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J. Serb. Chem. Soc. 80 (5) S147–S165 (2015) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Double catalytic effect of $(PhNH_3)_2CuCl_4$ in a novel, highly efficient synthesis of 2-oxo- and thioxo-1,2,3,4-tetra-hydopyrimidines

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COPIES OF ^{1}H- AND ^{13}C-NMR SPECTRA

*Ethyl 6-methyl-4-(3-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carbo-xylate (**7a**)*

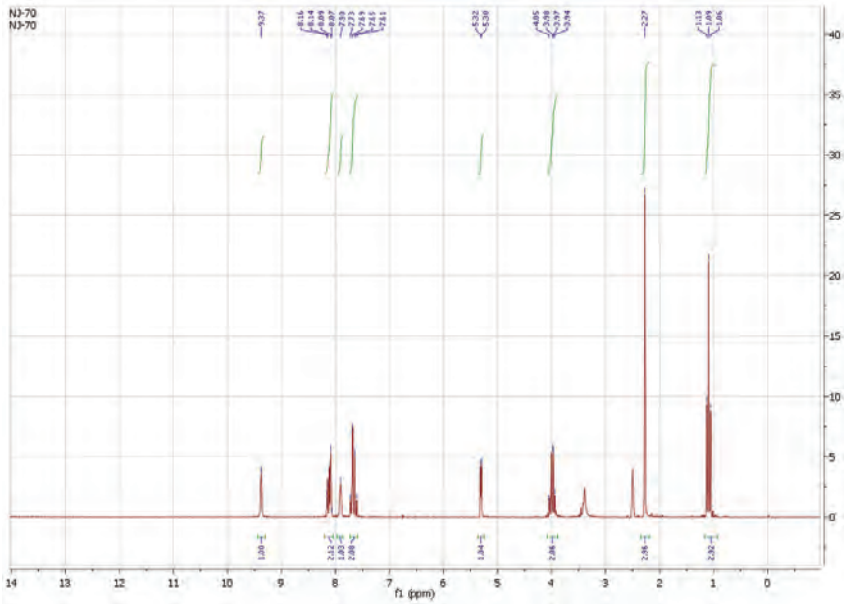

Fig. S-1. ^{1}H-NMR spectrum for **7a**.

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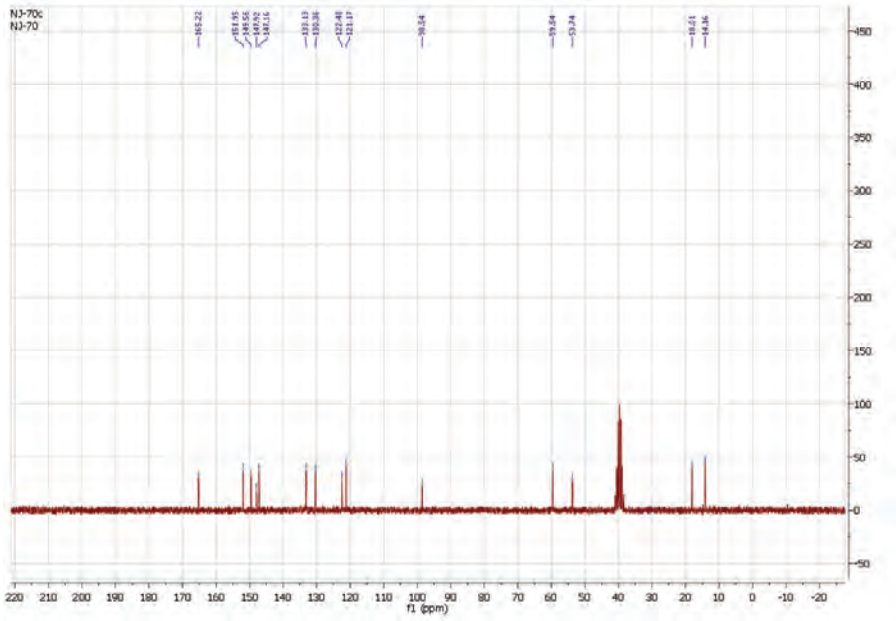

Fig. S-2. ^{13}C-NMR spectrum for **7a**.

*Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7b**)*

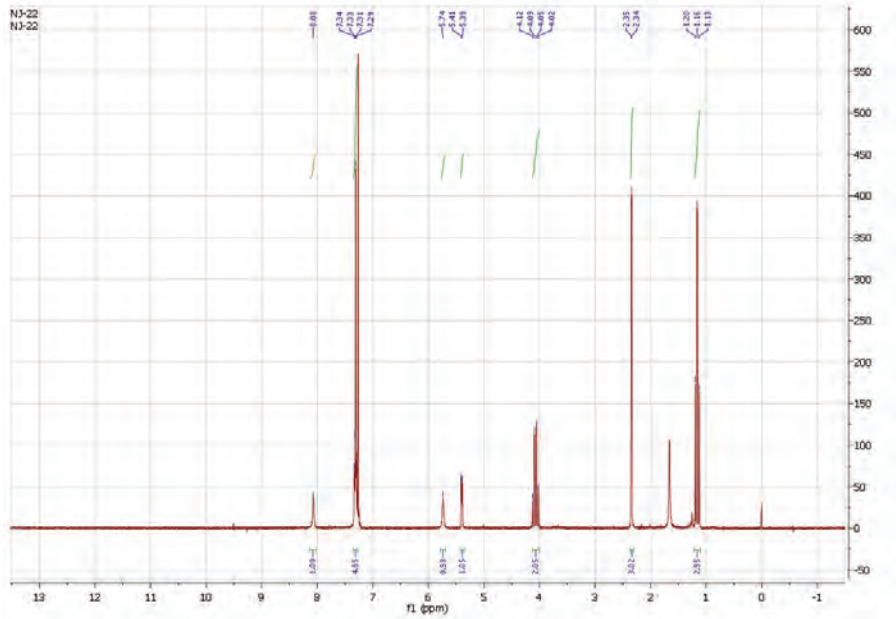

Fig. S-3. ^{1}H-NMR spectrum for **7b**.

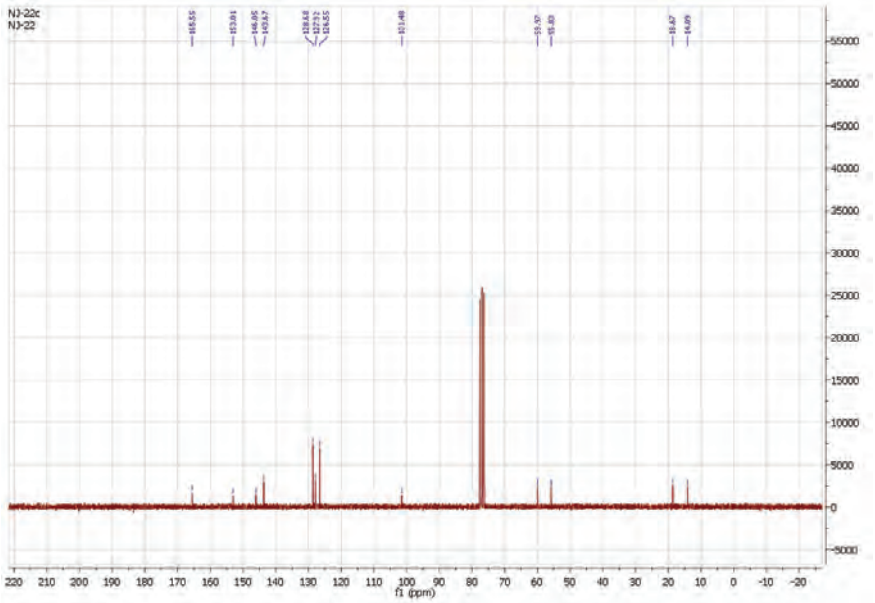

Fig. S-4. ^{13}C-NMR spectrum for **7b**.

*Ethyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7c**)*

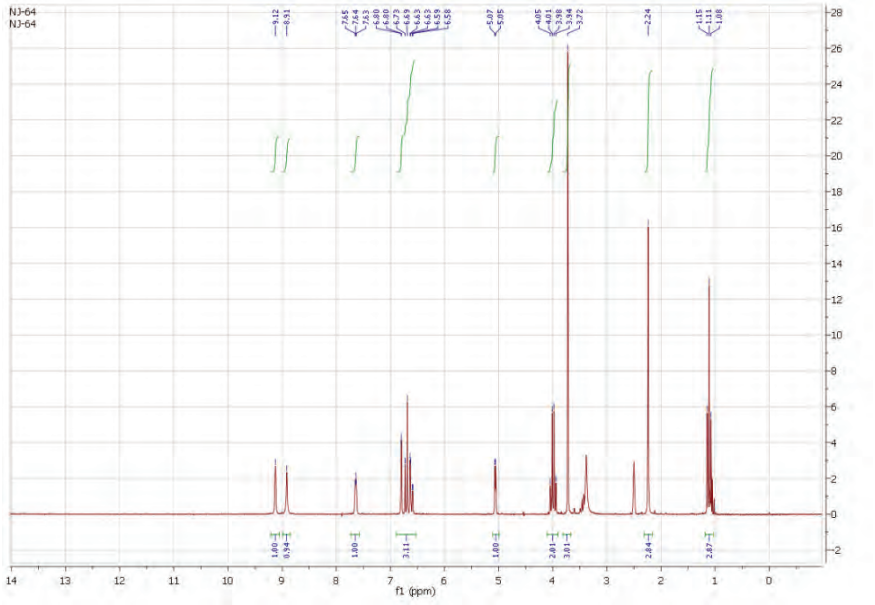

Fig. S-5. ^{1}H-NMRspectrum for **7c**.

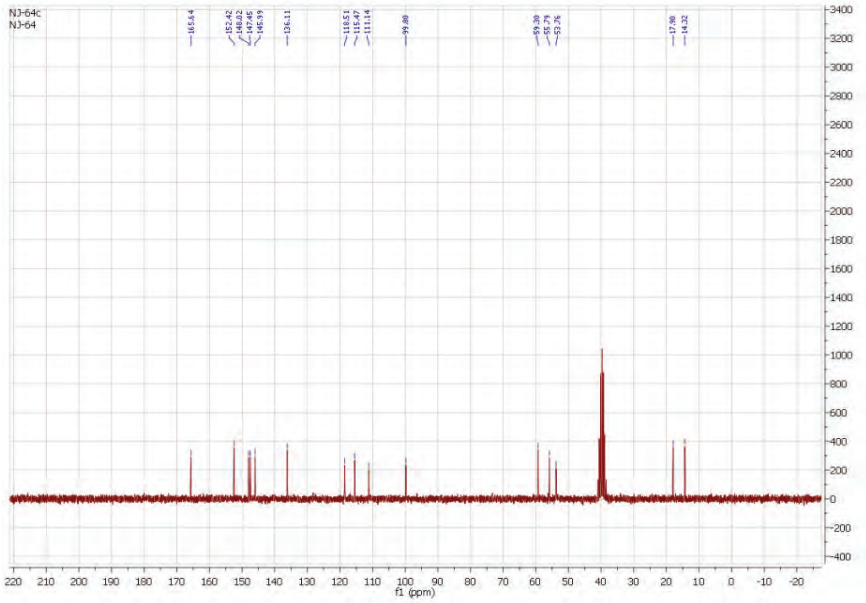

Fig. S-6. ^{13}C-NMR spectrum for **7c**.

*Ethyl 6-methyl-2-oxo-4-[(Z)-2-phenylvinyl]-1,2,3,4- tetrahydropyrimidine-5-carboxylate (**7d**)*

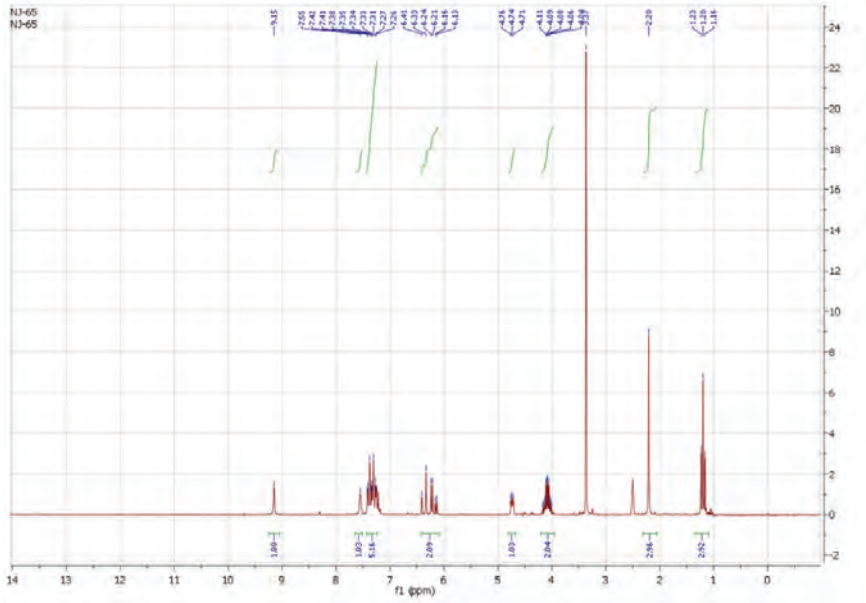

Fig. S-7. ^{1}H-NMR spectrum for **7d**.

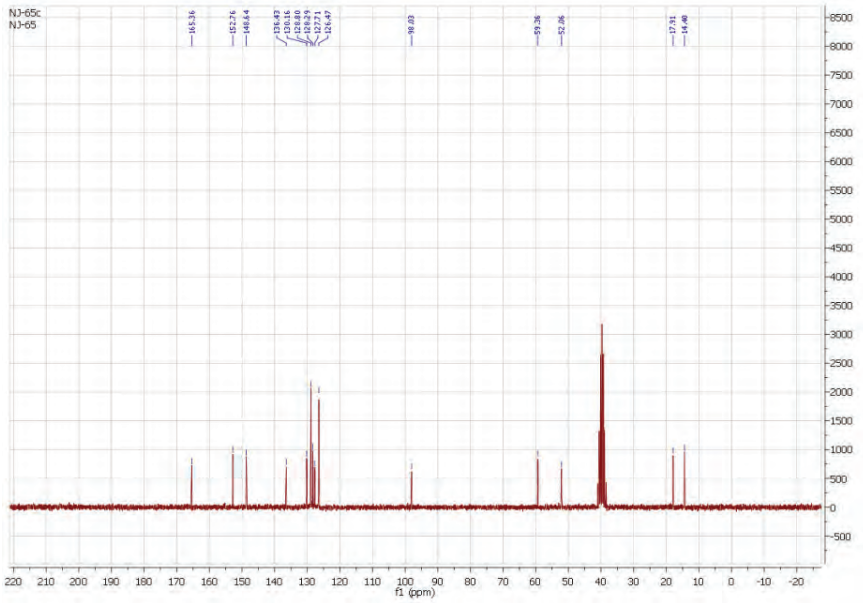

Fig. S-8. ^{13}C-NMR spectrum for **7d**.

*Ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7e**)*

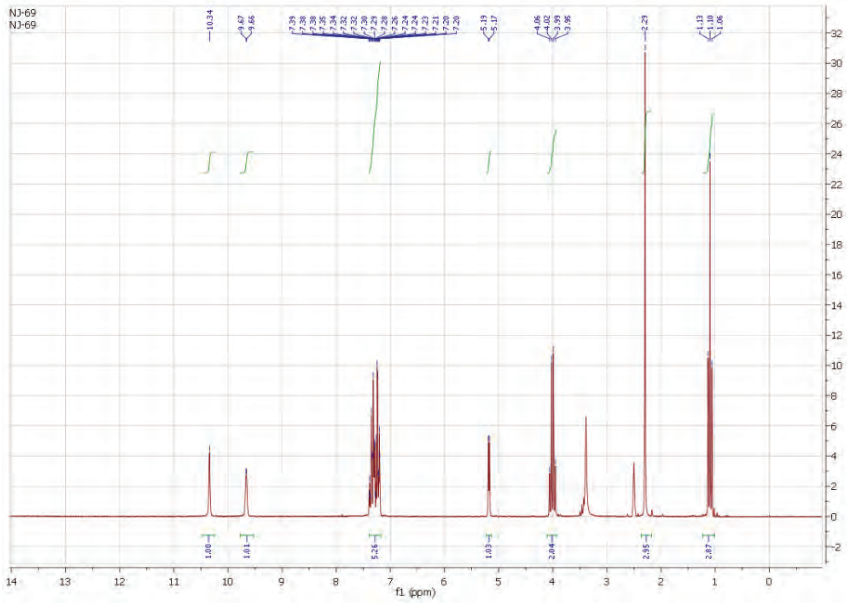

Fig. S-9. ^{1}H-NMR spectrum for **7e**.

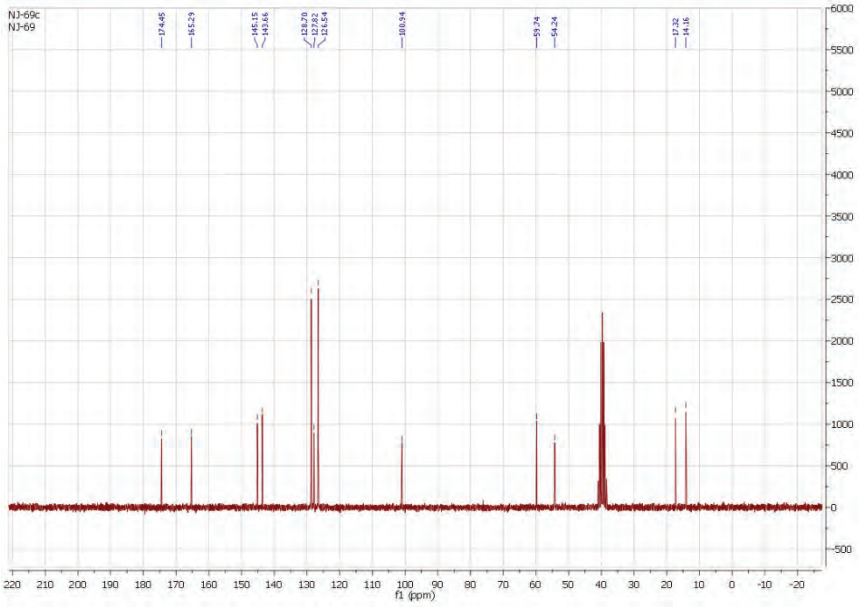

Fig. S-10. ^{13}C-NMR spectrum for **7e**.

*Ethyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7f**)*

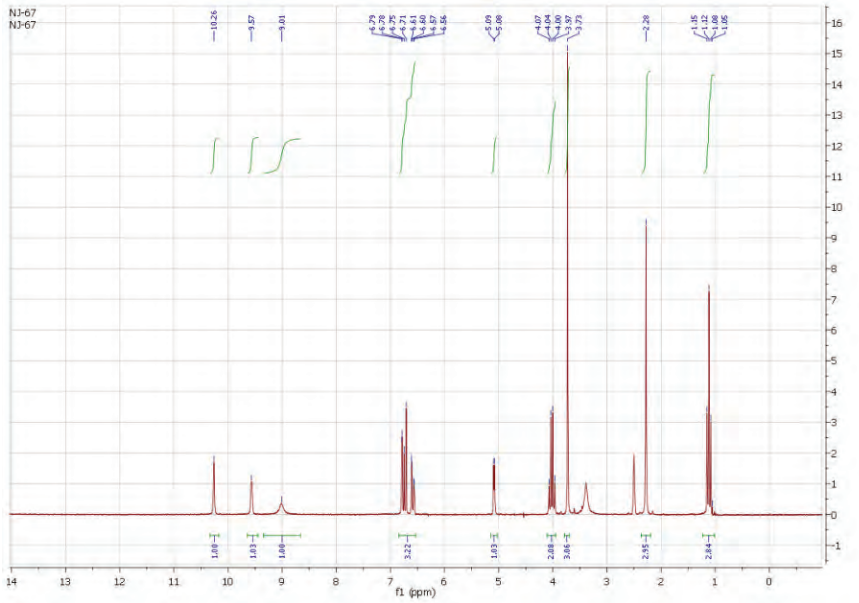

Fig. S-11. ^{1}H-NMR spectrum for **7f**.

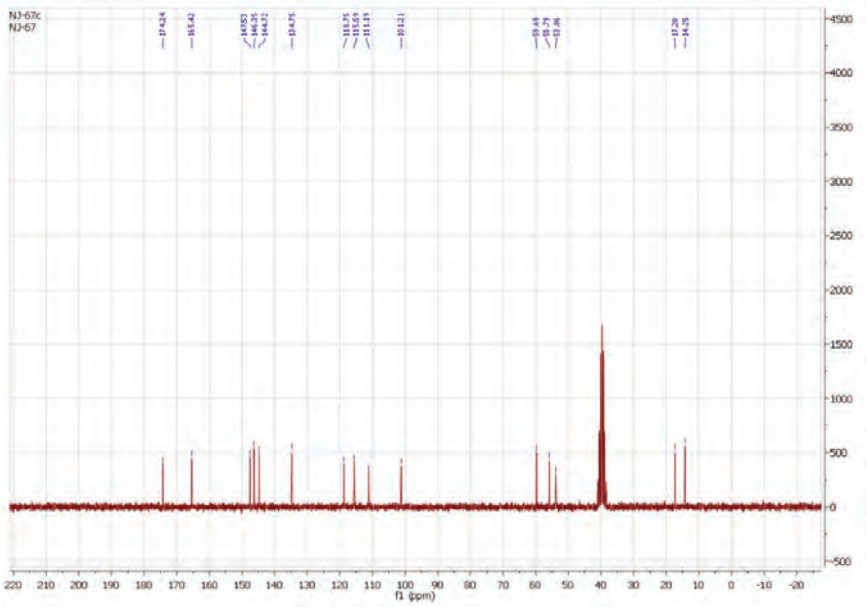

Fig. S-12. ^{13}C-NMR spectrum for **7f**.

*Methyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7h**)*

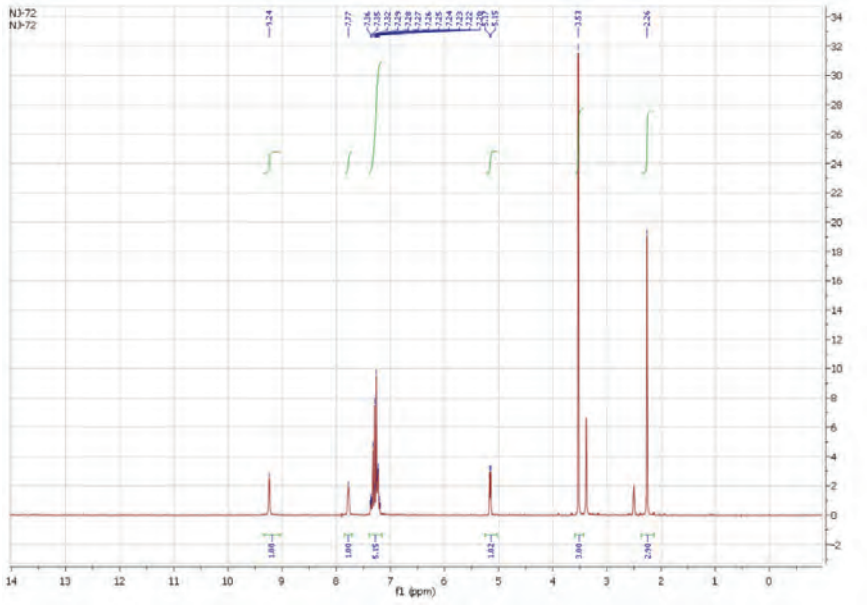

Fig. S-13 ^{1}H-NMR spectrum for **7h**.

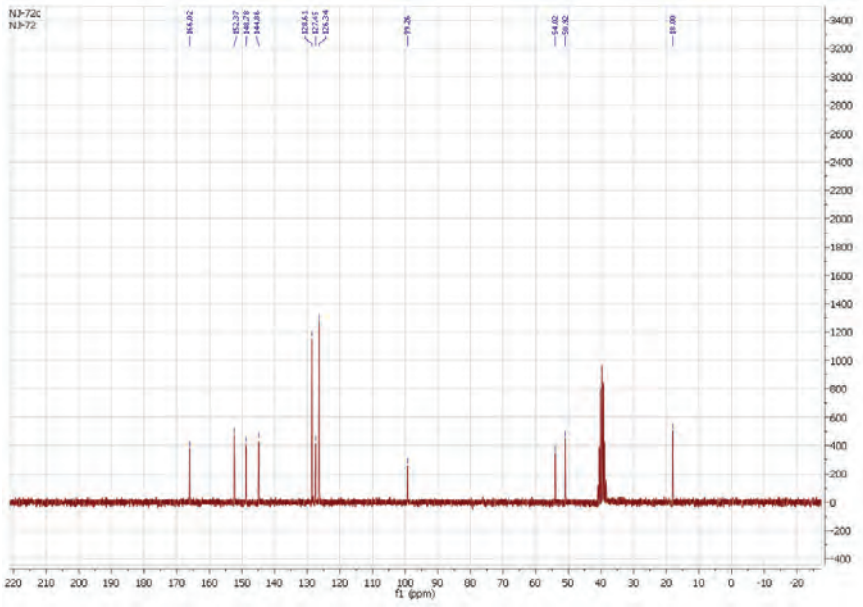

Fig. S-14. ^{13}C-NMR spectrum for **7h**.

*Methyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7i**)*

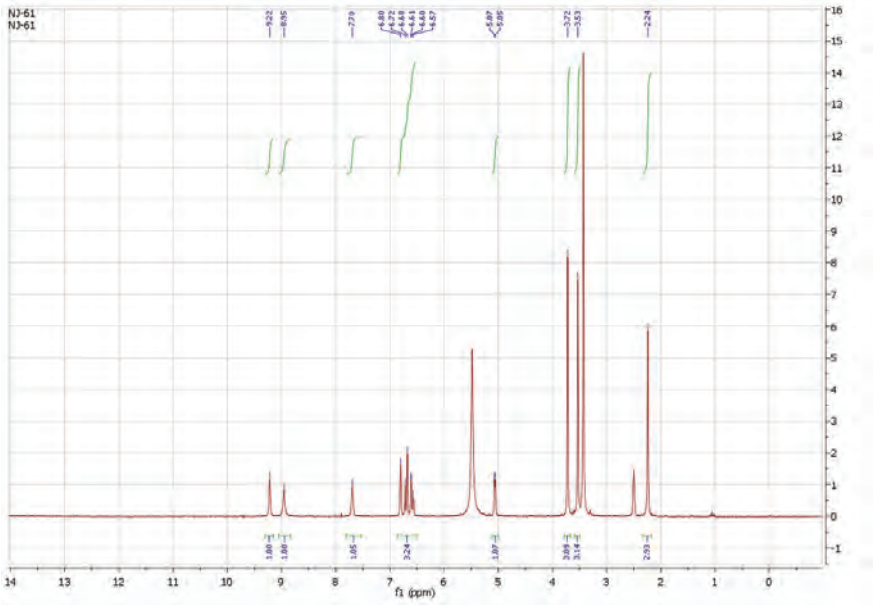

Fig. S-15. ^{1}H-NMR spectrum for **7i**.

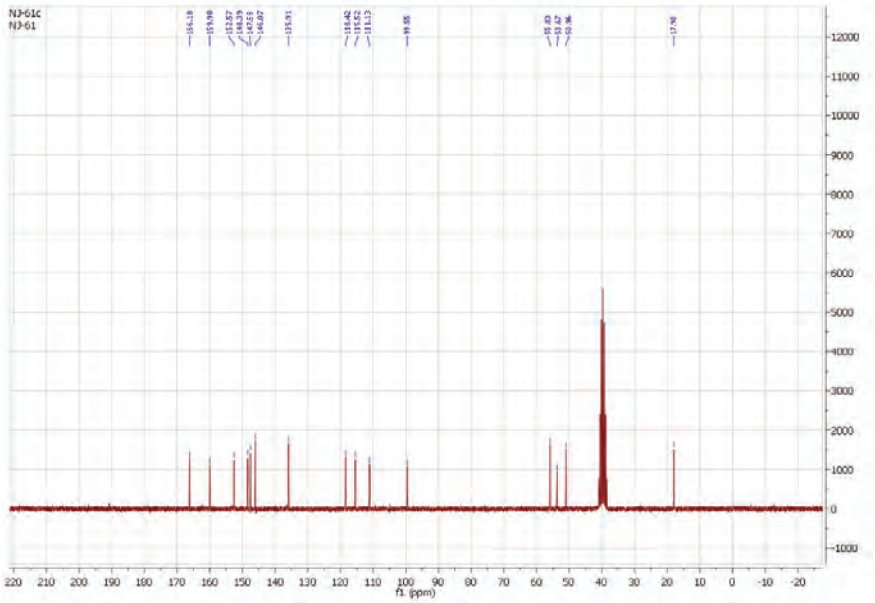

Fig. S-16. ^{13}C-NMR spectrum for **7i**.

*Methyl 6-methyl-2-oxo-4-[(*E*)-2-phenylvinyl]-1,2,3,4-tetrahydropyrimidine-5--carboxylate (**7j**)*

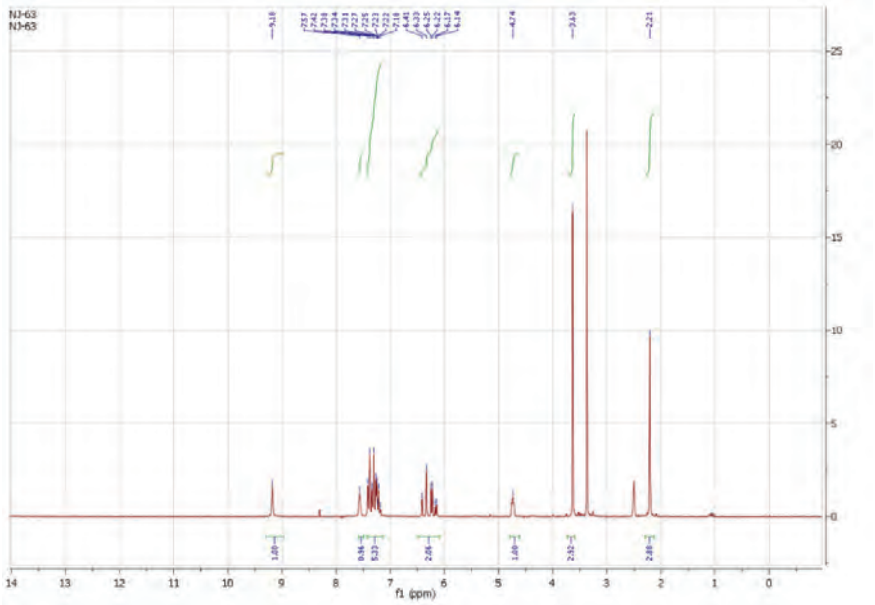

Fig. S-17. ^{1}H-NMR spectrum for **7j**.

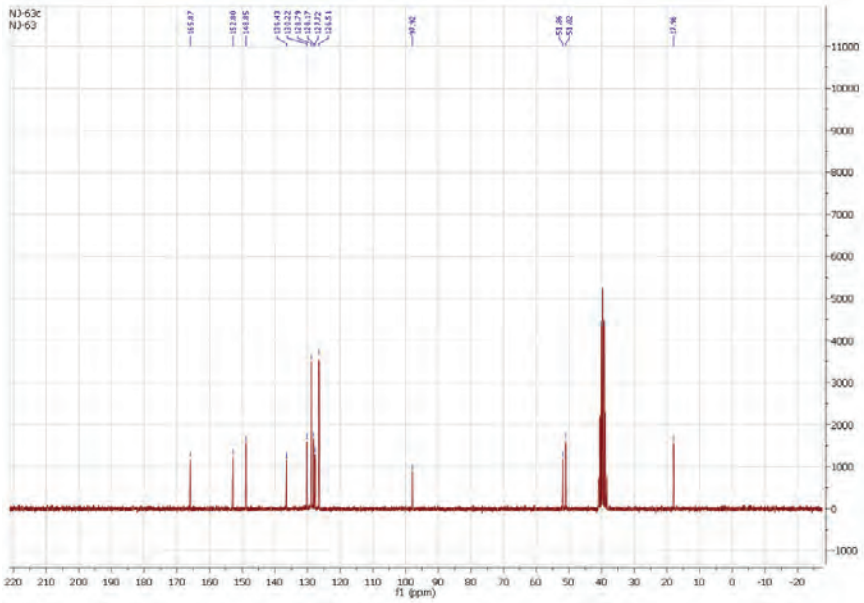

Fig. S-18. ^{13}C-NMR spectrum for **7j**.

*Methyl 6-methyl-4-(3-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7k**)*

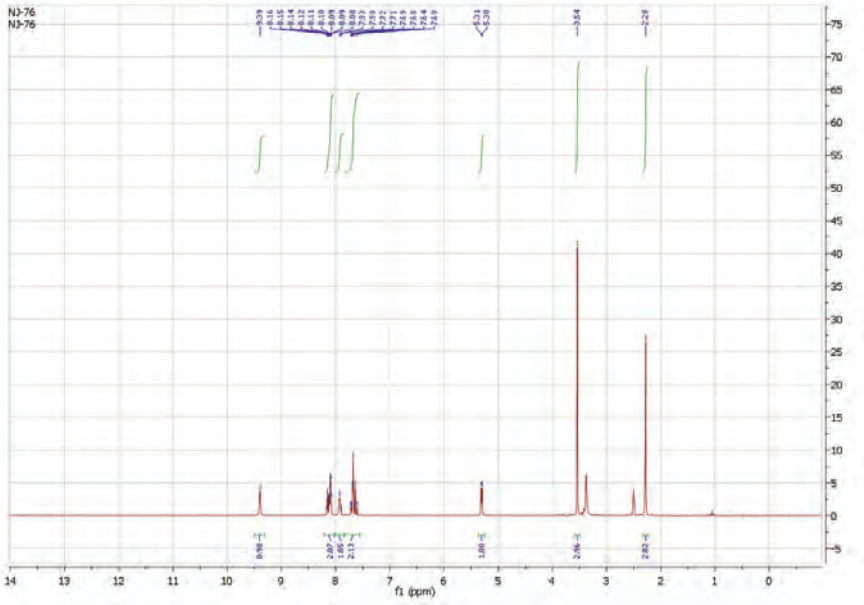

Fig. S-19. ^{1}H-NMR spectrum for **7k**.

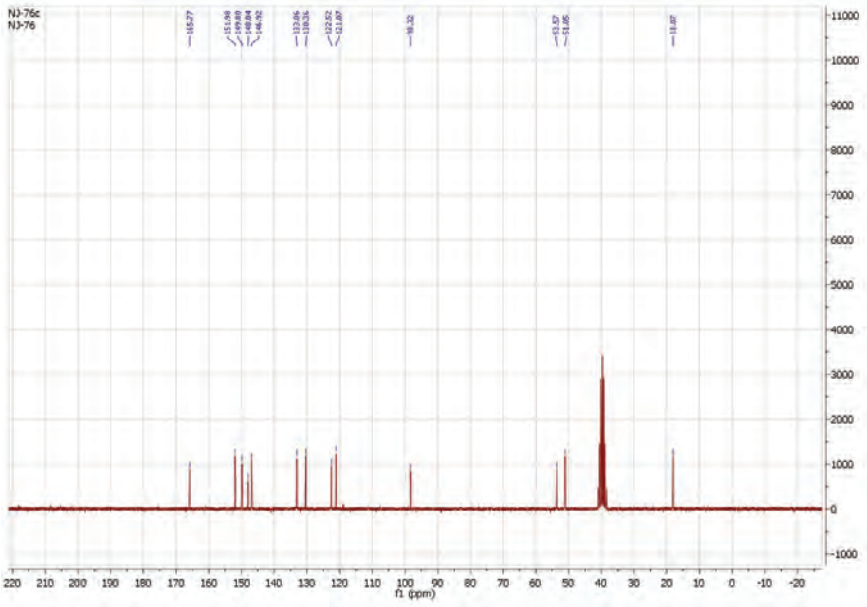

Fig. S-20. ^{13}C-NMR spectrum for **7k**.

*Methyl 4-(2-furyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7l**)*

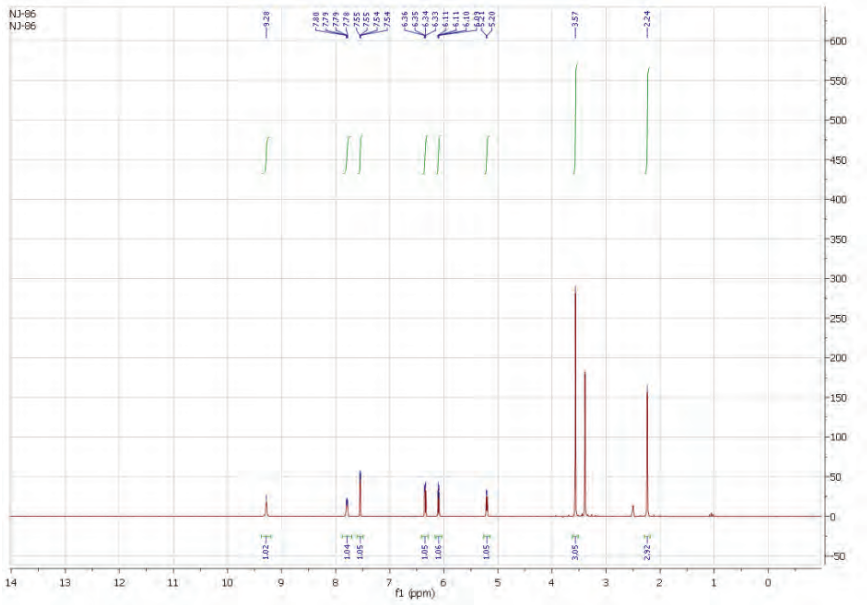

Fig. S-21. ^{1}H-NMR spectrum for **7l**.

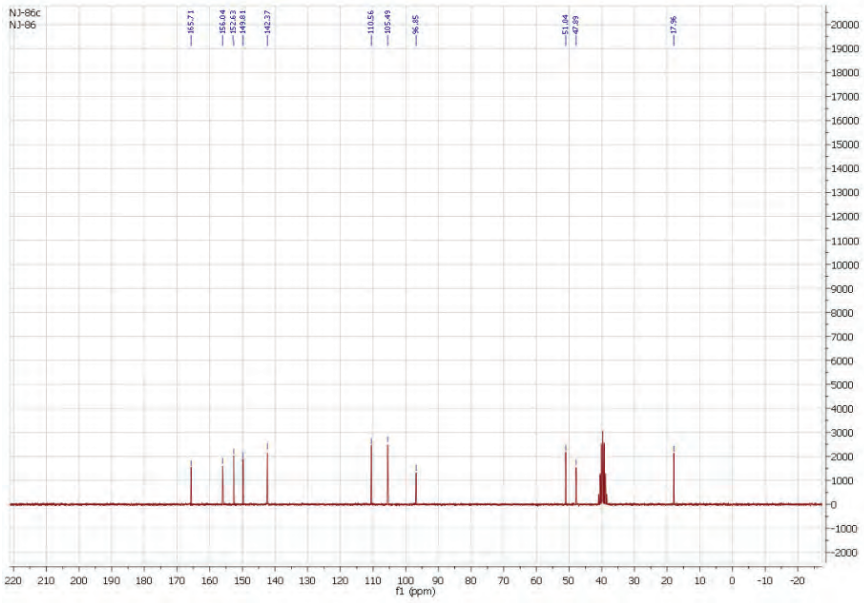

Fig. S-22. ^{13}C-NMR spectrum for **7l**.

*Methyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylate (**7m**)*

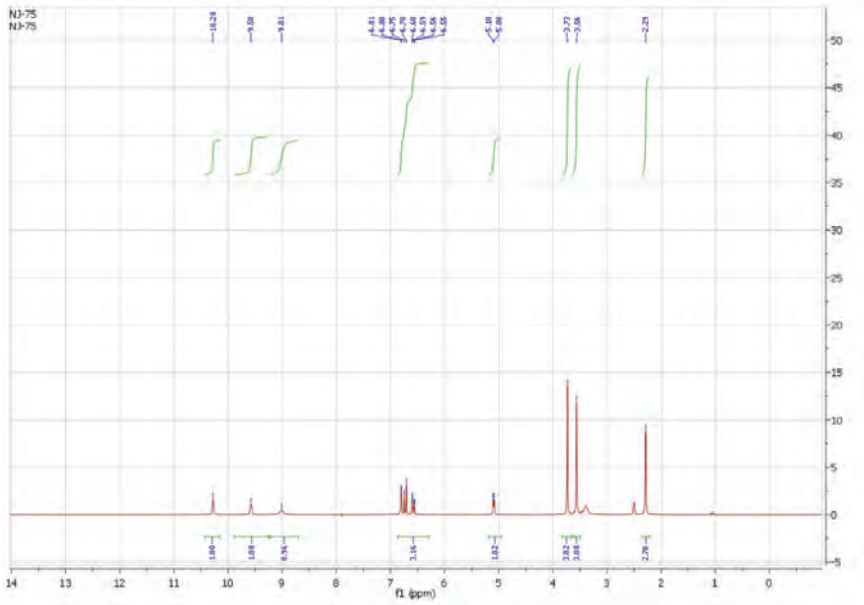

Fig. S-23. ^{1}H-MR spectrum for **7m**.

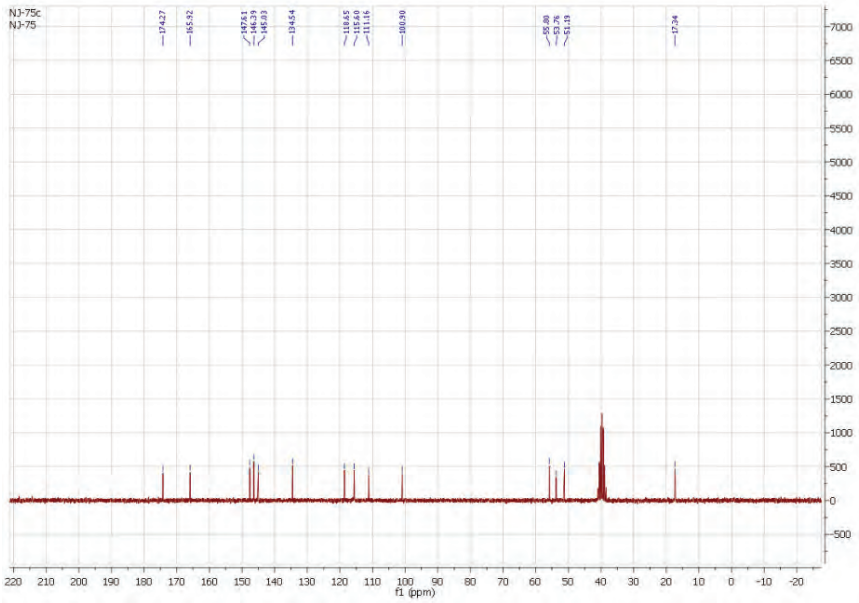

Fig. S-24. ^{13}C-NMR spectrum for **7m**.

*Methyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7n**)*

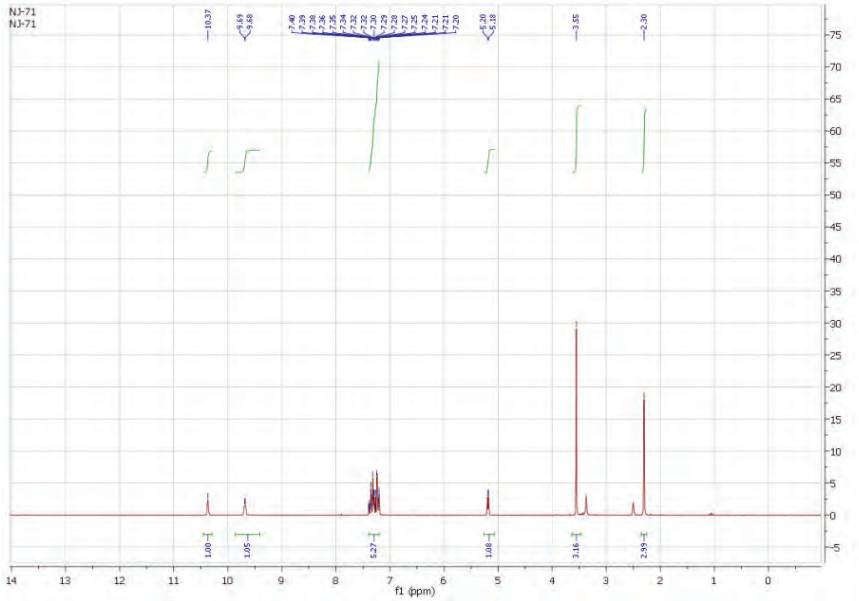

Fig. S-25. ^{1}H-NMR spectrum for **7n**.

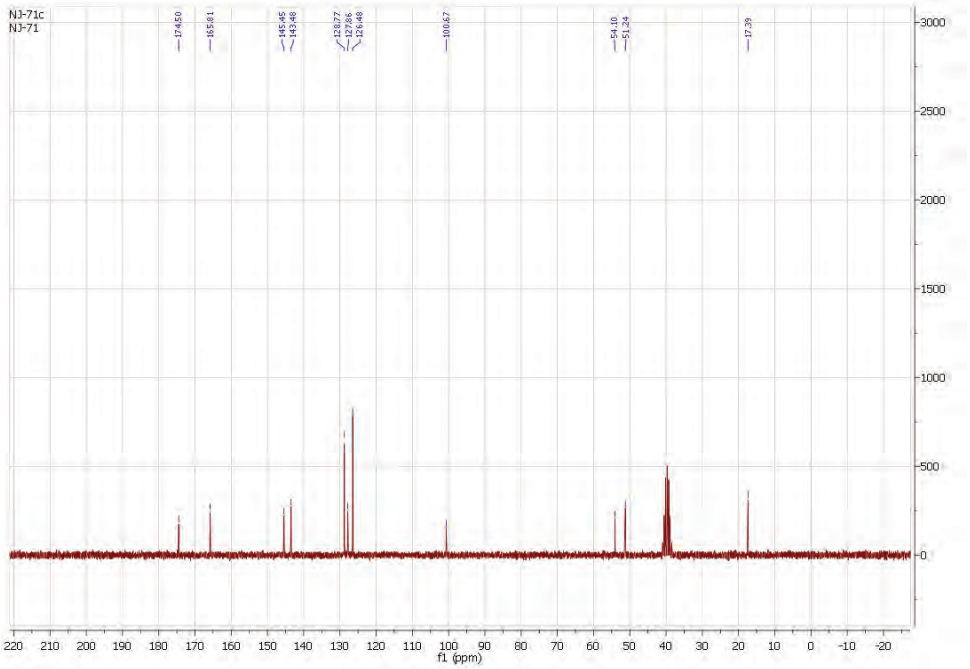

Fig. S-26. ^{13}C-NMR spectrum for **7n**.

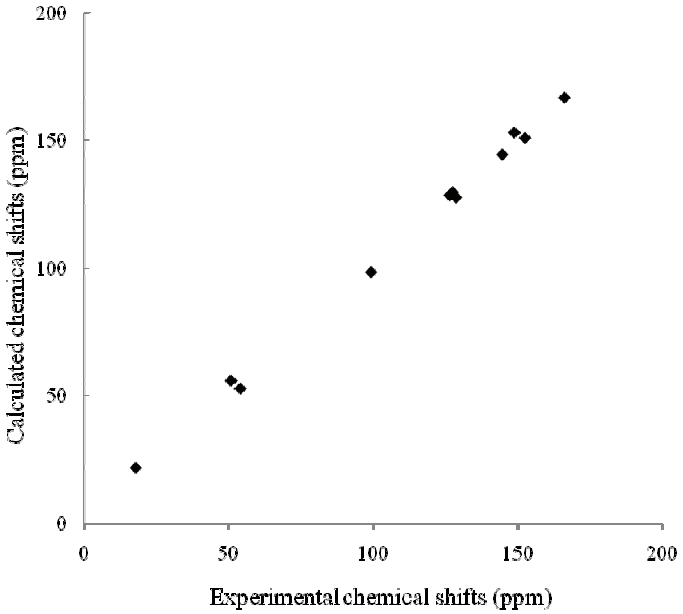

Fig. S-27. Plot of the calculated *versus* experimental chemical shifts of the carbon atoms of **7h** in DMSO.

ANALYTICAL AND SPECTRAL DATA FOR COMPOUNDS **7a–n**

*Ethyl 6-methyl-4-(3-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7a**).* M.p.: 227–229 °C (Lit. 230–232 °C[1]); Anal. Calcd. for $C_{14}H_{15}N_3O_5$: C, 55.08; H, 4.95; N, 13.76 %. Found: C, 55.15; H, 5.01; N, 13.79 %; IR (KBr, cm^{-1}): 3324, 3085, 2961, 1701, 1684, 1624, 1527, 1446, 1315.1, 1300, 1261, 1221, 1086; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 1.07 (3H, *t*, *J* = 7.1 Hz, CH_3), 2.27 (3H, *s*, CH_3), 4.00 (2H, *m*, CH_2O), 5.28 (1H, *d*, *J* = 3.4 Hz, CH), 7.64–7.69 (2H, *m*, Ar), 7.90 (1H, *bs*, NH), 8.07–8.15 (2H, *m*, Ar), 9.37 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, *δ* / ppm): 14.2, 18.2, 53.7, 59.5, 98.6, 121.2, 122.5, 130.4, 133.1, 147.2, 147.9, 149.6, 151.9, 165.2.

*Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7b**).* M.p.: 201–204 °C (Lit. 204 °C[1]); Anal. Calcd. for $C_{14}H_{16}N_2O_3$: C, 64.60; H, 6.19; N, 10.76 %. Found: C, 64.62; H, 6.22; N, 10.86 %; IR (KBr, cm^{-1}): 3333, 3220, 3107, 2951, 1696, 1667, 1651, 1340, 1239, 1094; ^{1}H-NMR (200 MHz, DMSO-d_6 / *δ* ppm): 1.16 (3H, *t*, *J* = 7.1 Hz, CH_3), 2.34 (3H, *s*, CH_3), 4.06 (2H, *q*, *J* = 7.1 Hz, CH_2O), 5.39 (1H, *d*, *J* = 2.3 Hz, CH), 5.74 (1H, *bs*, NH), 7.26–7.34 (5H, *m*, Ar), 8.07 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, *δ* / ppm): 14.0, 18.6, 55.8, 59.9, 101.4, 126.6, 127.9, 128.7, 143.7, 146.1, 153.0, 165.6.

*Ethyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7c**).* M.p.: 233–236 °C (Lit. 233–235 °C[1]); Anal. Calcd. for $C_{15}H_{18}N_2O_5$: C, 58.82; H, 5.92; N, 9.15 %. Found: C, 58.94; H, 5.94; N, 9.18 %; IR (KBr, cm^{-1}): 3450, 3246, 3122, 1698, 1645, 1513, 1277, 1222, 1093; ^{1}H-NMR (200 MHz, DMSO-d_6, *δ* / ppm): 1.11 (3H, *t*, *J* = 7.3 Hz, CH_3), 2.23 (3H, *s*, CH_3), 3.73 (3H, *s*, CH_3O), 4.01 (2H, *q*, *J* = 7.1 Hz, CH_2O), 5.06 (1H, *d*, *J* = 3.2 Hz, CH), 6.58–6.80 (3H, *m*, Ar), 7.64 (1H, *bs*, NH), 8.91 (1H, *s*, OH), 9.12 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, *δ* / ppm): 14.3, 17.9, 53.7, 55.8, 59.3, 99.8, 111.1, 115.5, 118.5, 136.1, 146.0, 147.5, 148.1, 152.4, 165.7.

*Ethyl 6-methyl-2-oxo-4-[(*E*)-2-phenylvinyl]-1,2,3,4- tetrahydropyrimidine-5--carboxylate (**7d**).* M.p.: 235–237 °C (Lit. 234–236 °C[4]); Anal. Calcd. for $C_{16}H_{18}N_2O_3$: C, 67.12; H, 6.34; N, 9.78 %. Found: C, 67.10; H, 6.35; N, 9.82 %; IR (KBr, cm^{-1}): 3232, 3087, 2975, 2891, 1722, 1687, 1654, 1526, 1493, 14525, 1339, 1072; ^{1}H-NMR (200 MHz, DMSO-d_6, *δ* / ppm): 1.19 (3H, *t*, CH_3), 2.21 (3H, *s*, CH_3), 4.11 (2H, *m*, CH_2O), 4.72 (1H, *d*, *J* = 2.8 Hz, CH), 6.13–6.41 (2H, *m*, 2×CH=), 7.22–7.42 (5H, *m*, Ar), 7.55 (1H, *bs*, NH), 9.14 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, *δ* / ppm): 14.4, 17.9, 52.0, 59.3, 98.1, 126.5, 127.7, 128.3, 128.8, 130.2, 136.4, 148.7, 152.7, 165.4.

*Ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**7e**).* M.p.: 206–207 °C (Lit. 208–209 °C[4]); Anal. Calcd. for $C_{14}H_{16}N_2O_2S$: C, 60.85; H, 5.84; N, 10.14 %. Found: C, 60.86; H, 5.88; N, 10.18 %; IR (KBr,

cm^{-1}): 3324, 3170, 2980, 1666, 1572, 1464, 1370, 1326, 1283, 1192, 1175, 1114, 1002; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 1.09 (3H, *t*, *J* = 7.1 Hz, CH_3), 2.29 (3H, *s*, CH_3), 4.02 (2H, *q*, *J* = 7.1 Hz CH_2O), 5.18 (1H, *s*, *J* = 3.7 Hz, CH), 7.19–7.35 (5H, *m*, Ar), 9.66 (1H, *d*, *J* = 1.9 Hz, NH), 10.34 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 14.2, 17.3, 54.2, 59.7, 100.9, 126.5, 127.8, 128.7, 143.7, 145.2, 165.3, 174.5.

Ethyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (***7f***). M.p: 205–208 °C (Lit. 206–208 °C[2]); Anal. Calcd. for $C_{15}H_{18}N_2O_4S$: C, 55.88; H, 5.63; N, 8.69 %. Found: C, 55.92; H, 5.67; N, 8.70 %; IR (KBr, cm^{-1}): 3417, 3154, 2999, 2960, 1678, 1593, 1575, 1518, 1461, 1194, 1113; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 1.15 (3H, *t*, *J* = 7.1 Hz, CH_3), 2.28 (3H, *s*, CH_3), 3.72 (3H, *s*, CH_3O), 4.04 (2H, *q*, *J* = 7.0 Hz, CH_2O), 5.08 (1H, *d*, *J* = 3.6 Hz, CH), 6.56–6.79 (3H, *m*, Ar), 9.01 (1H, *s*, OH), 9.56 (1H, *bs*, NH), 10.25 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 14.2, 17.3, 53.9, 55.8, 59.7, 101.2, 111.1, 115.6, 118.7, 134.8, 144.7, 146.4, 147.5, 165.4, 174.3.

Ethyl 4-(2-furyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (***7g***). M.p.: 206–207 °C (Lit. 208–209 °C[1]); Anal. Calcd. for $C_{12}H_{14}N_2O_4$: C, 57.59; H, 5.64; N, 11.19 %. Found: C, 57.62; H, 5.64; N, 11.23 %; IR (KBr, cm^{-1}): 3315, 3118, 1708, 1672, 1651, 1432, 1339, 1239, 1088; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 1.15 (3H, *t*, *J* = 7.2 Hz, CH_3), 2.34 (3H, *s*, CH_3), 4.06 (2H, *q*, *J* = 7.0 Hz, CH_2O), 5.15 (1H, *d*, *J* = 3.2 Hz, CH), 6.18–6.21 (1H, *m*, Ar), 6.30–6.34 (1H, *m*, Ar), 7.58–7.61 (1H, *m*, Ar), 7.94 (1H, *bs*, NH), 9.08 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 14.5, 18.7, 53.3, 56.6, 96.4, 105.4, 110.7, 143.7, 149.5, 152.7, 156.0, 165.4.

Methyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (***7h***). M.p.: 210–213 °C (Lit. 212–213 °C[3]); Anal. Calcd. for $C_{13}H_{14}N_2O_3$: C, 63.40; H, 5.73; N, 11.37 %. Found: C, 63.44; H, 5.73; N, 11.39 %; IR (KBr, cm^{-1}): 3365, 3221, 3078, 3020, 2925, 1749, 1708, 1654, 1423, 1074; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.26 (3H, *s*, CH_3), 3.53 (3H, *s*, CH_3O), 5.15 (1H, *d*, *J* = 3.4 Hz, CH), 7.22–7.32 (5H, *m*, Ar), 7.77 (1H, *bs*, NH), 9.24 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, the calculated values are given in brackets, δ / ppm): 18.0 (21.8), 50.9 (56.0), 54.0 (52.8), 99.3 (98.3), 126.4 (128.4), 127.4 (129.6), 128.6 (127.6), 144.7 (144.3), 148.8 (153.1), 152.4 (150.9), 166.0 (166.7).

Methyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (***7i***). M.p.: 253–255 °C (Lit. 253–254 °C[5]); Anal. Calcd. for $C_{14}H_{16}N_2O_5$: C, 57.53; H, 5.52; N, 9.58 %. Found: C, 57.54; H, 5.53; N, 9.60 %; IR (KBr, cm^{-1}): 3363, 3230, 3069, 3033, 2941, 1746, 1707, 1647, 1430, 1107; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.24 (3H, *s*, CH_3), 3.53 (3H, *s*, CH_3O), 3.72 (3H, *s*, CH_3O), 5.06 (1H, *d*, *J* = 3.2 Hz, CH), 6.57–6.81 (3H,

m, Ar), 7.69 (1H, *bs*, NH), 8.95 (1H, *s*, OH), 9.22 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 17.9, 50.1, 55.8, 99.5, 111.1, 115.5, 118.4, 135.9, 146.1, 147.6, 148.4, 152.6, 159.9, 166.2.

Methyl 6-methyl-2-oxo-4-[(E*)-2-phenylvinyl]-1,2,3,4-tetrahydropyrimidine--5-carboxylate (**7j**)*. M.p.: 229–231 °C (Lit. 229–232 °C[5]); Anal. Calcd. for $C_{15}H_{16}N_2O_3$: C, 66.16; H, 5.92; N, 10.29 %. Found: C, 66.19; H, 5.96; N, 10.29 %; IR (KBr, cm^{-1}): 3245, 3116, 2952, 1722, 1712, 1685, 1645, 1434, 1249, 1099; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.20 (3H, *s*, CH_3), 3.63 (3H, *s*, CH_3O), 4.74 (1H, *d*, *J* = 3.2 Hz, CH), 6.14–6.41 (2H, *m*, 2×CH=), 7.22–7.41 (5H, *m*, Ar), 7.55 (1H, *bs*, NH), 9.12 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 17.9, 51.1, 51.8, 97.9, 126.5, 127.7, 128.2, 128.8, 130.2, 136.4, 148.9, 152.8, 165.9.

*Methyl 6-methyl-4-(3-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5--carboxylate (**7k**)*. M.p.: 281–283 °C (Lit. 280–283 °C[6]); Anal. Calcd. for $C_{13}H_{13}N_3O_5$: C, 53.61; H, 4.49; N, 14.42 %. Found: C, 53.62; H, 4.49; N, 14.45 %; IR (KBr, cm^{-1}): 3177, 2980, 1710, 1654, 1590, 1521, 1462, 1340, 1274, 1180, 1100; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.28 (3H, *s*, CH_3), 3.54 (3H, *s*, CH_3O), 5.30 (1H, *d*, *J* = 3.4 Hz, CH), 7.64–7.69 (2H, *m*, Ar), 7.90 (1H, *bs*, NH), 8.07–8.15 (2H, *m*, Ar), 9.37 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 18.0, 51.1, 53.6, 98.3, 121.0, 122.5, 130.4, 133.1, 146.9, 148.0, 149.8, 151.9, 165.8.

*Methyl 4-(2-furyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxyl-ate (**7l**)*. M.p.: 207–209 °C (Lit. 208–209 °C[7]); Anal. Calcd. for $C_{11}H_{12}N_2O_4$: C, 55.93; H, 5.12; N, 11.85 %. Found: C, 55.95; H, 5.15; N, 11.86 %; IR (KBr, cm^{-1}): 3245, 3118, 2975, 2940, 1709, 1701, 1650, 1435, 1318, 1296, 1234, 1100; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.24 (3H, *s*, CH_3), 3.56 (3H, *s*, CH_3O), 5.20 (1H, *d*, *J* = 3.3 Hz, CH), 6.08–6.11 (1H, *m*, Ar), 6.33–6.36 (1H, *m*, Ar), 7.54–7.56 (1H, *m*, Ar), 7.97 (1H, *t*, NH), 9.28 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 17.9, 47.8, 51.1, 96.8, 105.5, 110.6, 142.4, 149.8, 152.6, 156.1, 165.7.

*Methyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahyd-ropyrimidine-5-carboxylate (**7m**)*. M.p.: 257–260 °C (Lit. 258–260 °C[8]); Anal. Calcd. for $C_{14}H_{16}N_2O_4S$: C, 54.53; H, 5.23; N, 9.08 %. Found: C, 54.55; H, 5.28; N, 9.10 %; IR (KBr, cm^{-1}): 3411, 3164, 3002, 1692, 1661, 1584, 1519, 1435, 1344, 1287, 1197; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.28 (3H, *s*, CH_3), 3.56 (3H, *s*, CH_3O), 3.73 (3H, *s*, CH_3O), 5.08 (1H, *d*, *J* = 3.7 Hz, CH), 6.55–6.80 (3H, *m*, Ar), 9.01 (1H, *s*, OH), 9.57 (1H, *bs*, NH), 10.28 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 17.3, 51.2, 53.8, 55.7, 100.9, 111.2, 115.6, 118.7, 134.5, 145.0, 146.4, 147.6, 165.9, 174.3.

*Methyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carbo-xylate (**7n**)*. M.p.: 207–210 °C (Lit. 237–239 °C[9]); Anal. Calcd. for

$C_{13}H_{14}N_2O_2S$: C, 59.52; H, 5.38; N, 10.68 %. Found: C, 59.52; H, 5.44; N, 10.71 %; IR (KBr, cm^{-1}): 3315, 3183, 2996, 1664, 1643, 1579, 1457, 1346, 1288, 1202, 1113; ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.30 (3H, *s*, CH_3), 3.55 (3H, *s*, CH_3), 5.18 (1H, *d*, J = 3.8 Hz, CH), 7.20–7.39 (5H, *m*, Ar), 9.66 (1H, *d*, J = 2.0 Hz, NH), 10.36 (1H, *bs*, NH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 17.4, 51.2, 54.1, 100.6, 126.5, 127.8, 128.8, 143.5, 145.4, 165.8, 174.5.

Table S-I. Cartesian coordinates of the product **7h**

Element	Coordinates		
C	–0.28524400	0.28629100	–0.98404300
C	1.02321100	0.06946900	–0.26491800
C	1.57184000	1.07011100	0.46901700
H	–1.25697000	1.98503200	–1.82013500
H	1.35716700	3.05638100	1.01588500
H	–0.21774700	–0.18955800	–1.96932900
C	–1.47976900	–0.31974600	–0.27008100
C	–2.43738400	–1.01671100	–0.99917600
C	–1.66766700	–0.14437700	1.09919900
C	–3.56931000	–1.52776400	–0.37641200
H	–2.29007800	–1.16391200	–2.06711900
C	–2.79802800	–0.65129700	1.72443700
H	–0.92142000	0.38888400	1.68378000
C	–3.75251600	–1.34352800	0.98750100
H	–4.30723500	–2.07331300	–0.95681300
H	–2.93396500	–0.50967300	2.79245600
H	–4.63519300	–1.74228700	1.47820400
N	0.95308300	2.30356800	0.47429900
N	–0.48858600	1.71740100	–1.21830100
C	–0.03605800	2.70345500	–0.41449400
O	–0.40880200	3.86389900	–0.45997400
C	1.56397200	–1.27559300	–0.42334000
O	0.99671600	–2.14735400	–1.05169400
O	2.75068300	–1.47736700	0.16662000
C	3.30637400	–2.78283400	0.02491000
H	3.47821400	–3.01760600	–1.02809900
H	4.25256400	–2.76457500	0.56323000
H	2.64282600	–3.53560900	0.45639800
C	2.80631900	1.01544400	1.30600400
H	2.82750500	0.12461300	1.93216300
H	3.69687300	0.98433100	0.67204200
H	2.87275800	1.89956300	1.94410800

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