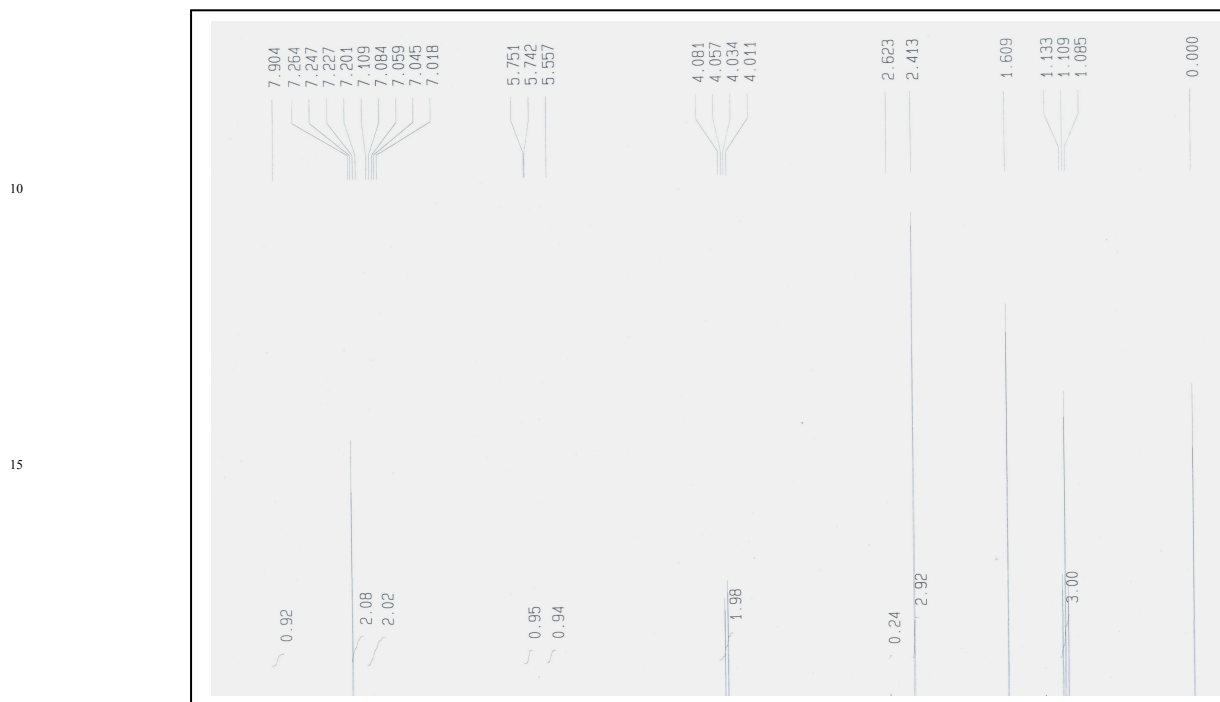


¹HNMR- Of these compounds provide evidence for purity of the samples before crystallization

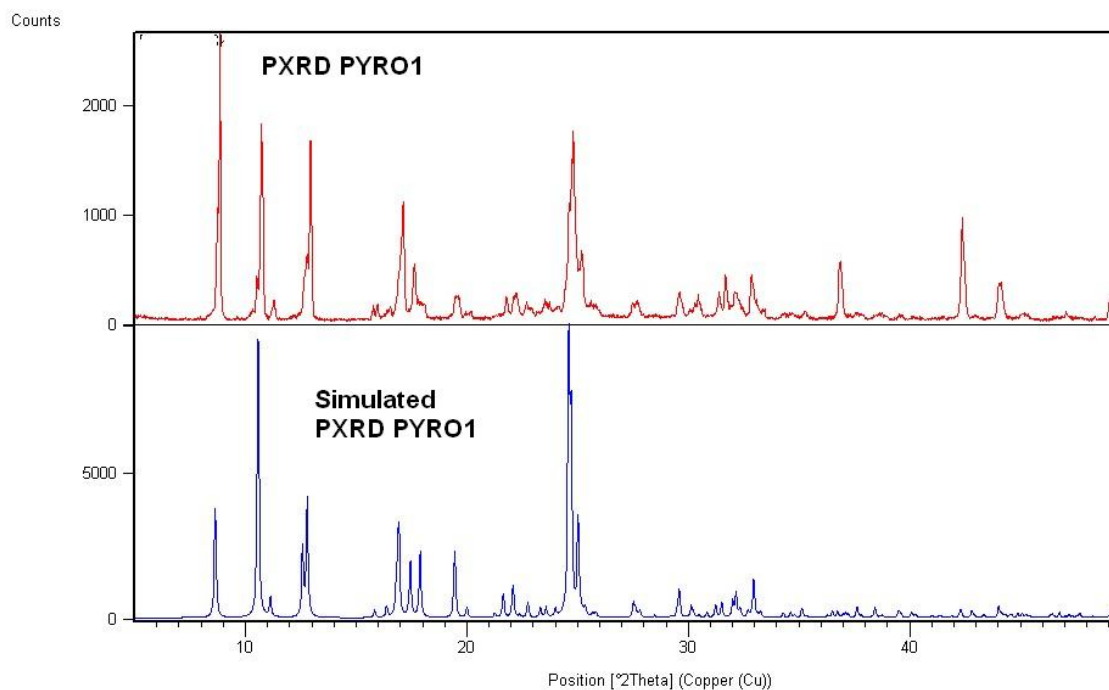
Comparison of Powder X-ray Data (PXRD) bulk samples with the simulated Powder X-ray data (simulated PXRD) of the solved crystal structures.

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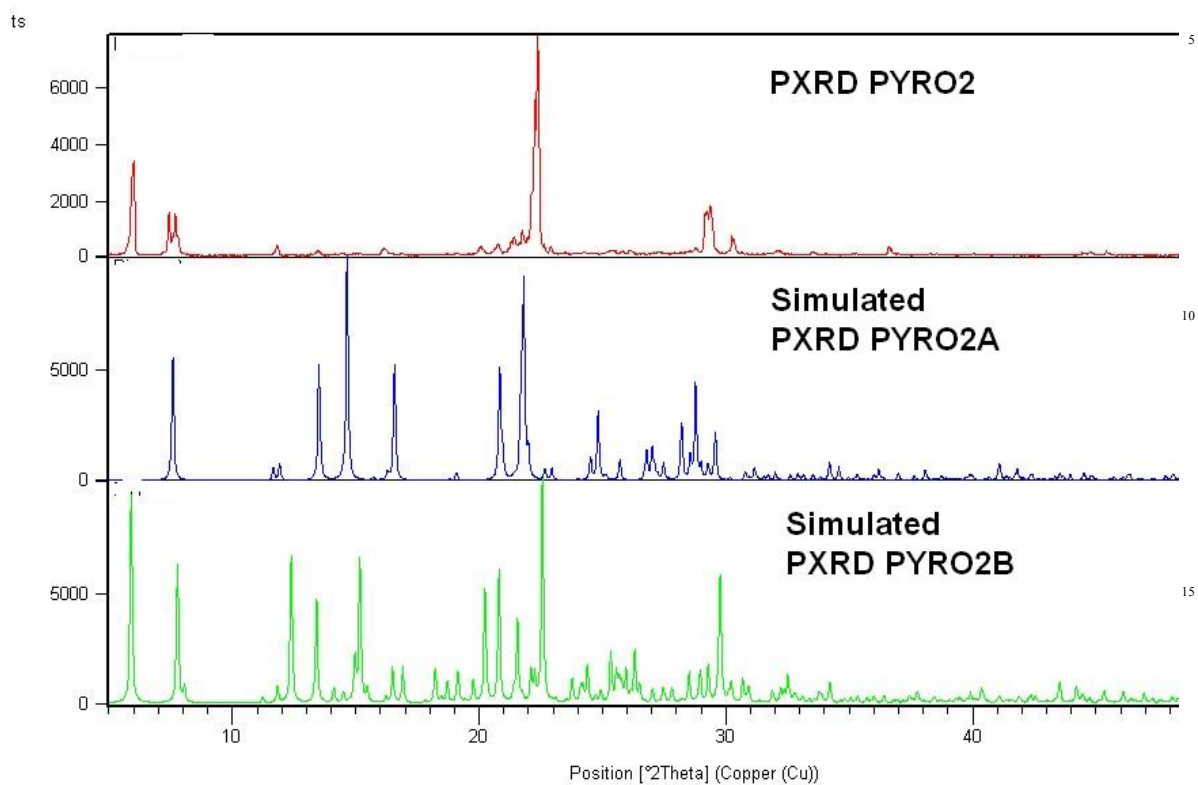
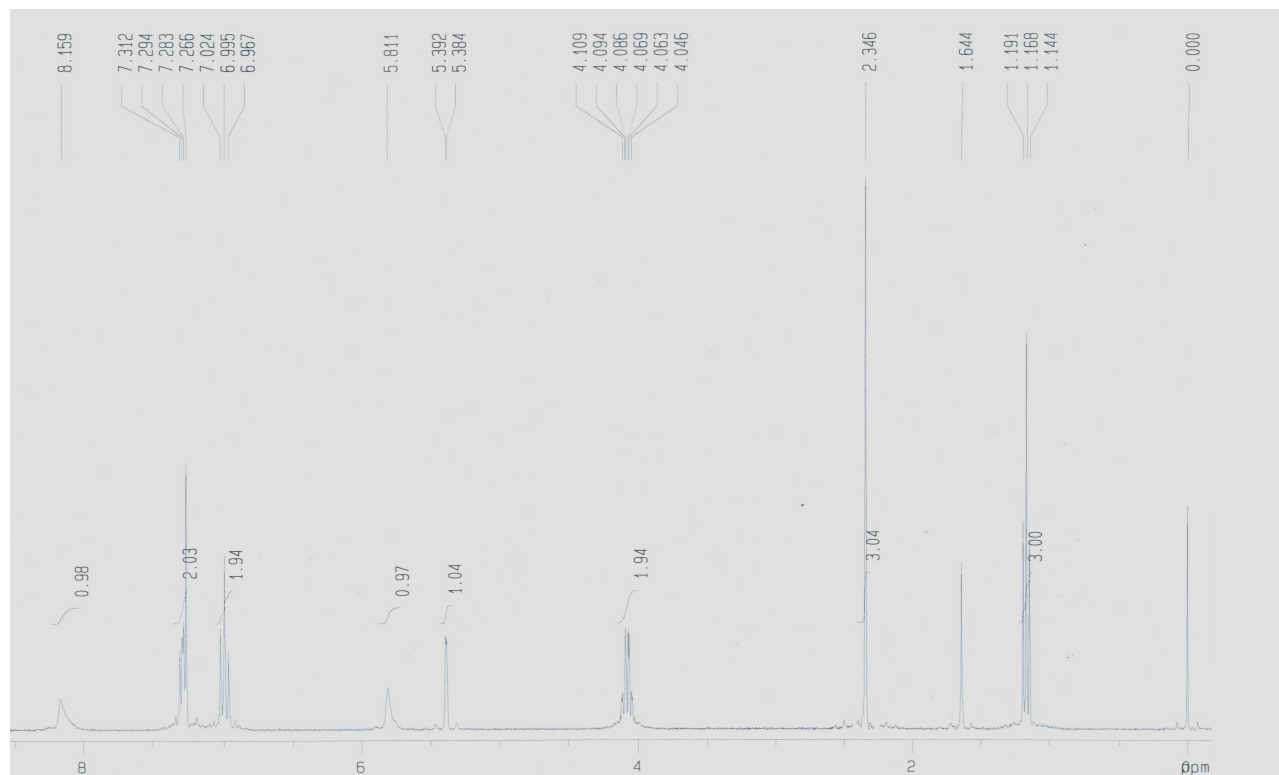
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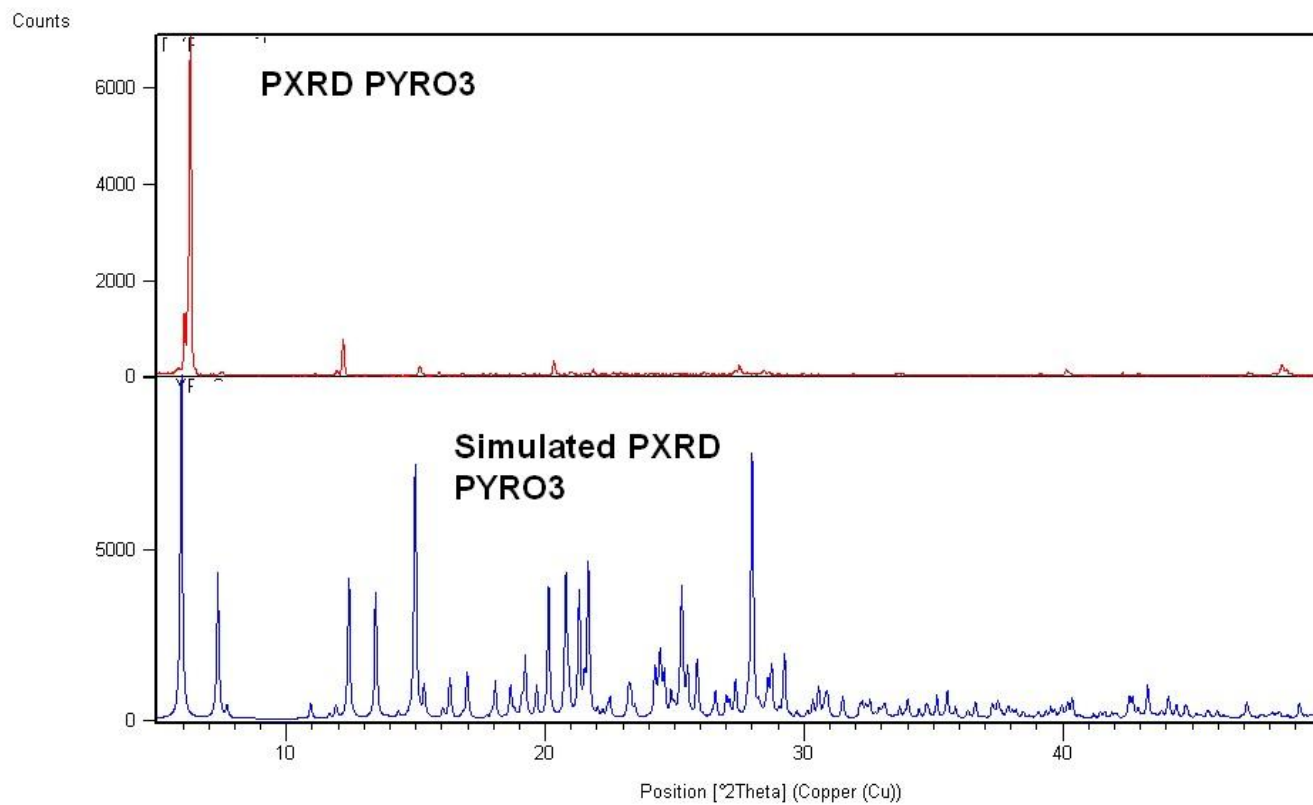
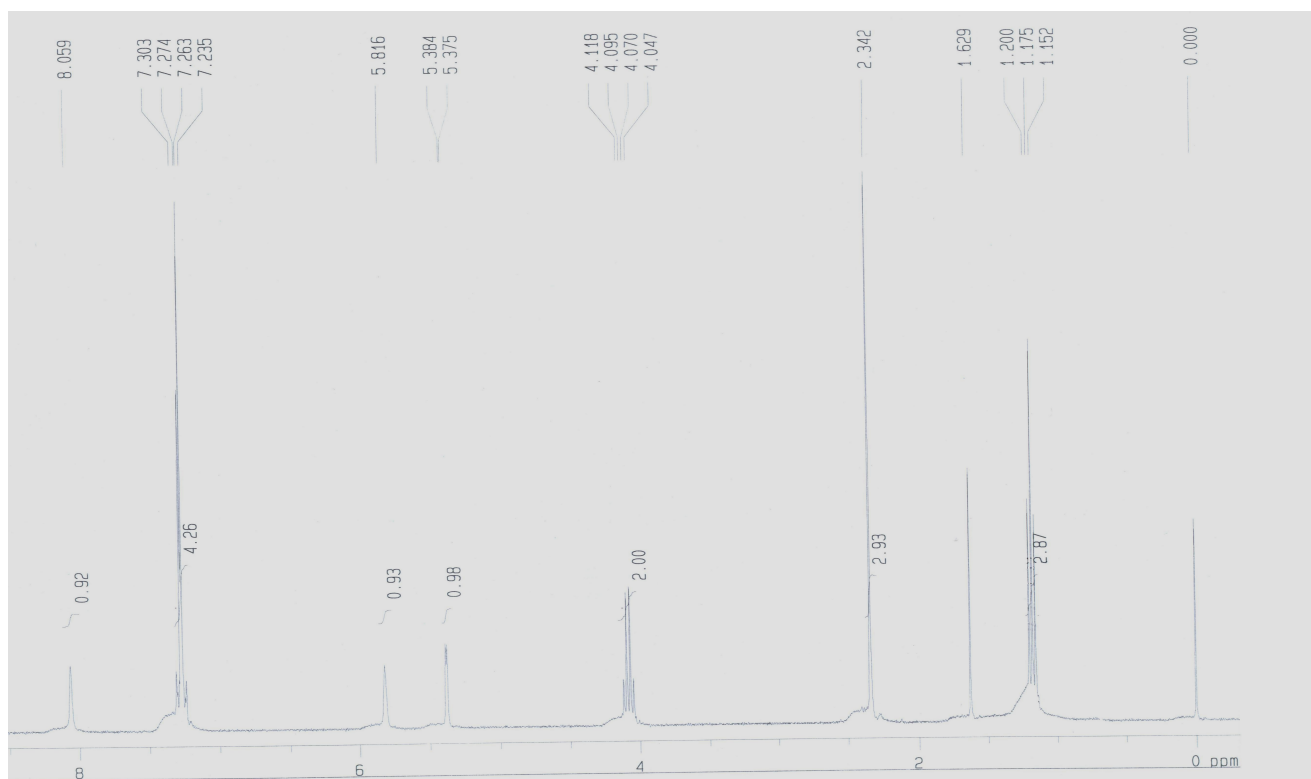
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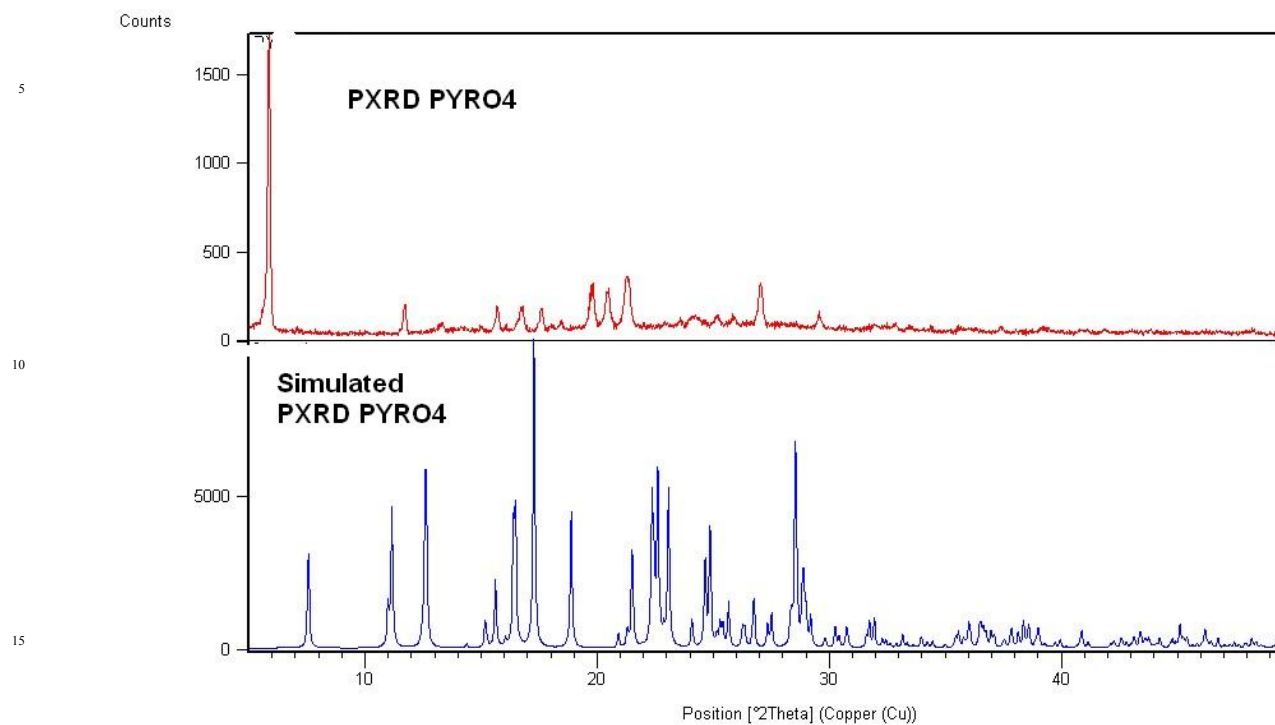
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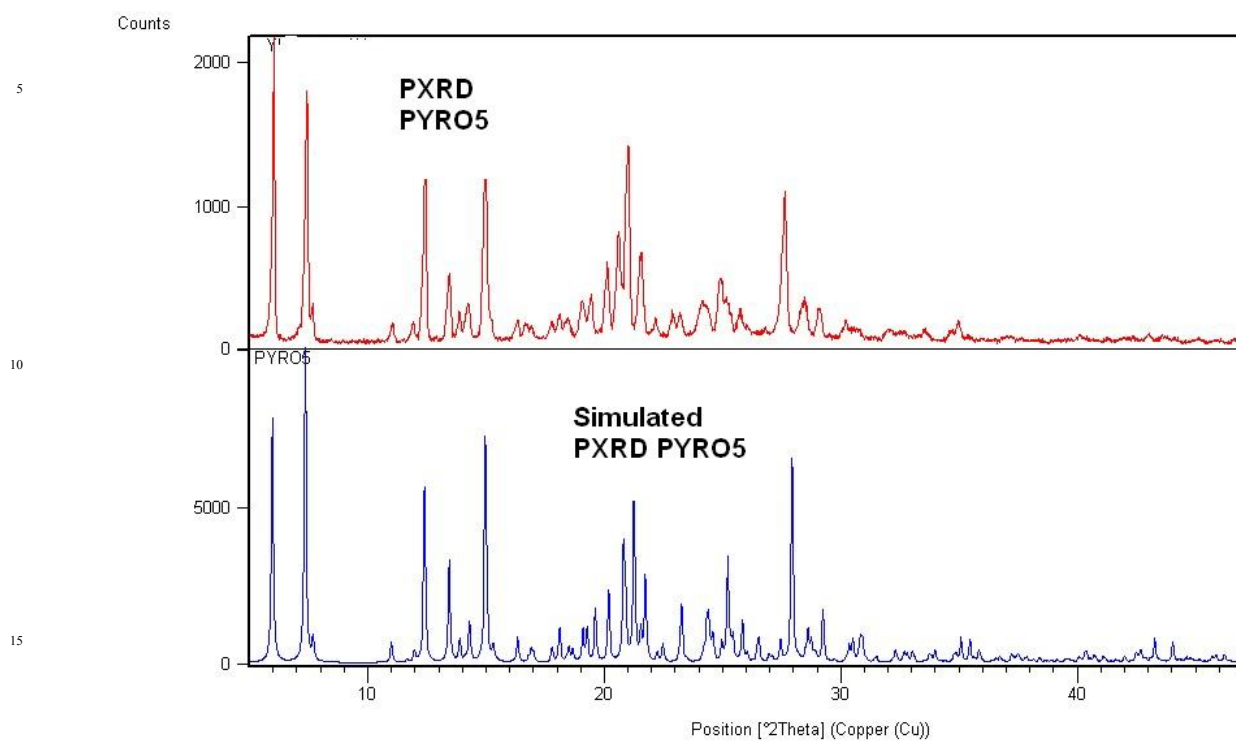
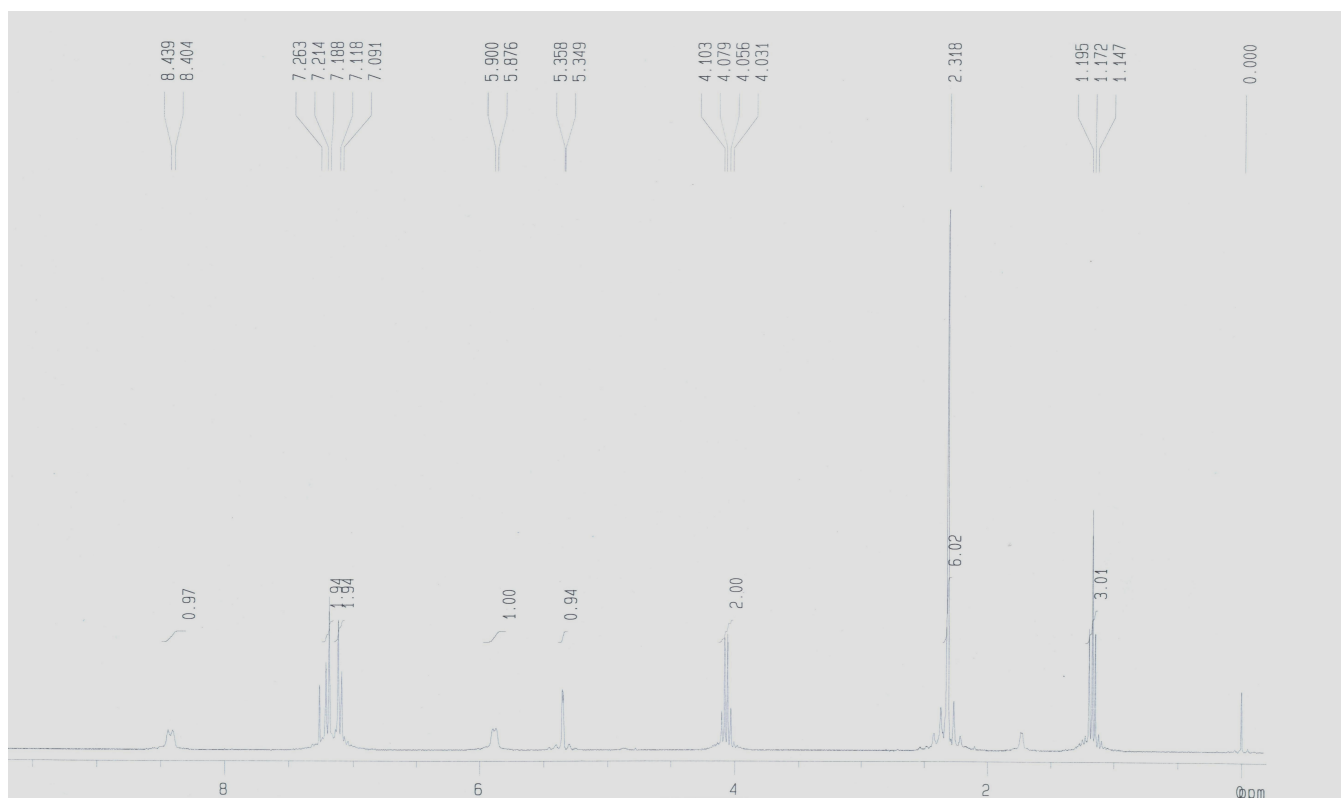
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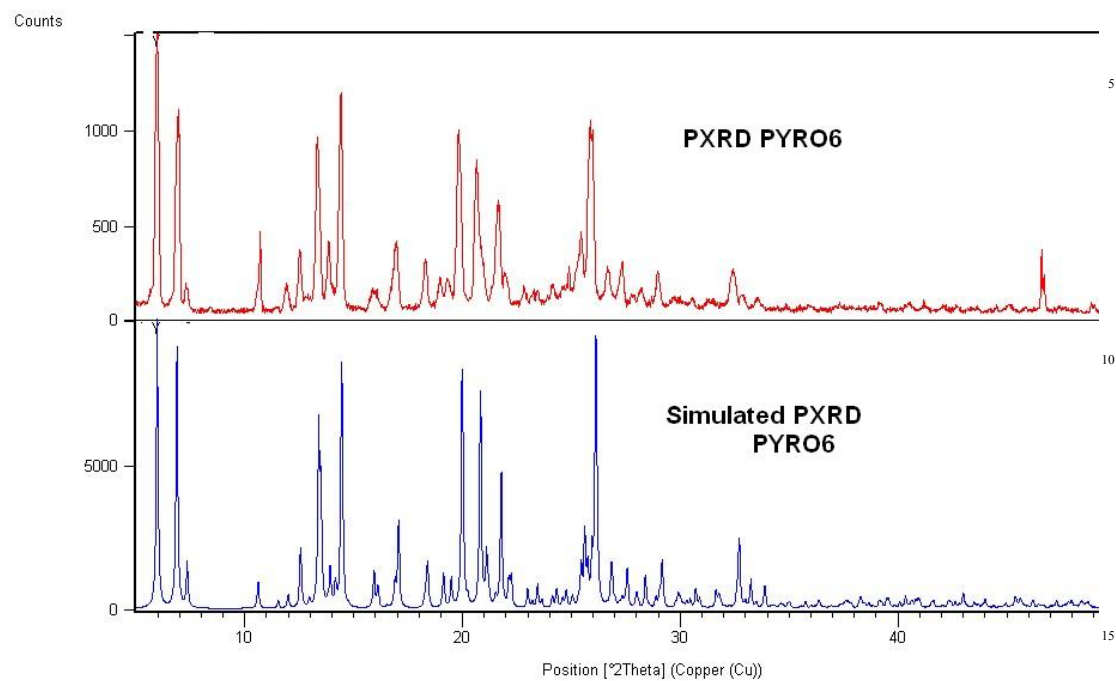
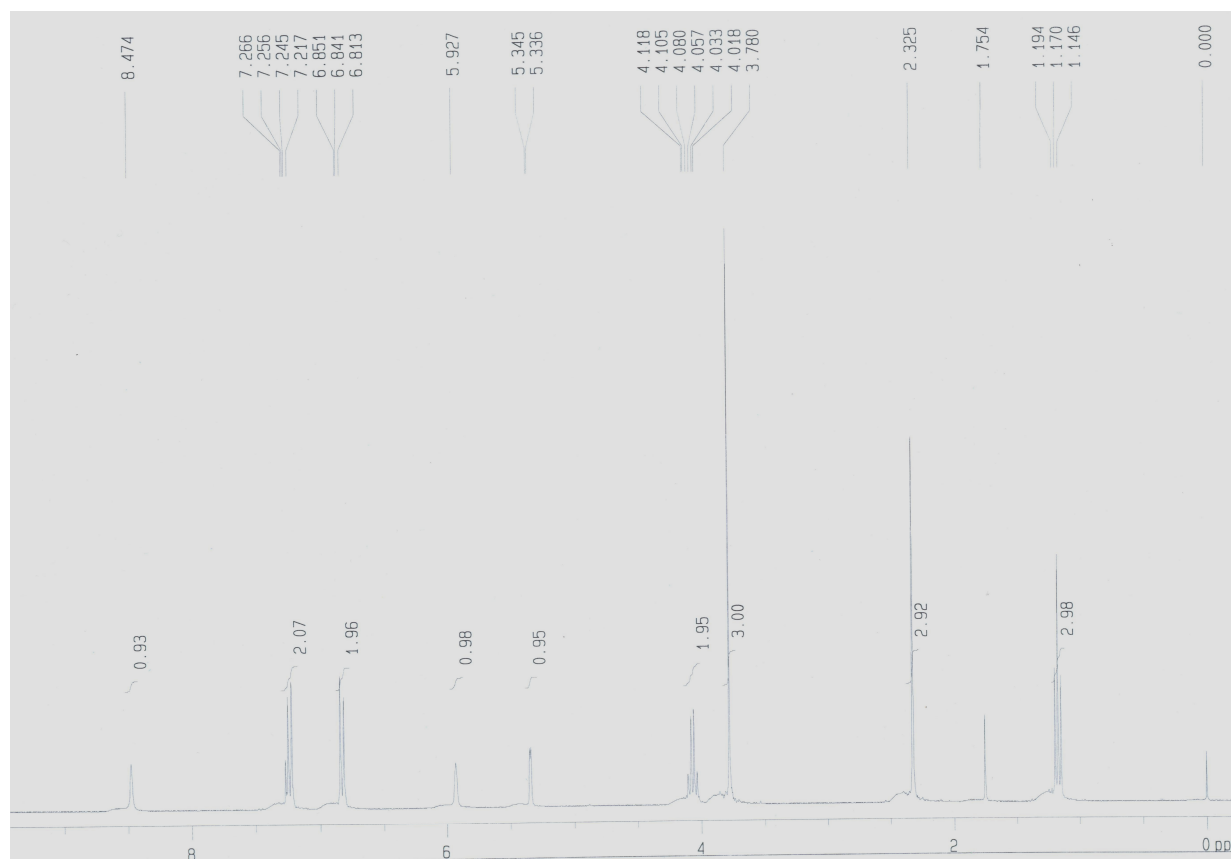
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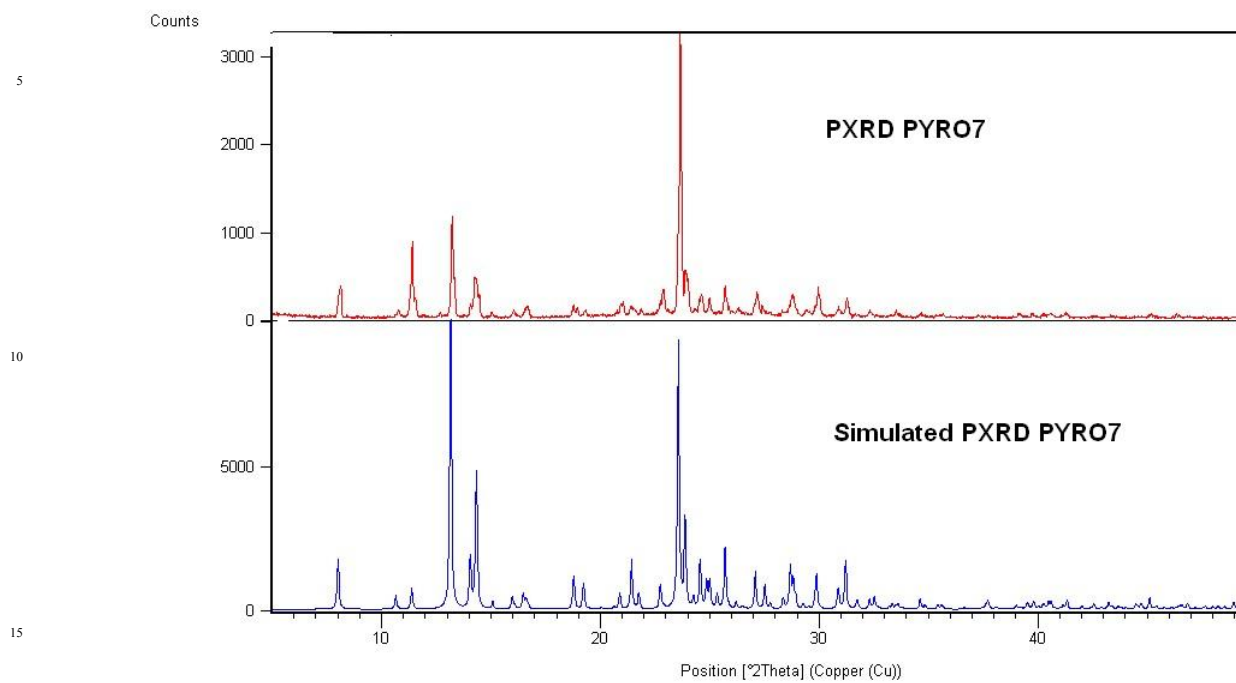
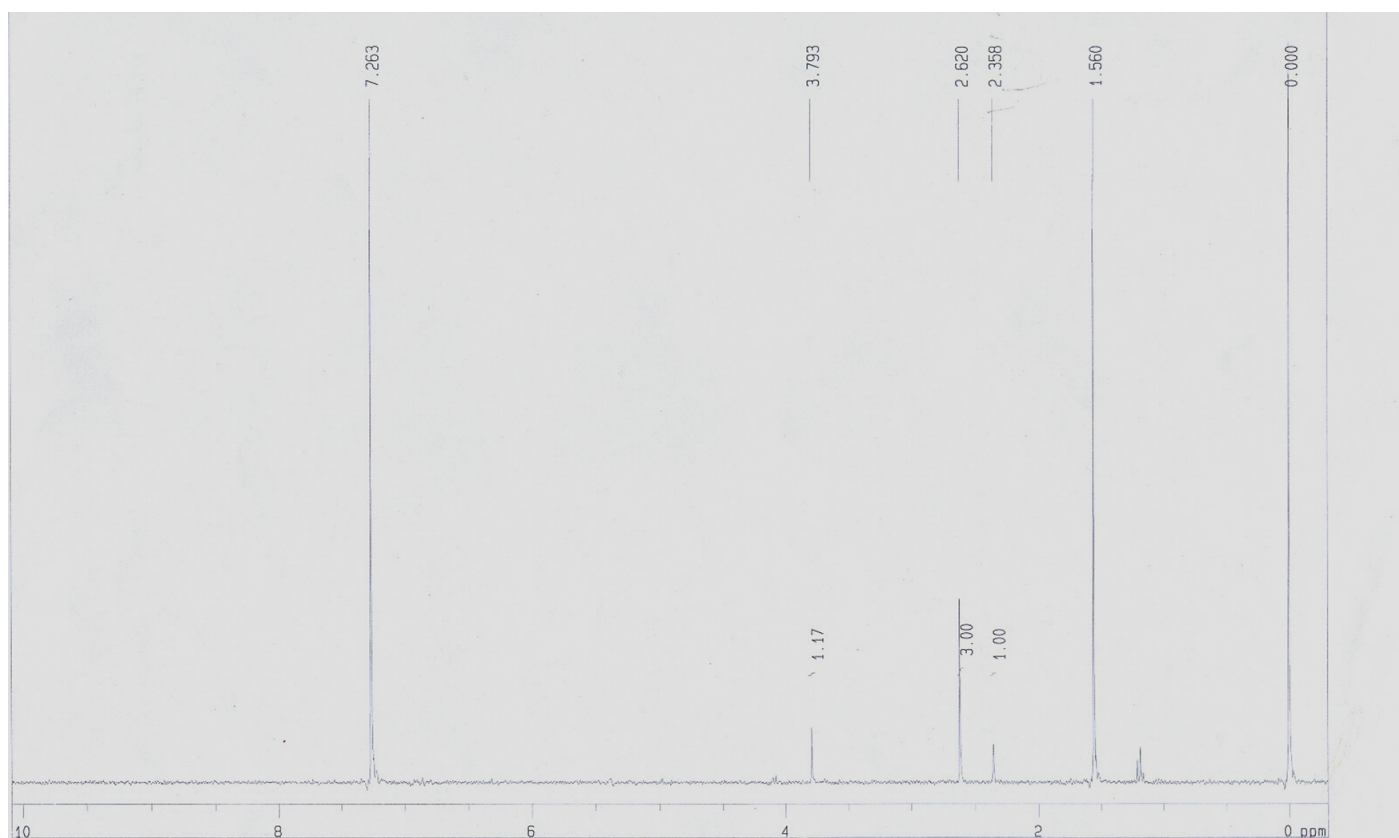
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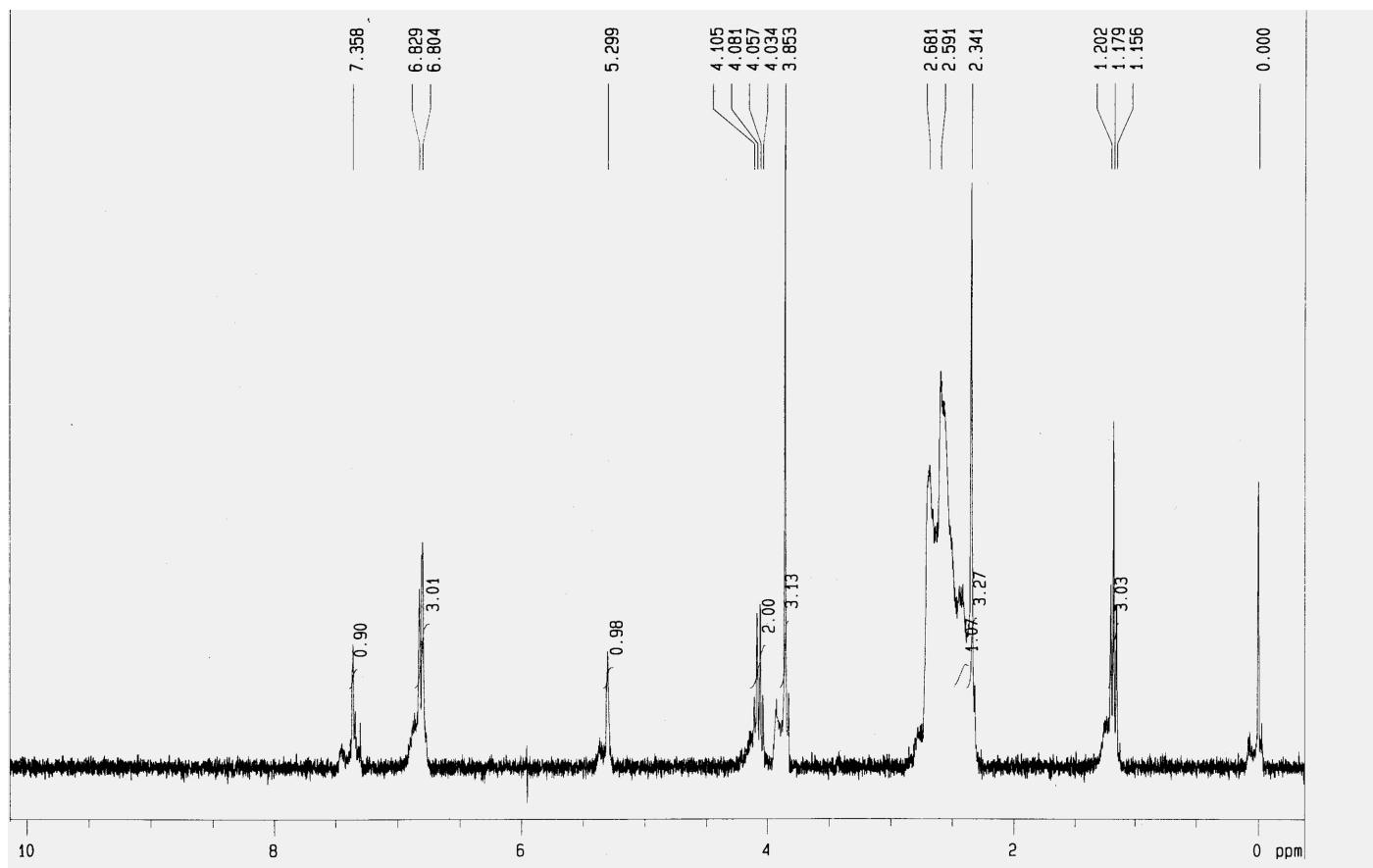
PYRO6:



PYRO7:



PYRO8:



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