Supplementary Information for

D-xylonic Acid: A Solvent and Effective Biocatalyst for Three-component Reaction

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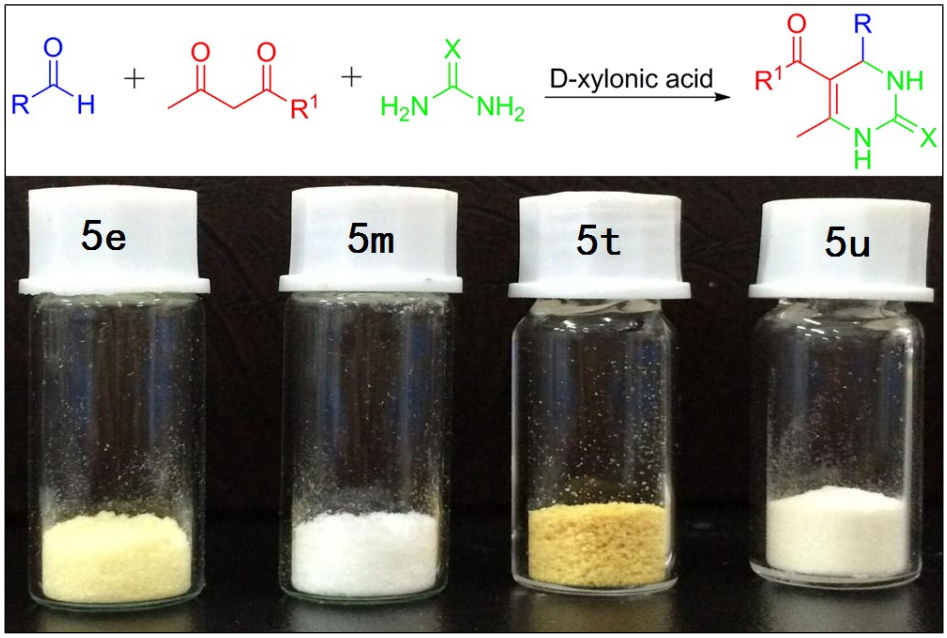
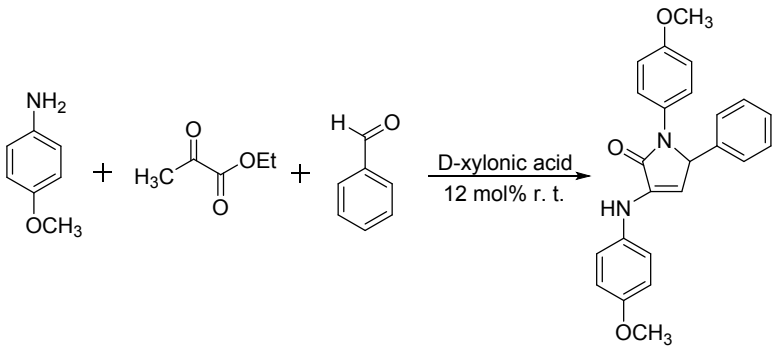
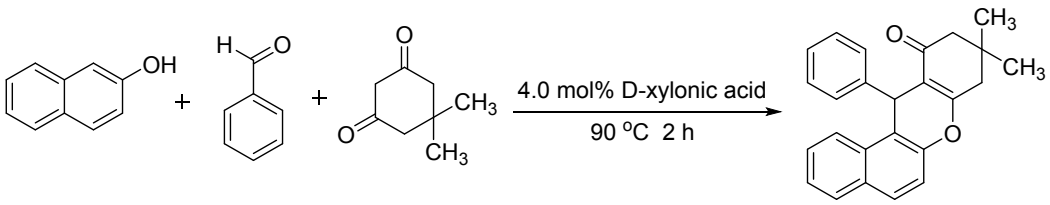


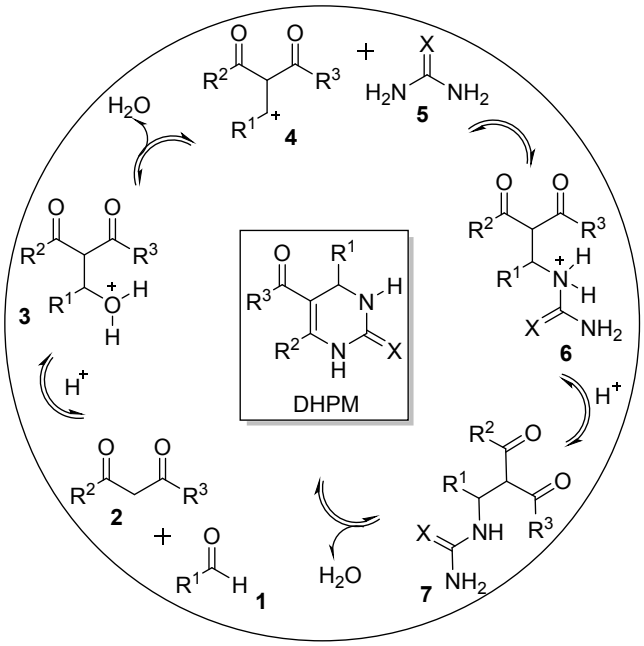
Summary



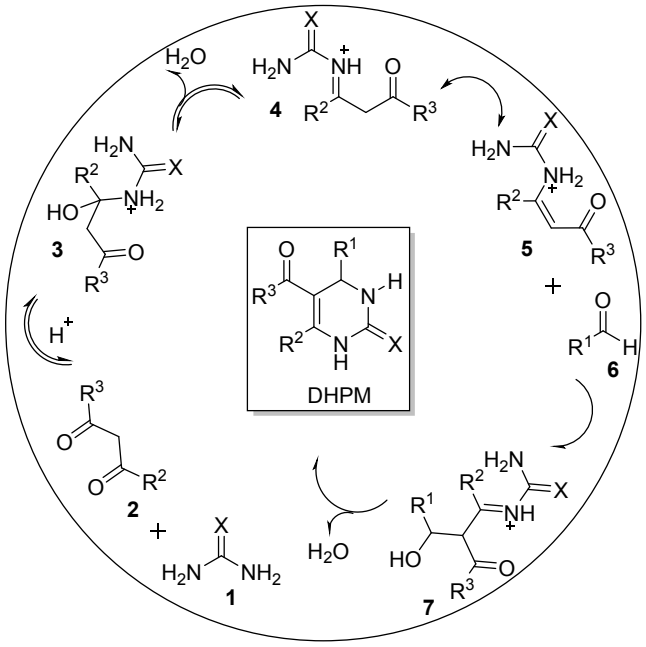
Scheme S1 D-xylonic acid catalyzed for the synthesis of 5-phenyl-1(4-methoxyphenyl)-3[(4-methoxyphenyl)-amino]-1*H*-pyrrol-2(5*H*)-one.



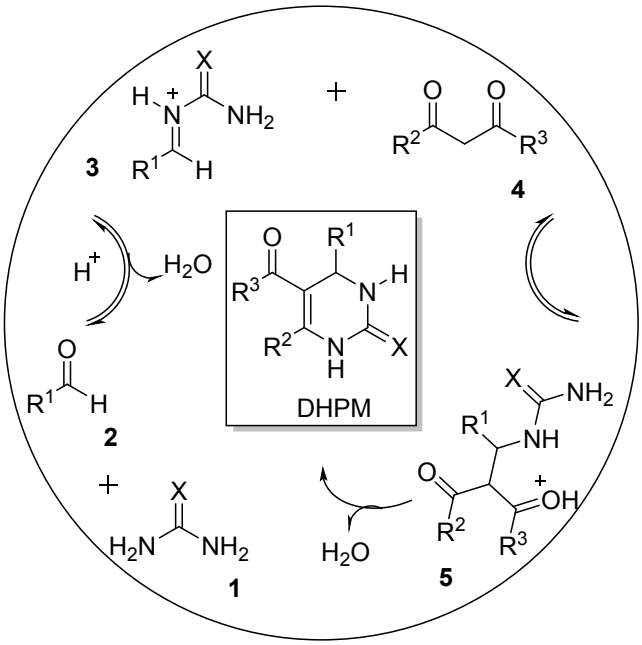
Scheme S2 D-xylonic acid catalyzed for the synthesis of 12-phenyl-9,9-dimethyl-8,9,10,12-tetrahydrobenzo[*a*]xanthen-11-one.



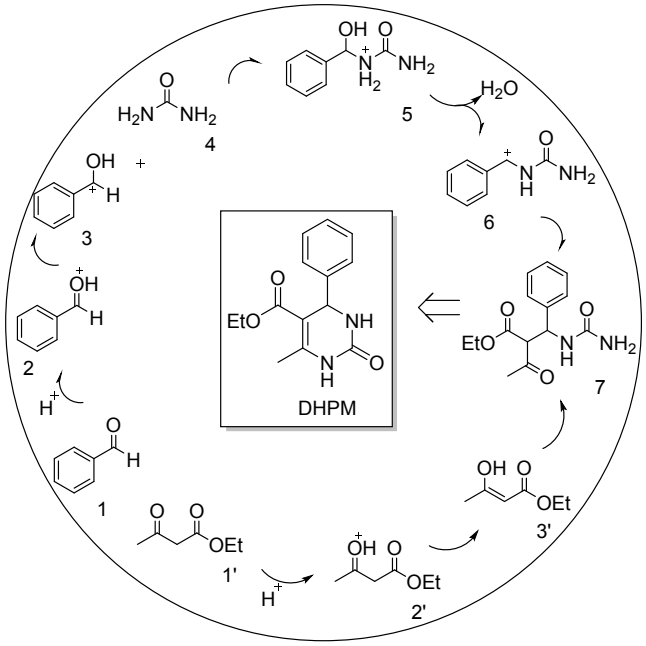
Scheme S3 The Knoevenagel mechanism for the Biginelli reaction.



Scheme S4 The enamine-based mechanism for the Biginelli reaction.

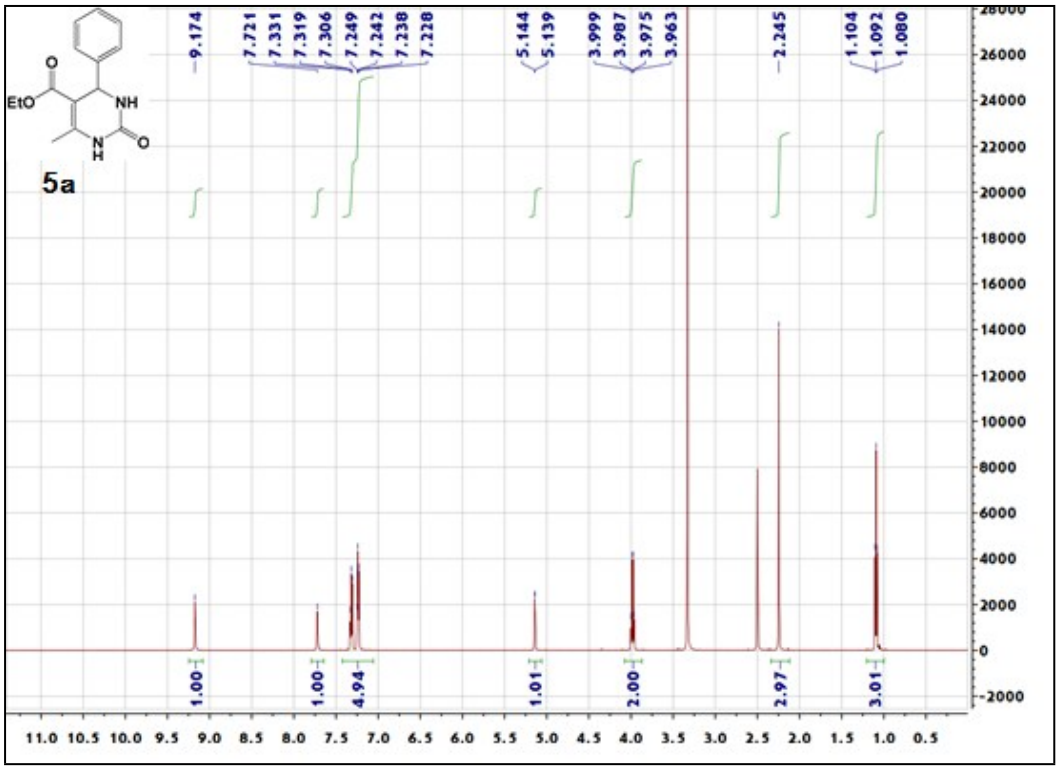


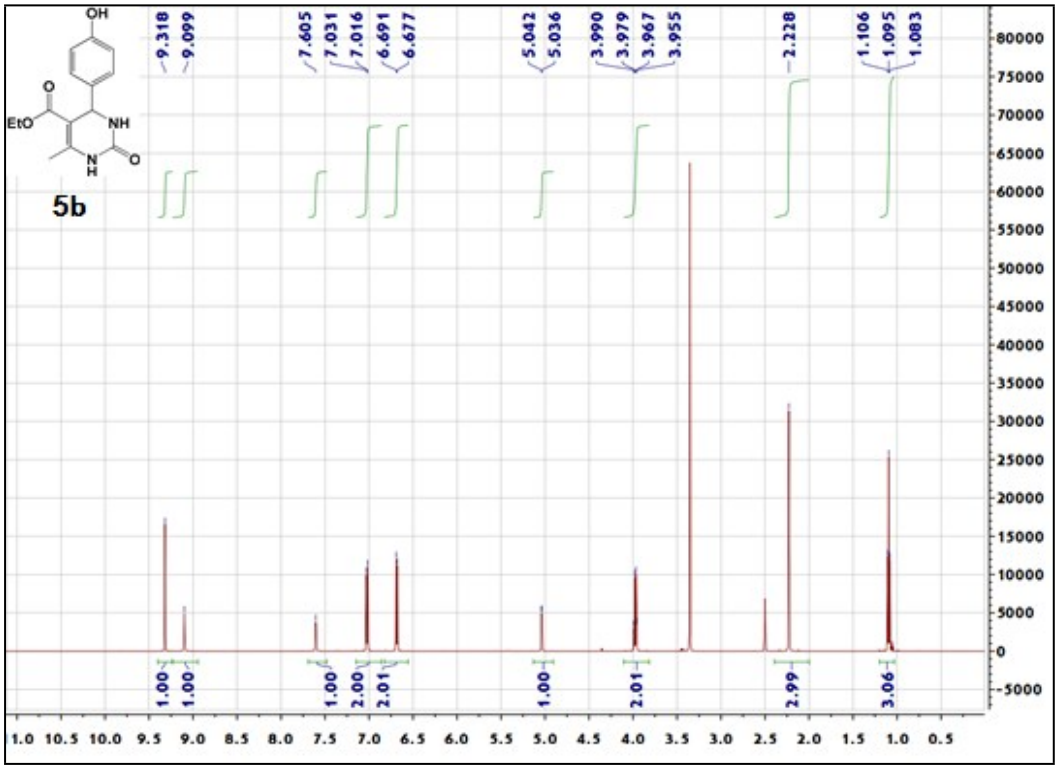
Scheme S5 The iminium mechanism for the Biginelli reaction .

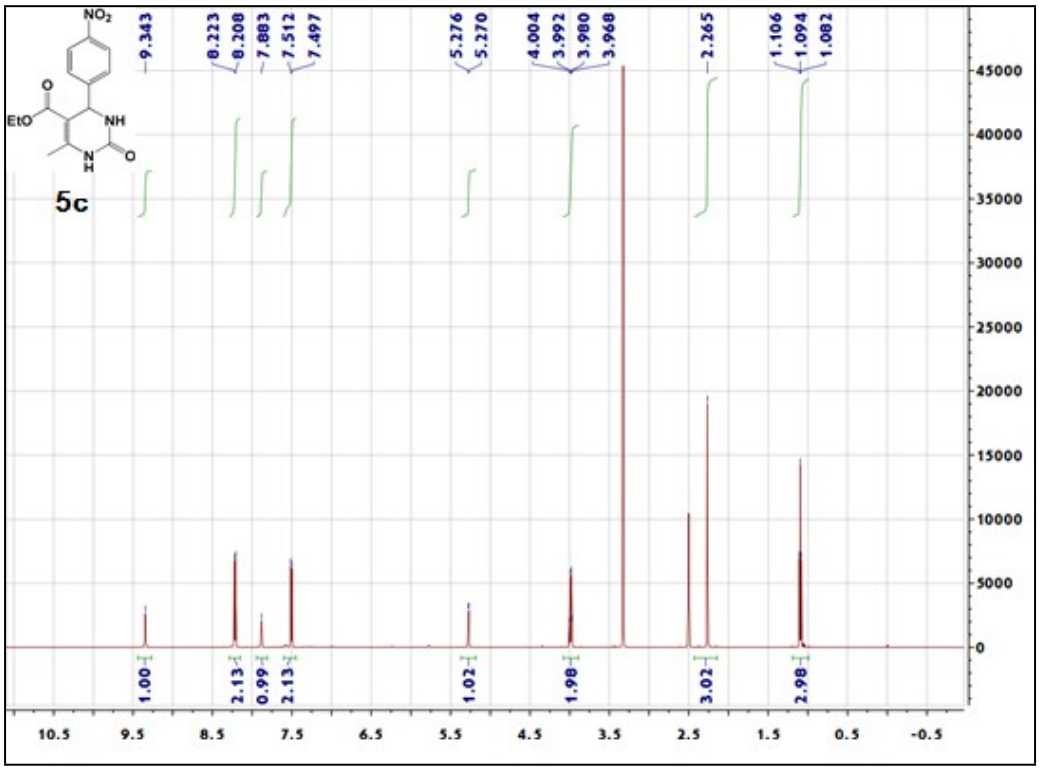


Scheme S6 A plausible mechanism of D-xylonic acid-catalyzed three-component Biginelli condensation reaction .

[1]H NMR for all compounds



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8.208
7.883
7.512
7.497
5.276
5.270
4.004
3.992
3.980
3.968
2.265
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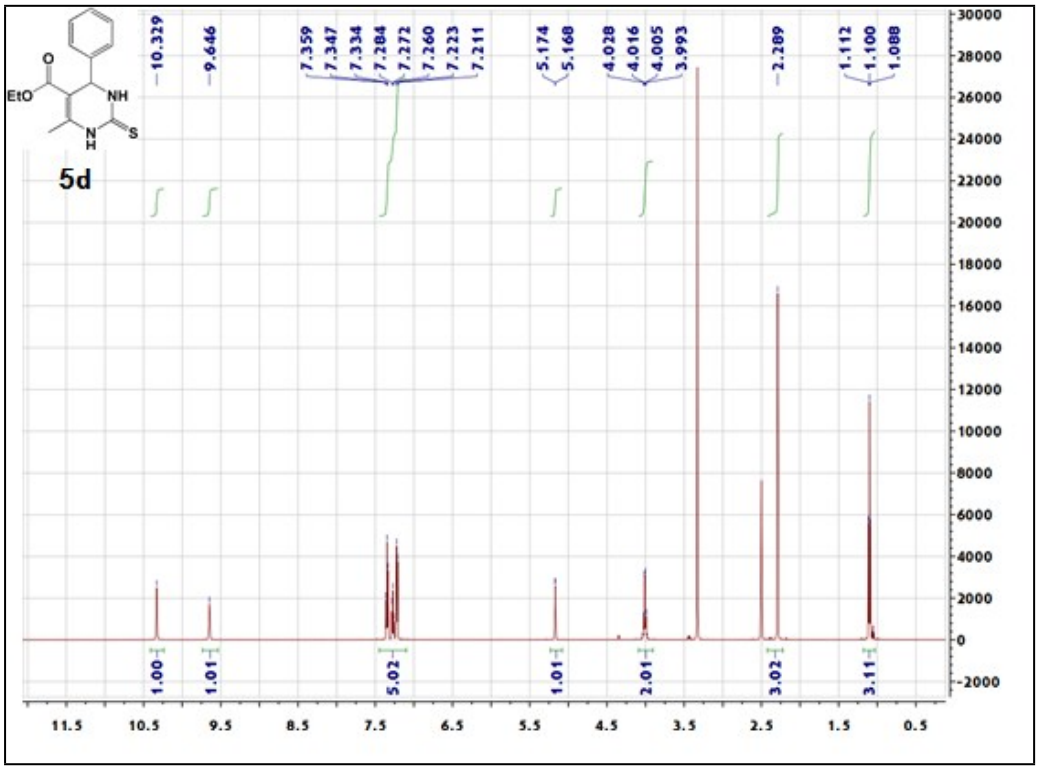
1.094
1.082
1.00
2.13
0.99
2.13
1.02
1.98
3.02
2.98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7.359
7.347
7.334
7.284
7.272
7.260
7.223
7.211
5.174
5.168
4.028
4.016
4.005
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1.00
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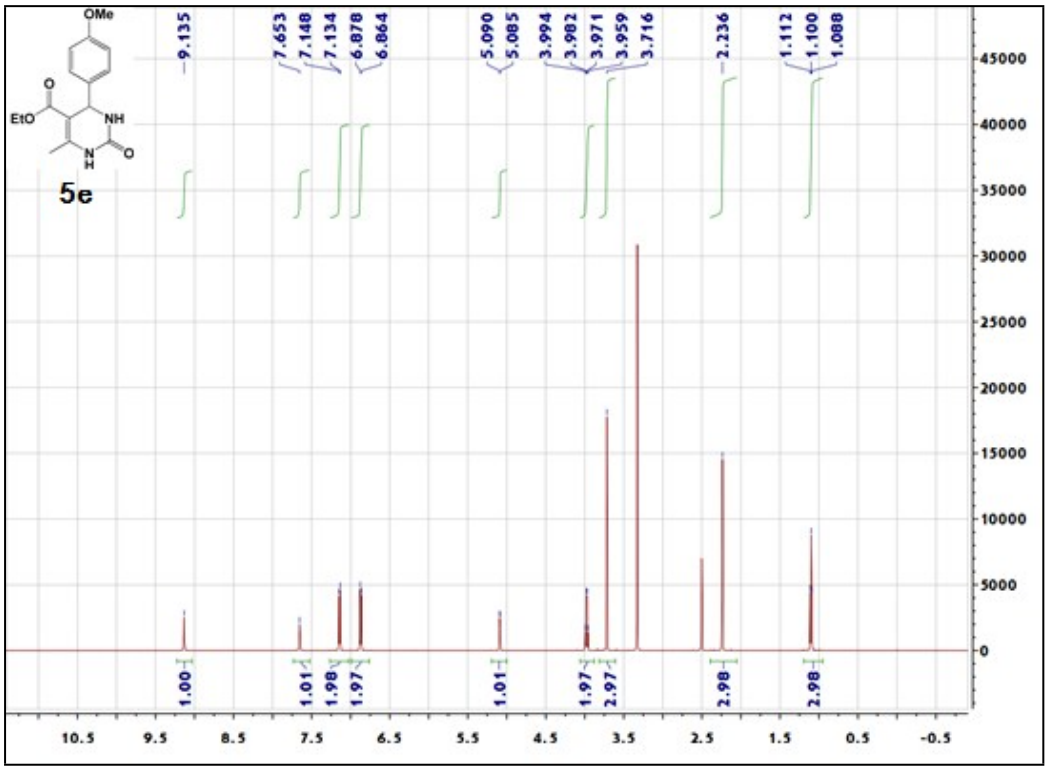
3.11



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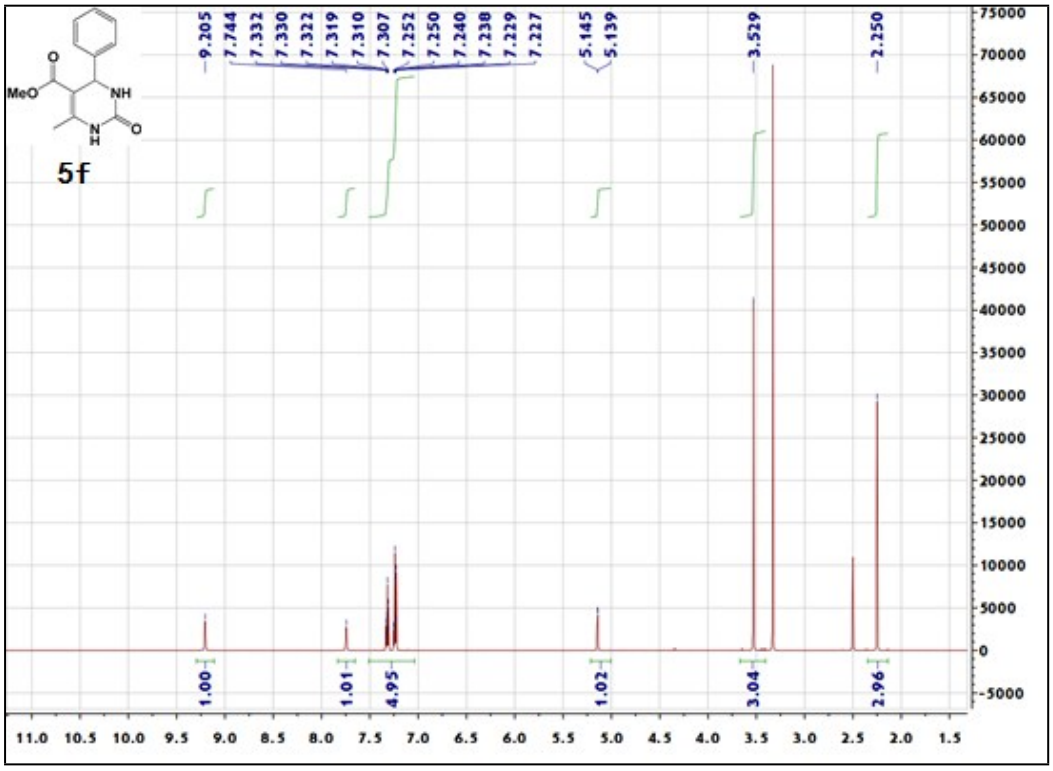

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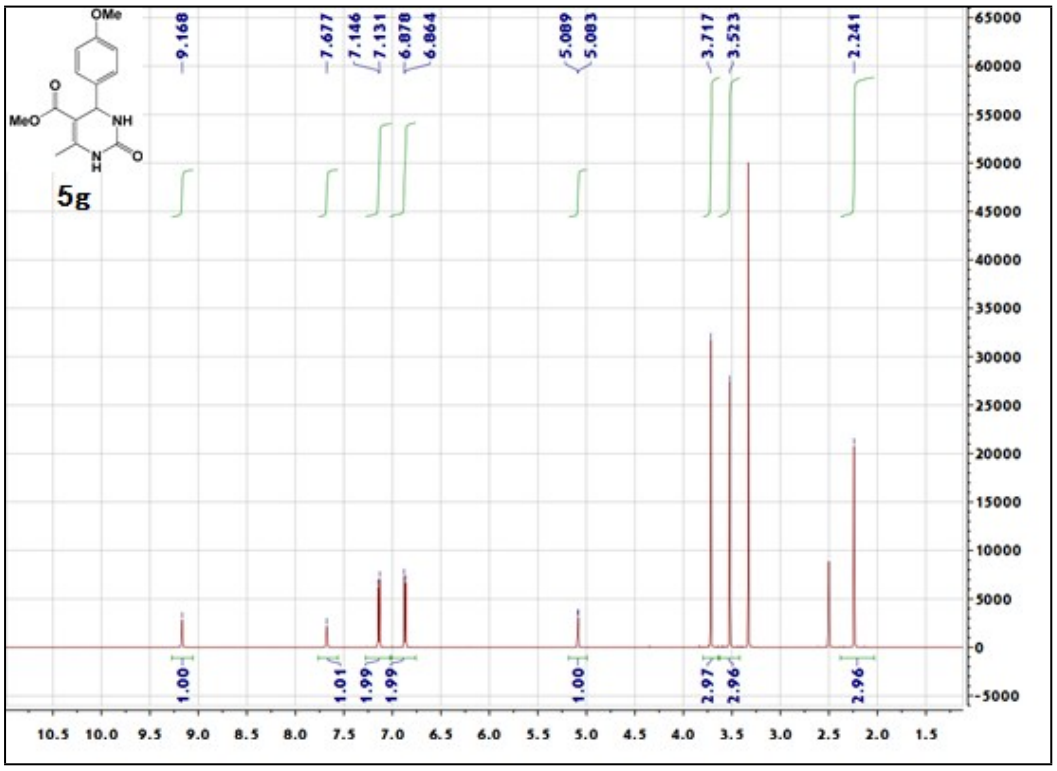

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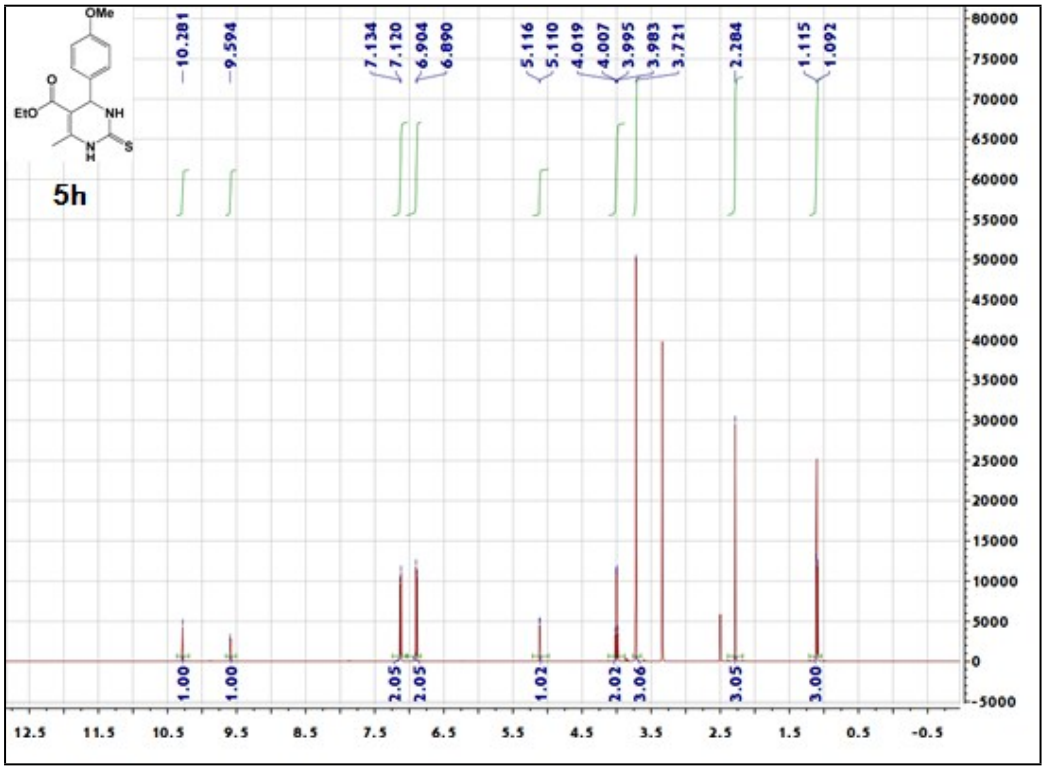

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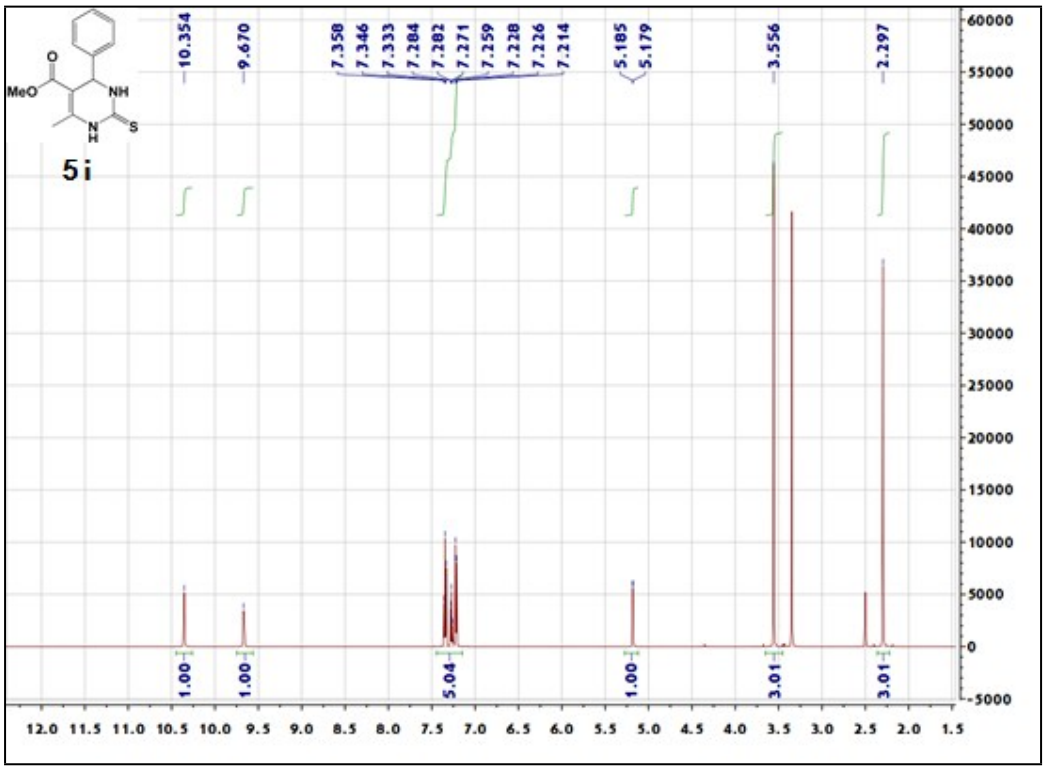

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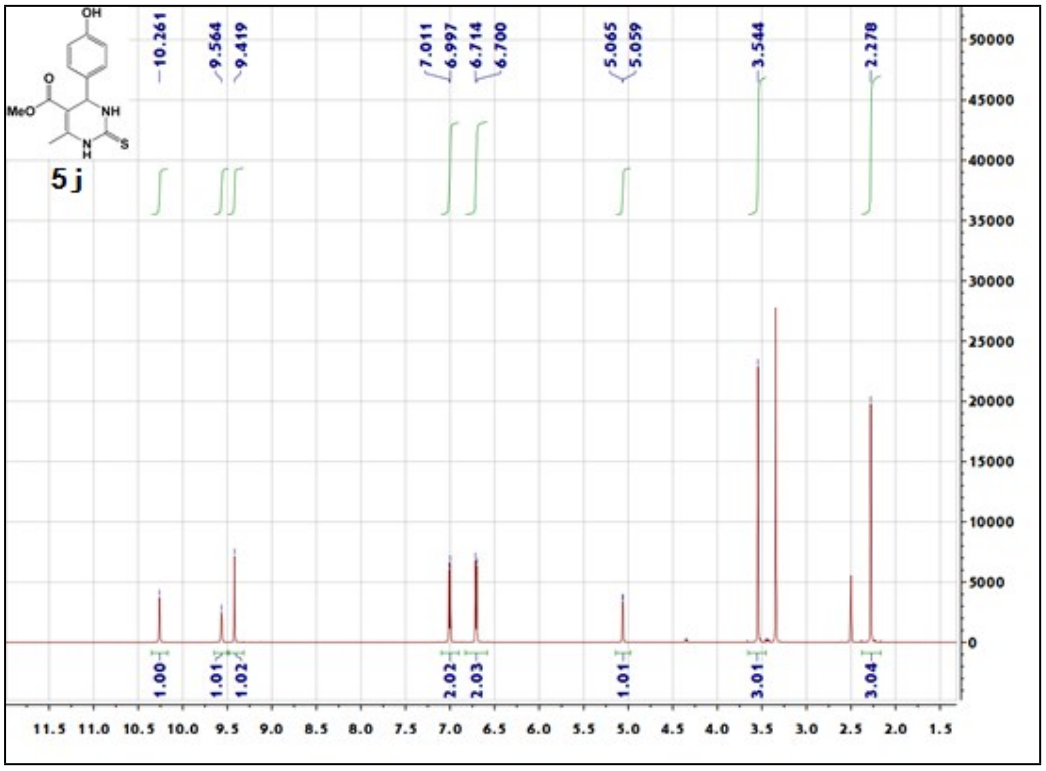

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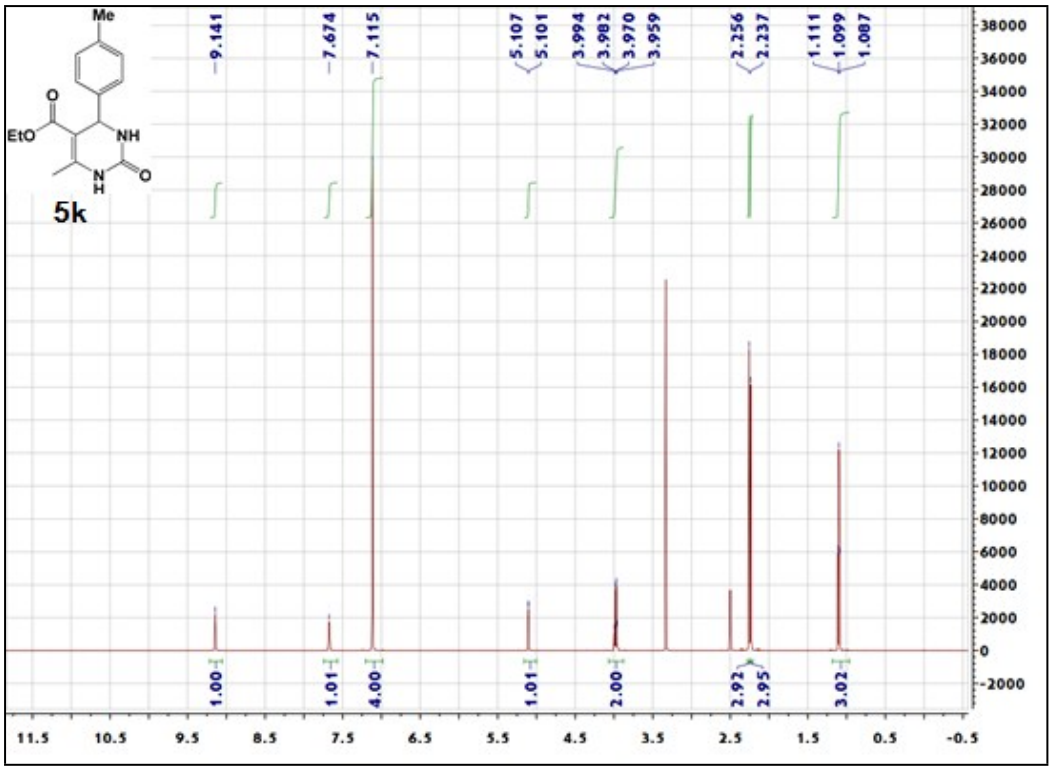

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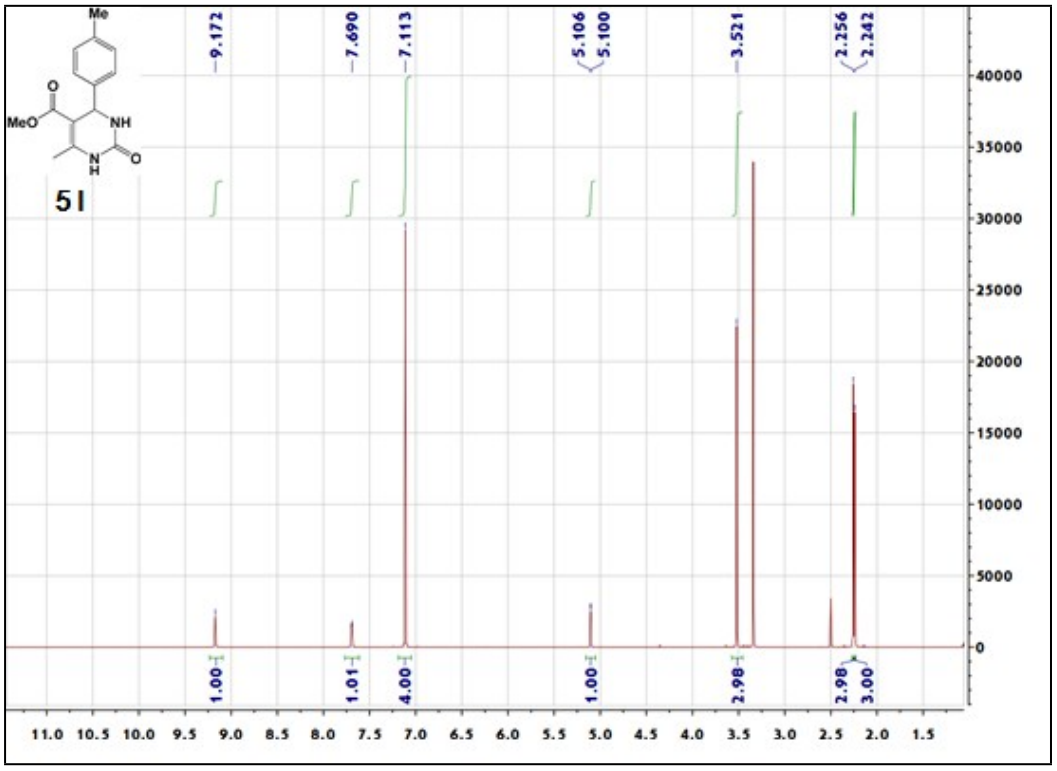

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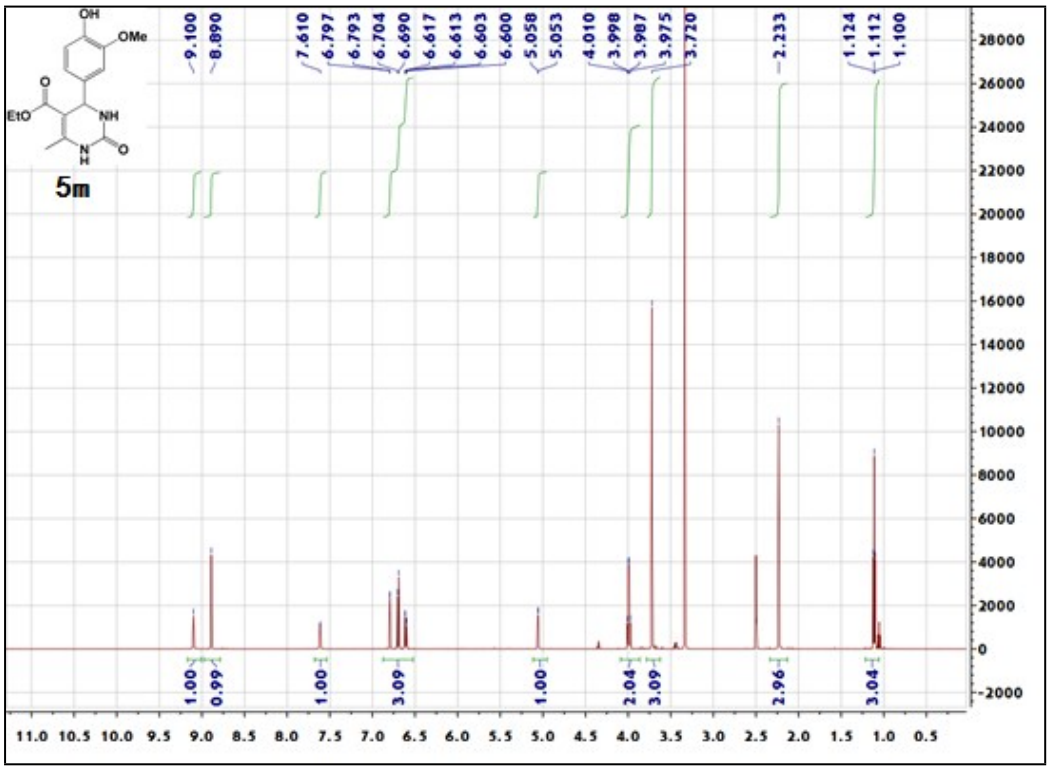

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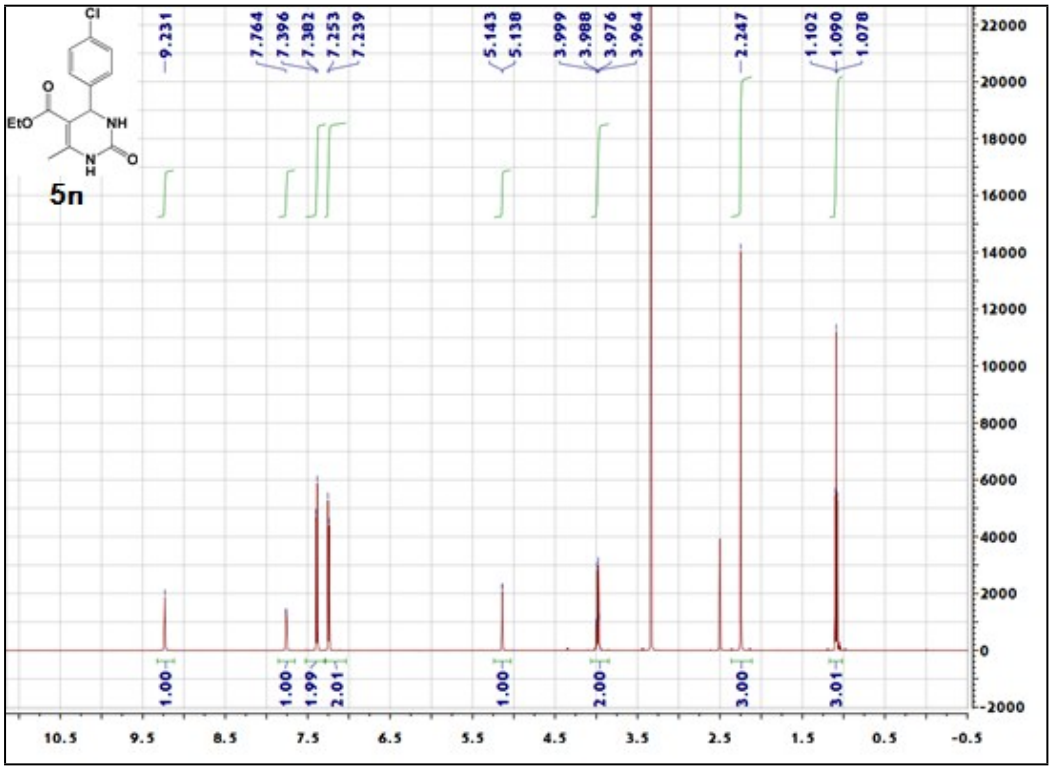

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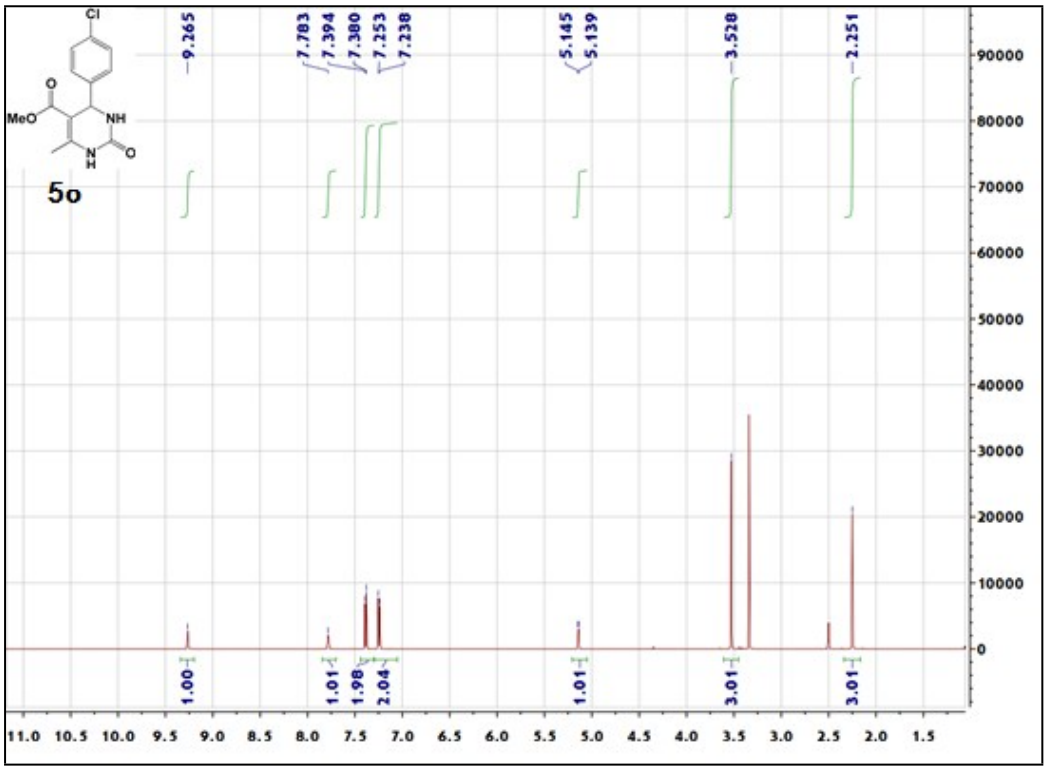
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1.98
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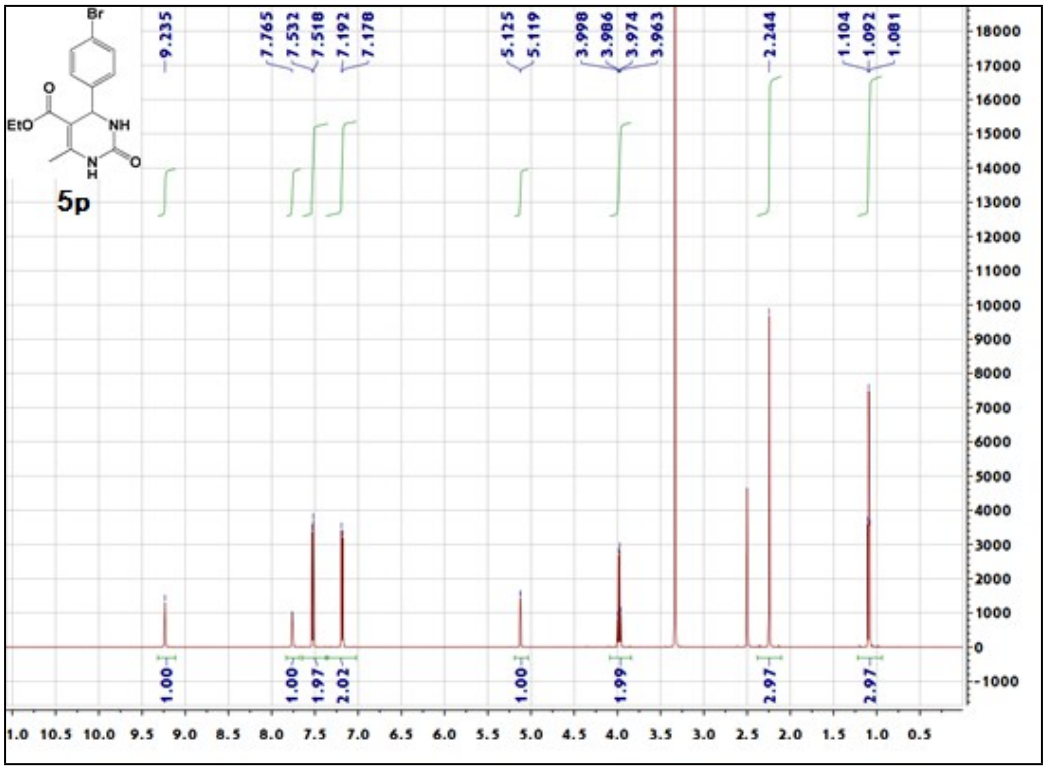
1.01
3.01
3.01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3.986
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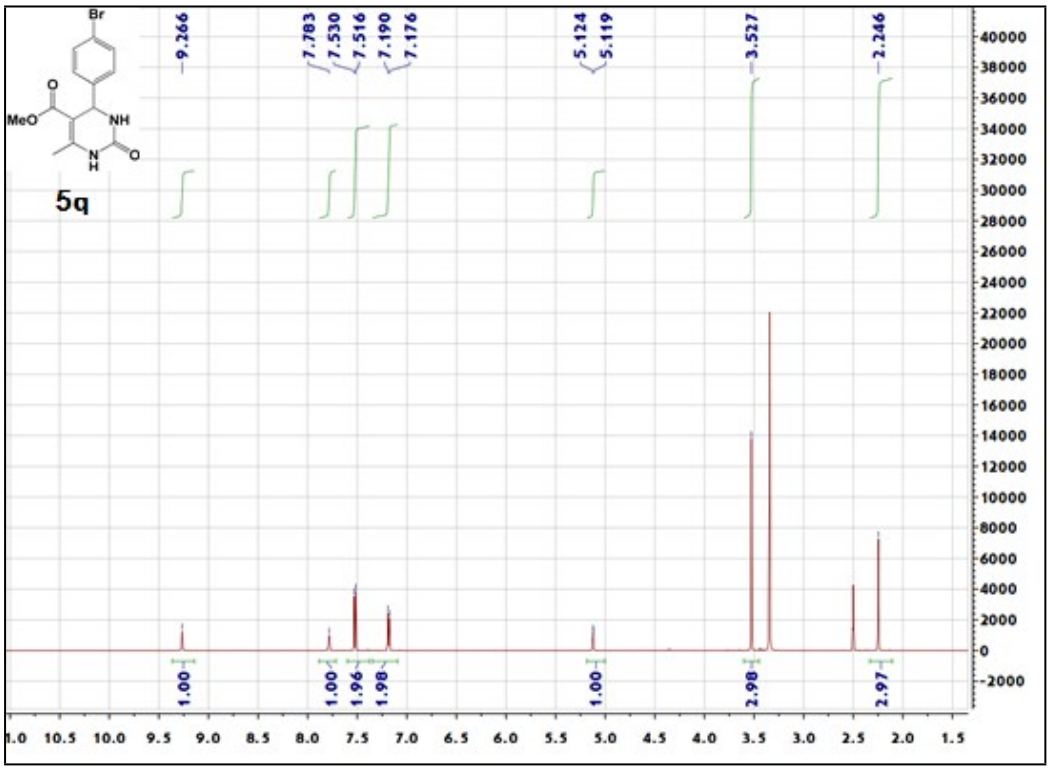

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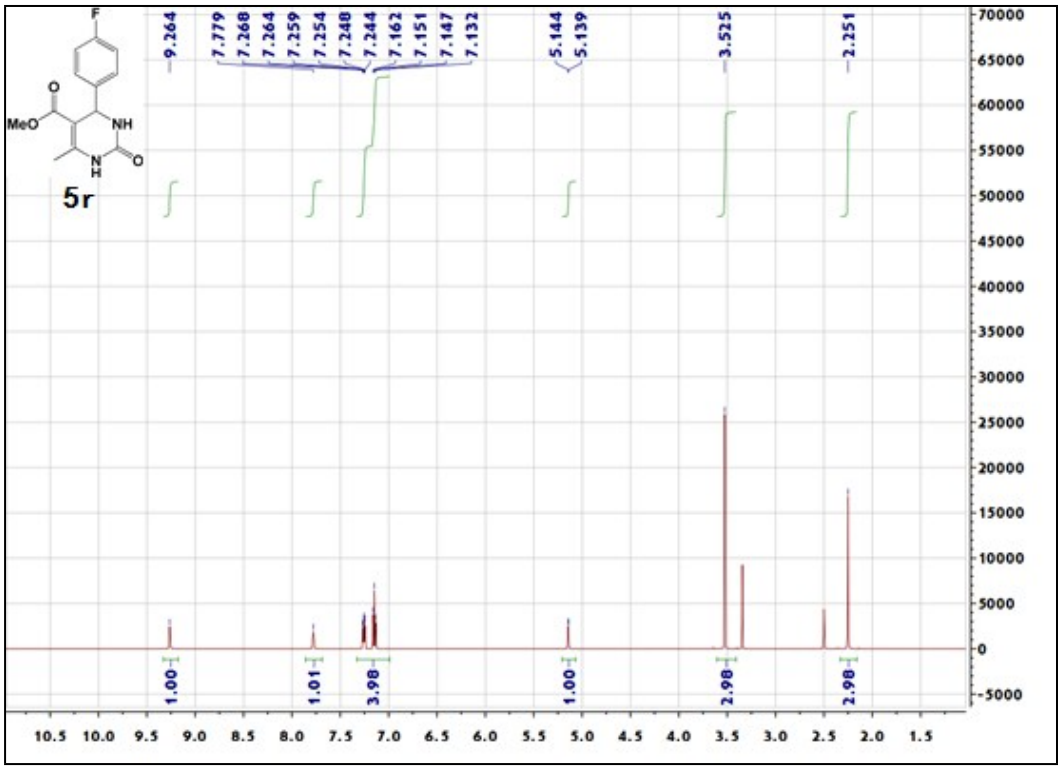

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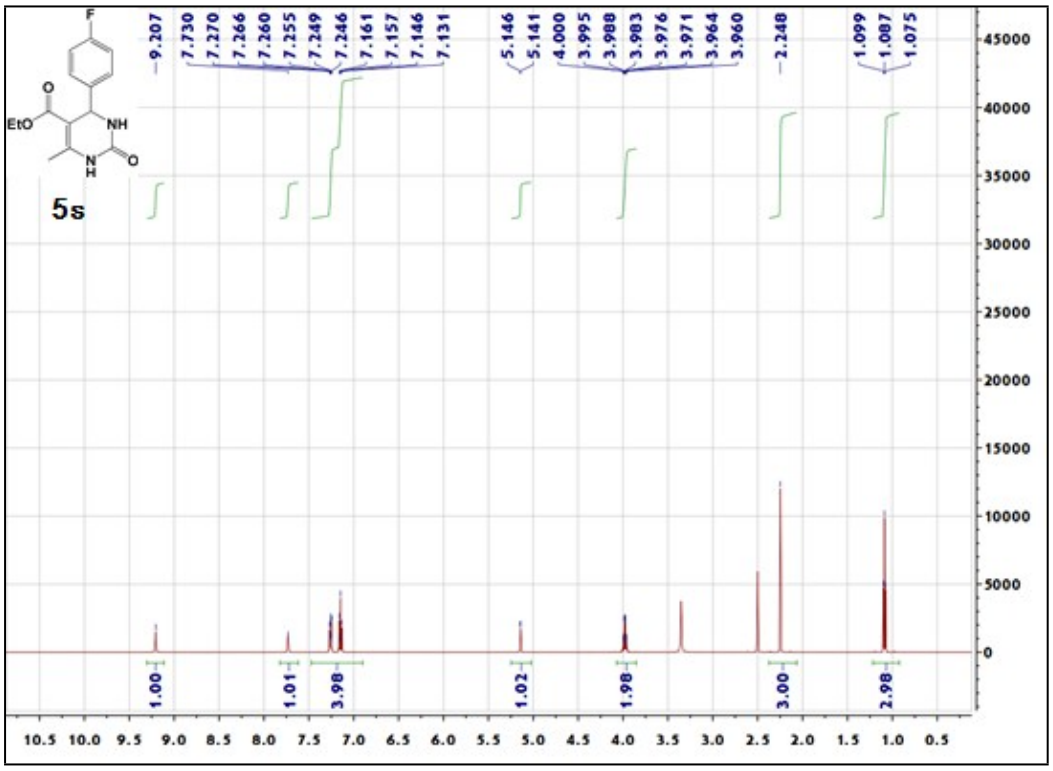

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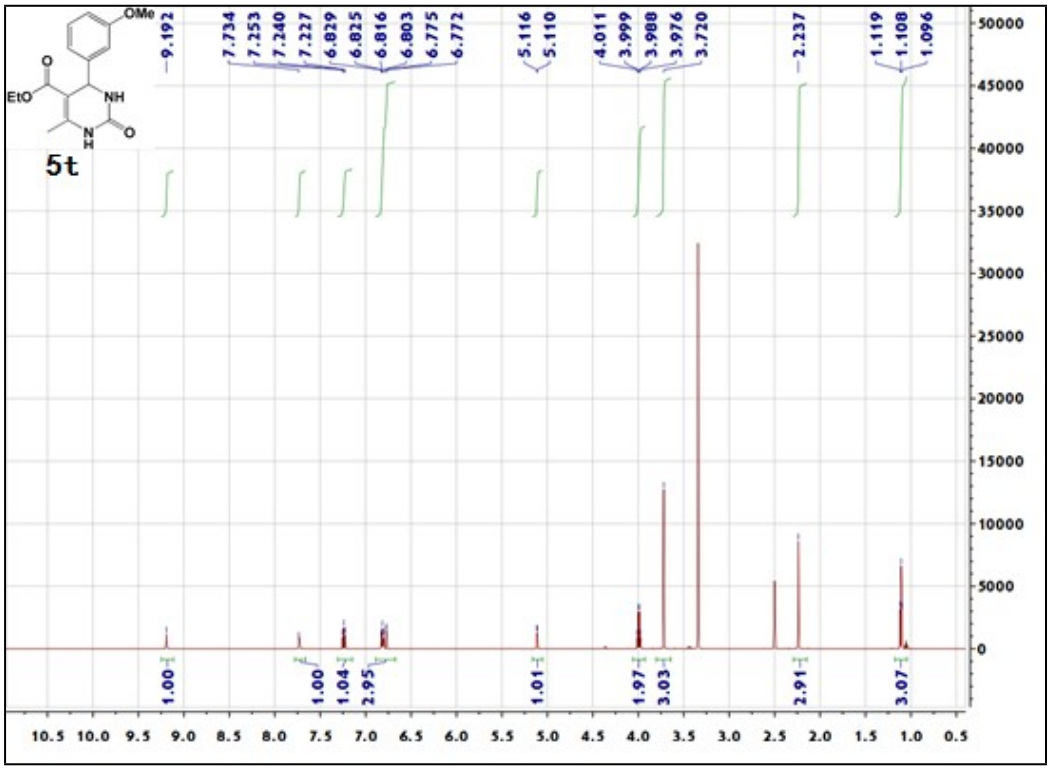

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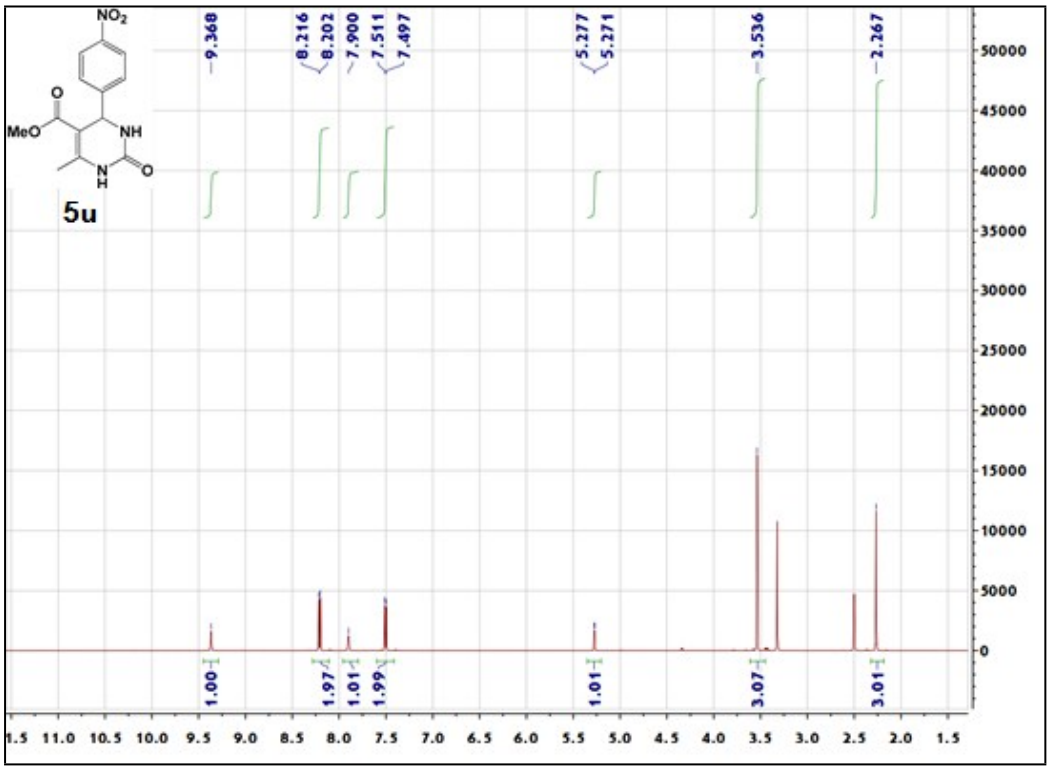

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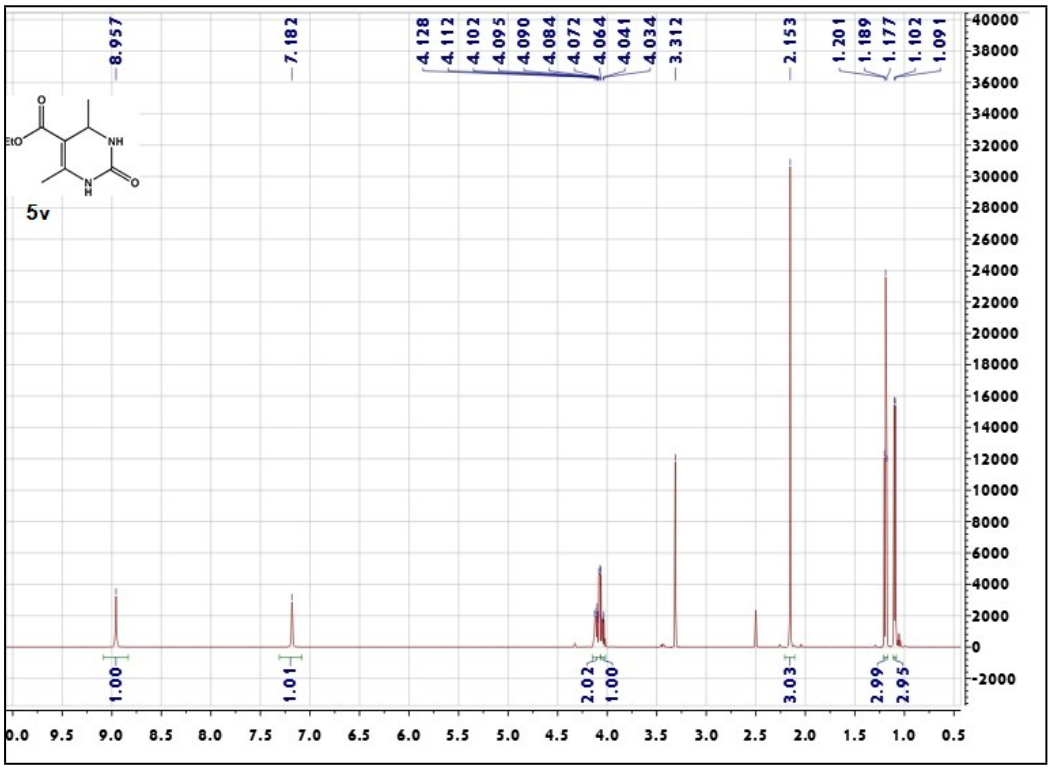

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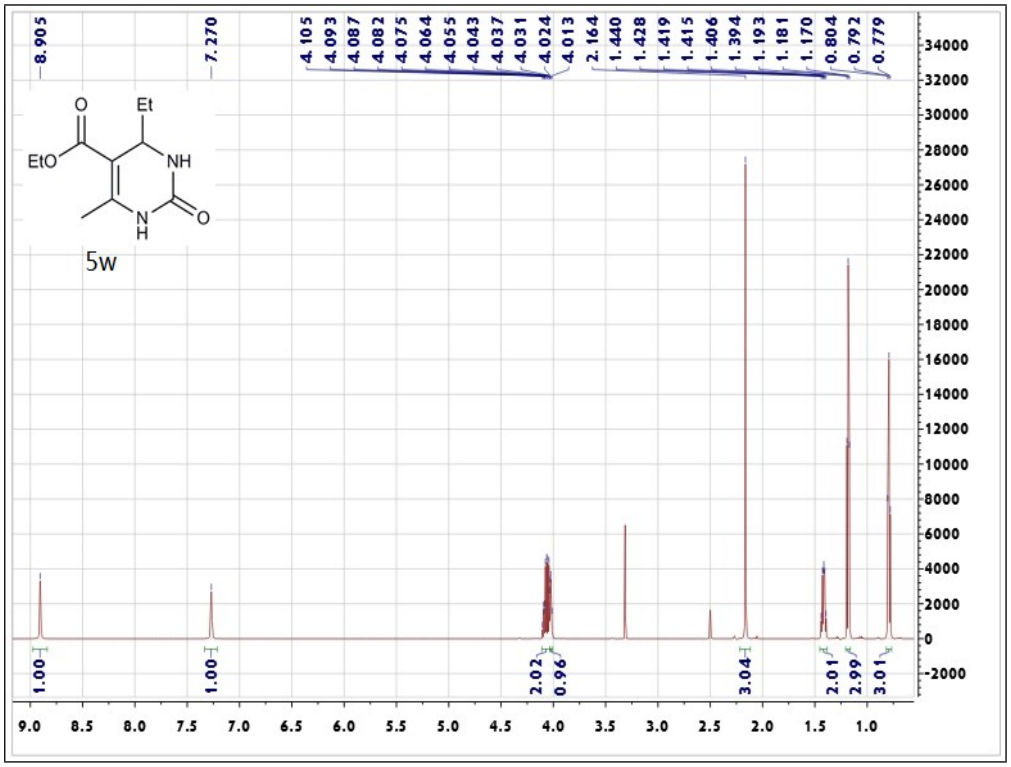

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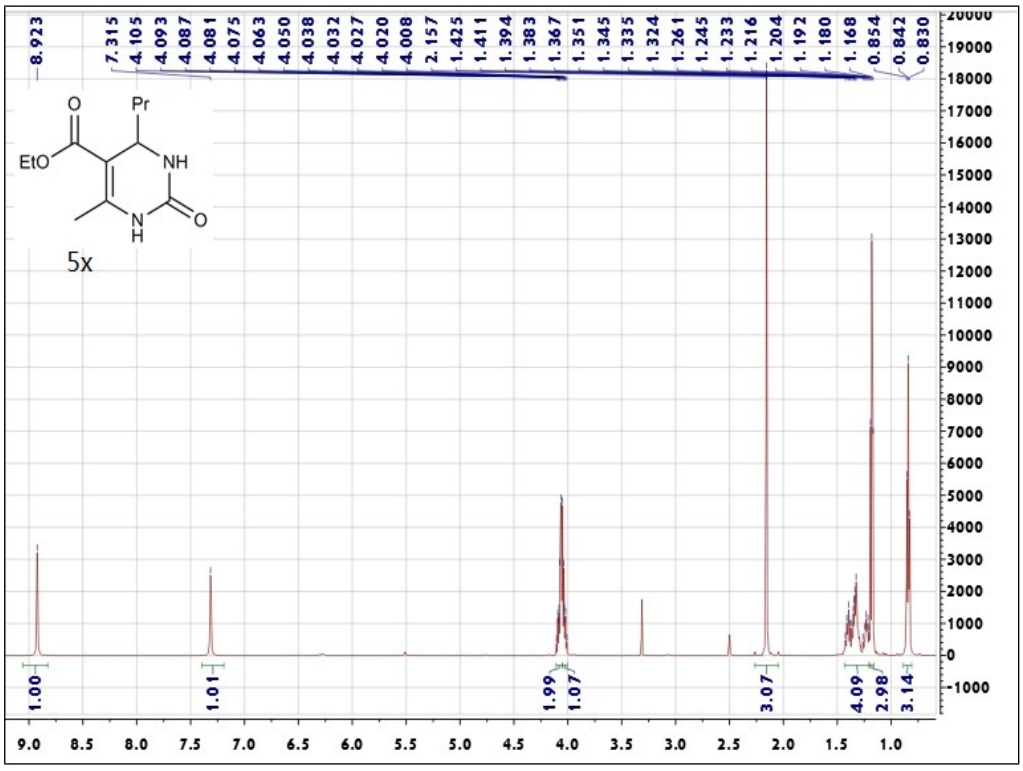

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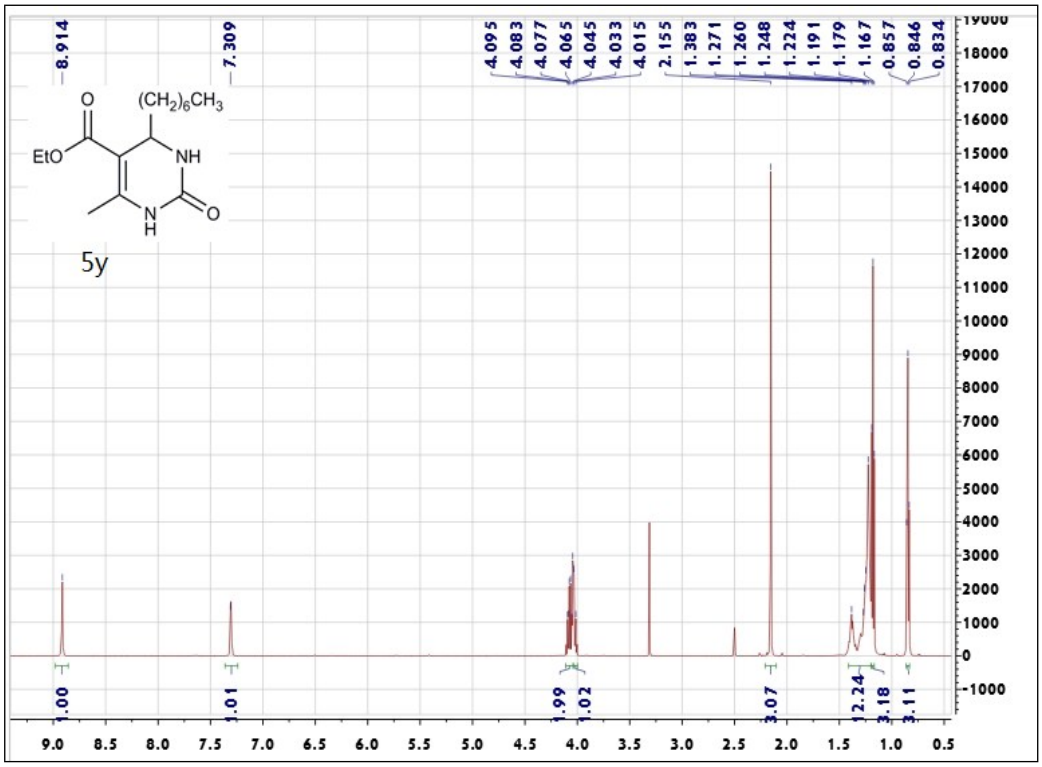

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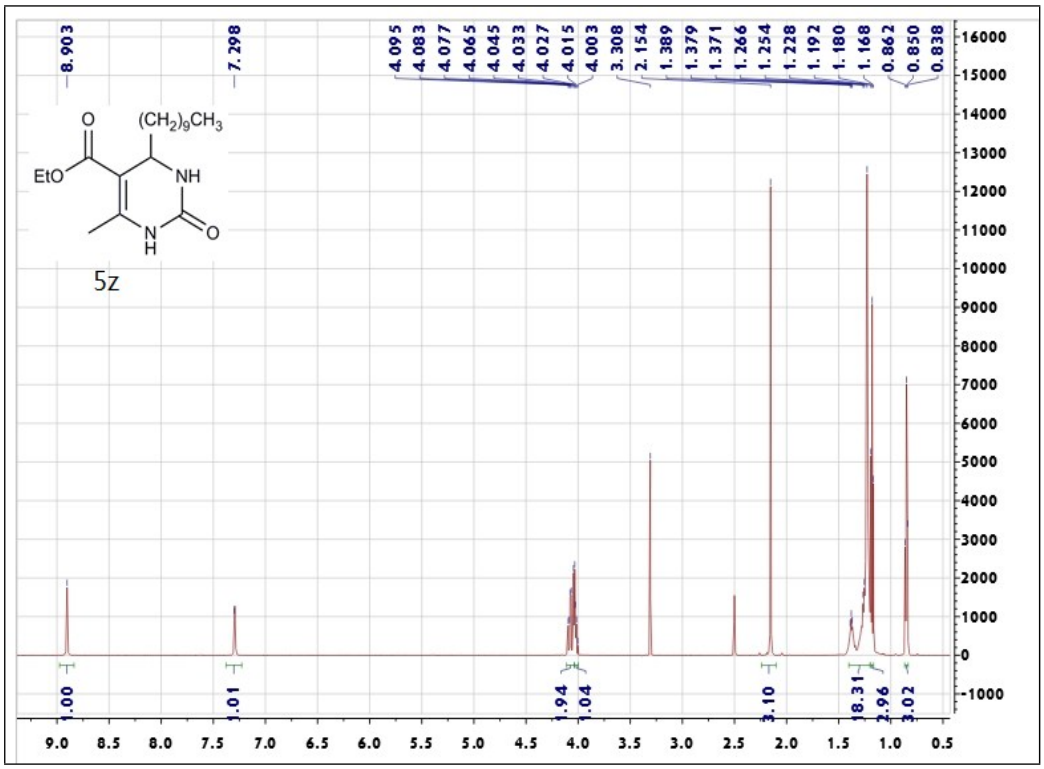

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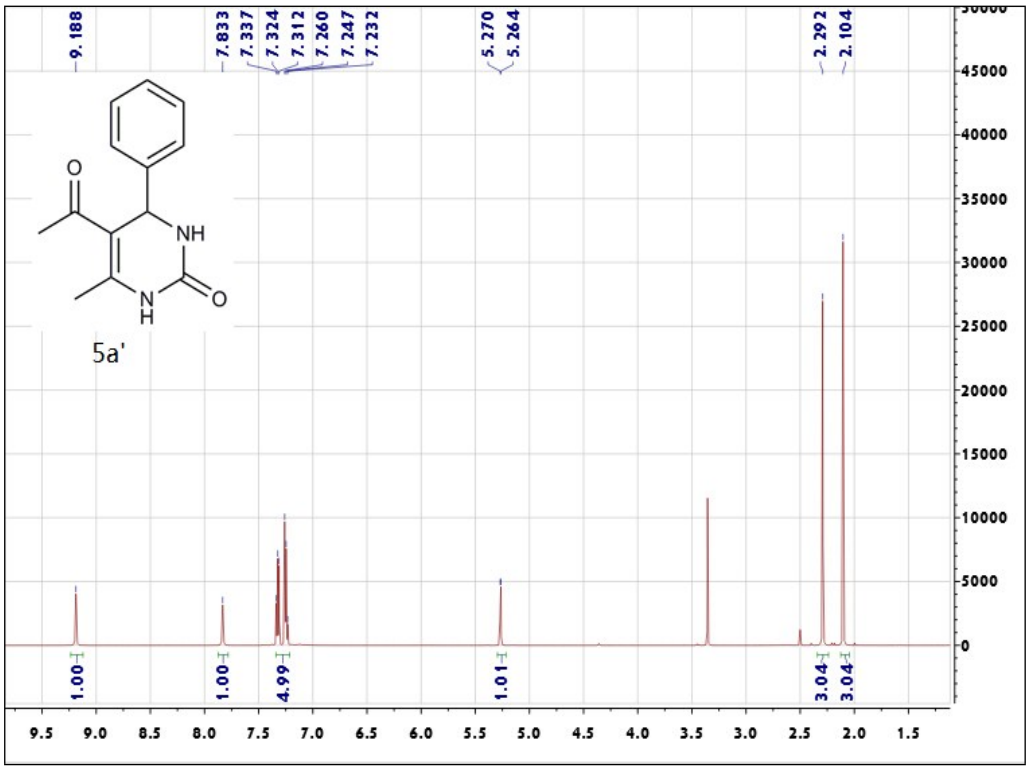

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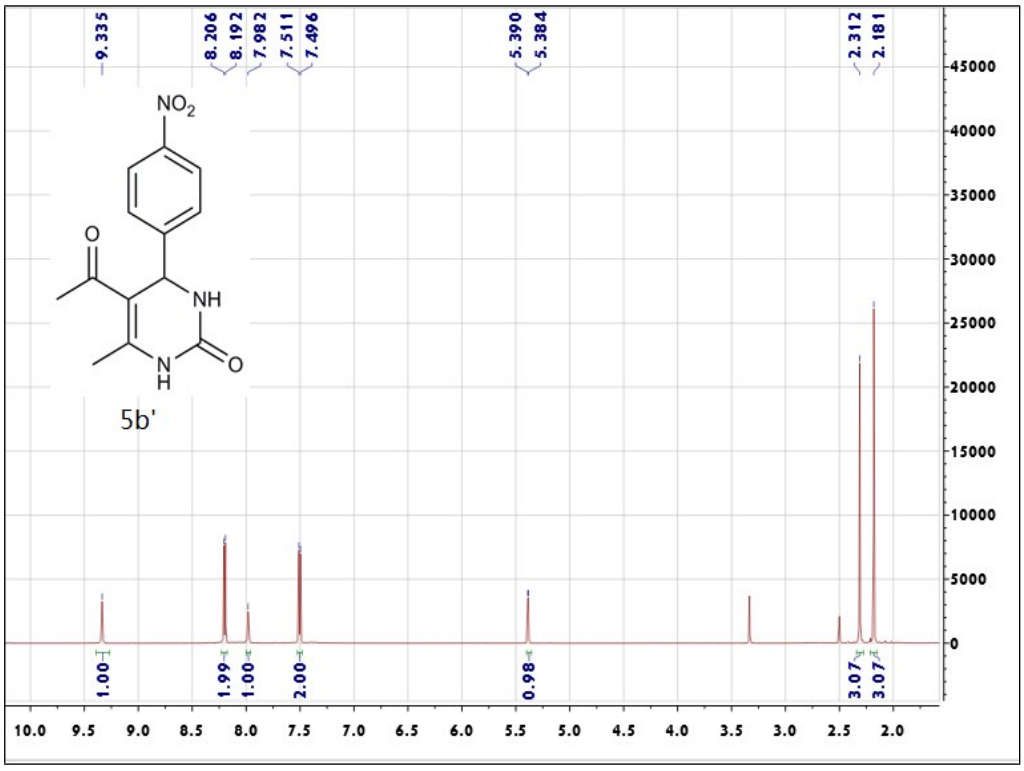

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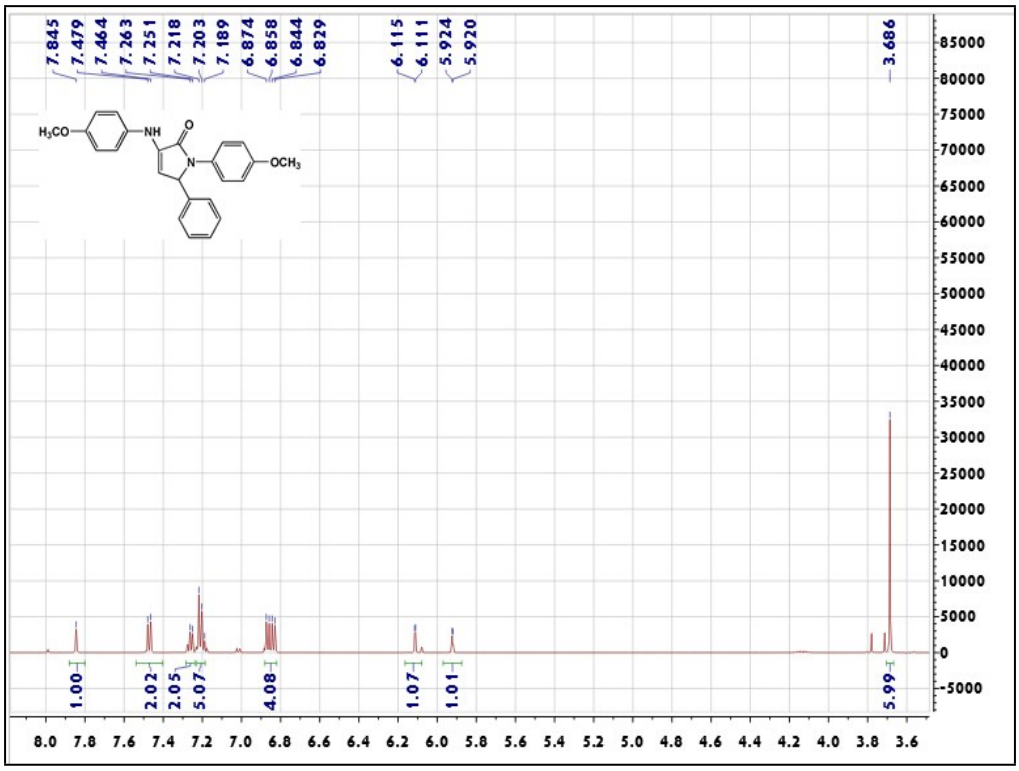

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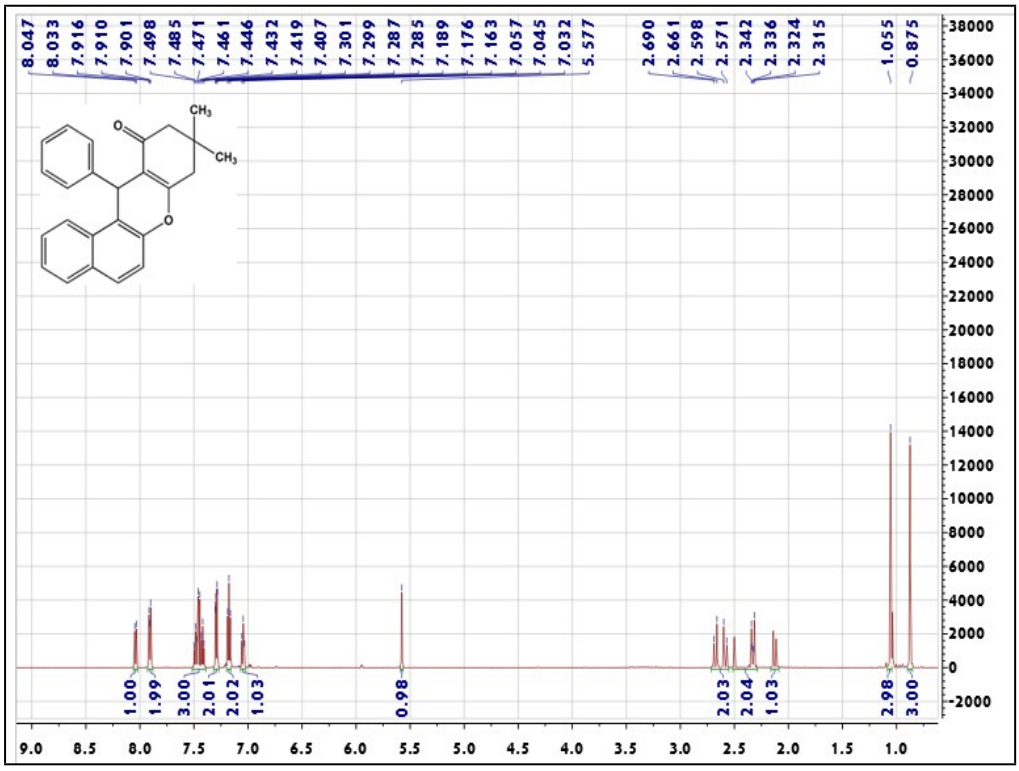

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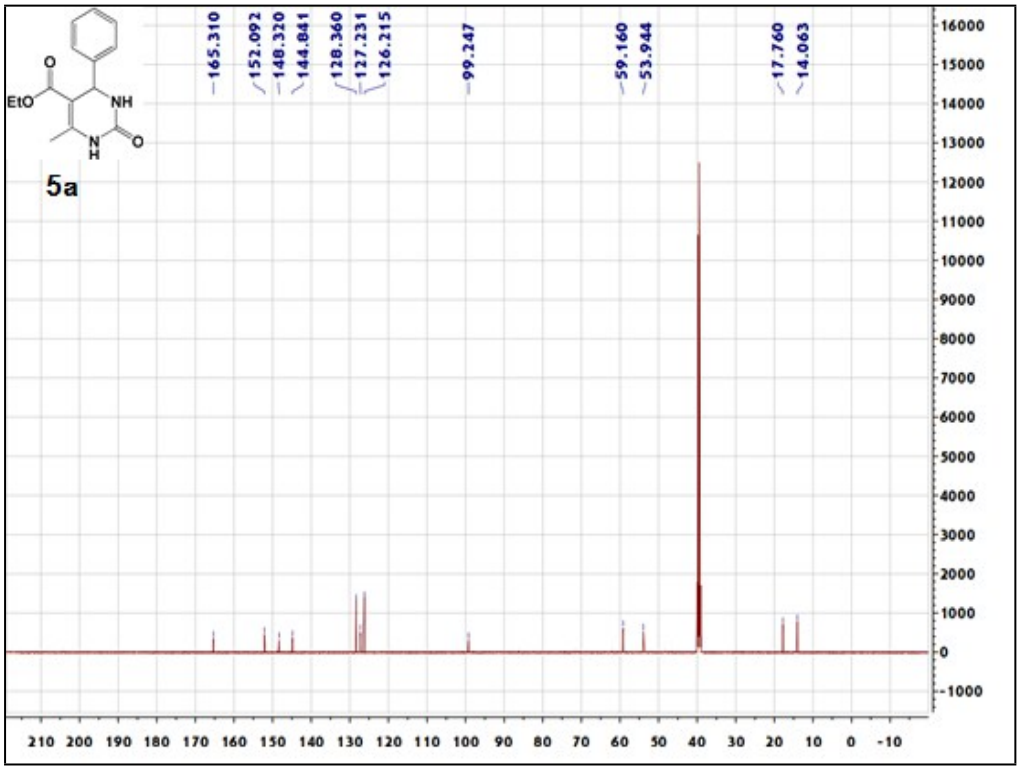
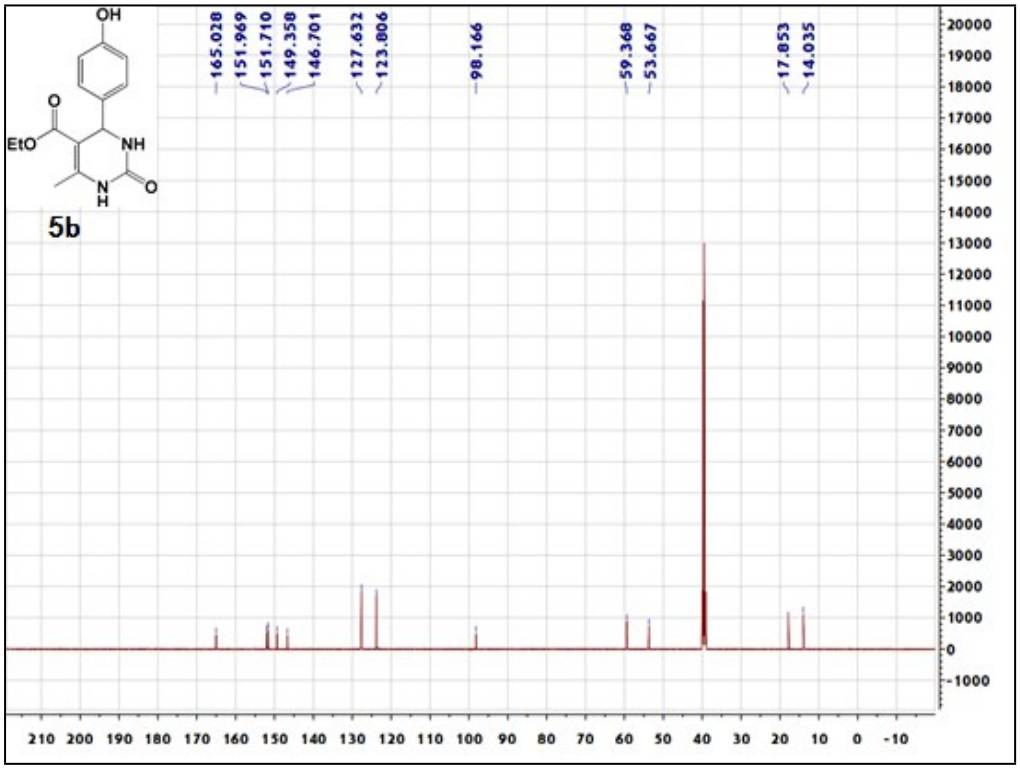
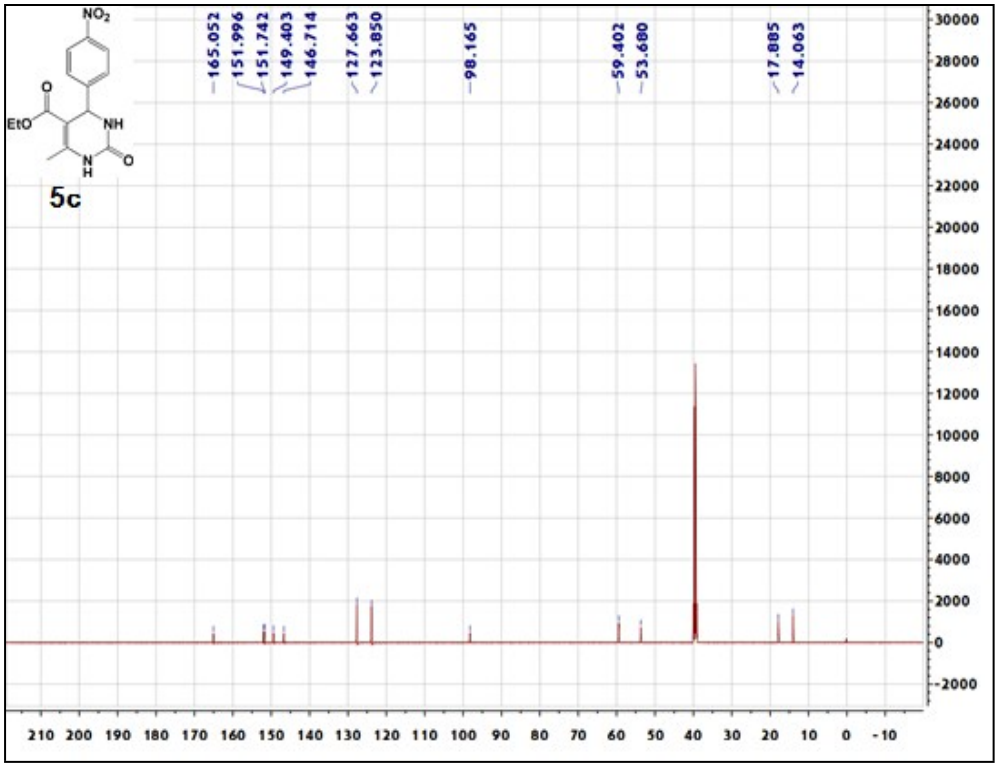
^{13}C NMR for all compounds







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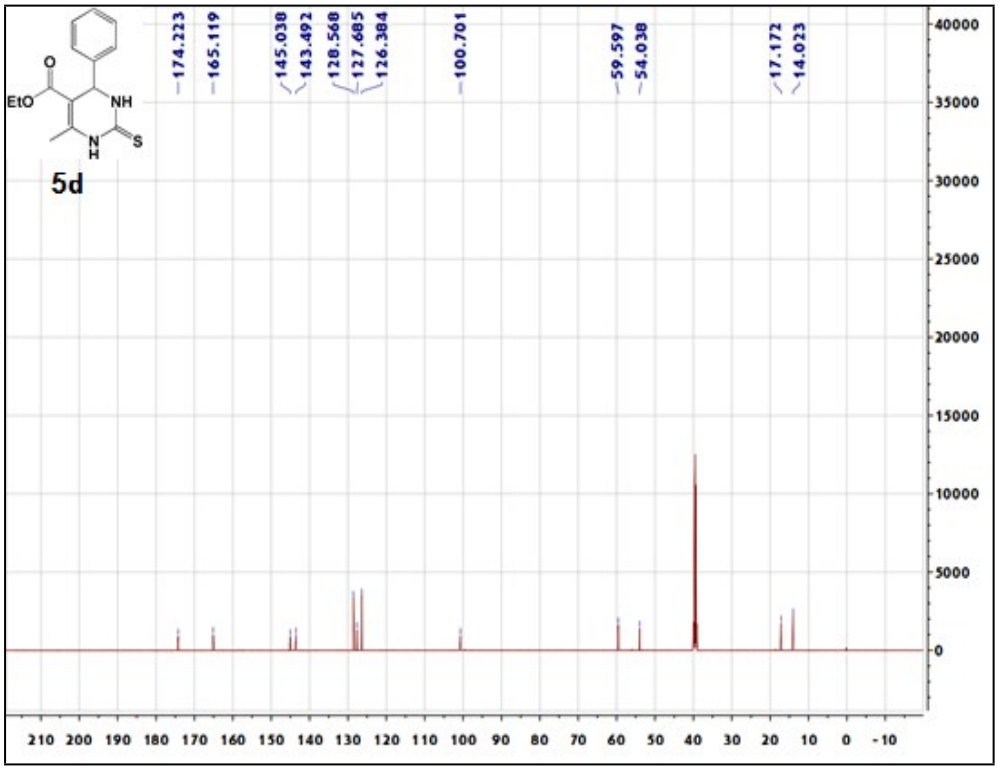

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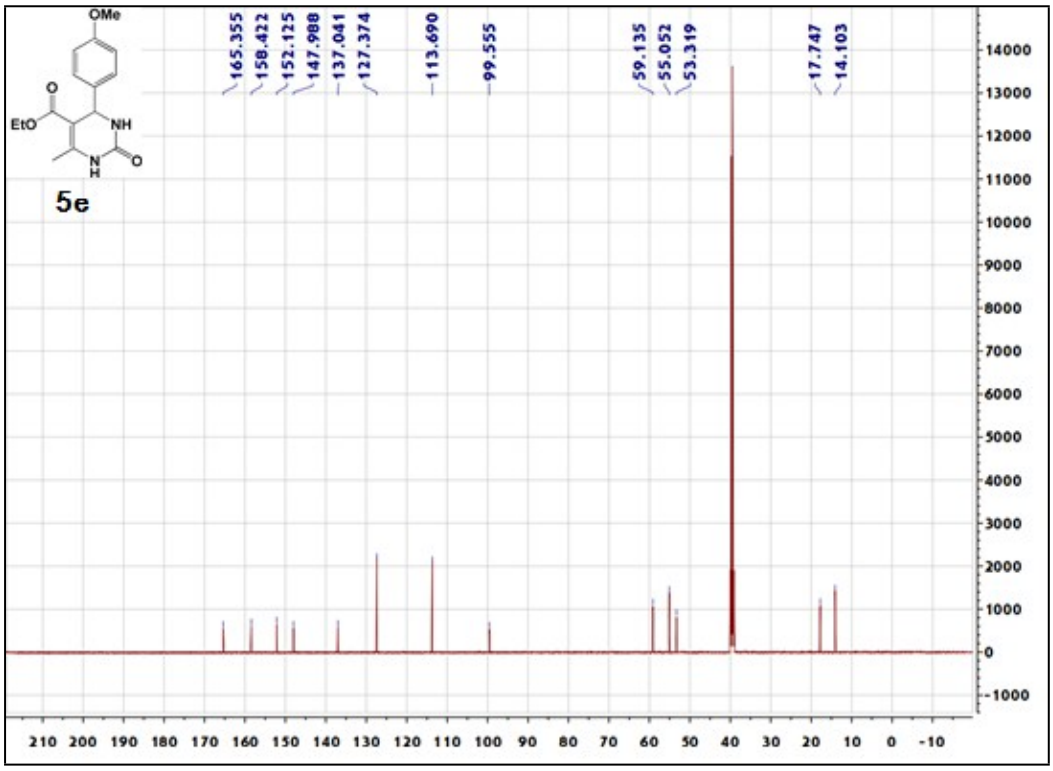

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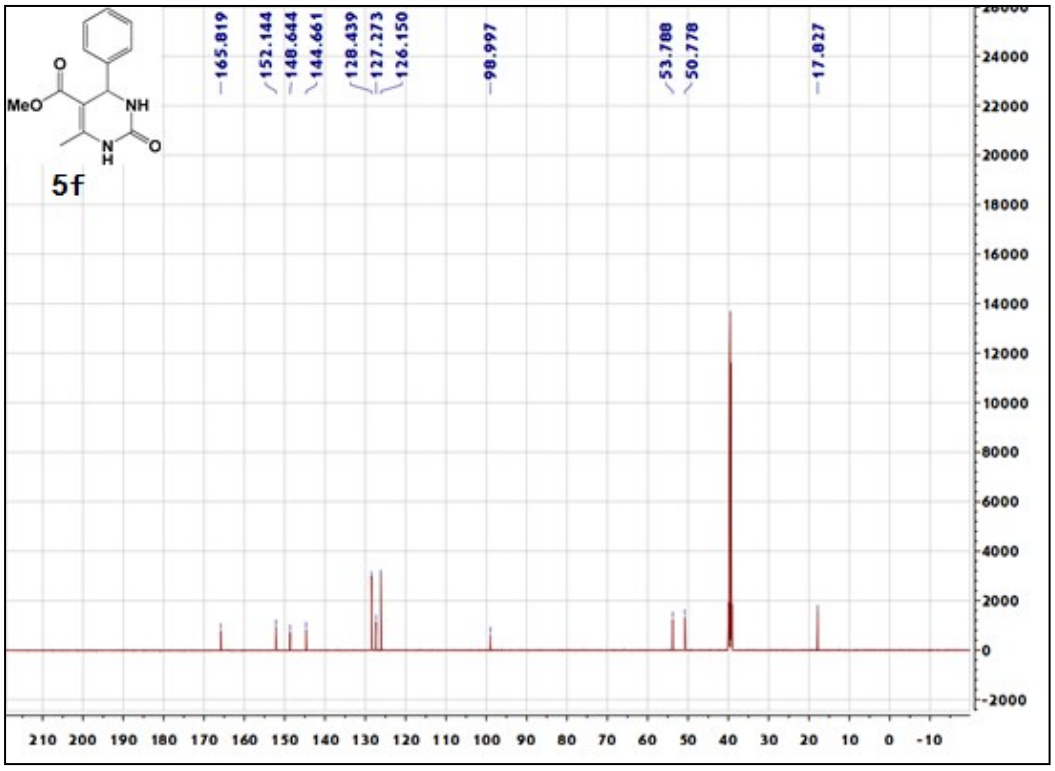

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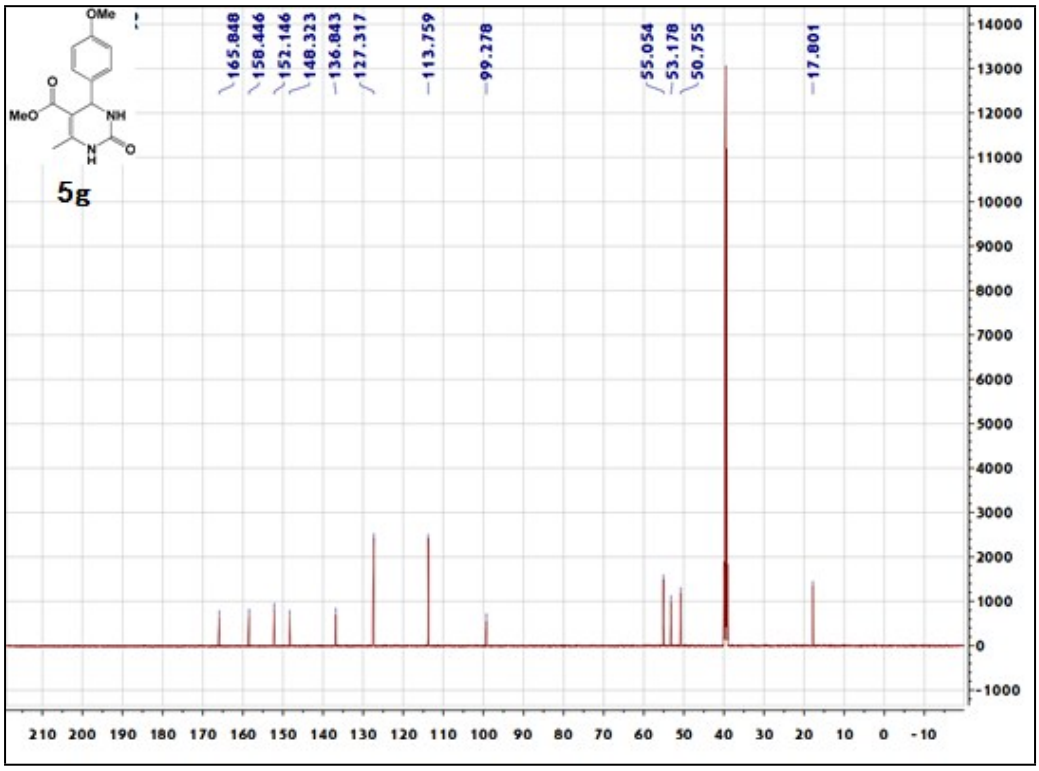

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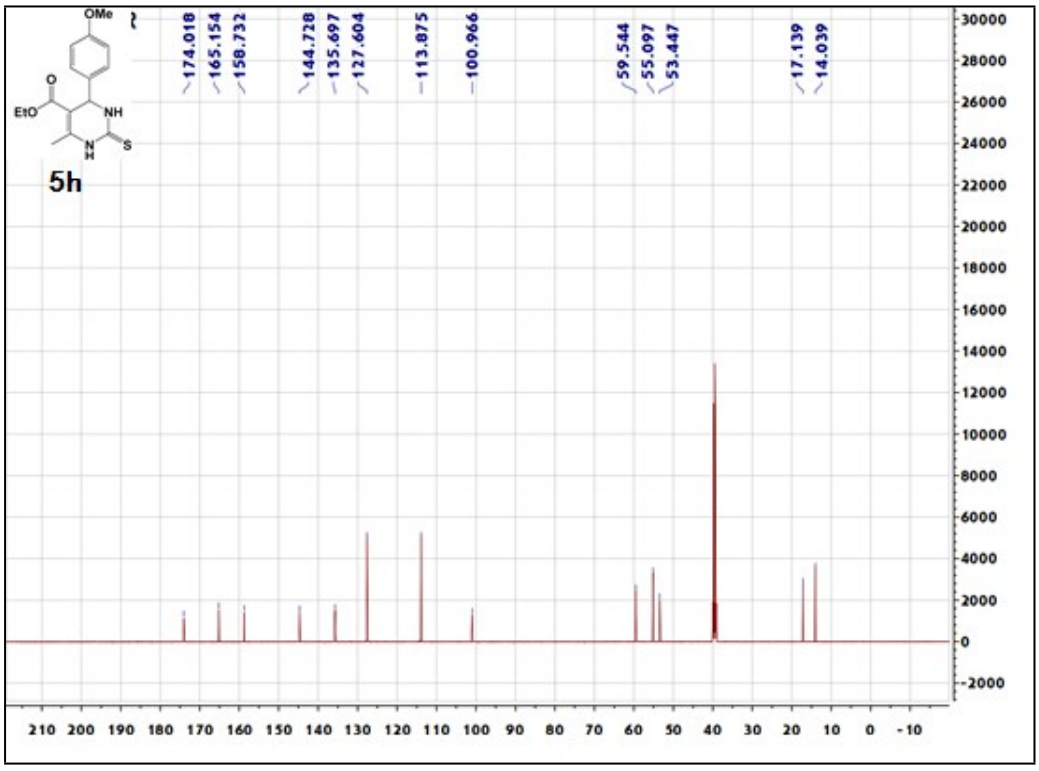

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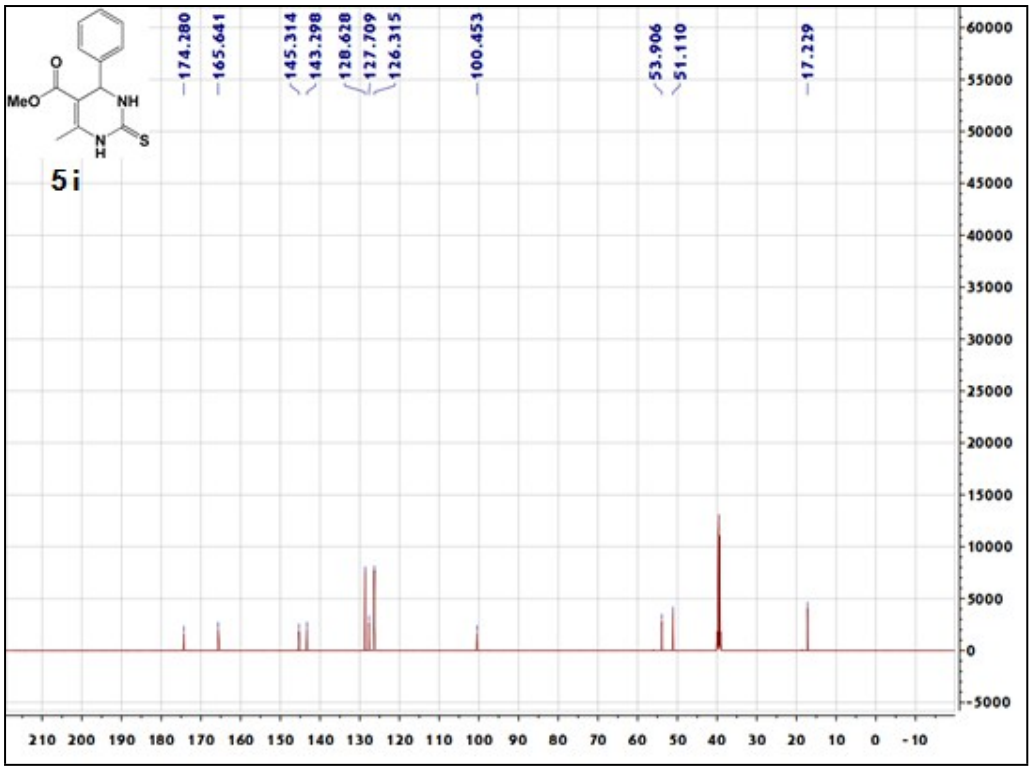

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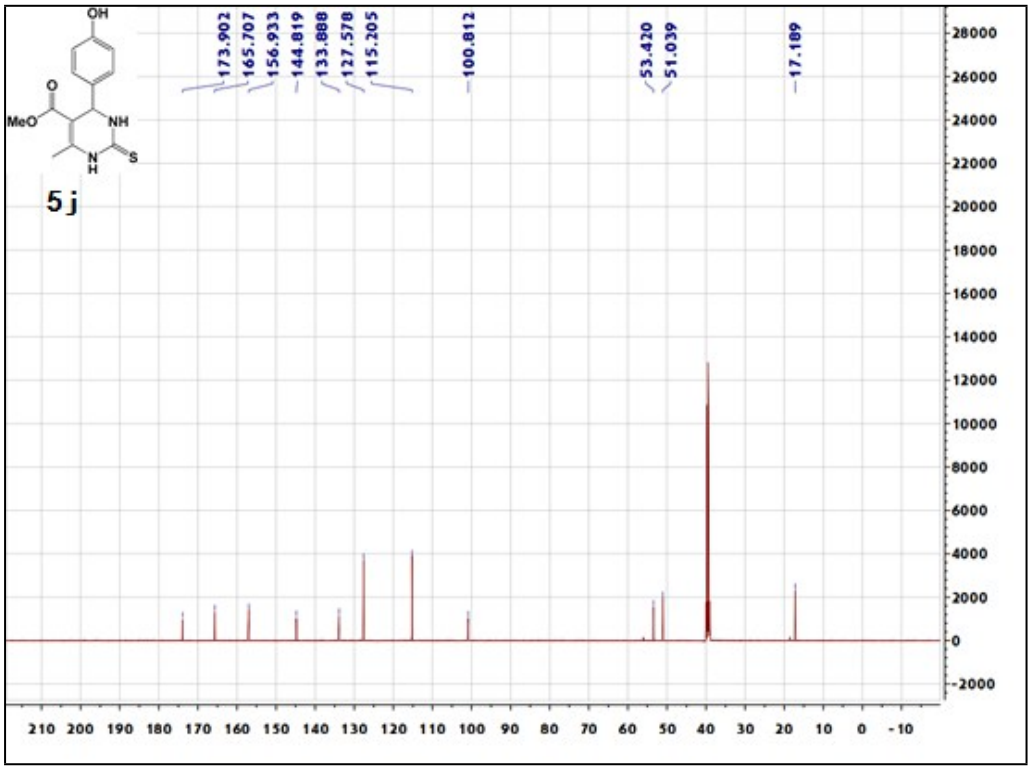

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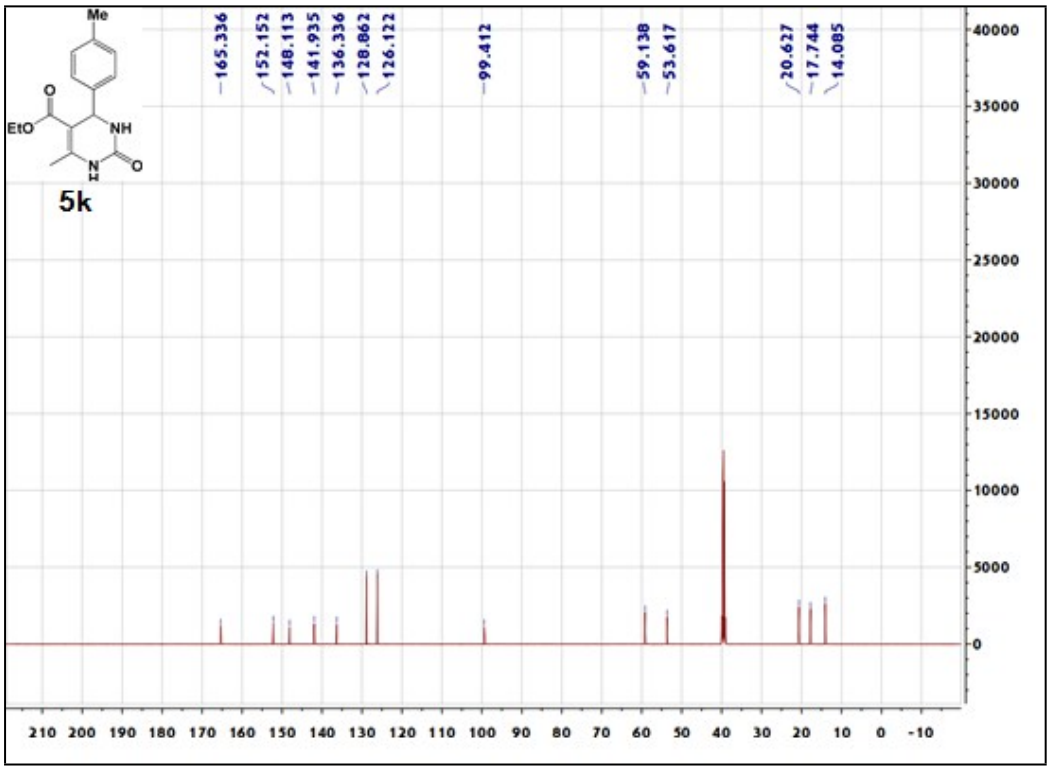

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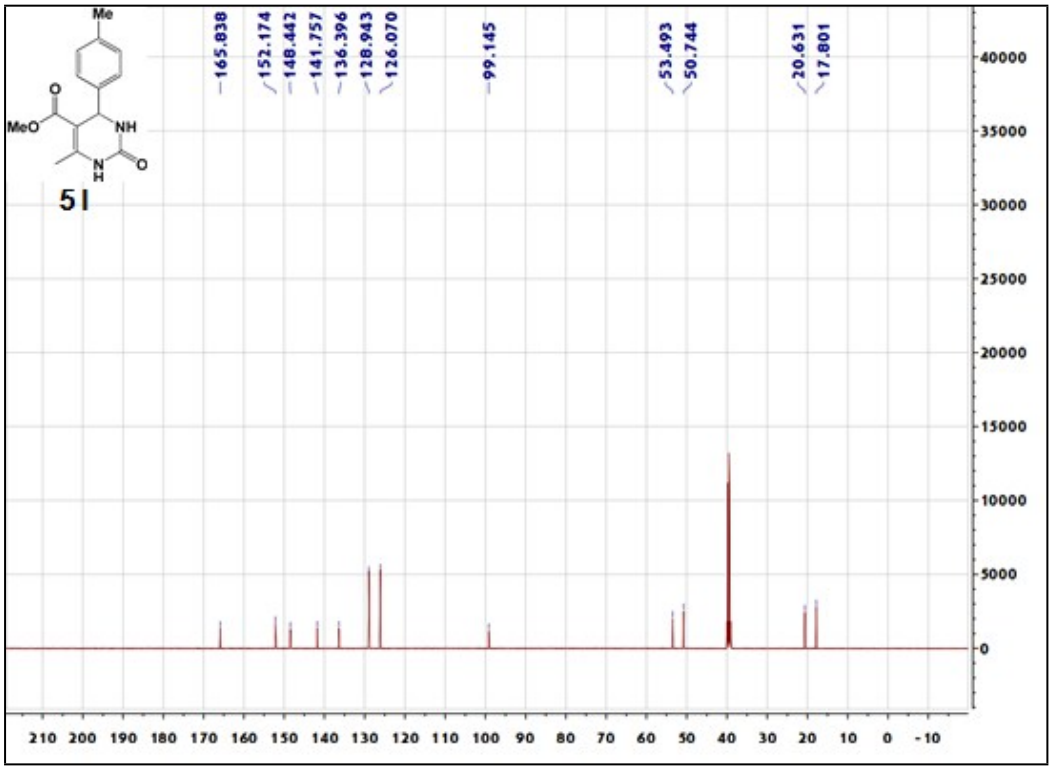

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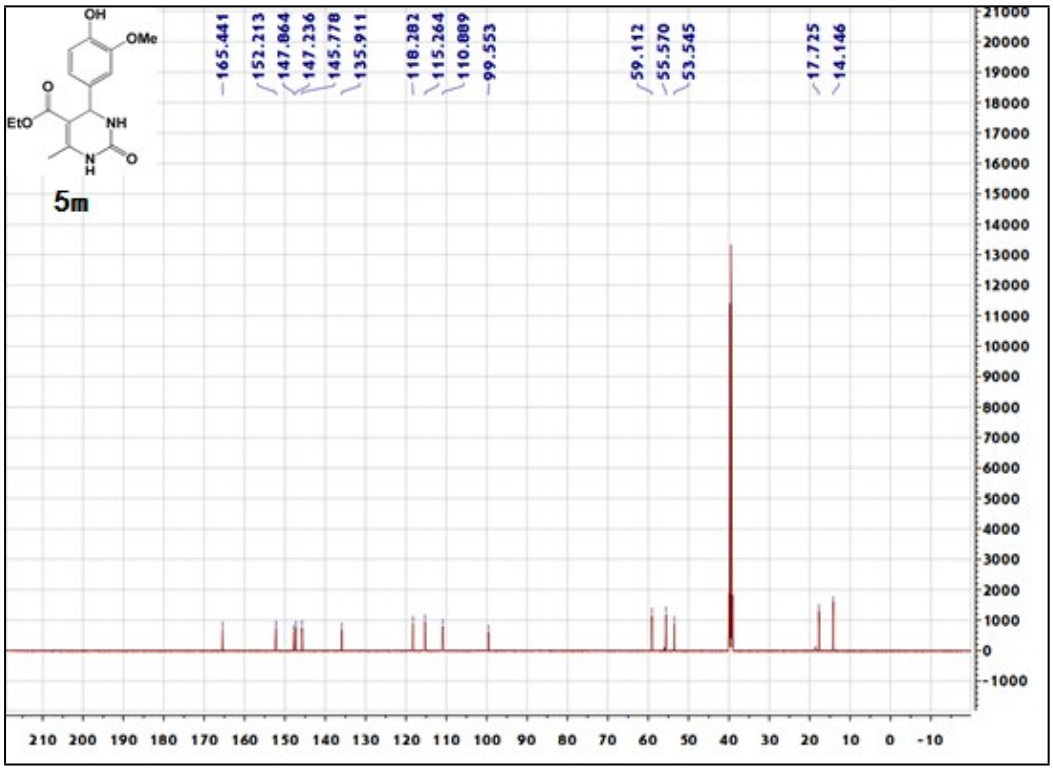

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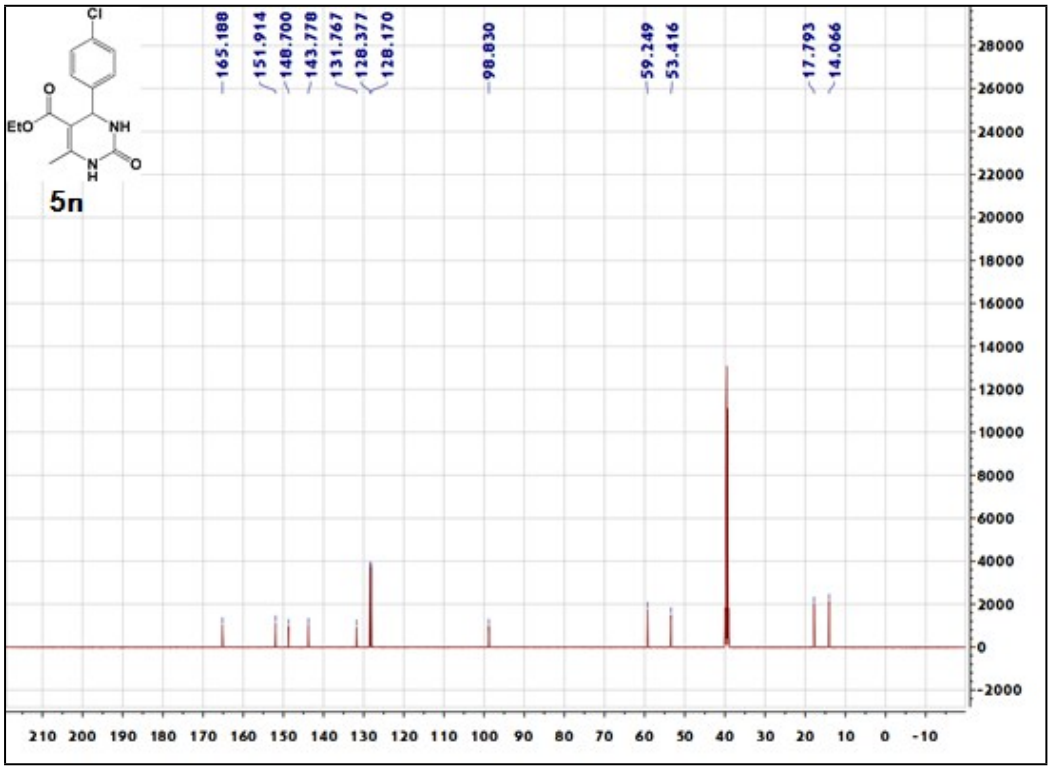

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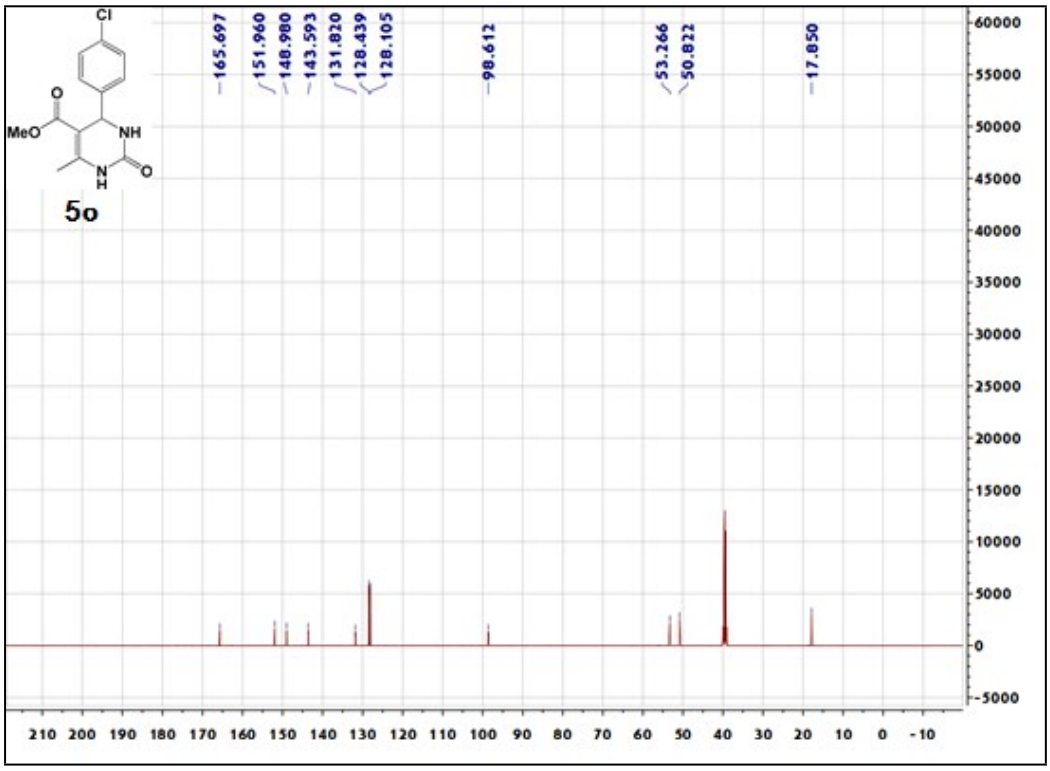

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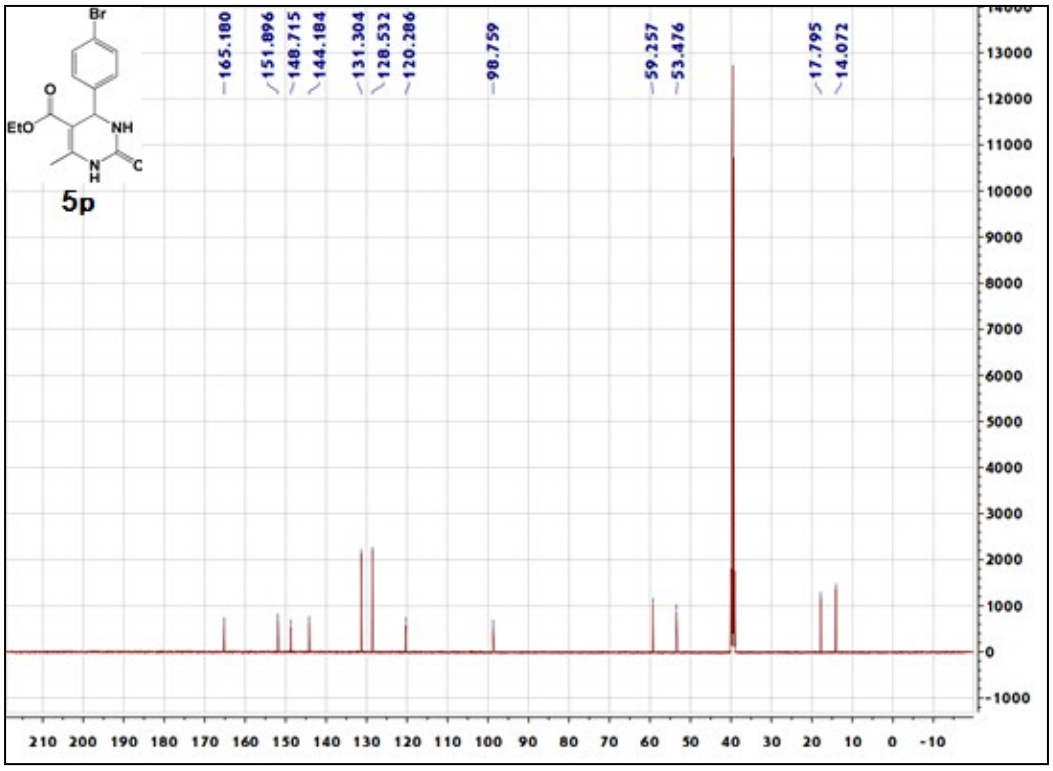

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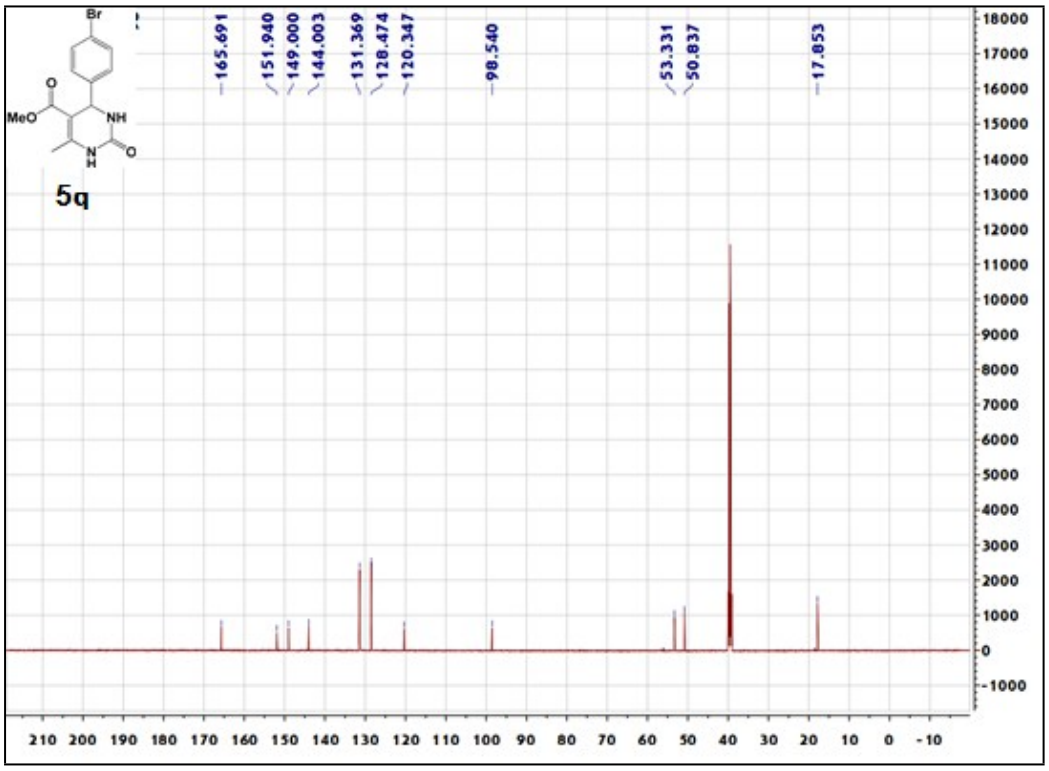

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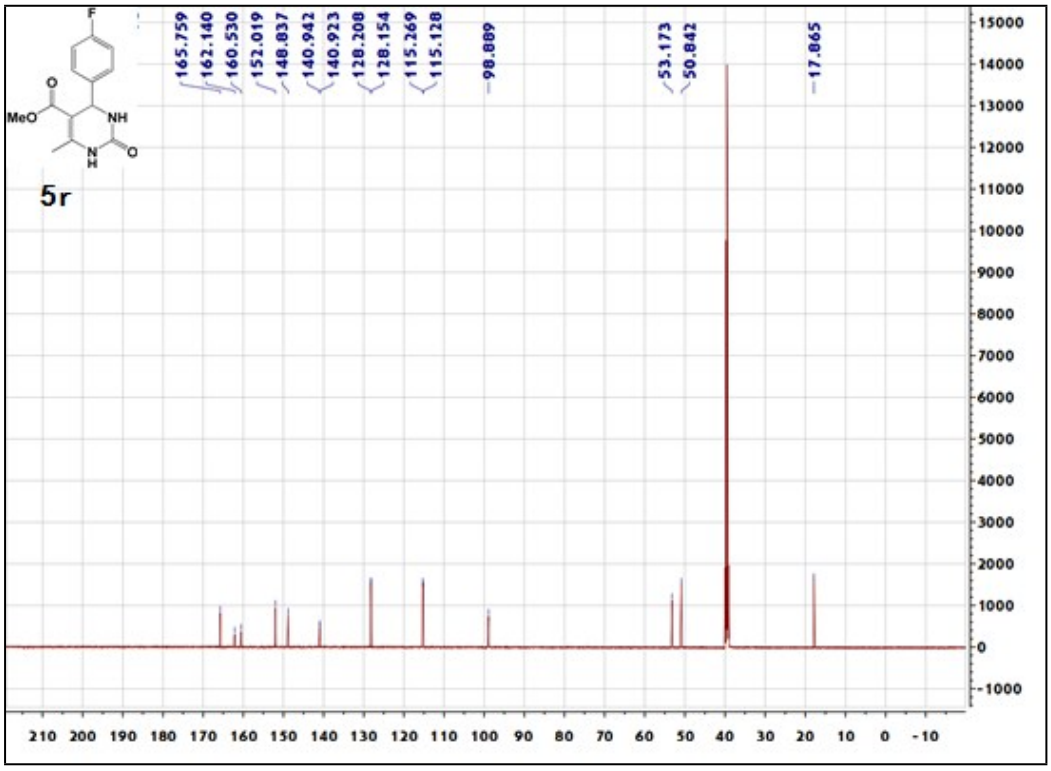

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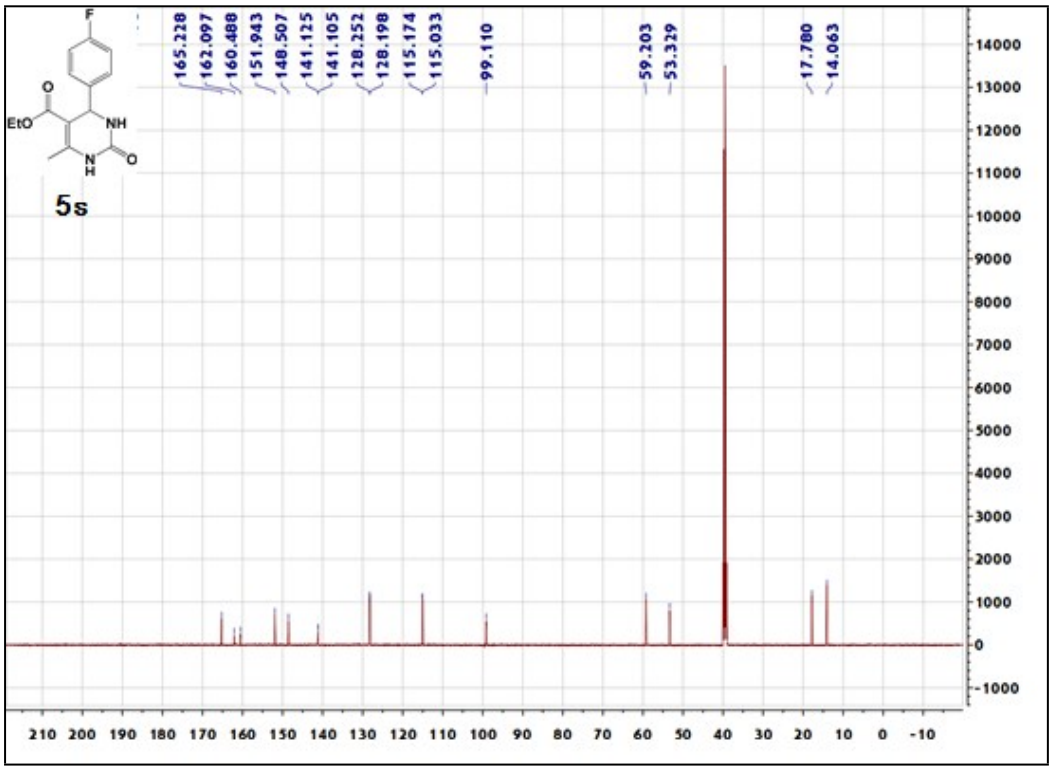

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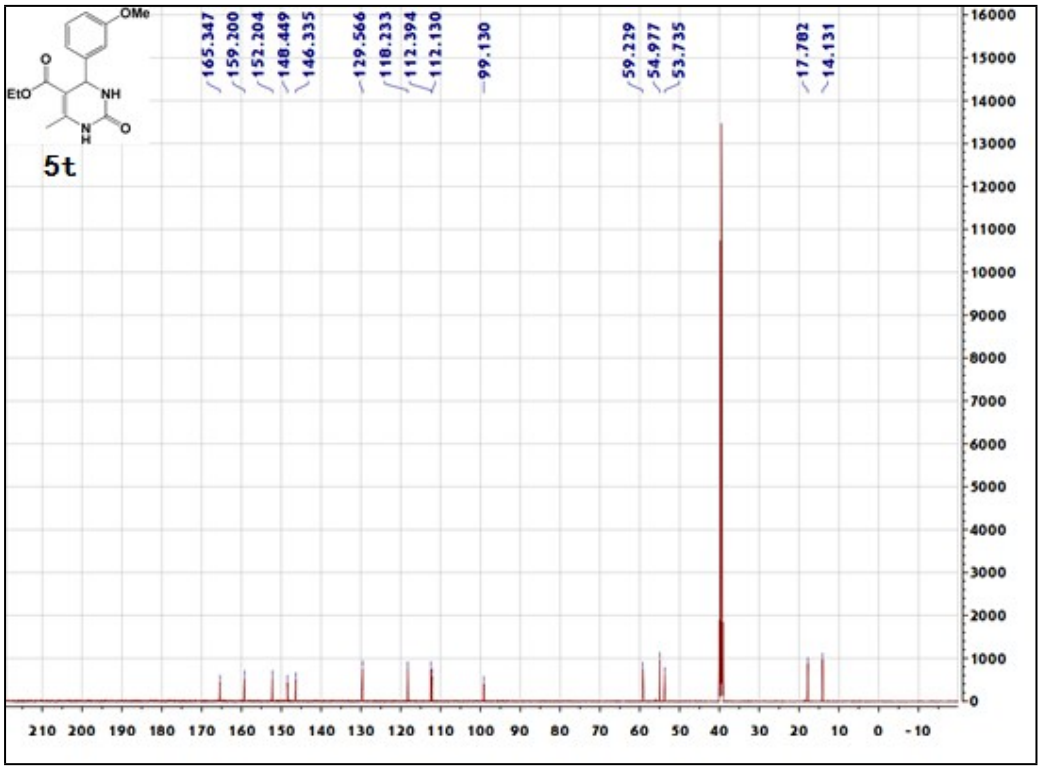

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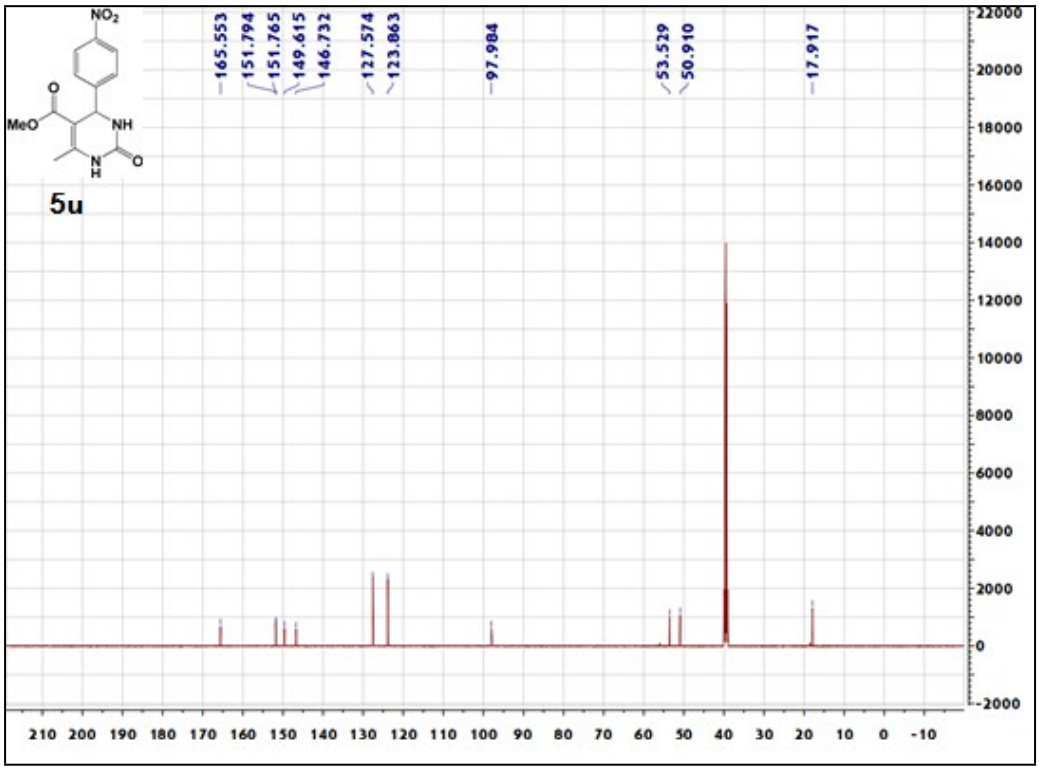

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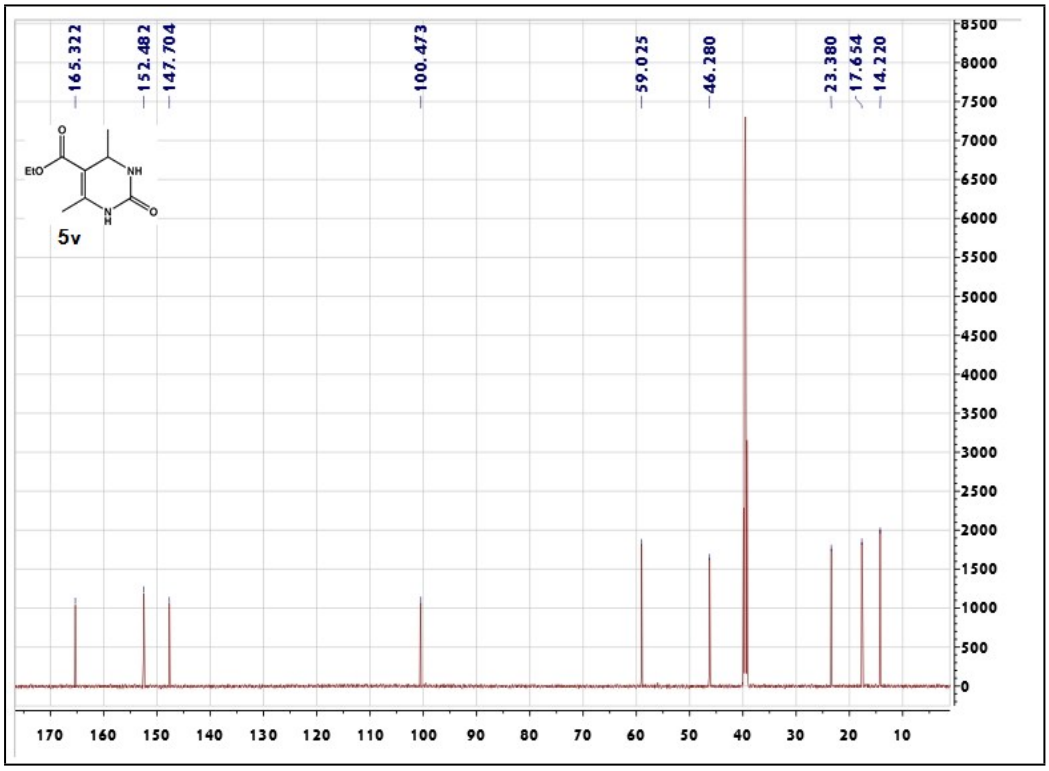

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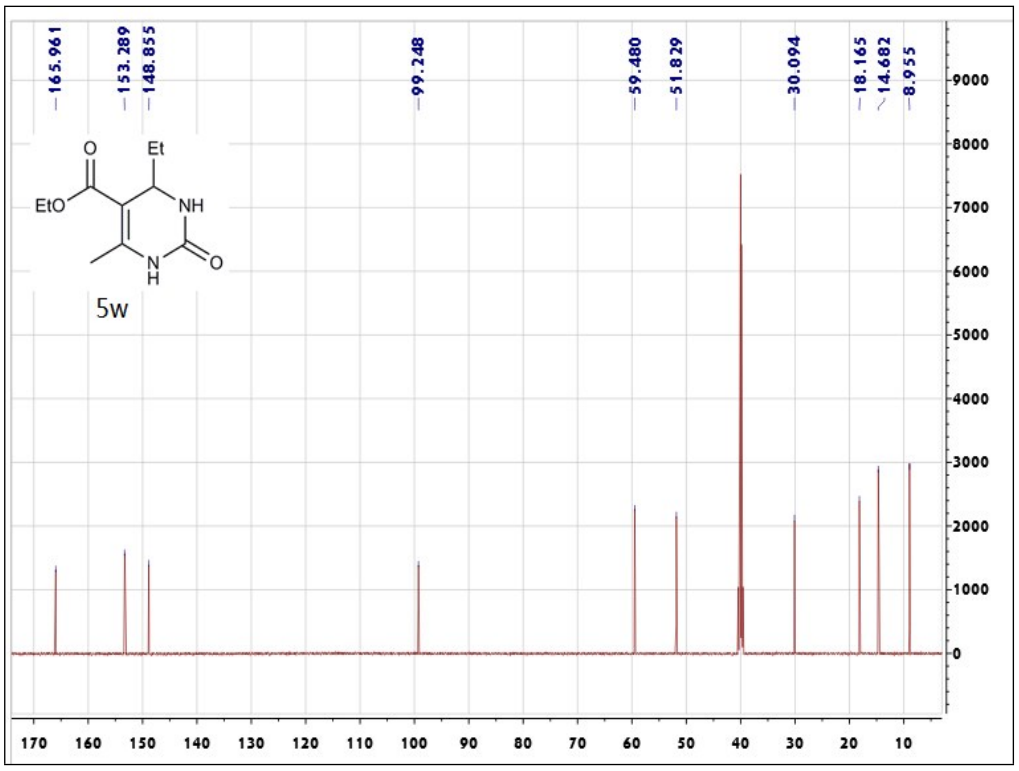

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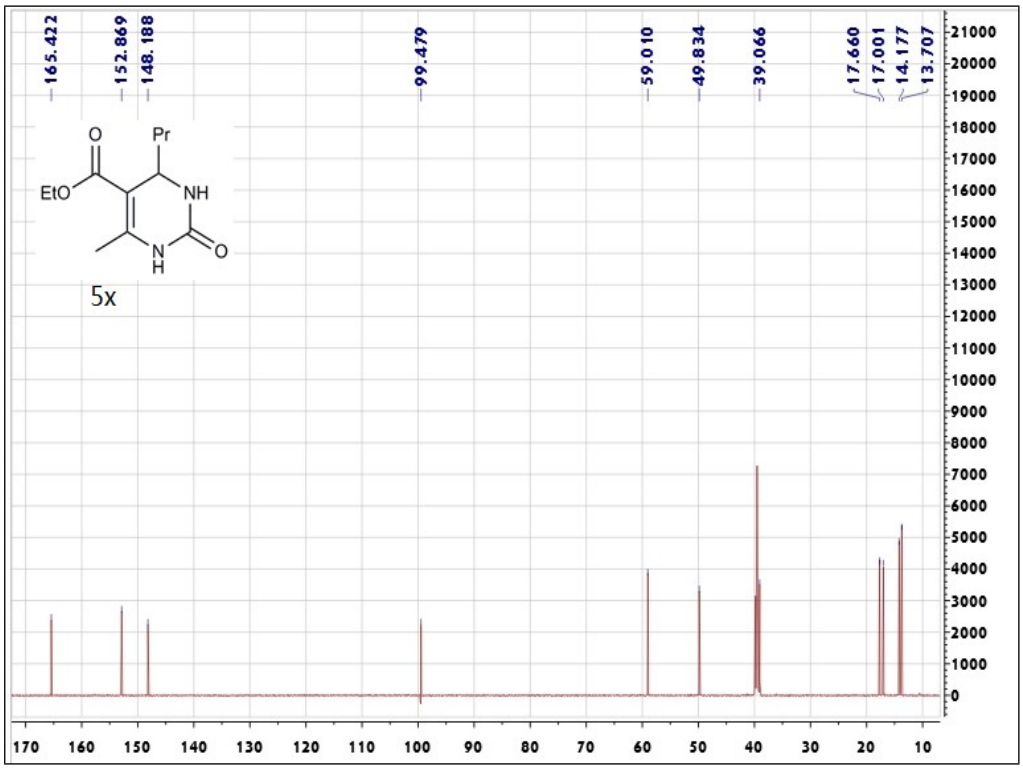

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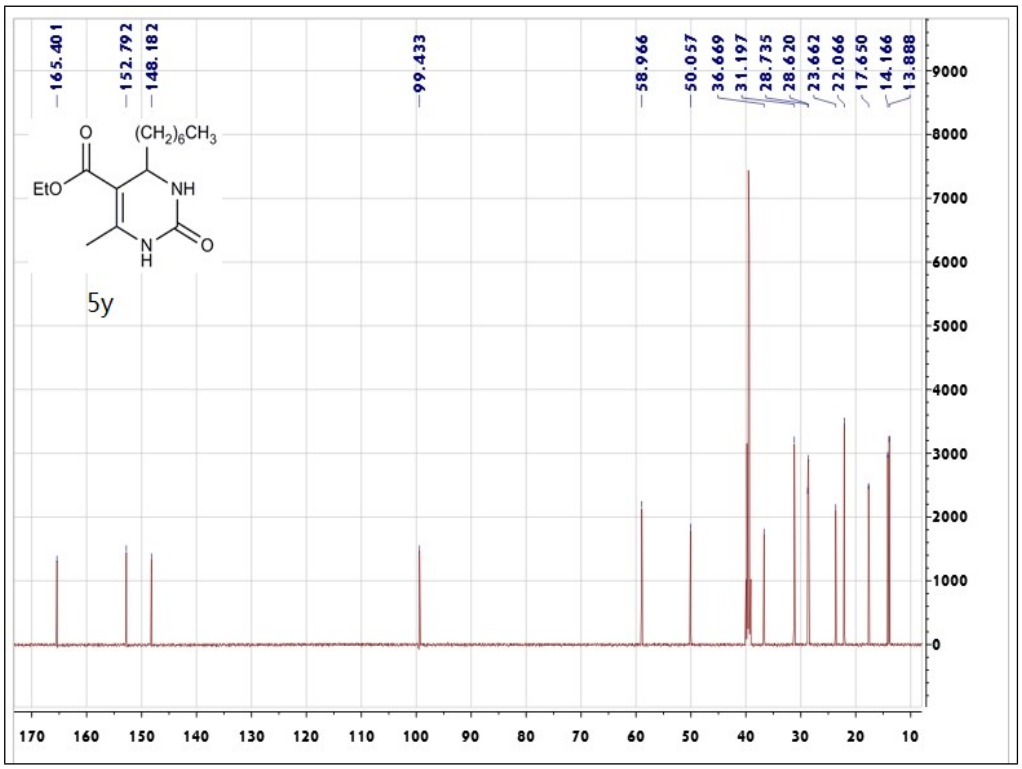

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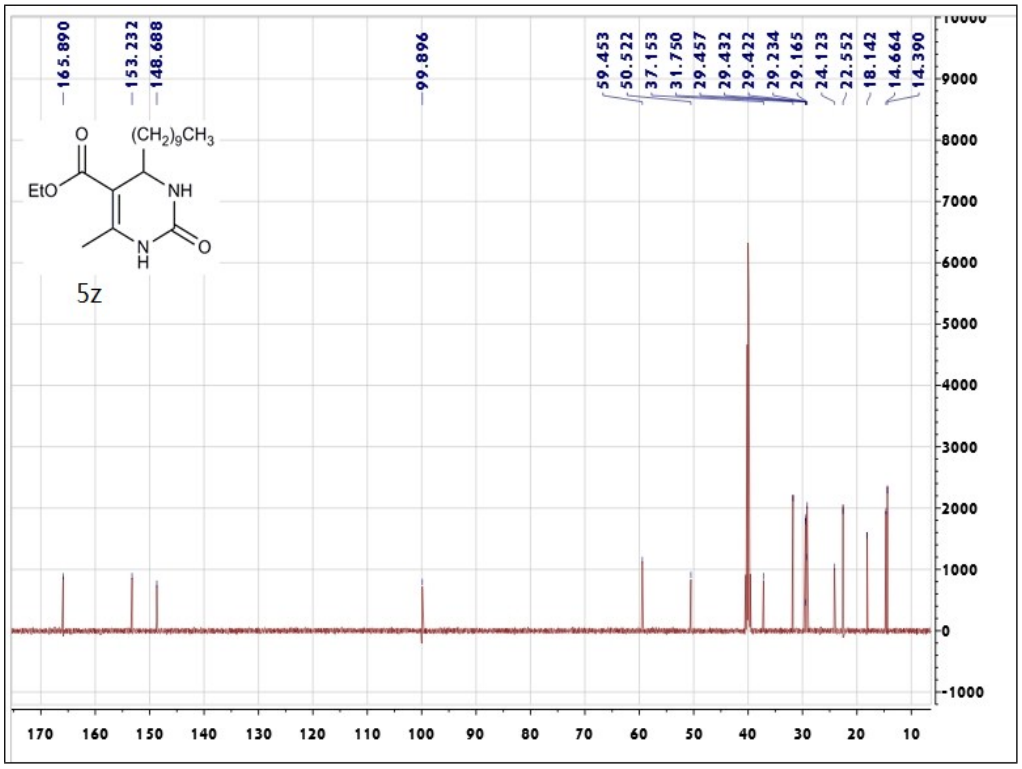

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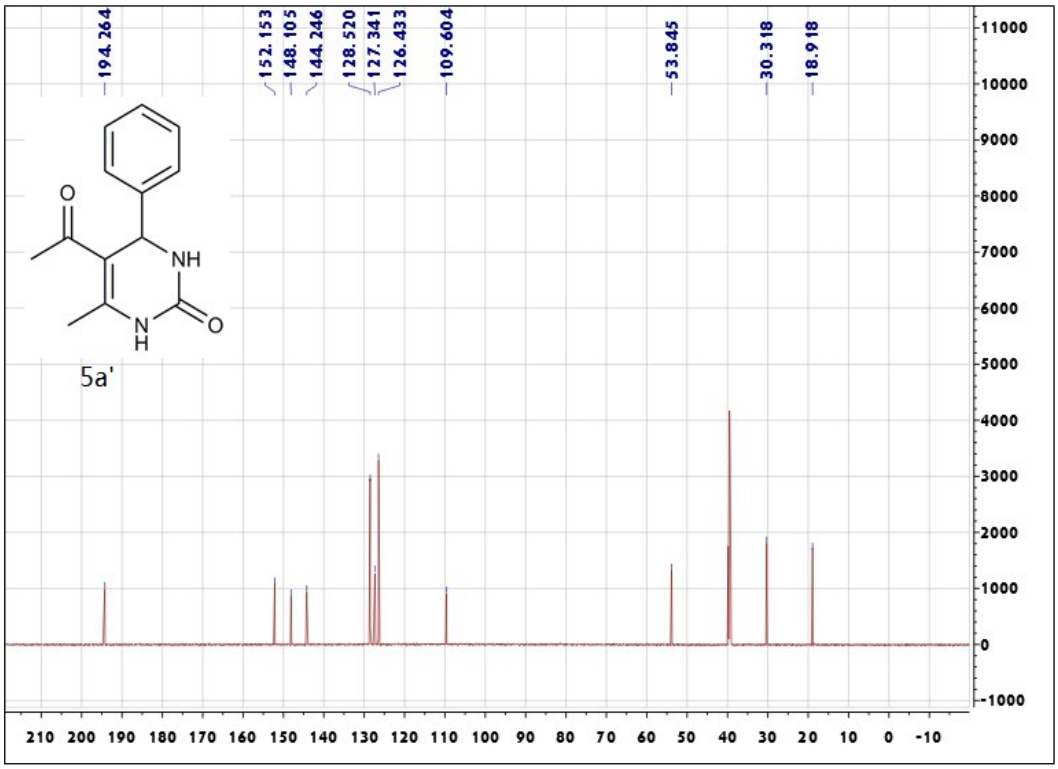

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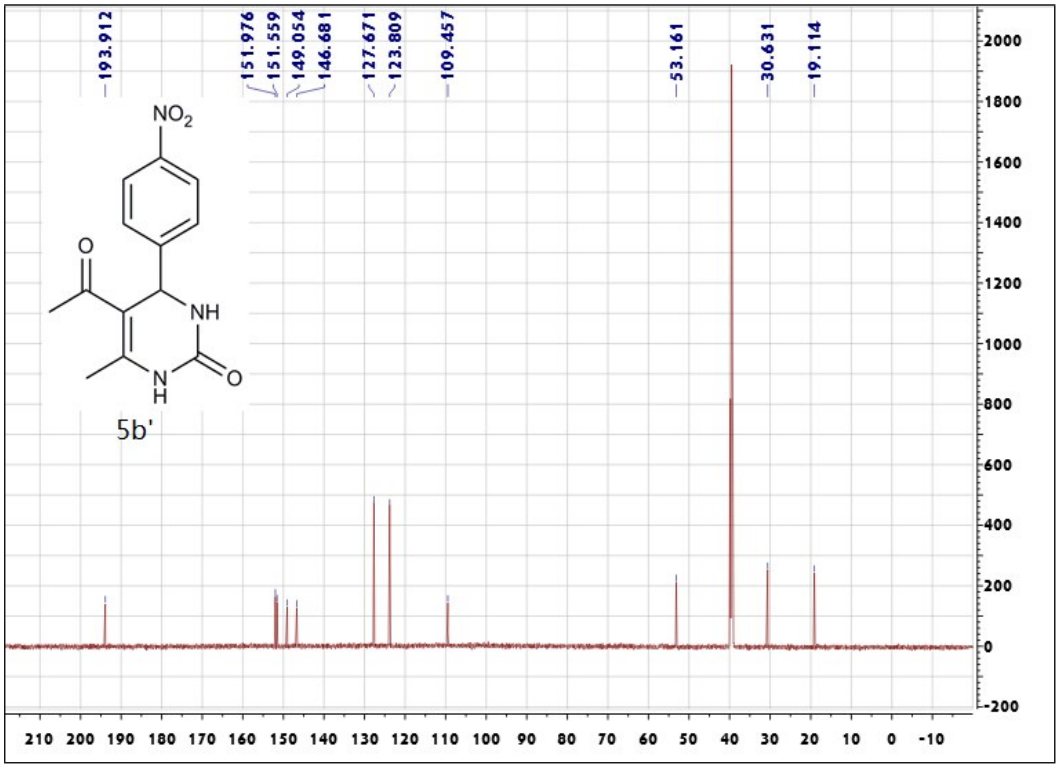

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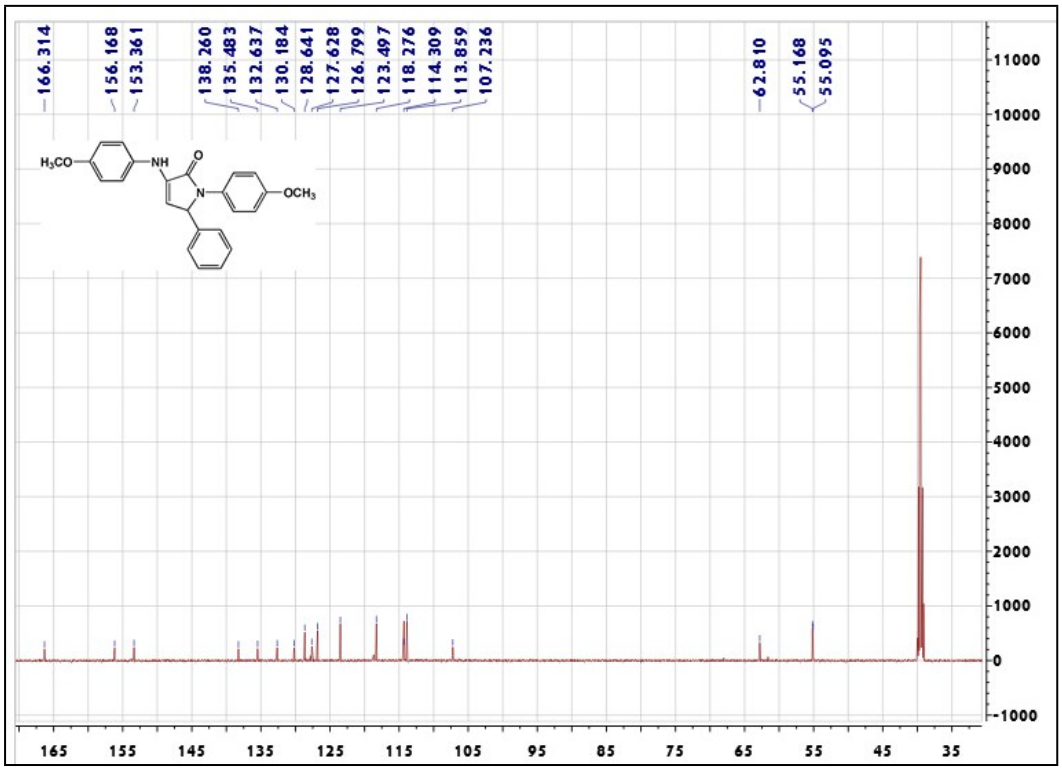
436 

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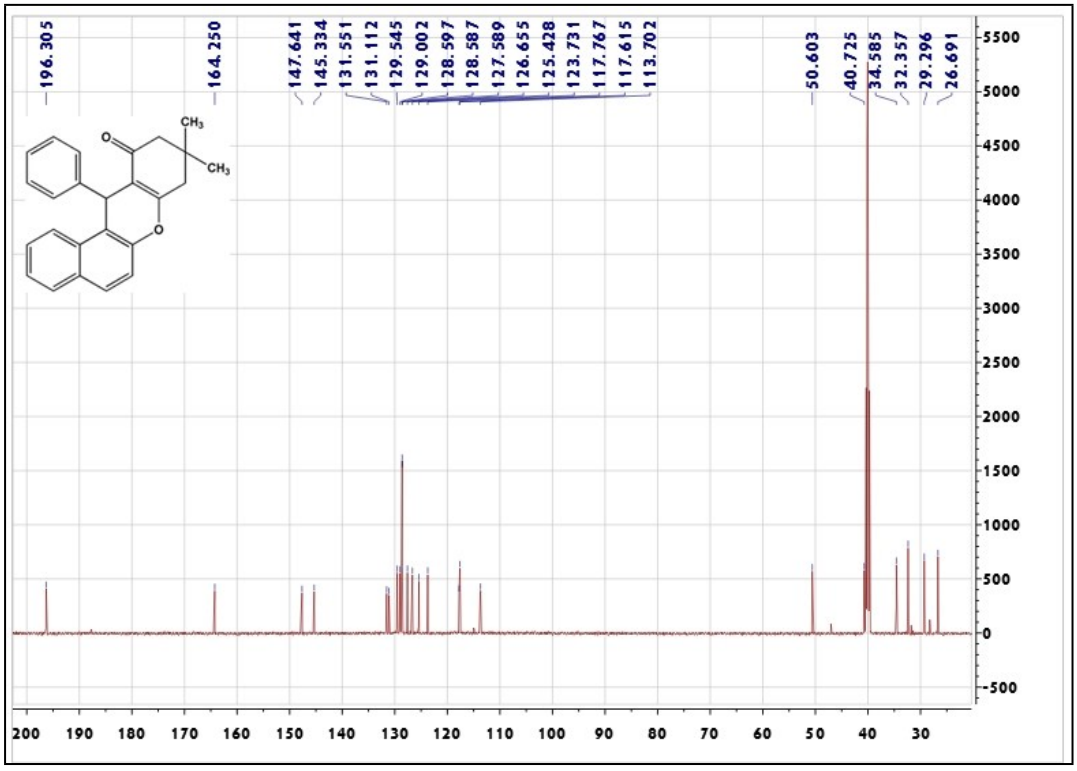
440 

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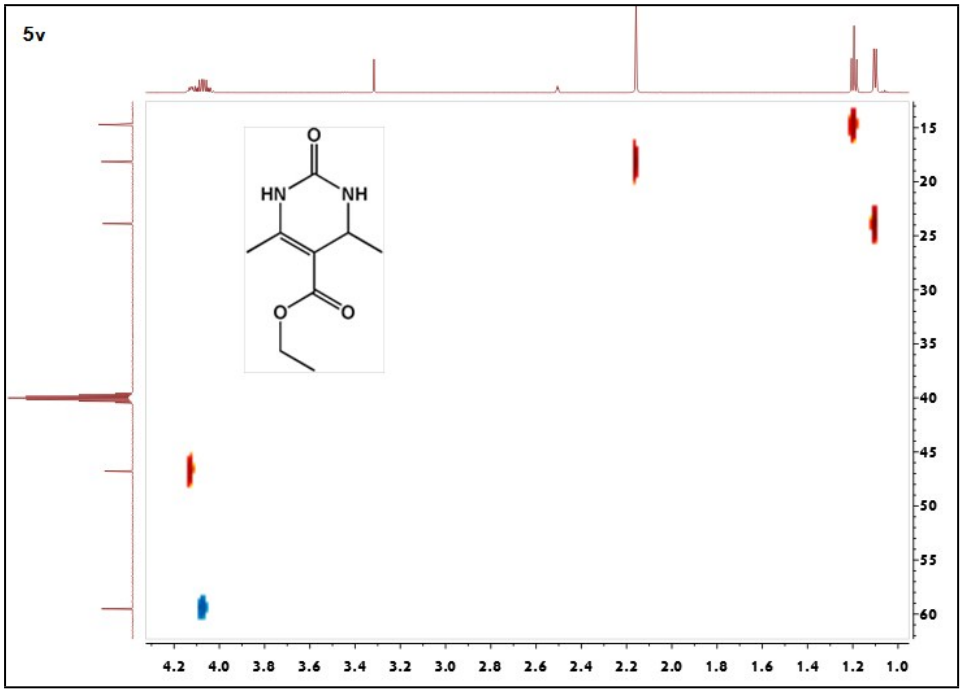
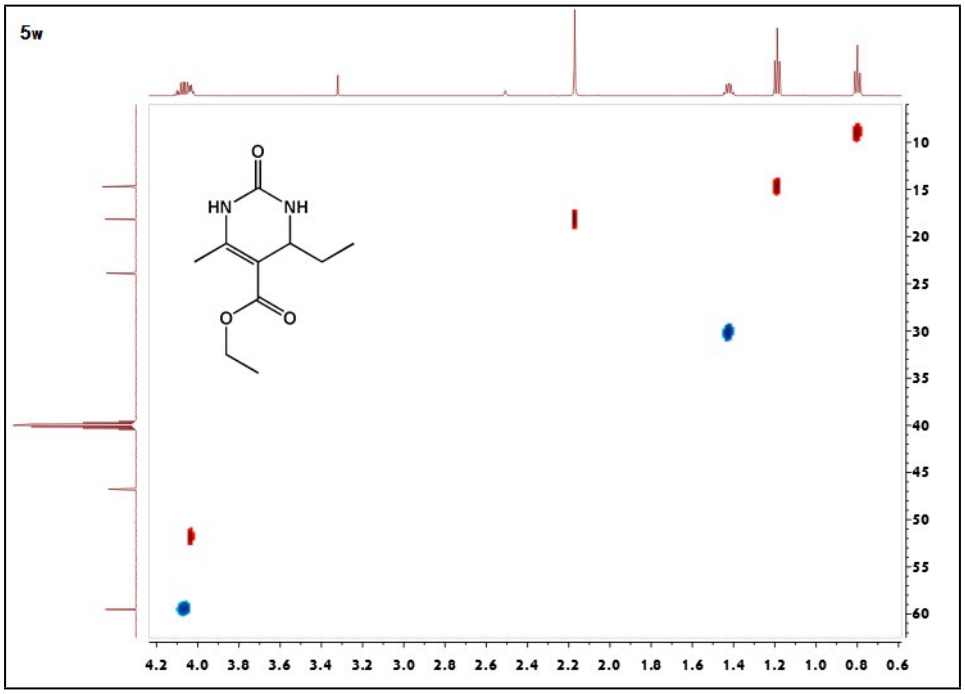
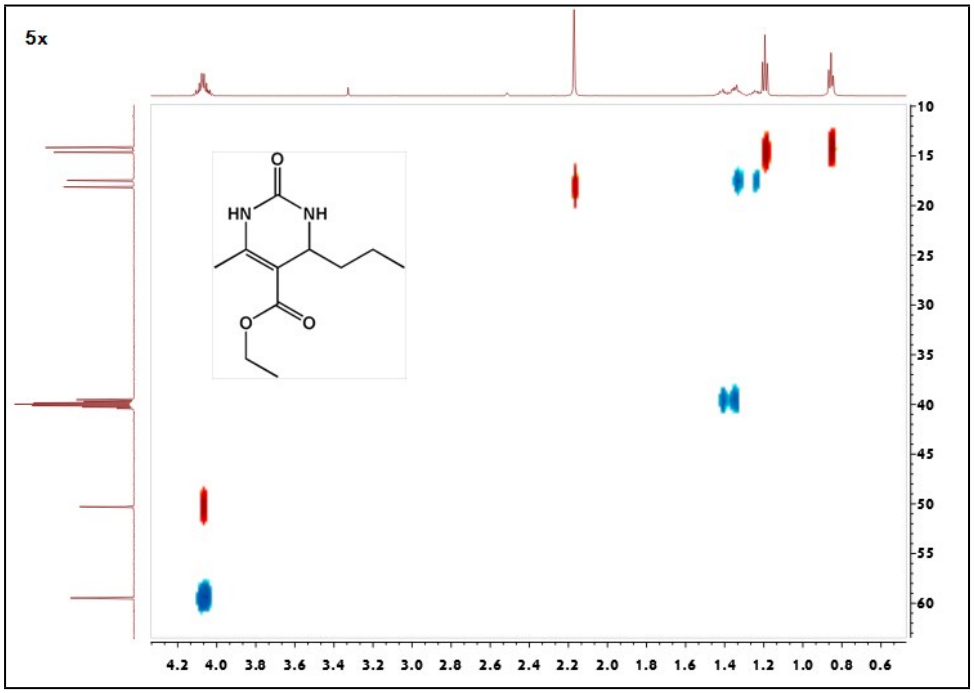
2D NMR of 5v-5z





449 

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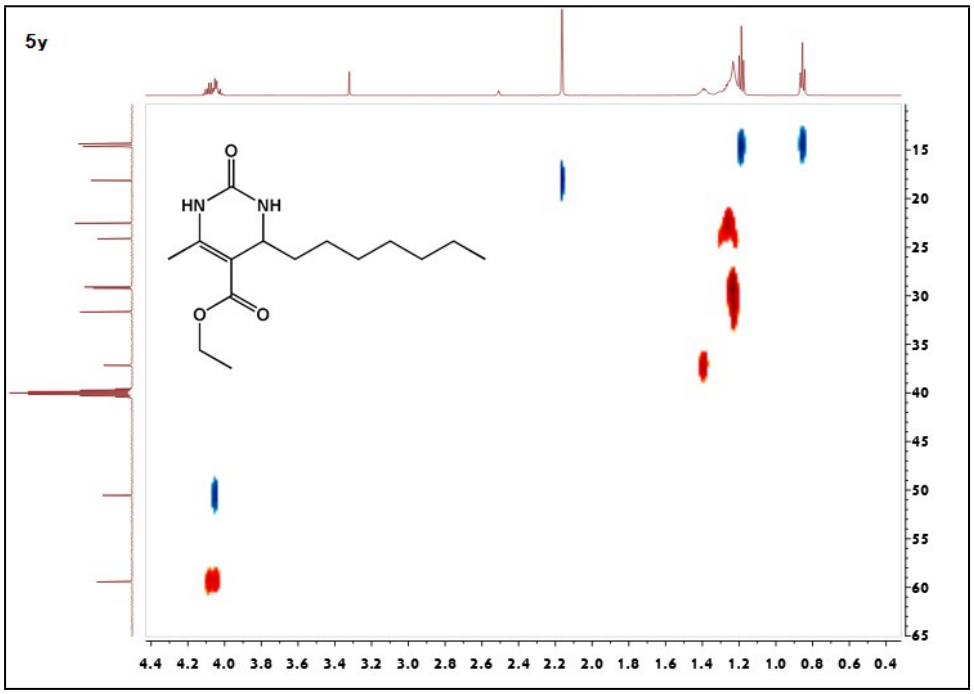
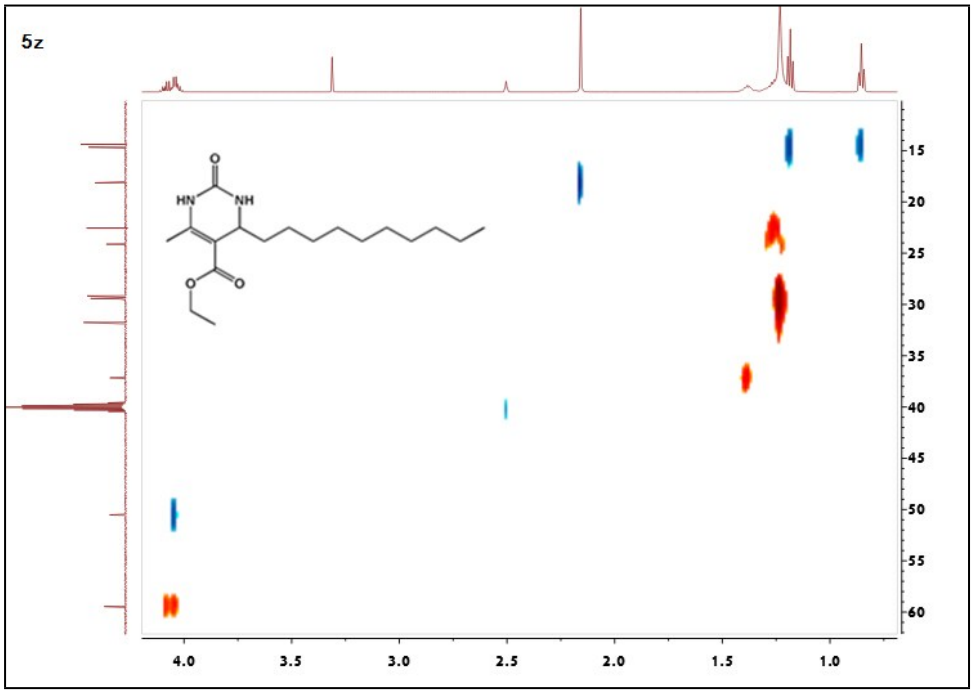
453 


5z
HN
NH
O
O
O
15
20
25
30
35
40
45
50
55
60
4.0
3.5
3.0
2.5
2.0
1.5
1.0

Spectroscopic data for all compounds

5-Ethoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one (5a)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.17 (brs, 1H, NH), 7.72 (brs, 1H, NH), 7.33-7.23 (m, 5H, Ar-H), 5.14 (d, J = 3.0 Hz, 1H, CH), 3.98 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.25 (s, 3H, CH_3), 1.08 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.31, 152.09, 148.32, 144.84, 128.36, 127.23, 126.22, 99.25, 59.16, 53.94, 17.76, 14.06; IR (KBr): v (cm^{-1}) 3245, 3115, 2979, 1725, 1702, 1649; mp (^{o}C): 208-210.

5-Ethoxycarbonyl-4-(4-hydroxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5b)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.32 (s, 1H, OH), 9.10 (brs, 1H, NH), 7.61 (brs, 1H, NH), 7.02 (d, J = 9.0 Hz, 2H, Ar-H), 6.68 (d, J = 8.4 Hz, 2H, Ar-H), 5.04 (d, J = 3.6 Hz, 1H, CH), 3.97 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.23 (s, 3H, CH_3), 1.09 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.03, 151.97, 151.71, 149.36, 146.70, 127.63, 123.81, 98.17, 59.37, 53.67, 17.85, 14.04; IR (KBr): v (cm^{-1}) 3284, 3111, 2973, 1691, 1652, 1606; mp (^{o}C): 232-234.

5-Ethoxycarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1*H*)-one (5c)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.34 (brs, 1H, NH), 8.22 (d, J = 9.0 Hz, 2H, Ar-H), 7.88 (brs, 1H, NH), 7.50 (d, J = 9.0 Hz, 2H, Ar-H), 5.27 (d, J = 3.6 Hz, 1H, CH), 3.99 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.27 (s, 3H, CH_3), 1.09 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.05, 152.00, 151.74, 149.40, 146.71, 127.66, 123.85, 98.17, 59.40, 53.68, 17.89, 14.06; IR (KBr): v (cm^{-1}) 3225, 3118, 2981, 1705, 1641, 1522; mp (^{o}C): 210-212.

5-Ethoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-thione (5d)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 10.33 (brs, 1H, NH), 9.65 (brs, 1H, NH), 7.36-7.21 (m, 5H, Ar-H), 5.17 (d, J = 3.6 Hz, 1H, CH), 4.01 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.29 (s, 3H, CH_3), 1.10 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 174.22, 165.12, 145.04, 143.49, 128.57, 127.69, 126.38, 100.70, 59.60, 54.04, 17.17, 14.02; IR (KBr): v (cm^{-1}) 3248, 3113, 2954, 1716, 1684,1652; mp (^{o}C): 205-206.

5-Ethoxycarbonyl-4-(4-methoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5e)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.14 (brs, 1H, NH), 7.65 (brs, 1H, NH), 7.14 (d, J = 8.4 Hz, 2H, Ar-H), 6.87 (d, J = 8.4 Hz, 2H, Ar-H), 5.09 (d, J = 3.0 Hz, 1H, CH), 3.98

(q, J = 7.2 Hz, 2H, OCH_2CH_3), 3.72 (s, 3H, OCH_3), 2.24 (s, 3H, CH_3), 1.10 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.36, 158.42, 152.13, 147.99, 137.04, 127.37, 113.69, 99.56, 59.14, 55.05, 53.32, 17.75, 14.10; IR (KBr): v (cm^{-1}) 3244, 3111, 2956, 1706, 1650, 1614; mp (°C): 203-205.

5-Methoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one (5f)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 9.21 (brs, 1H, NH), 7.74 (brs, 1H, NH), 7.33-7.23 (m, 5H, Ar-H), 5.14 (d, J = 3.6 Hz, 1H, CH), 3.53 (s, 3H, OCH_3), 2.25 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.82, 152.14, 148.64, 144.66, 128.44, 127.27, 126.15, 99.00, 53.77, 50.79, 17.83; IR (KBr): v (cm^{-1}) 3332, 3224, 3107, 2947, 1706, 1668; mp (°C): 212-213.

5-Methoxycarbonyl-4-(4-methoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5g)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 9.17 (brs, 1H, NH), 7.68 (brs, 1H, NH), 7.14 (d, J = 9.0 Hz, 2H, Ar-H), 6.87 (d, J = 8.4 Hz, 2H, Ar-H), 5.09 (d, J = 3.6 Hz, 1H, CH), 3.72 (s, 3H, OCH_3), 3.52 (s, 3H, OCH_3), 2.24 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.85, 158.45, 152.15, 148.32, 136.84, 127.32, 113.76, 99.28, 55.05, 53.18, 50.76, 17.80; IR (KBr): v (cm^{-1}) 3246, 3111, 2949, 2840, 1720, 1655; mp (°C): 197-200.

5-Ethoxycarbonyl-4-(4-methoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-thione (5h)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 10.28 (brs, 1H, NH), 9.59 (brs, 1H, NH), 7.13 (d, J = 8.4 Hz, 2H, Ar-H), 6.90 (d, J = 8.4 Hz, 2H, Ar-H), 5.11 (d, J = 3.6 Hz, 1H, CH), 4.00 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 3.72 (s, 3H, OCH_3), 2.28 (s, 3H, CH_3), 1.10 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 174.02, 165.15, 158.73, 144.73, 135.70, 127.60, 113.86, 100.97, 59.54, 55.10, 53.45, 17.14, 14.04; IR (KBr): v (cm^{-1}) 3313, 3172, 2984, 1669, 1572, 1458; mp (°C): 151-153.

5-Methoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-thione (5i)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 10.35 (brs, 1H, NH), 9.67 (brs, 1H, NH), 7.36-7.21 (m, 5H, Ar-H), 5.18 (d, J = 3.6 Hz, 1H, CH), 3.56 (s, 3H, OCH_3), 2.30 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm: 174.28, 165.64, 145.31, 143.30, 128.63, 127.71, 126.32, 100.45, 53.91, 51.11, 17.23; IR (KBr) : v (cm^{-1}) 3313, 3184, 3000, 1667, 1575, 1448; mp (°C): 226-228.

4-(4-Hydroxyphenyl)-5-methoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-thione (5j)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm =10.26 (brs, 1H, NH), 9.56 (brs, 1H, NH), 9.42 (s, 1H, OH), 7.01 (d, J = 8.4 Hz, 2H, Ar-H), 6.71 (d, J = 8.4 Hz, 2H, Ar-H), 5.06 (d, J = 3.6 Hz, 1H, CH), 3.54 (s, 3H,OCH_3), 2.28 (s, 3H,CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 173.90, 165.71, 156.93, 144.82, 133.89, 127.58, 115.21, 100.81, 53.42, 51.04, 17.19; IR (KBr): v (cm^{-1}) 3310, 3124, 1665, 1567, 1448, 1341, 1192; mp (^{o}C): 246-248.

5-Ethoxycarbonyl-4-(4-methylphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5k)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.14 (brs, 1H, NH), 7.67 (brs, 1H, NH), 7.12 (s, 4H, Ar-H), 5.10 (d, J = 3.6 Hz, 1H, CH), 3.98 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.26 (s, 3H, CH_3), 2.24 (s, 3H, CH_3), 1.10 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.34, 152.15, 148.11, 141.94, 136.34, 128.86, 126.12, 99.41, 59.14, 53.62, 20.63, 17.74, 14.09; IR (KBr): v (cm^{-1}) 3246, 3115, 2972, 1716, 1644, 1460; mp (^{o}C): 216-218.

5-Methoxycarbonyl-4-(4-methylphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5l)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.17 (brs, 1H, NH), 7.69 (brs, 1H, NH), 7.11 (s, 4H, Ar-H), 5.10 (d, J = 3.6 Hz, 1H, CH), 3.52 (s, 3H, OCH3), 2.26 (s, 3H, CH_3), 2.24 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ pp): 165.84, 152.17, 148.44, 141.76, 136.40, 128.94, 126.07, 99.15, 53.49, 50.74, 20.63, 17.80; IR (KBr): v (cm^{-1}) 3242, 3113, 2934, 1703, 1644, 1514; mp (^{o}C): 234-236.

5-Ethoxycarbonyl-4-(4-hydroxyphenyl-3-methoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5m)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.10 (s, 1H, OH), 8.89 (brs, 1H, NH), 7.61 (brs, 1H, NH), 6.80-6.60 (m, 3H, Ar-H), 5.06 (d, J = 3.0 Hz, 1H, CH), 3.99 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 3.72 (s, 3H, OCH_3), 2.23 (s, 3H, CH_3), 1.11 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.44, 152.21, 147.86, 147.24, 145.78, 135.91, 118.28, 115.26, 110.89, 99.55, 59.11, 55.57, 53.55, 17.73, 14.15; IR (KBr): v (cm^{-1}) 3245, 3114, 2948, 1717, 1647, 1433; mp (^{o}C): 225-226.

4-(4-Chlorophenyl)-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5n)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C) : δ ppm = 9.23 (brs, 1H, NH), 7.76 (brs, 1H, NH), 7.39 (d, J = 8.4 Hz, 2H, Ar-H), 7.25 (d, J = 8.4 Hz, 2H, Ar-H), 5.14 (d, J = 3.0 Hz, 1H, CH), 3.98 (q, J = 7.2 Hz, 2H, OCH_2CH_3), 2.25 (s, 3H, CH_3), 1.09 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.19, 151.91, 148.70, 143.78, 131.77, 128.38, 128.17, 98.83,

59.25, 53.42, 17.79, 14.07; IR (KBr): v (cm^{-1}) 3241, 3114, 2968, 1713, 1645, 1469; mp (^oC): 215-217.

4-(4-Chlorophenyl)-5-methoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5o)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^oC): δ ppm = 9.27 (brs, 1H, NH), 7.78 (brs, 1H, NH), 7.39 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.25 (d, *J* = 9.0 Hz, 2H, Ar-H), 5.14 (d, *J* = 3.6 Hz, 1H, CH), 3.53 (s, 3H, OCH_3), 2.25 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.70, 151.96, 148.98, 143.59, 131.82, 128.44, 128.11, 98.61, 53.27, 50.82, 17.85; IR (KBr): v (cm^{-1}) 3362, 3226, 3108, 2964, 1722, 1630; mp (^oC): 209-212.

4-(4-Bromophenyl)-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5p)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^oC): δ ppm = 9.24 (brs, 1H, NH), 7.77 (brs, 1H, NH), 7.53 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.19 (d, *J* = 8.4 Hz, 2H, Ar-H), 5.12 (d, *J* = 3.6 Hz, 1H, CH), 3.98 (q, *J* = 7.2 Hz, 2H, OCH_2CH_3), 2.24 (s, 3H, CH_3), 1.09 (t, *J* = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.18, 151.90, 148.72, 144.18, 131.30, 128.53, 120.29, 98.76, 59.26, 53.48, 17.80, 14.07; IR (KBr) : v (cm^{-1}) 3244, 3116, 2968, 1717, 1648, 1471; mp (^oC): 223-225.

4-(4-Bromophenyl)-5-methylcarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5q)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^oC): δ ppm = 9.27 (brs, 1H, NH), 7.78 (brs, 1H, NH), 7.52 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.18 (d, *J* = 8.4 Hz, 2H, Ar-H), 5.12 (d, *J* = 3.0 Hz, 1H, CH), 3.53 (s, 3H, OCH_3), 2.25 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.69, 151.94, 149.00, 144.00, 131.37, 128.47, 120.35, 98.54, 53.33, 50.84, 17.85; IR (KBr): v (cm^{-1}) 3363, 3222, 3106, 2953, 1720, 1633; mp (^oC): 225-227.

4-(4-Fluorophenyl)-5-methylcarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5r)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^oC): δ ppm = 9.26 (brs, 1H, NH), 7.78 (brs, 1H, NH), 7.27-7.13 (m, 4H, Ar-H), 5.14 (d, *J* = 3.0 Hz, 1H, CH), 3.53 (s, 3H, OCH_3), 2.25 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.76, 162.14, 160.53, 152.02, 148.84, 140.93 (d, J=2.87 Hz), 128.18 (d, *J* = 8.15 Hz), 115.20 (d, *J*=21.29 Hz), 98.89, 53.17, 50.84, 17.87; IR (KBr) : v (cm^{-1}) 3327, 3223, 3106, 2948, 1680, 1423; mp (^oC): 202-203.

4-(4-Fluorophenyl)-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5s)

^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^oC): δ ppm = 9.21 (brs, 1H, NH), 7.73 (brs, 1H, NH), 7.27-7.13 (m, 4H, Ar-H), 5.14 (d, *J* = 3.0 Hz, 1H, CH), 3.98 (m, 2H, OCH_2CH_3), 2.25 (s, 3H,

593 CH_3), 1.09 (t, J = 7.2 Hz, 3H, OCH_2CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.23,
594 162.10, 160.49, 151.94, 148.51, 141.12 (d, J = 3.02 Hz), 128.23 (d, J = 8.15 Hz), 115.10 (d, J =
595 21.29 Hz), 99.11, 59.20, 53.33, 17.78, 14.06; IR (KBr): v (cm^{-1}) 3243, 3120, 2971, 1717, 1646,
596 1461; mp (°C): 184-186.

597 **5-Ethoxycarbonyl-4-(3-methoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one (5t)**

598 ^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 9.19 (brs, 1H, NH), 7.73 (brs, 1H, NH),
599 7.24 (t, 1H, J = 7.8 Hz, Ar-H), 6.80 (m, 3H, Ar-H), 5.11 (d, J = 3.0 Hz, 1H, CH), 3.99 (q, J = 7.2
600 Hz, 2H, OCH_2CH_3), 3.72 (s, 3H, OCH_3), 2.24 (s, 3H, CH_3), 1.11 (t, J = 7.2 Hz, 3H, OCH_2CH_3);
601 ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.35, 159.20, 152.20, 148.45, 146.34, 129.57, 118.23,
602 112.39, 112.13, 99.13, 59.23, 54.98, 53.74, 17.78, 14.13; IR (KBr): v (cm^{-1}) 3254, 3109, 2952,
603 1704, 1638, 1451; mp (°C): 229-231.

604 **5-Methylcarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1*H*)-one (5u)**

605 ^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm = 9.37 (brs, 1H, NH), 8.21 (d, J = 8.4 Hz,
606 2H, Ar-H), 7.90 (brs, 1H, NH), 7.50 (d, J = 8.4 Hz, 2H, Ar-H), 5.27 (d, J = 3.6 Hz, 1H, CH), 3.54
607 (s, 3H, OCH_3), 2.27 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.55, 151.79,
608 151.77, 149.62, 146.73, 127.57, 123.86, 97.98, 53.53, 50.91, 17.92; IR (KBr): v (cm^{-1}) 3364, 3223,
609 3113, 2958, 1714, 1638, 1516; mp (°C): 241-243.

610 **5-Ethoxycarbonyl-4,6-dimethyl-3,4-dihydropyrimidin-2(1*H*)-one (5v)**

611 ^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm= 8.96 (s, 1H, NH), 7.18 (s, 1H, NH), 4.13-
612 4.06 (m, 2H, OCH_2CH_3), 4.06-4.03 (m, 1H, CH), 2.15 (s, 3H, CH_3), 1.19 (t, J = 7.2 Hz, 3H,
613 OCH_2CH_3), 1.10 (d, J = 6.6 Hz, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.32,
614 152.48, 147.70, 100.47, 59.03, 46.28, 23.38, 17.65, 14.22; IR (KBr): v (cm^{-1}) 3251, 3116, 2978,
615 2937, 1705, 1656; mp (°C): 288-290.

616 **5-Ethoxycarbonyl-6-methyl-4-ethyl-3,4-dihydropyrimidin-2(1*H*)-one (5w)**

617 ^1H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm= 8.91 (s, 1H, NH), 7.27 (s, 1H, NH), 4.11-
618 4.06 (m, 2H, OCH_2CH_3), 4.06-4.01 (m, 1H, CH), 2.16 (s, 3H, CH_3), 1.44-1.39 (m, 2H, CH_2CH_3),
619 1.18 (t, J = 7.2 Hz, 3H, OCH_2CH_3), 0.79 (t, J = 7.2 Hz, 3H, CH_2CH_3); ^{13}C NMR (151 MHz,
620 DMSO-d_6, δ ppm): 165.96, 153.29, 148.86, 99.25, 59.48, 51.83, 30.09, 18.17, 14.68, 9.00; IR
621 (KBr): v (cm^{-1}) 3249, 3121, 2961, 2936, 1724, 1704; mp (°C): 191-192.

622 **5-Ethoxycarbonyl-6-methyl-4-propyl-3,4-dihydropyrimidin-2(1*H*)-one (5x)**

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm= 8.92 (s, 1H, NH), 7.32 (s, 1H, NH), 4.11-4.06 (m, 2H, OCH_2CH_3), 4.06-4.01 (m, 1H, CH), 2.16 (s, 3H, CH_3), 1.43-1.20 (m, 4H, $(CH_2)_2CH_3$), 1.18 (t, J = 7.2 Hz, 3H, OCH_2CH_3), 0.84 (t, J = 7.2 Hz, 3H, $(CH_2)_2CH_3$); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.42, 152.87, 148.19, 99.48, 59.01, 49.83, 39.07, 17.66, 17.00, 14.18, 13.71; IR (KBr): v (cm^{-1}) 3251, 3120, 2958, 2935, 1721, 1704; mp (^{o}C): 192-193.

5-Ethoxycarbonyl-6-methyl-4-heptyl-3,4-dihydropyrimidin-2(1*H*)-one (5y)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm= 8.91 (s, 1H, NH), 7.31 (s, 1H, NH), 4.10-4.07 (m, 2H, OCH_2CH_3), 4.07-4.02 (m, 1H, CH), 2.16 (s, 3H, CH_3), 1.38-1.22 (m, 12H, $(CH_2)_6CH_3$), 1.18 (t, J = 7.2 Hz, 3H, OCH_2CH_3), 0.85 (t, J = 7.2 Hz, 3H, $(CH_2)_6CH_3$); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.40, 152.79, 148.18, 99.43, 59.00, 50.06, 36.67, 31.20, 28.74, 28.62, 23.66, 22.07, 17.65, 14.17, 13.89; IR (KBr): v (cm^{-1}) 3240, 3113, 2952, 2927, 2859, 1706; mp (^{o}C): 138-139.

5-Ethoxycarbonyl-6-methyl-4-decyl-3,4-dihydropyrimidin-2(1*H*)-one (5z)

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm= 8.90 (s, 1H, NH), 7.30 (s, 1H, NH), 4.10-4.03 (m, 2H, OCH_2CH_3), 4.03-4.00 (m, 1H, CH), 2.15 (s, 3H, CH_3), 1.39-1.23 (m, 18H, $(CH_2)_9CH_3$), 1.18 (t, J = 7.2 Hz, 3H, OCH_2CH_3), 0.85 (t, J = 7.2 Hz, 3H, $(CH_2)_9CH_3$); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 165.89, 153.23, 148.69, 99.90, 59.45, 50.52, 37.15, 31.75, 29.46, 29.43, 29.42, 29.23, 29.17, 24.12, 22.55, 18.14, 14.66, 14.39; IR (KBr): v (cm^{-1}) 3244, 3122, 2921, 2852, 1730, 1706; mp (^{o}C): 142-143.

5,6-Dimethyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one (5a')

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.19 (brs, 1H, NH), 7.83 (brs, 1H, NH), 7.34-7.23 (m, 5H, Ar-H), 5.27 (d, J = 3.6 Hz, 1H, CH), 2.29 (s, 3H, CH_3), 2.10 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 194.26, 152.15, 148.11, 144.25, 128.52, 127.34, 126.43, 109.60, 53.85, 30.32, 18.92; IR (KBr): v (cm^{-1}) 3408, 2936, 1745, 1636, 1510, 1458; mp (^{o}C): 239-241.

5,6-Dimethyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1*H*)-one (5b')

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 ^{o}C): δ ppm = 9.34 (brs, 1H, NH), 8.20 (d, J = 8.4 Hz, 2H, Ar-H), 7.98 (brs, 1H, NH), 7.50 (d, J = 9.0 Hz, 2H, Ar-H), 5.39 (d, J = 3.6 Hz, 1H, CH), 2.31 (s, 3H, CH_3), 2.18 (s, 3H, CH_3); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 193.91, 151.98, 151.56, 149.05, 146.68, 127.67, 123.81, 109.46, 53.16, 30.63, 19.11; IR (KBr): v (cm^{-1}) 3269, 2943, 1716,

1670, 1591, 1524; mp (°C): 254-256.

5-Phenyl-1(4-methoxyphenyl)-3[(4-methoxyphenyl)-amino]-1*H*-pyrrol-2(5*H*)-one

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm= 7.85 (s, 1H), 7.47 (d, J = 9.0 Hz, 2H), 7.26 (d, J = 7.2 Hz, 2H), 7.22-7.19 (m, 5H), 6.85 (dd, J_1 = 9.6 Hz, J_2 = 9.0 Hz, 4H), 6.11 (d, J = 2.4 Hz, 1H), 5.92 (d, J = 2.4 Hz, 1H), 3.69 (s, 6H); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 166.31, 156.17, 153.36, 138.26, 135.48, 132.64, 130.18, 128.64, 127.63, 126.80, 123.50, 118.28, 114.31, 113.86, 107.24, 62.81, 55.17, 55.10; mp (°C): 197-199.

12-Phenyl-9,9-dimethyl-8,9,10,12-tetrahydrobenzo[*a*]xanthen-11-one

^{1}H NMR (DMSO-d_6, 600 MHz, Me_4Si, 25 °C): δ ppm= 8.04 (d, J = 8.4 Hz, 2H), 7.92-7.90 (m, 2H), 7.50-7.41 (m, 3H), 7.30-7.29 (m, 2H), 7.19-7.16 (m, 2H), 7.06-7.03 (m, 1H), 5.58 (s, 1H), 2.63 (dd, J_1 = 17.4 Hz, J_2 = 16.2 Hz, 2H), 2.34-2.32 (m, 2H), 1.06 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (151 MHz, DMSO-d_6, δ ppm): 196.31, 164.25, 147.64, 145.33, 131.55, 131.11, 129.55, 129.00, 128.60, 128.59, 127.60, 126.66, 125.43, 123.73, 117.77, 117.62, 113.70, 50.60, 40.73, 34.59, 32.36, 29.30, 26.69; mp (°C): 151-153.