$([Cu_3(DMAP)_8(\mu_3\text{-}CO_3)_2]I_2)_n \cdot xH_2O$: Synthesis of a $\mu_3\text{-}CO_3$ bridged linear polymeric Cu-complex, characterization and catalytic applications in the synthesis of phenoxypyrimidines and arylthiopyrimidines via C-O and C-S cross-coupling reactions

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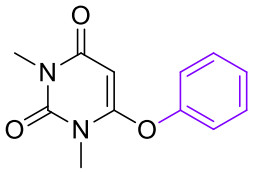
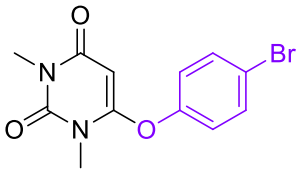
Contents:

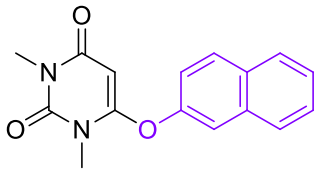
1. Spectral data of synthesized compounds



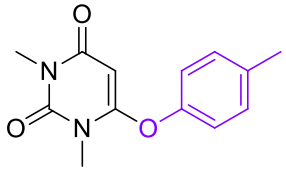
1,3-Dimethyl-6-phenoxypyrimidine-2,4(1*H*,3*H*)-dione (3a): Creamy white solid (86 %); mp: 105 °C – 109 °C; R_f = 0.3 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.43 (t, *J* = 8 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 2H), 4.77 (s, 1H), 3.52 (s, 3H), 3.30 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 163.3, 161.7, 151.6, 151.6, 130.6, 127.4, 121.3, 81.1, 29.6, 28.2 ppm; HRMS(ESI): calcd. for $C_{12}H_{12}N_2O_3$ $[M+H]^+$ 233.0926; found: 233.0923.



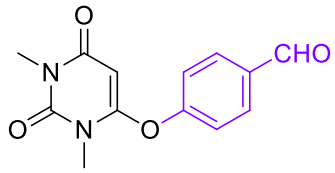
6-(4-bromophenoxy)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3b): White solid (94 %); mp: 150 °C – 151 °C; R_f = 0.3in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.73 (d, *J* = 8.8 Hz, 2H), 7.31(d, *J* = 8.8 Hz, 2H), 4.53(s, 1H), 3.39(s, 3H), 3.14(s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 161.8, 161.1, 150.9, 150.8, 133.4,123.5, 119.3, 80.3, 29.2, 27.5 ppm; HRMS(ESI): calcd. for $C_{12}H_{11}BrN_2O_3$ $[M+H]^+$ 311.0031.



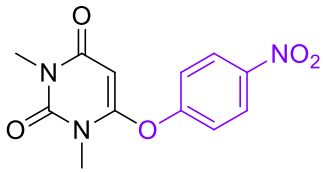
1,3-Dimethyl-6-(naphthalen-2-yloxy)pyrimidine-2,4(1*H*,3*H*)-dione (3c): Light yellow solid (90 %); mp: 134 °C – 136 °C, R_f = 0.2 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.92 (d, *J* = 8.8 Hz, 1H), 7.88 (m, 2H), 7.81 (m, 3H), 7.22 (dd, J= 2.4 Hz, 8.8 Hz, 1H), 4.82 (s, 1H), 3.58(s, 3H), 3.32 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 163.2, 161.7, 151.6, 149.1, 134.0, 132.0, 131.0, 128.2, 127.8, 127.6, 126.8, 120.0, 118.7, 81.5, 29.6, 28.2 ppm; HRMS(ESI): calcd. for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1083; found: 283.1082.



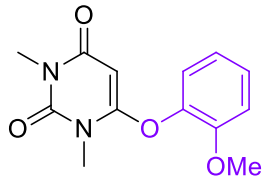
1,3-dimethyl-6-(p-tolyloxy)pyrimidine-2,4(1*H*,3*H*)-dione (3d): Light red solid (88 %); mp: 106 °C – 108 °C; R_f = 0.3 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.21 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 4.76 (s, 1H), 3.51 (s, 3H), 3.29 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 163.3, 161.9, 151.6, 149.4, 137.3, 131.0, 121.0, 81.0, 29.5, 28.2, 21.1 ppm; HRMS(ESI): calcd. for $C_{13}H_{14}N_2O_3$ $[M+H]^+$ 247.1083; found: 247.1081.



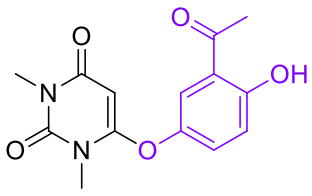
4-((1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)oxy)benzaldehyde (3e): Brown solid (80%); mp: 113 °C – 114 °C; R_f = 0.2 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.01(s, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.30(d, *J* = 8.4 Hz, 2H), 4.82(s, 1H), 3.53(s, 3H), 3.31(s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 190.5, 162.9, 160.7, 156.0, 151.4, 135.2, 132.3, 122.0, 82.0, 29.7, 28.3 ppm; HRMS(ESI): calcd. for $C_{13}H_{12}N_2O_4$ $[M+H]^+$ 261.0875.



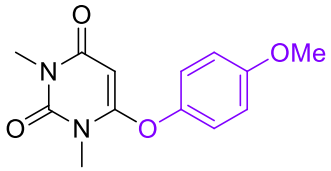
1,3-dimethyl-6-(4-nitrophenoxy)pyrimidine-2,4(1*H*,3*H*)-dione (3f): White solid (82 %); mp: 179 °C – 181 °C; R_f = 0.2 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* = 9.2 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 4.81 (s, 1H), 3.52 (s, 3H), 3.30 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 162.6, 160.3, 156.2, 151.3, 146.3, 126.5, 122.1, 82.3, 29.8, 28.3 ppm; HRMS(ESI): calcd. for $C_{12}H_{11}N_3O_5$ $[M+H]^+$ 278.0777; found: 278.0774.



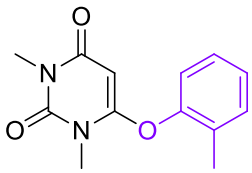
6-**(2-methoxyphenoxy)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3g)**: White solid (93 %); mp: 141 °C – 144 °C; R_f = 0.3 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.39 (dt, *J* = 1.65 & 8.2 Hz, 1H), 7.30 (ddd, *J* = 1.5 & 8.2Hz, 2H), 7.08 (dt, *J* = 1.5 & 7.7 Hz, 1H), 4.42 (s, 1H), 3.81 (s, 3H), 3.42 (s, 3H), 3.13 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 161.8, 160.9, 150.7, 150.5, 139.6, 128.4, 122.6, 121.2, 113.8, 79.0, 56.0, 29.1, 27.5 ppm; HRMS(ESI): calcd. for $C_{13}H_{14}N_2O_4$ $[M+H]^+$ 263.1032; found:263.1028.



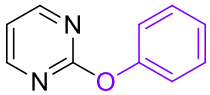
6-(3-acetyl-4-hydroxyphenoxy)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3h): Light yellow solid (66 %); mp: 193 °C – 197 °C; R_f = 0.2 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.5 (s, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 6.71 (s, 1H), 6.66 (d, *J* = 7.2 Hz, 1H), 4.91 (s, 1H), 3.48 (s, 3H), 3.30 (s, 3H), 2.63 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 203.7, 164.6, 162.9, 160.2, 157.2, 151.4, 133.2, 118.6, 111.8, 110.7, 82.3, 29.7, 28.3, 27.0 ppm; HRMS(ESI): calcd. for $C_{14}H_{14}N_2O_5$ $[M+H]^+$ 291.0981; found: 291.0978.



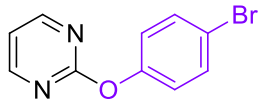
6-(4-methoxyphenoxy)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3i): White solid (90 %); mp: 125 °C – 129 °C; R_f = 0.3 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.25 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 9.2 Hz, 2H), 4.42 (s, 1H), 3.79 (s, 3H), 3.40 (s, 3H), 3.13 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 162.0, 161.9, 157.7, 150.8, 144.8, 122.3, 115.3, 79.5, 55.6, 29.1, 27.5 ppm; HRMS(ESI): calcd. for $C_{13}H_{14}N_2O_4$ $[M+H]^+$ 263.1032; found: 263.1027.



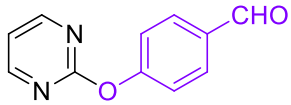
1,3-dimethyl-6-(o-tolyloxy)pyrimidine-2,4(1*H*,3*H*)-dione (3j): White solid (85 %); mp: 112 °C – 114 °C; R_f = 0.4 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.28 (m, 3H), 7.01 (dd, *J* = 2 & 7.4 Hz, 1H), 4.67 (s, 1H), 3.54 (s, 3H), 3.30 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 163.3, 160.8, 151.6, 149.9, 132.3, 130.2, 128.1, 127.5, 121.5, 80.5, 29.4, 28.2, 15.9 ppm; HRMS(ESI): calcd. for $C_{13}H_{14}N_2O_3$ $[M+H]^+$ 247.1083; found: 247.1080.



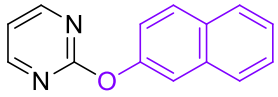
2-Phenoxypyrimidine (3k): White solid (84 %); mp: 87 °C – 89 °C; R_f = 0.5 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (d, *J* = 4.8 Hz, 2H), 7.46 (t, *J* = 8 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 2H), 7.06 (t, *J* = 4.8 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 165.5, 159.9, 153.0, 129.9, 125.7, 121.8, 116.3 ppm; HRMS(ESI): calcd. for $C_{10}H_8N_2O$ $[M+H]^+$ 173.0715.



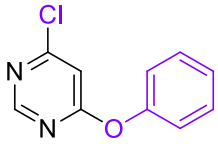
2-(4-Bromophenoxy)pyrimidine (3l): Brown solid (82 %); mp: 110 °C – 113 °C; R_f = 0.5 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.55 (d, *J* = 4.8 Hz, 2H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.09 (d, *J* = 8.8 Hz, 2H), 7.04 (t, *J* = 4.8 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 165.2, 160.0, 152.0, 132.9, 123.7, 118.8, 116.7 ppm; HRMS(ESI): calcd. for $C_{10}H_7BrN_2O$ $[M+H]^+$ 250.9820.



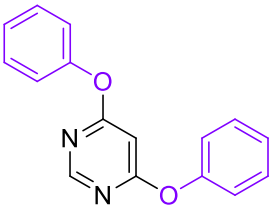
4-(pyrimidin-2-yloxy)benzaldehyde (3m): Yellow solid (60 %); mp: 81 °C – 82 °C; R_f = 0.3 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.99 (s, 1H), 8.58 (d, *J* = 4.8 Hz, 2H), 7.96(d, *J* = 8.8 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.09 (t, *J* = 4.8 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 191.1, 164.8, 160.1, 157.9, 133.8, 131.7, 122.4, 117.1 ppm; HRMS(ESI): calcd. for $C_{11}H_8N_2O_2$ $[M+H]^+$ 201.0664.



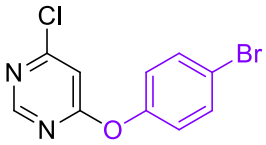
2-(naphthalen-2-yloxy)pyrimidine (3n): Creamy White solid (84 %); mp: 86 °C – 89 °C; R_f = 0.5 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.54 (d, *J* = 4.4 Hz, 2H), 7.90 (d, *J*= 9.2 Hz, 1H). 7.86 (d, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.2 Hz, 1H), 7.64 (s, 1H), 7.46 (m, 2H), 7.34 (dd, *J* = 2.4 Hz & 6.4 Hz, 1H), 7.01(t, *J* = 4.6 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 165.7, 159.9, 150.6, 134.3, 131.6, 129.8, 128.0, 127.8, 126.7, 125.8, 121.7, 118.5, 116.4 ppm; HRMS(ESI): calcd. for $C_{14}H_{10}N_2O$ $[M+H]^+$ 223.0871; found: 223.0869.



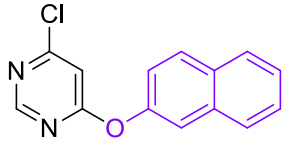
4-chloro-6-phenoxypyrimidine (3o): White solid (88 %); mp: 38°C – 39.5 °C; R_f = 0.7 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.65 (s, 1H), 7.48 (t, *J* =8 Hz, 2H), 7.38 (s, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.26 (d, *J* = 8.8 Hz, 2H) ppm; ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 169.9, 160.9, 158.6, 151.9, 129.9, 126.0, 121.6, 108.1 ppm; HRMS(ESI): calcd. for $C_{10}H_7ClN_2O$ $[M+H]^+$ 207.0325; found: 207.0320.



4,6-diphenoxypyrimidine (3p): White solid (86 %); mp: 107 °C – 109 °C; R_f = 0.5 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.41 (s, 1H), 7.46 (t, *J* = 8 Hz, 4H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 8 Hz, 4H), 6.50 (s, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 171.0, 158.1, 152.3, 129.9, 125.7, 121.5, 92.1 ppm; HRMS(ESI): calcd. for $C_{16}H_{12}N_2O_2$ $[M+H]^+$ 265.0977; found: 265.0974.

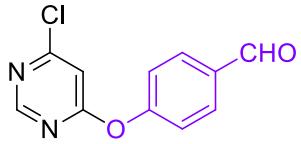


4-(4-bromophenoxy)-6-chloropyrimidine (3q): White solid (86 %); mp: 59 °C – 61 °C; R_f = 0.7 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (s, 1H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 9.2 Hz, 2H), 6.94 (s, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 170.1, 162.3, 158.7, 151.1, 133.2, 123.5, 119.6, 108.3 ppm; HRMS(ESI): calcd. for $C_{10}H_6BrClN_2O$ $[M+H]^+$ 284.9430.

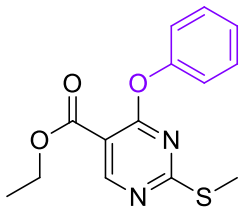


4-chloro-6-(naphthalen-2-yloxy)pyrimidine (3r): Creamy White solid (92 %); mp: 113 °C – 114 °C; R_f = 0.7 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58 (s, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 9.2 Hz, 1H), 7.82 (d, *J* =

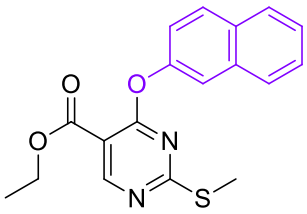
6.8 Hz, 1H), 7.59 (s, 1H), 7.50 (m, 2H), 7.27 (dd, *J* = 2.2 Hz & 6.4 Hz, 1H), 6.94 (s, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 170.7, 162.2, 158.8, 149.7, 134.1, 131.8, 130.3, 128.1, 127.9, 127.1, 126.3, 120.9, 118.6, 108.1 ppm; HRMS(ESI): calcd. for $C_{14}H_9ClN_2O$ $[M+H]^+$ 257.0482; found: 257.0480.



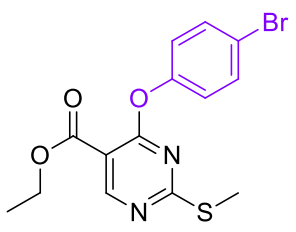
4-((6-chloropyrimidin-4-yl)oxy)benzaldehyde (3s): White solid (74 %); mp: 113 °C – 115 °C; R_f = 0.4 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.01 (s, 1H), 8.57 (s, 1H), 7.98 (d, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 10.8 Hz, 2H), 7.01 (s, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 190.9, 169.6, 162.6, 158.6, 156.8, 134.4, 131.8, 122.4, 108.7 ppm; HRMS(ESI): calcd. for $C_{11}H_7ClN_2O_2$ $[M+H]^+$ 235.0274; found: 235.0272.



Ethyl 2-(methylthio)-4-phenoxypyrimidine-5-carboxylate (3t): White solid (80 %); mp: 72 °C – 75 °C; R_f = 0.6 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.91 (s, 1H), 7.47 (t, *J* = 8 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 2H), 4.35 (q, *J* = 7.0 Hz, 2H), 2.26 (s, 3H), 1.31 (t, *J* = 7.0 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6): δ = 175.2, 165.8, 162.5, 160.9, 151.8, 129.6, 125.8, 121.8, 107.5, 61.0, 14.1, 13.5 ppm; HRMS(ESI): calcd. for $C_{14}H_{14}N_2O_3S$ $[M+H]^+$ 291.0803.

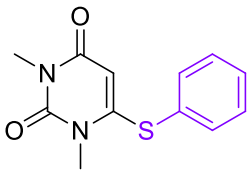


Ethyl 2-(methylthio)-4-(naphthalen-2-yloxy)pyrimidine-5-carboxylate (3u): Light Brown solid (84 %); mp: 78 °C – 80 °C; R_f = 0.5 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.94 (s, 1H), 7.87 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 6.8 Hz, 1H), 7.61 (s, 1H), 7.48 (m, 2H), 7.31 (dd, *J* = 2.4 Hz & 6.4 Hz, 1H), 4.44 (q, *J* = 7.0 Hz, 2H), 2.16 (s, 3H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 176.6, 166.8, 163.4, 161.3, 149.9, 134.0, 131.6, 129.3, 128.0, 127.8, 126.8, 125.9, 121.9, 118.8, 107.6, 61.7, 14.5, 14.3 ppm; HRMS(ESI): calcd. for $C_{18}H_{16}N_2O_3S$ $[M+H]^+$ 341.0960; found: 341.0958.

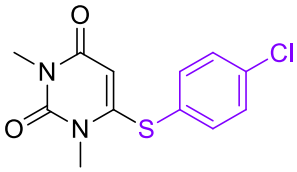


Ethyl 4-(4-bromophenoxy)-2-(methylthio)pyrimidine-5-carboxylate (3v): White solid (76 %); mp: 114 °C – 116 °C; R_f = 0.6 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.90 (s, 1H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 4.40 (q, *J* = 7.0 Hz, 2H), 2.26 (s, 3H), 1.37 (t, *J* = 7.0 Hz, 3H)

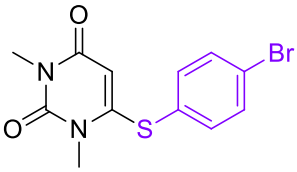
ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 176.6, 166.3, 163.2, 161.3, 151.3, 132.6, 124.0, 119.0, 107.6, 61.6, 14.4, 14.4 ppm; HRMS(ESI): calcd. for $C_{14}H_{13}BrN_2O_3S$ $[M+H]^+$ 368.9909.



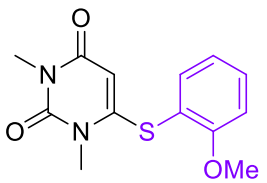
1,3-dimethyl-6-(phenylthio)pyrimidine-2,4(1*H*,3*H*)-dione (3w): White solid (94 %); mp: 132 °C – 134 °C; R_f = 0.2 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.65 (m, 5H), 4.73 (s, 1H), 3.45 (s, 3H), 3.11 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6): δ = 159.9, 157.2, 151.1, 135.5, 131.1, 130.6, 126.4, 96.5, 32.2, 27.5 ppm; HRMS(ESI): calcd. for $C_{12}H_{12}N_2O_2S$ $[M+H]^+$ 249.0698; found: 249.0694.



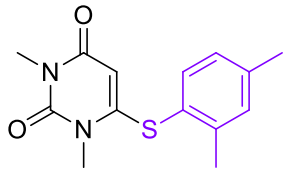
6-((4-chlorophenyl)thio)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3x): White solid (81 %); mp: 164 °C – 166°C; R_f = 0.3 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.45 (s, 4H), 4.96 (s, 1H), 3.54 (s, 3H), 3.27 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 161.2, 157.4, 151.9, 138.3, 137.5, 131.1, 124.6, 97.7, 32.5, 28.2 ppm; HRMS(ESI): calcd. for $C_{12}H_{11}ClN_2O_2S$ $[M+H]^+$ 283.0308; found: 283.0307.



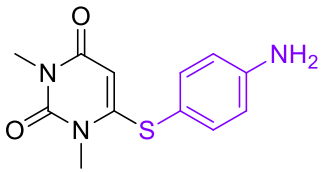
6-((4-bromophenyl)thio)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3y): White solid (87 %); mp: 172 °C –173°C; R_f = 0.3 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.61 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 8.4 Hz, 2H), 4.97 (s, 1H), 3.54 (s, 3H), 3.27 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 161.2, 157.3, 151.9, 137.6, 134.0, 126.6, 125.2, 97.8, 32.5, 28.2 ppm; HRMS(ESI): calcd. for $C_{12}H_{11}BrN_2O_2S$ $[M+H]^+$ 326.9803; found: 326.9800.



6-((2-methoxyphenyl)thio)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3z): White solid (90 %); mp: 184 °C –187 °C; R_f = 0.2 in EtOAc-Hexane (1:4); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.52 (m, 2H), 7.03 (m, 2H), 4.97 (s, 1H), 3.84 (s, 3H), 3.58 (s, 3H), 3.27 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 161.5, 160.2, 157.0, 152.1, 138.2, 133.8, 122.2, 113.6, 112.4, 96.6, 56.3, 32.4, 28.1 ppm; HRMS(ESI): calcd. for $C_{13}H_{14}N_2O_3S$ $[M+H]^+$ 279.0803; found: 279.0801.



6-((2,4-dimethylphenyl)thio)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3aa): White solid (84 %); mp: 114 °C – 117 °C; R_f = 0.6 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.36 (d, *J* = 8 Hz, 1H), 7.17 (s, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 4.84 (s, 1H), 3.57 (s, 3H), 3.27 (s, 3H), 2.35 (s, 6H) ppm; ^{13}C{^{1}H NMR (100 MHz, $CDCl_3$): δ = 161.4, 157.6, 152.1, 143.3, 142.7, 137.4, 132.9, 129.0, 121.8, 96.0, 32.3, 28.1, 21.5, 20.6 ppm; HRMS(ESI): calcd. for $C_{14}H_{16}N_2O_2S$ $[M+H]^+$ 277.1011.



6-((4-aminophenyl)thio)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3ab): Yellow solid (76 %); mp: 196 °C – 199°C; R_f = 0.2 in EtOAc-Hexane (3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.24 (d, *J* = 8.8 HZ, 2H), 6.69 (d, *J* = 8.8 Hz, 2H), 5.00 (s, 1H), 4.04 (s, 2H), 3.53 (s, 3H), 3.27 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 161.5, 160.2, 152.1, 149.6, 137.9, 116.4, 112.1, 96.5, 32.2, 28.1 ppm; HRMS(ESI): calcd. for $C_{12}H_{13}N_3O_2S$ $[M+H]^+$ 264.0807; found: 264.0808.

2. Representative spectra of synthesized compounds

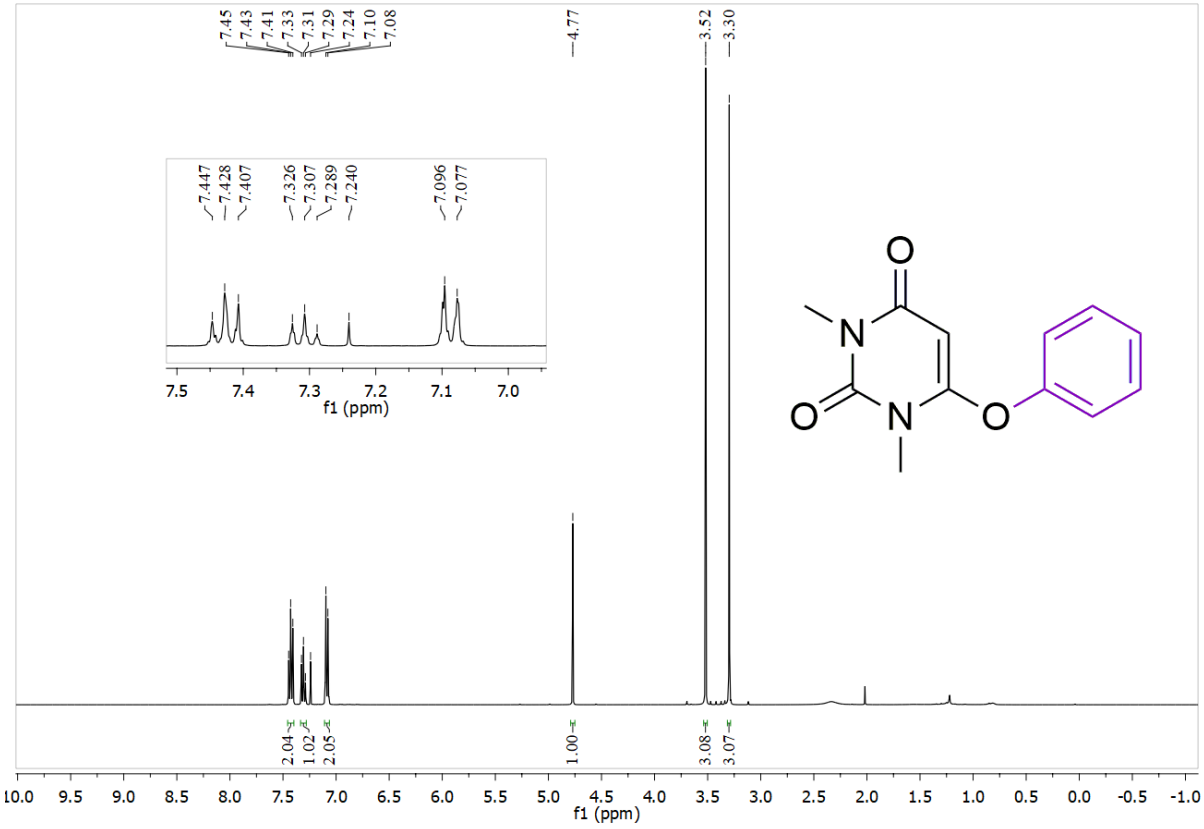


Fig. S1: ^{1}H NMR (400 MHz) spectra of **3a**

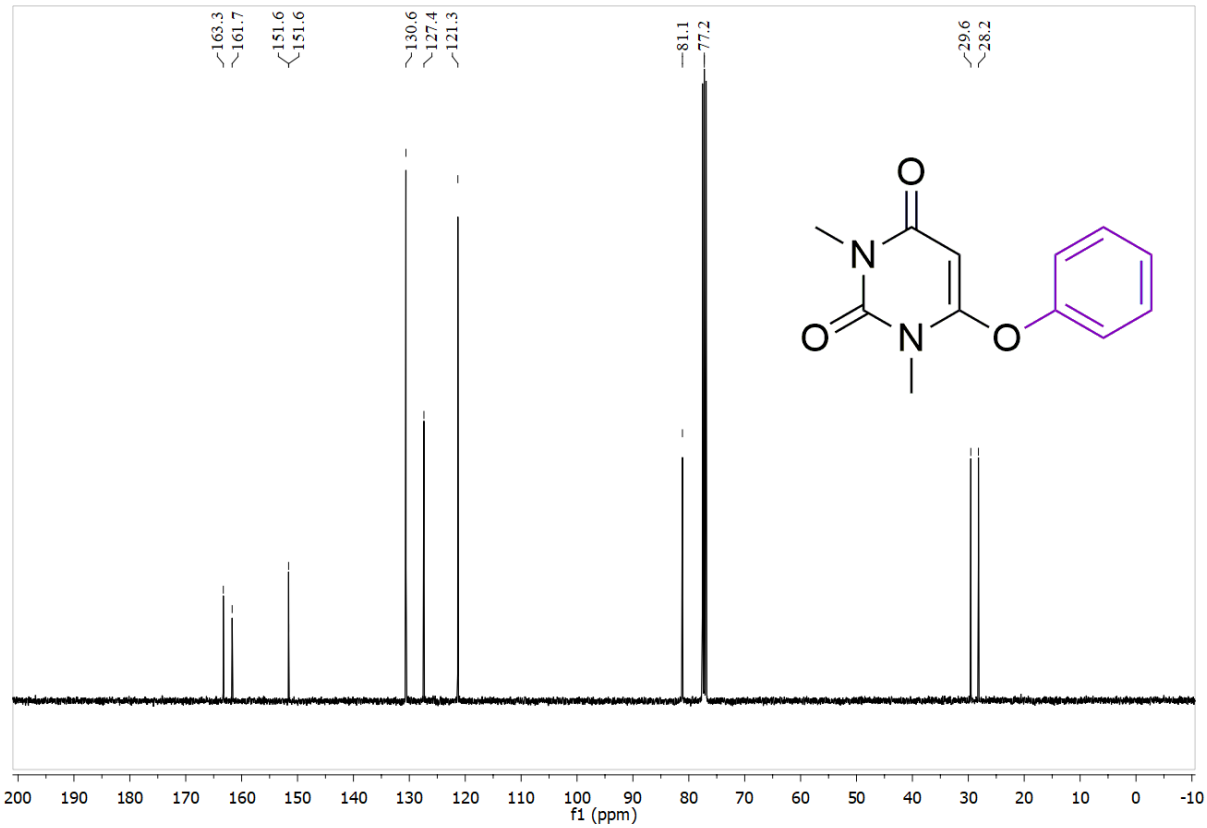


Fig. S2: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3a**

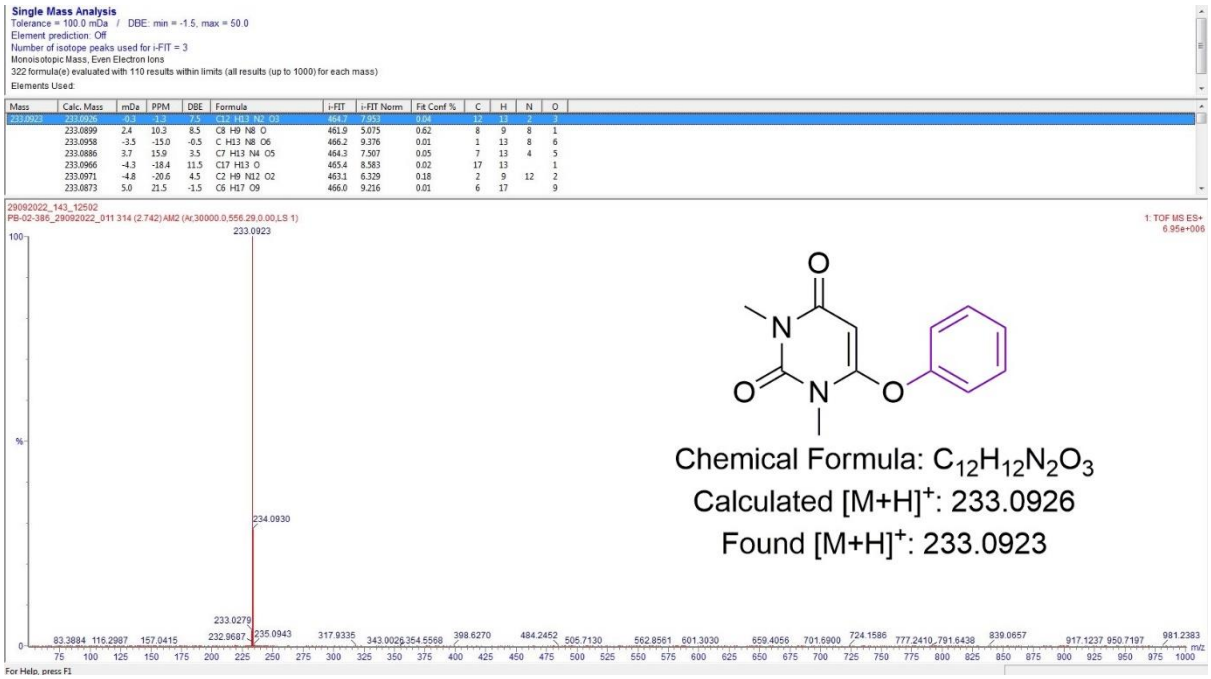


Fig. S3: HRMS spectrum of **3a**

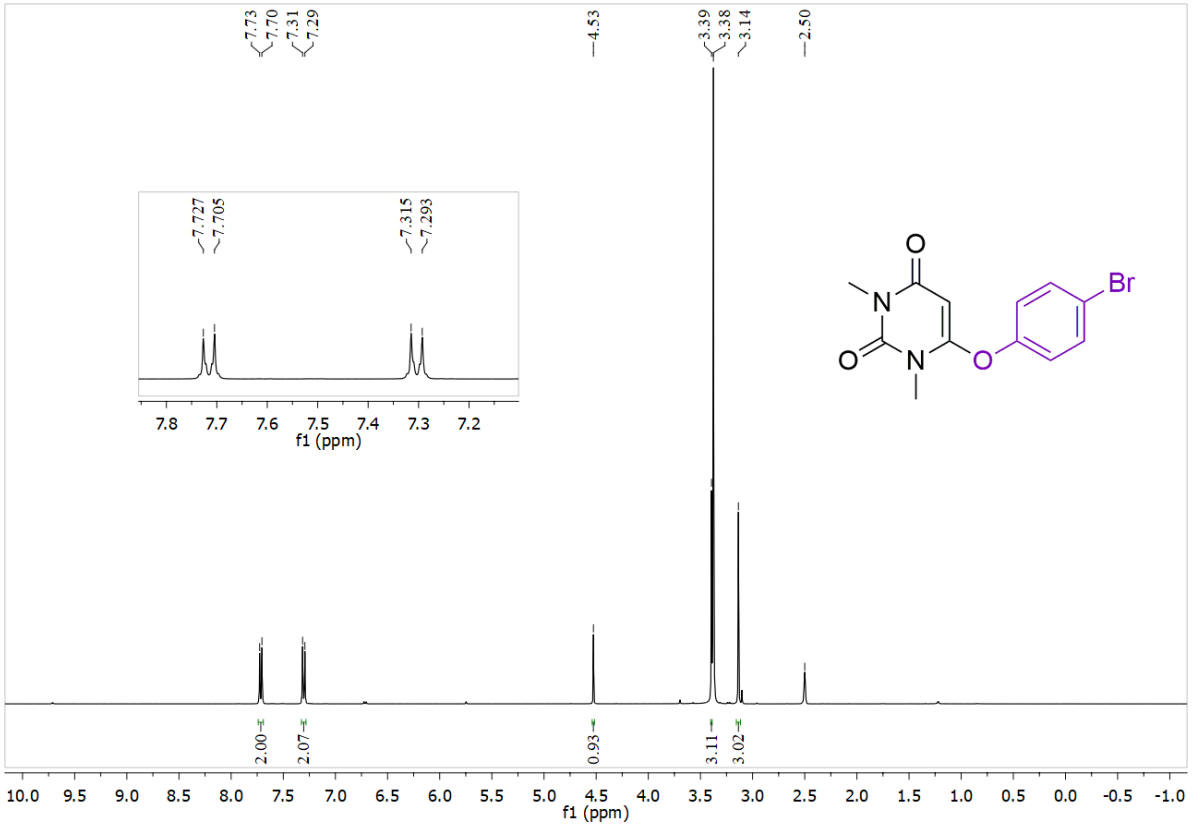


Fig. S4: ^{1}H NMR (400 MHz) spectra of **3b**

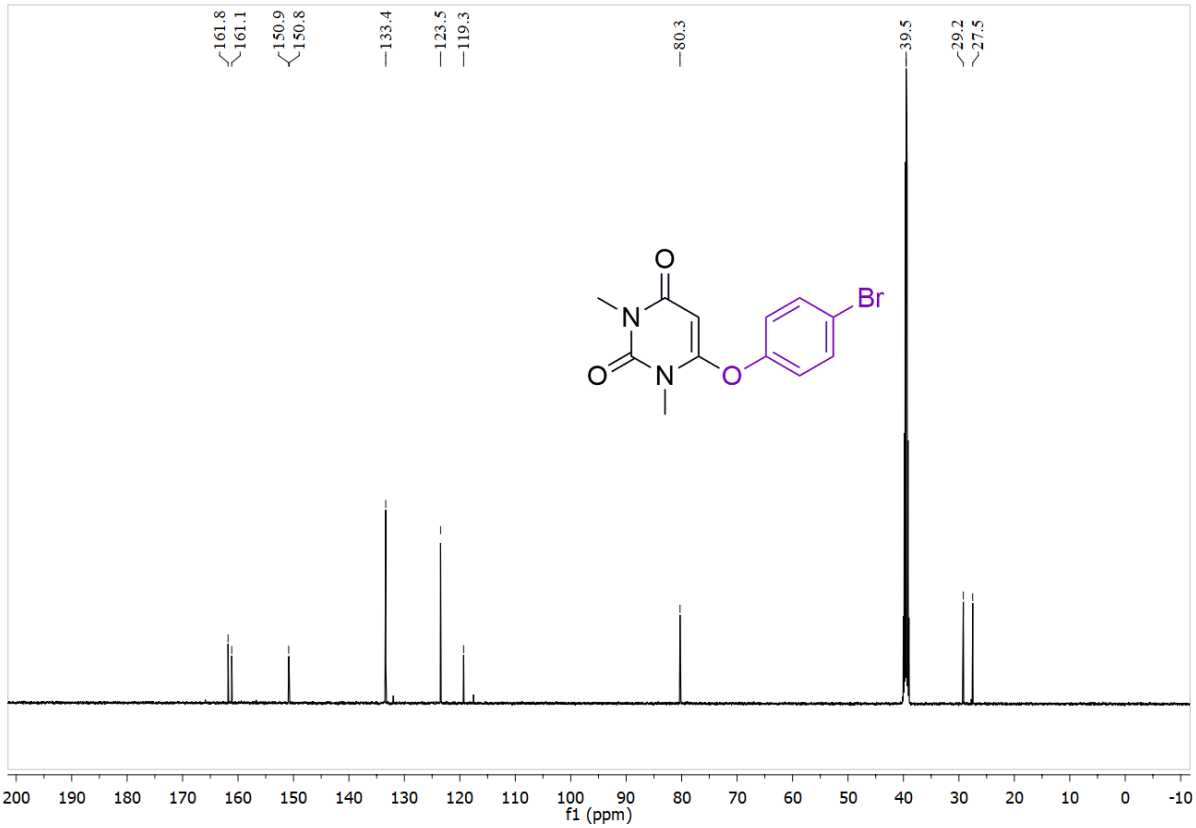


Fig. S5: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3b**

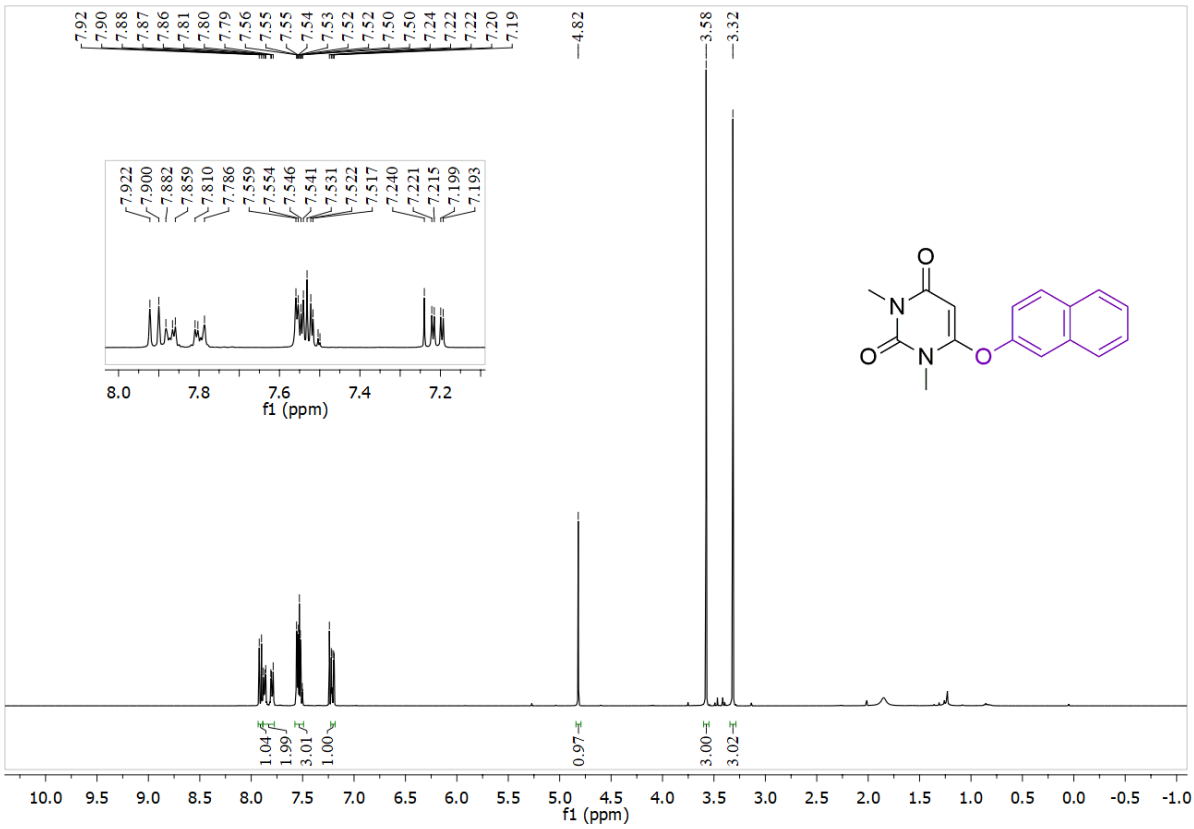


Fig. S6: ^{1}H NMR (400 MHz) spectra of **3c**

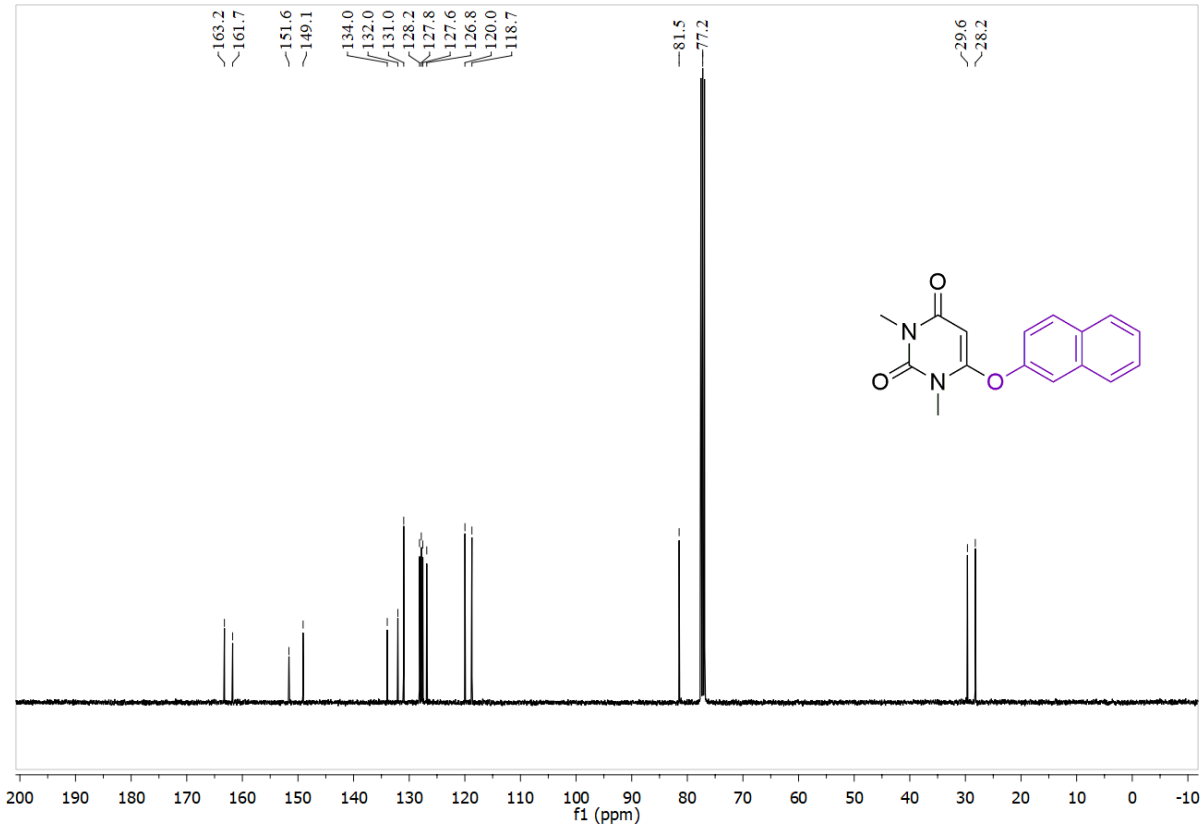


Fig. S7: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3c**

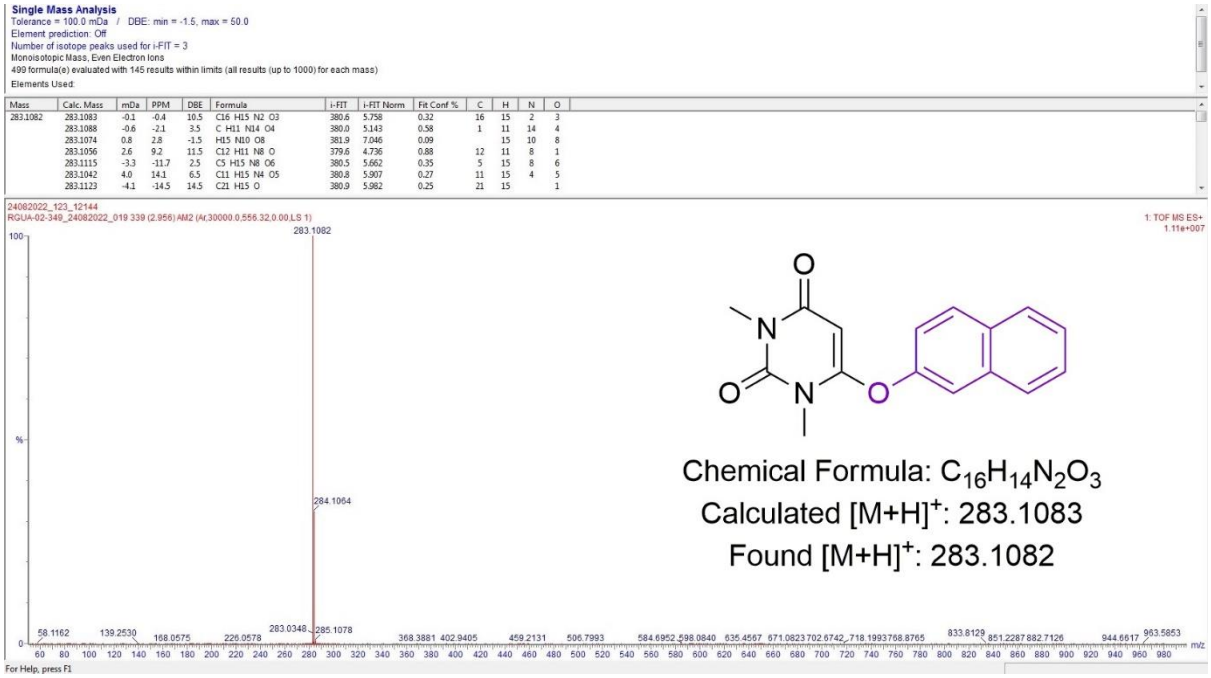


Fig. S8: HRMS spectrum of **3c**

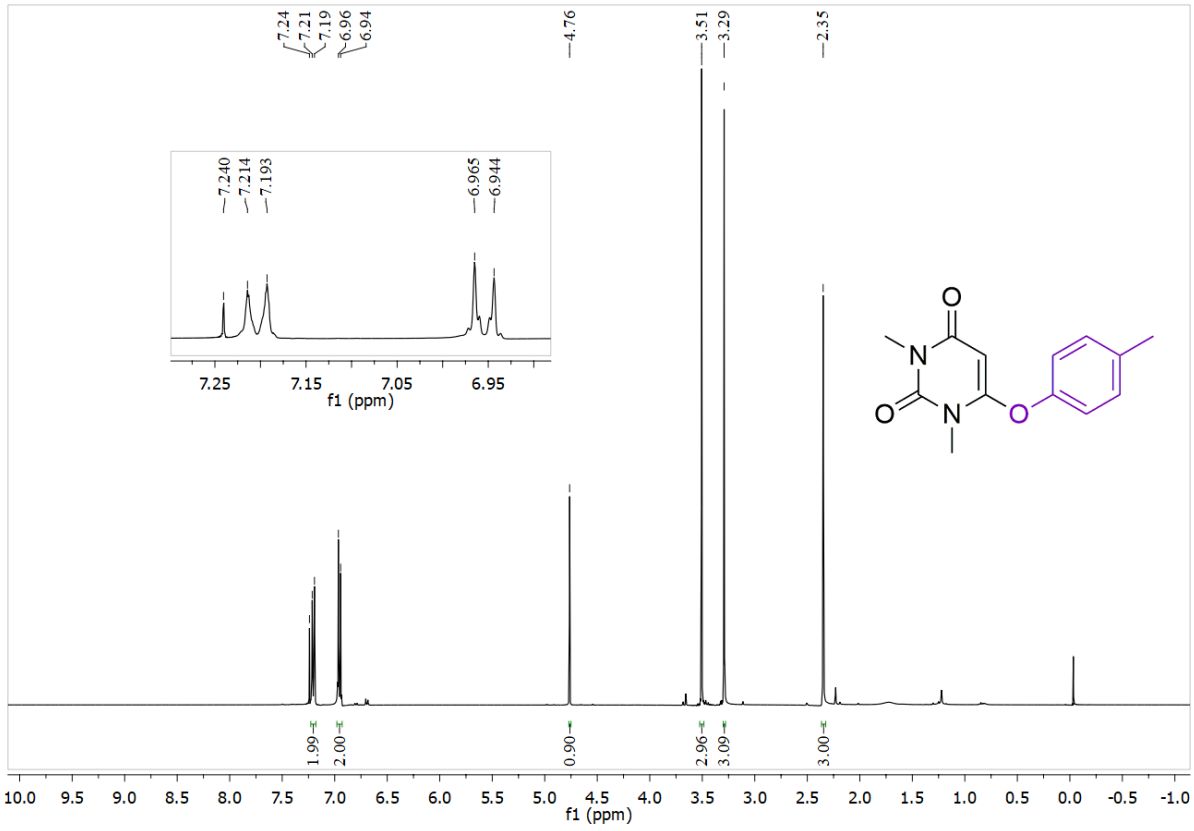


Fig. S9: ^{1}H NMR (400 MHz) spectra of **3d**

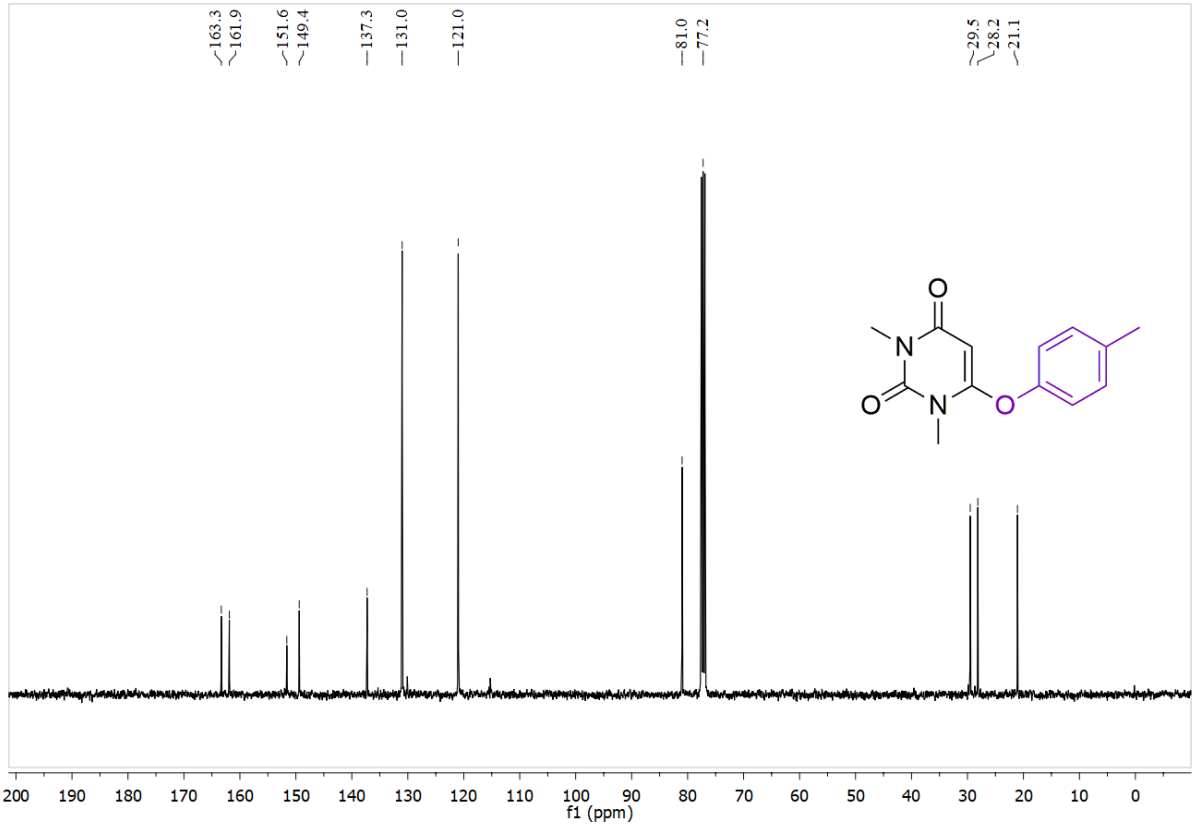


Fig. S10: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3d**

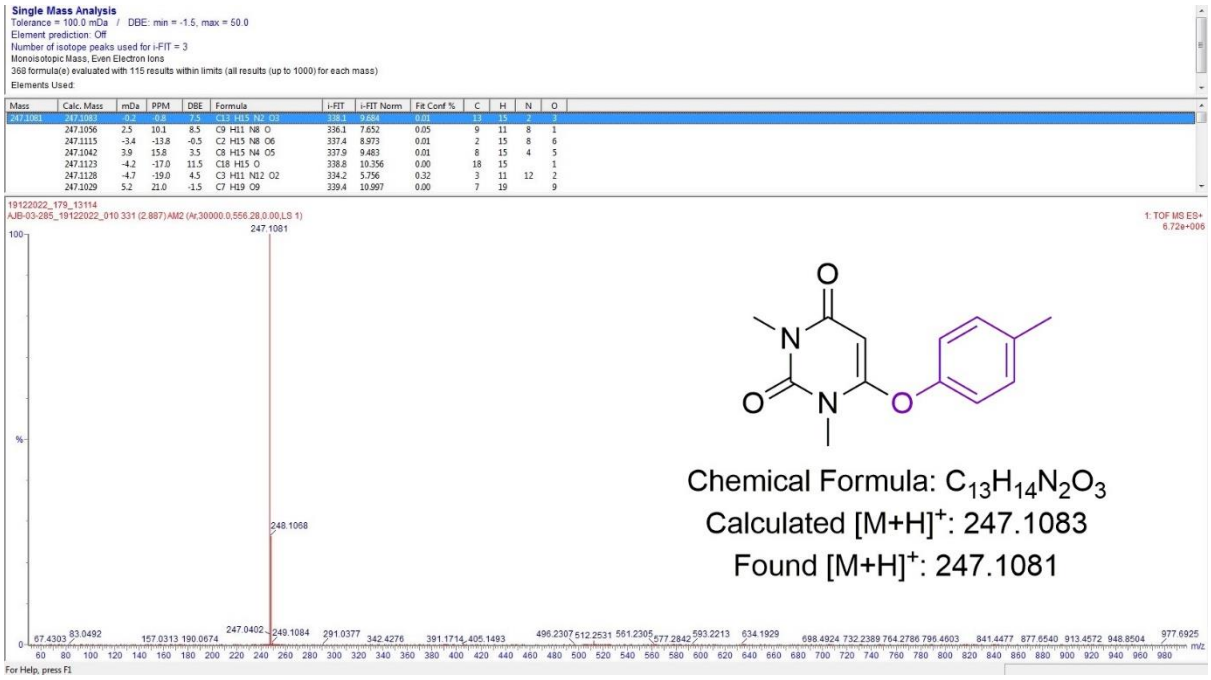


Fig. S11: HRMS spectrum of **3d**

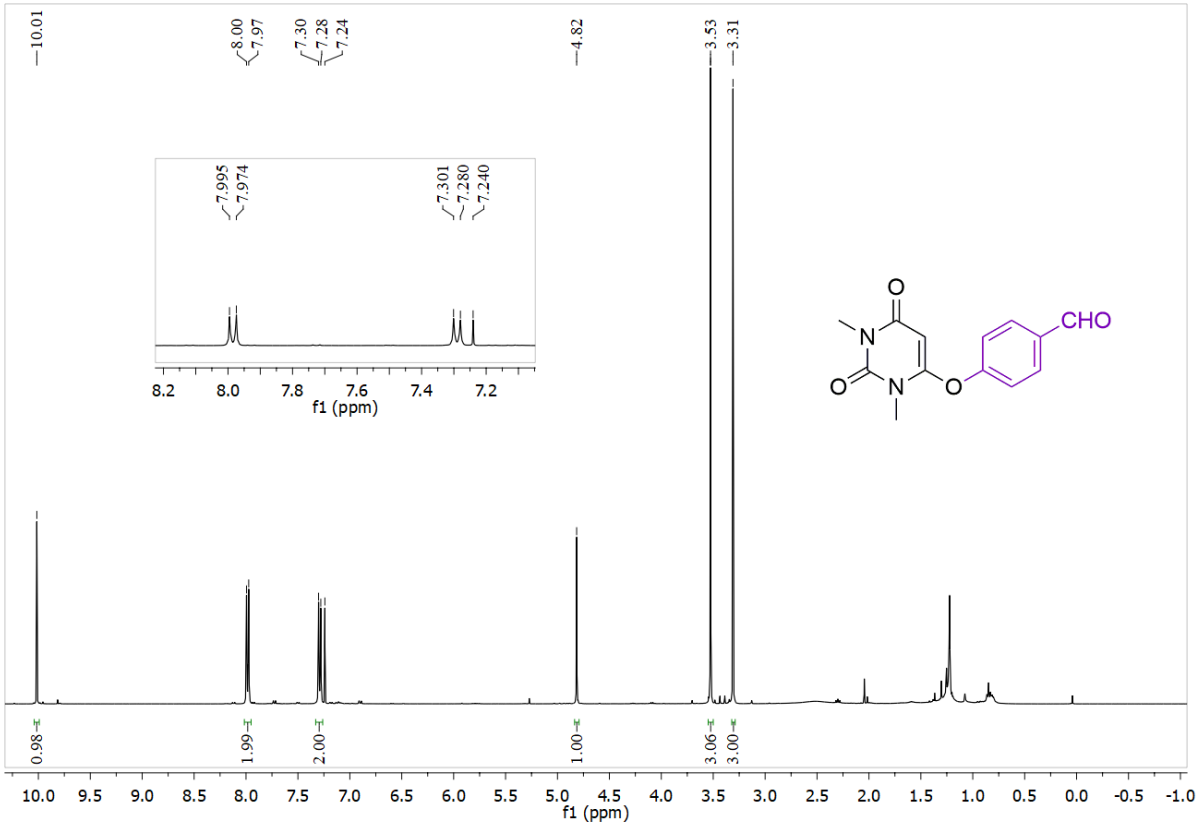


Fig. S12: ^{1}H NMR (400 MHz) spectra of **3e**

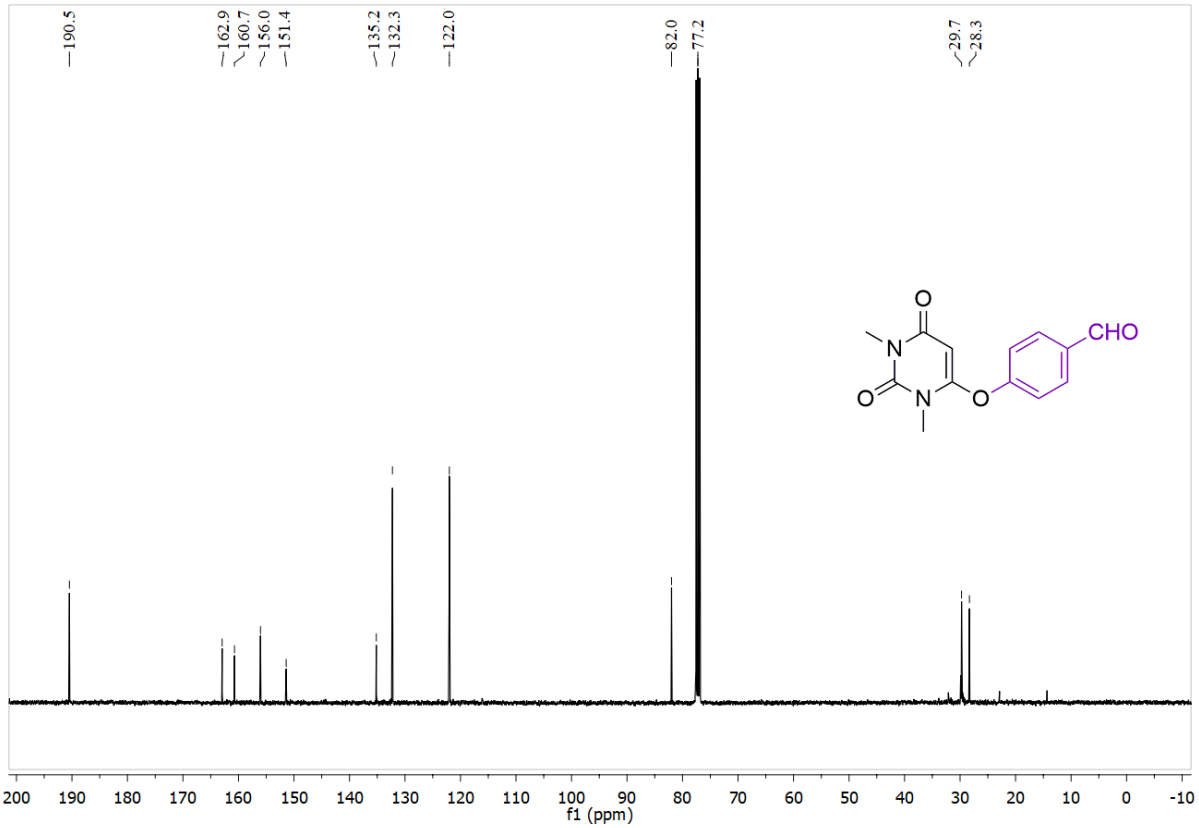


Fig. S13: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3e**

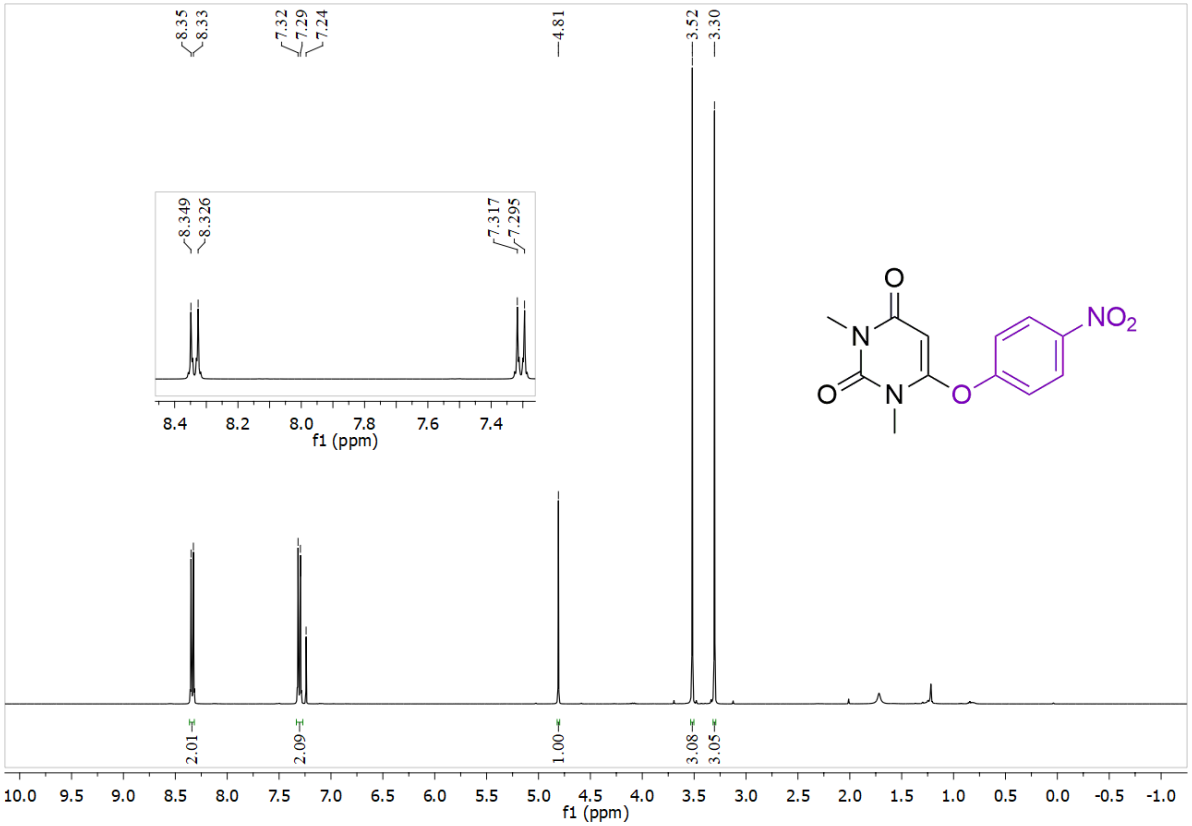


Fig. S14: ^{1}H NMR (400 MHz) spectra of **3f**

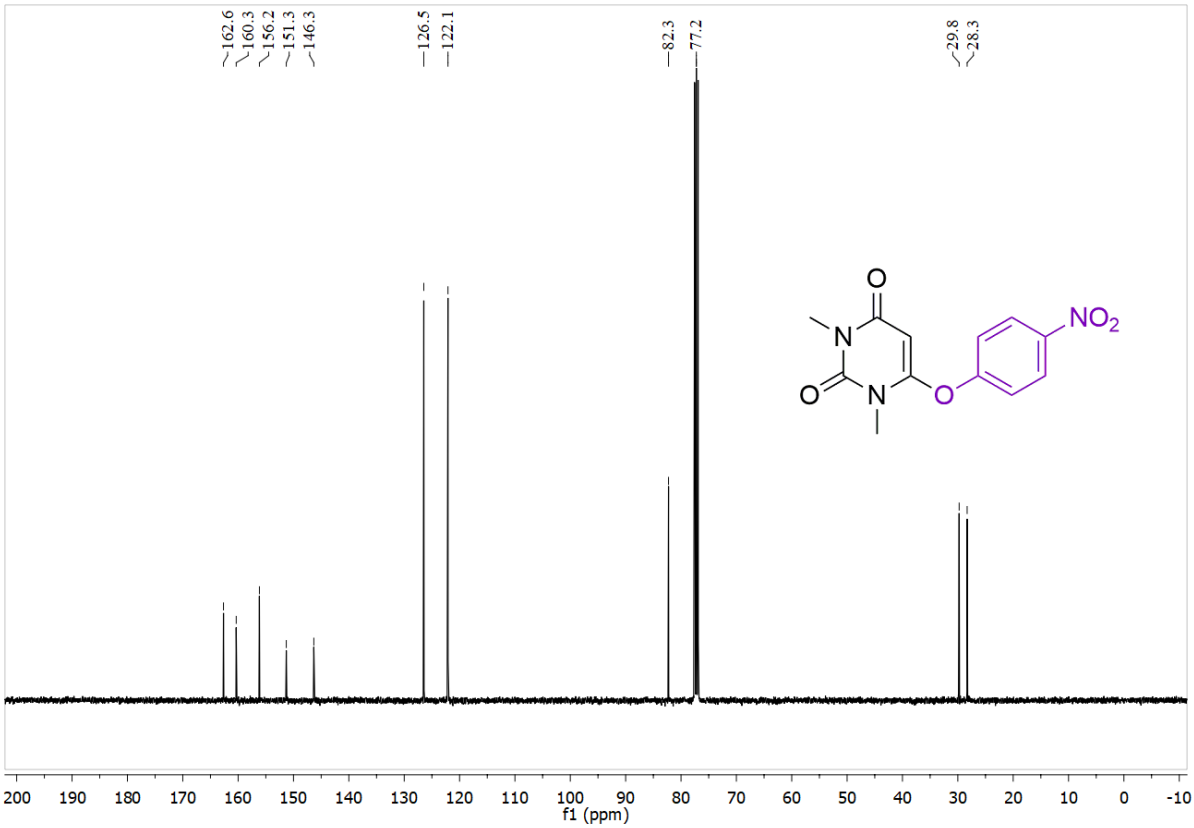


Fig. S15: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3f**

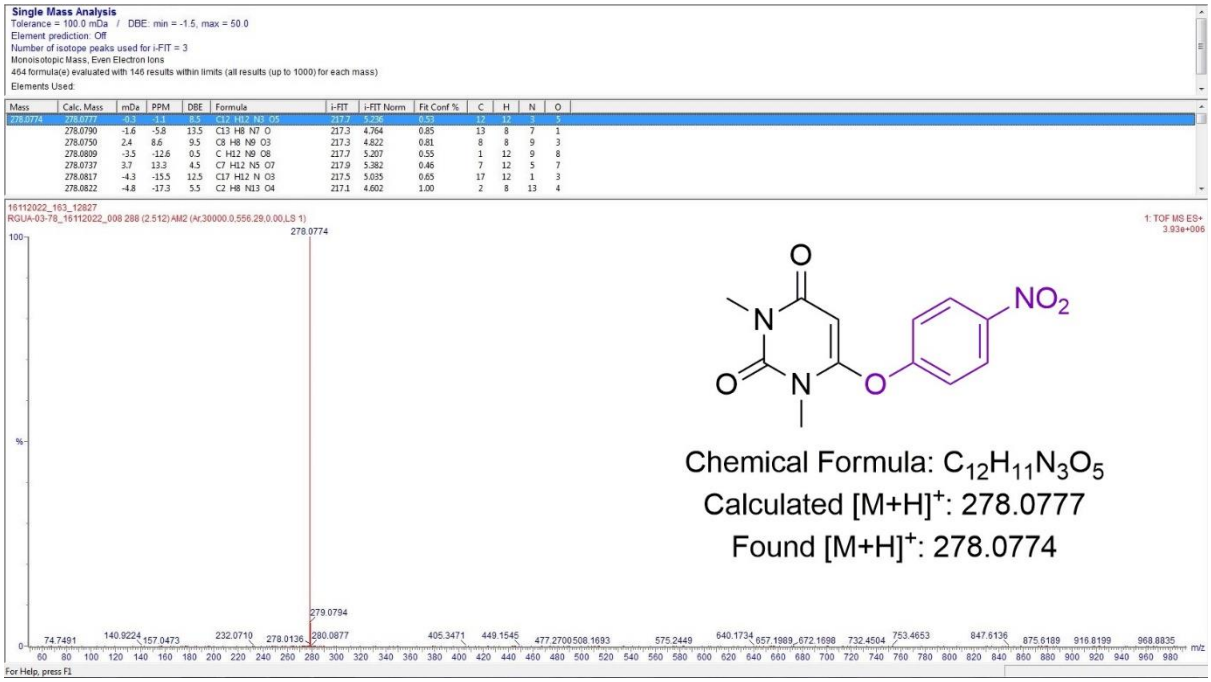


Fig. S16: HRMS spectrum of **3f**

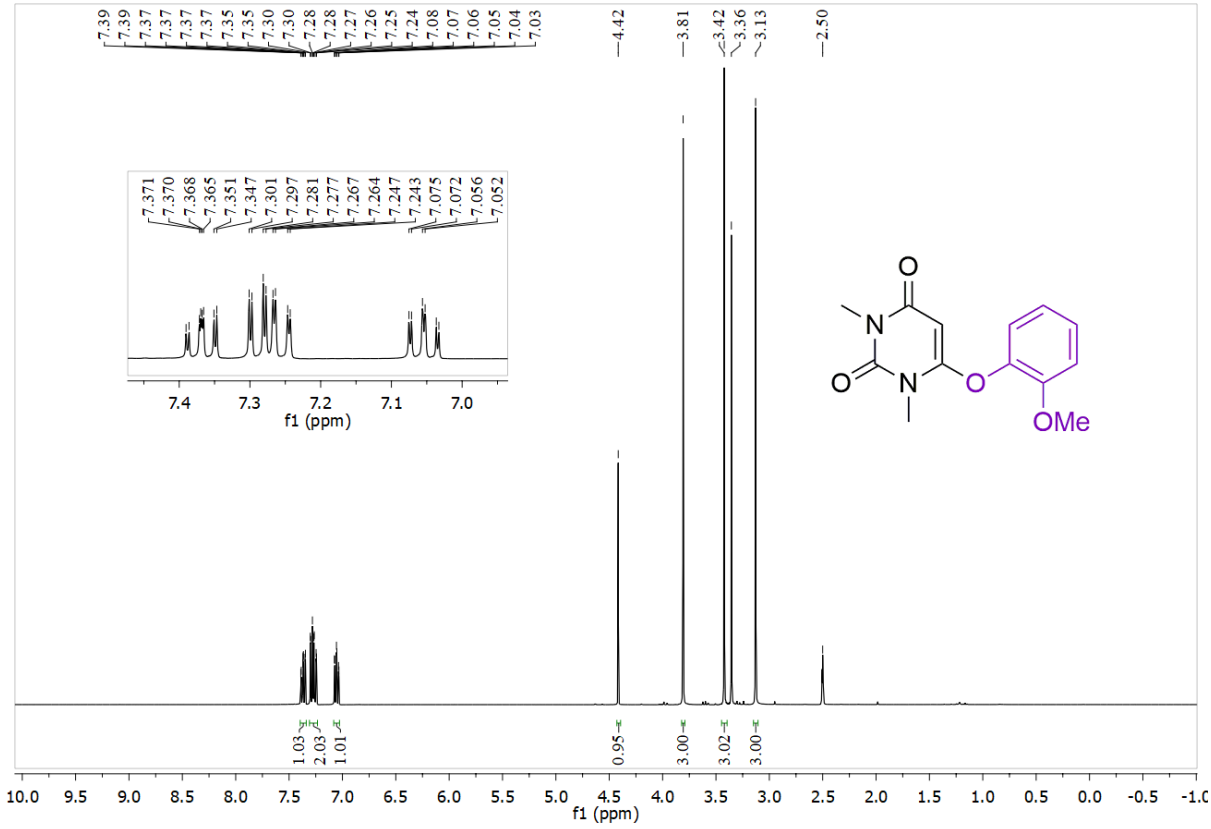


Fig. S17: ^{1}H NMR (400 MHz) spectra of **3g**

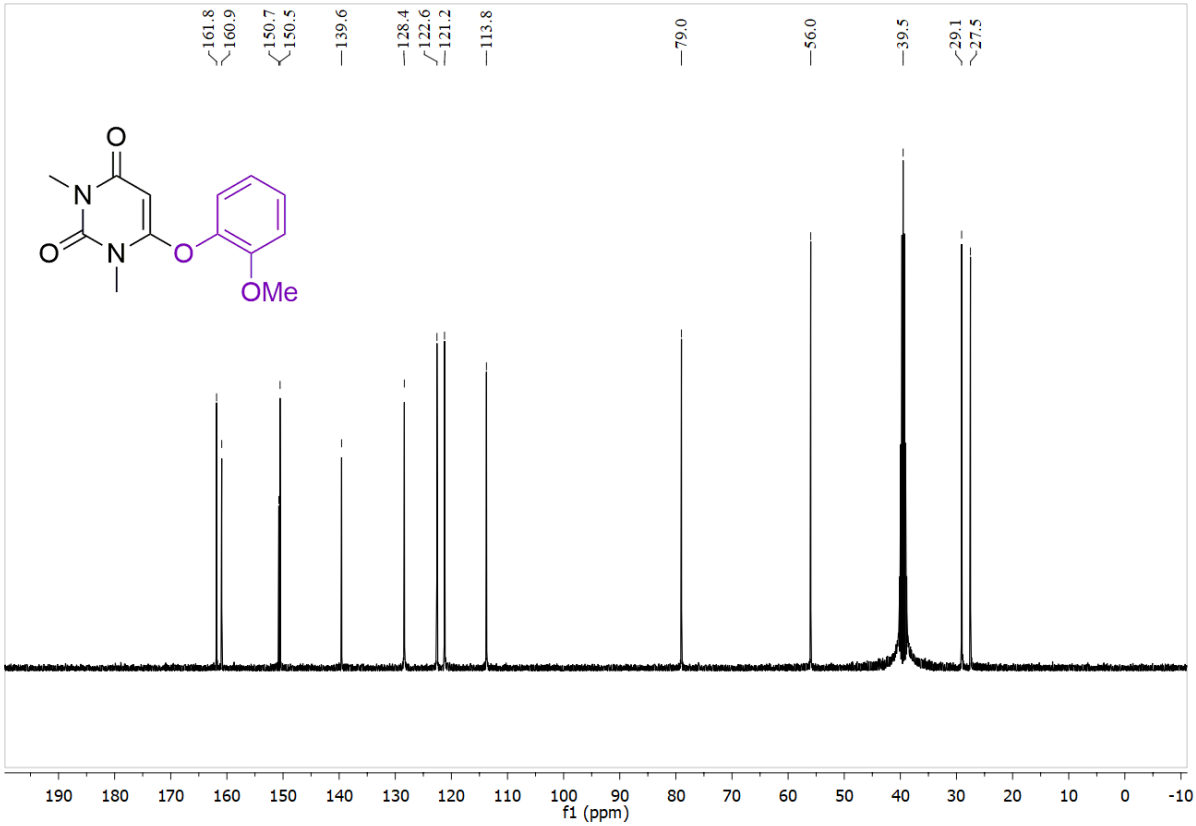


Fig. S18: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3g**

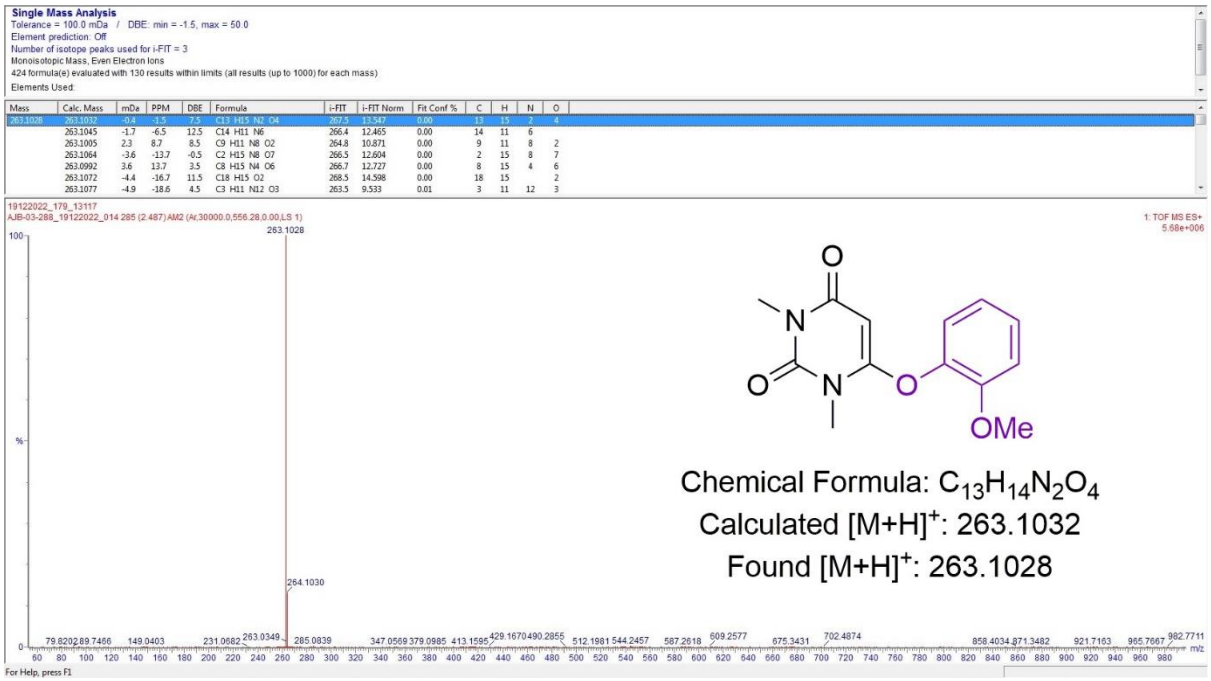


Fig. S19: HRMS spectrum of **3g**

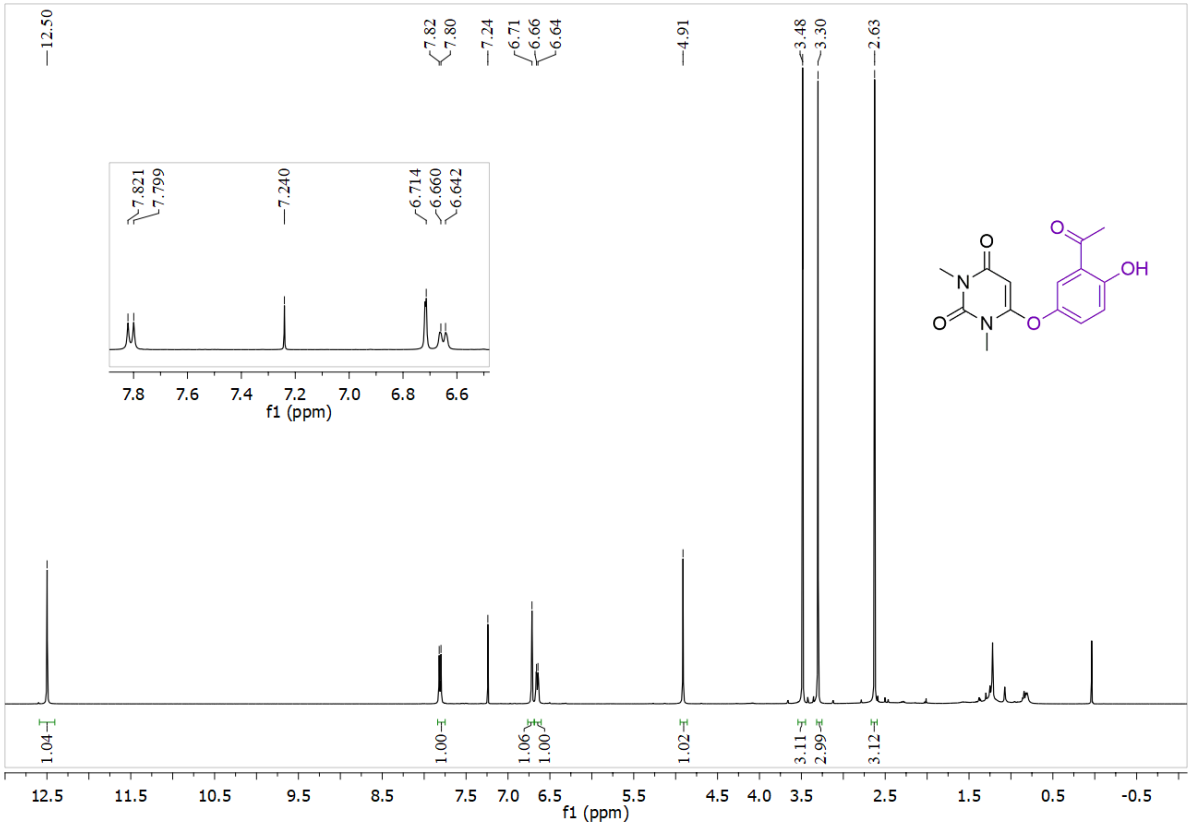


Fig. S20: ^{1}H NMR (400 MHz) spectra of **3h**

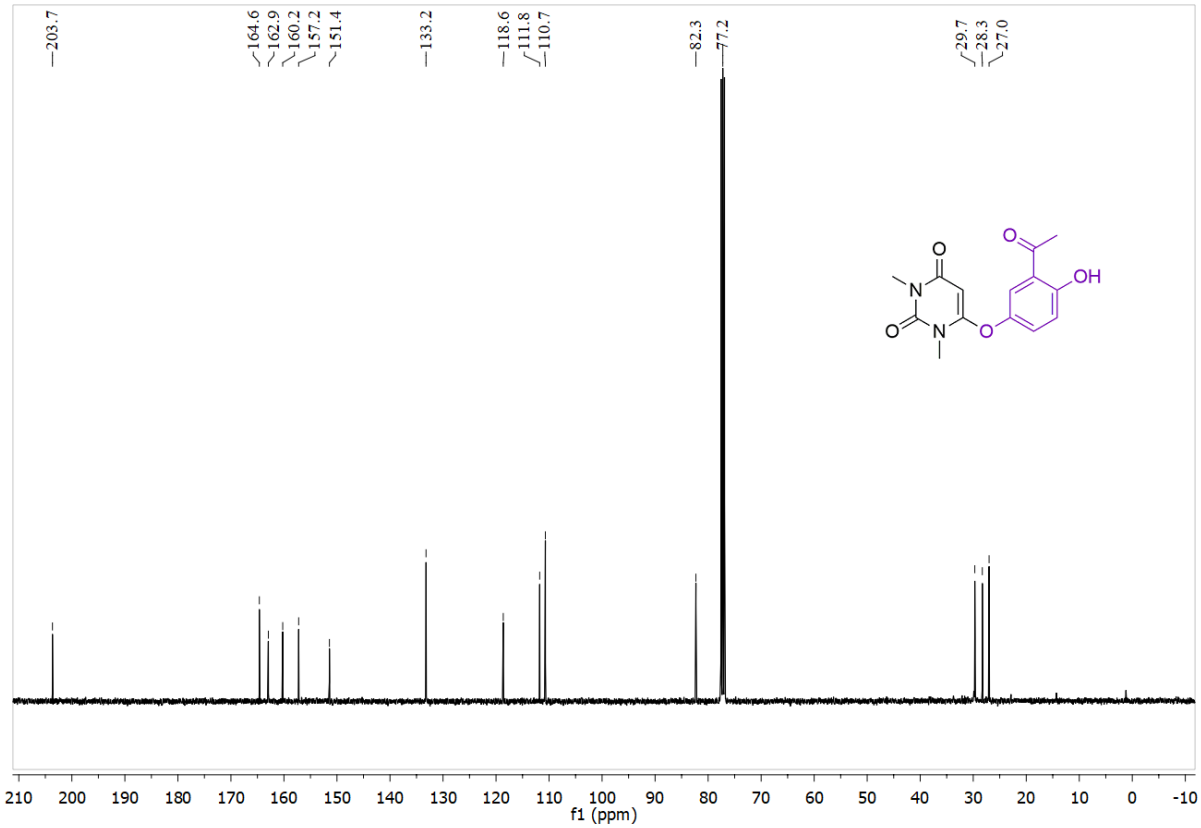


Fig. S21: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3h**

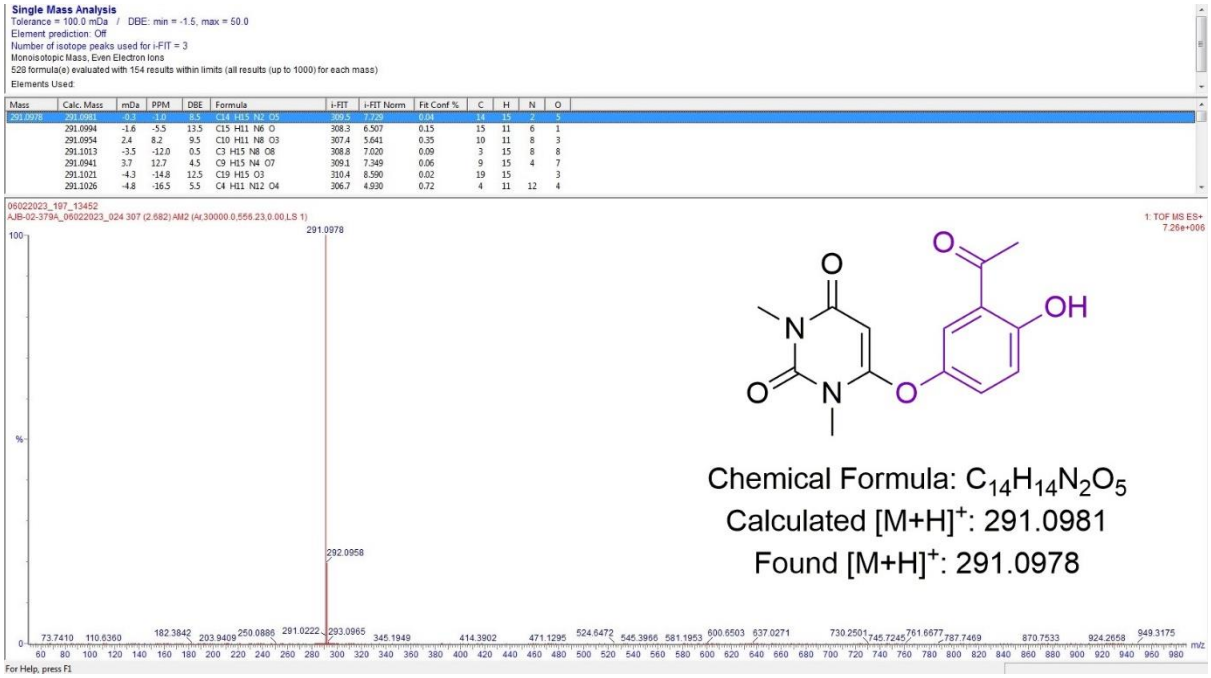


Fig. S22: HRMS spectrum of **3h**

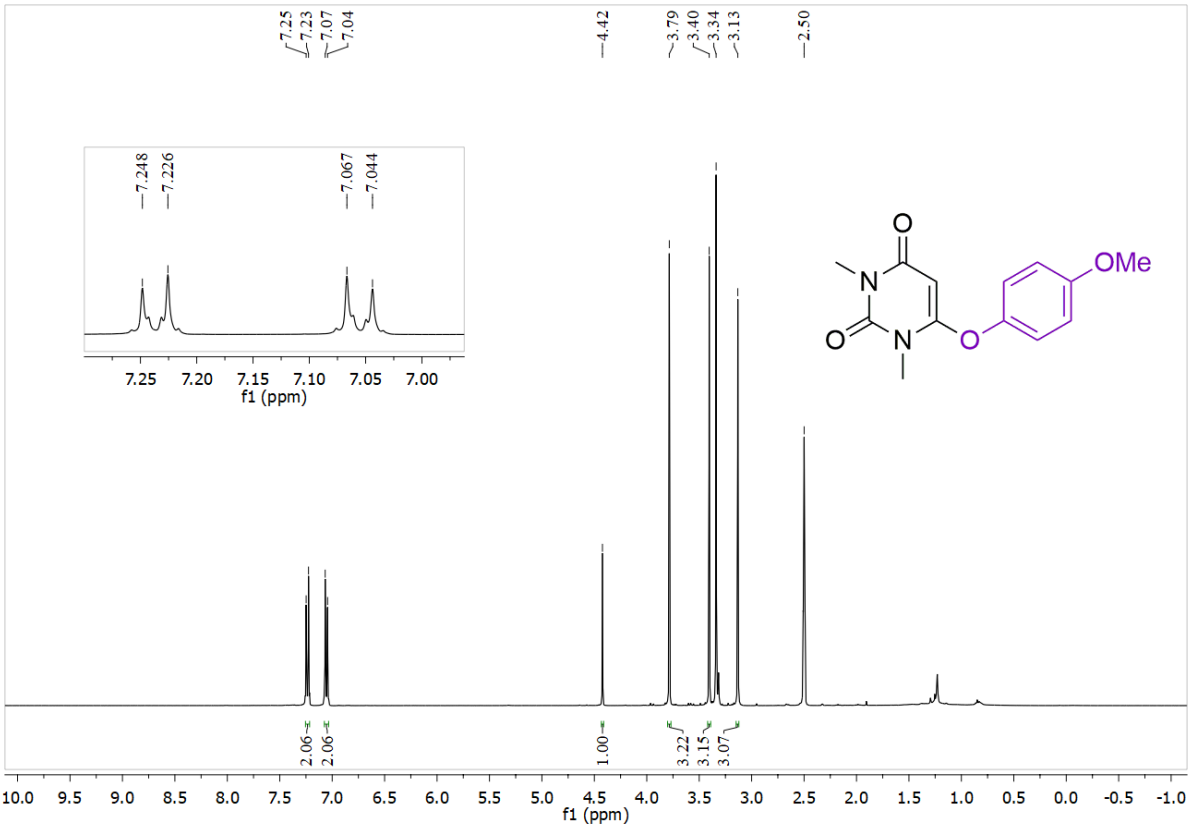


Fig. S23: ^{1}H NMR (400 MHz) spectra **3i**

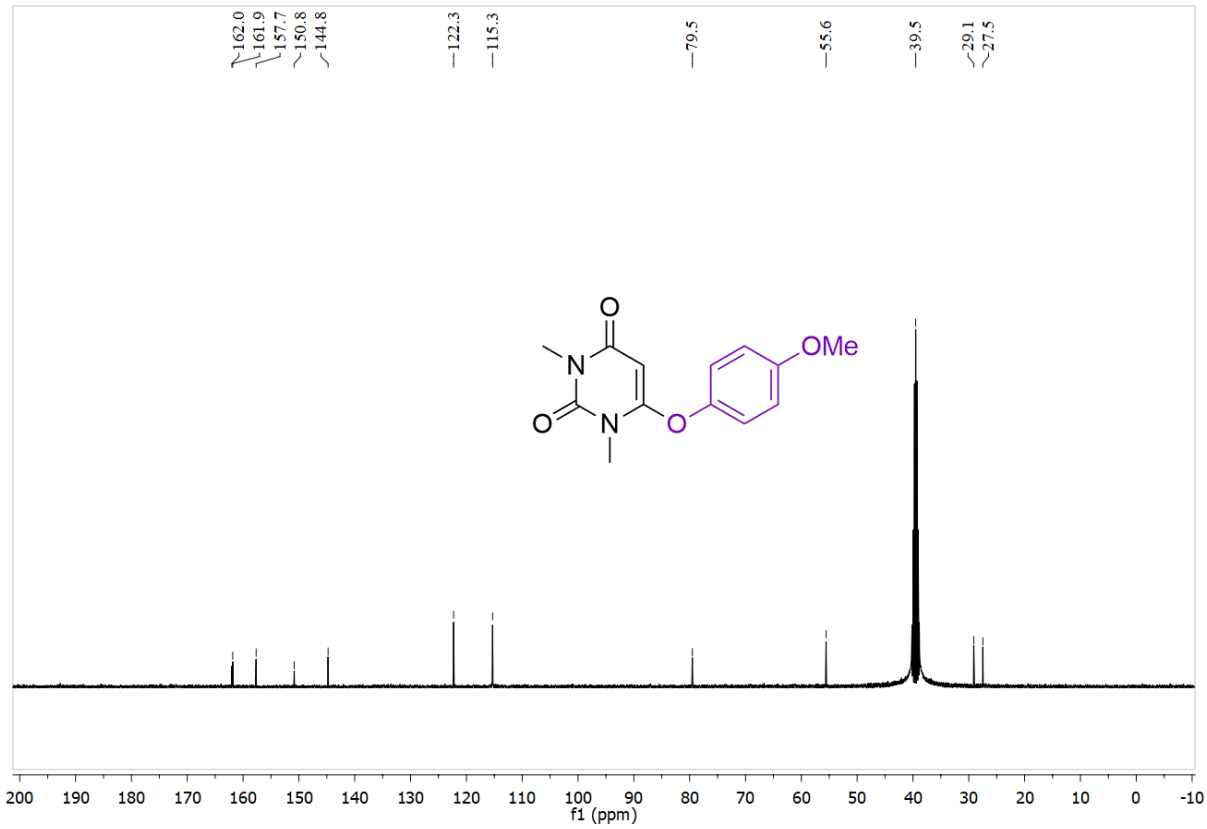


Fig. S24 $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3i**

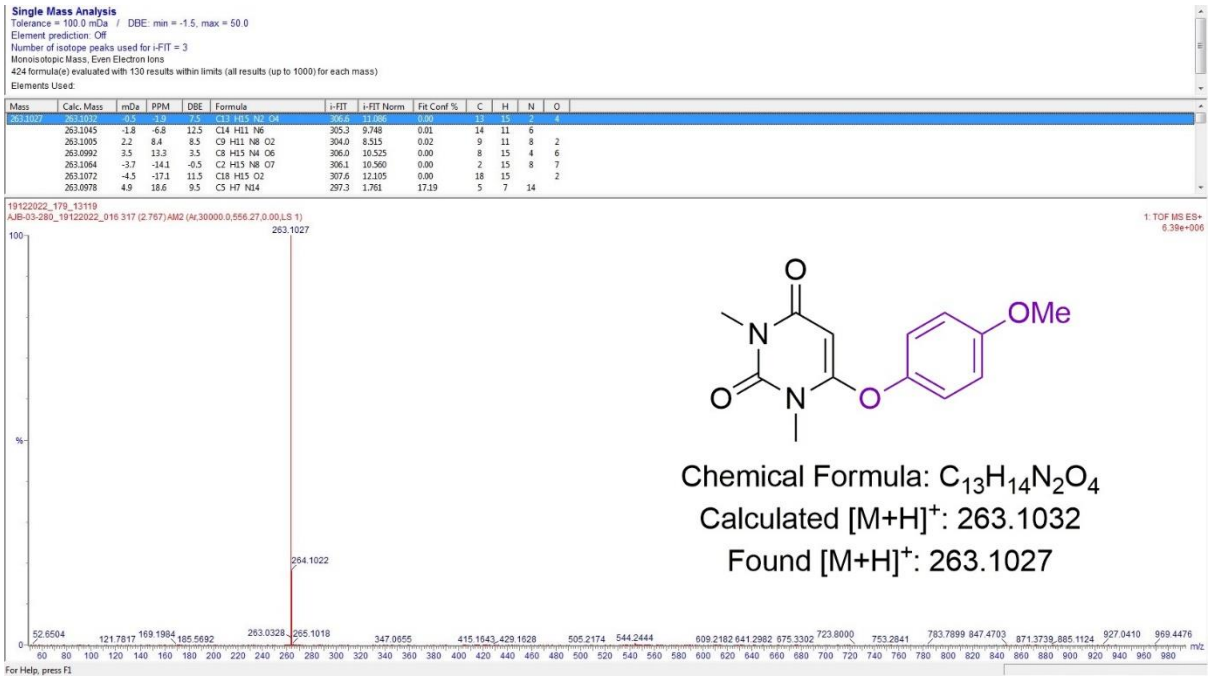


Fig. S25: HRMS spectrum of **3i**

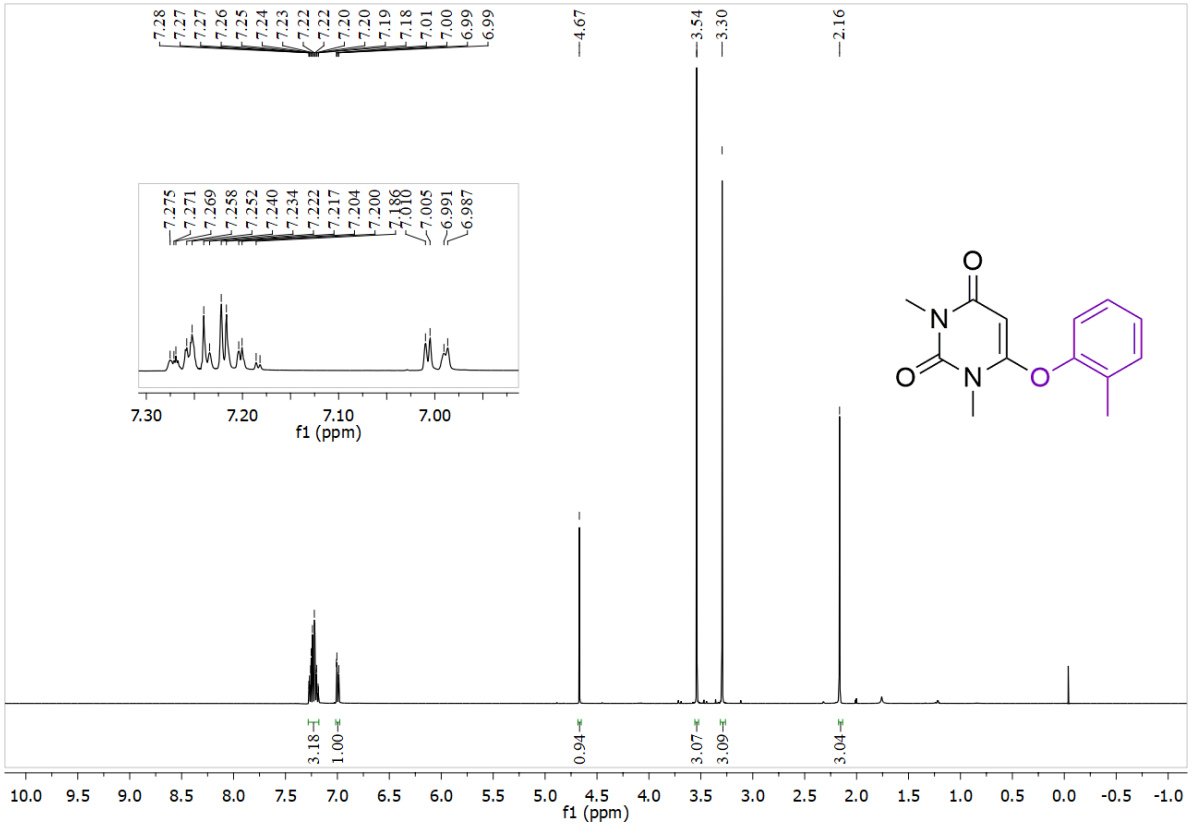


Fig. S26: ^{1}H NMR (400 MHz) spectra **3j**

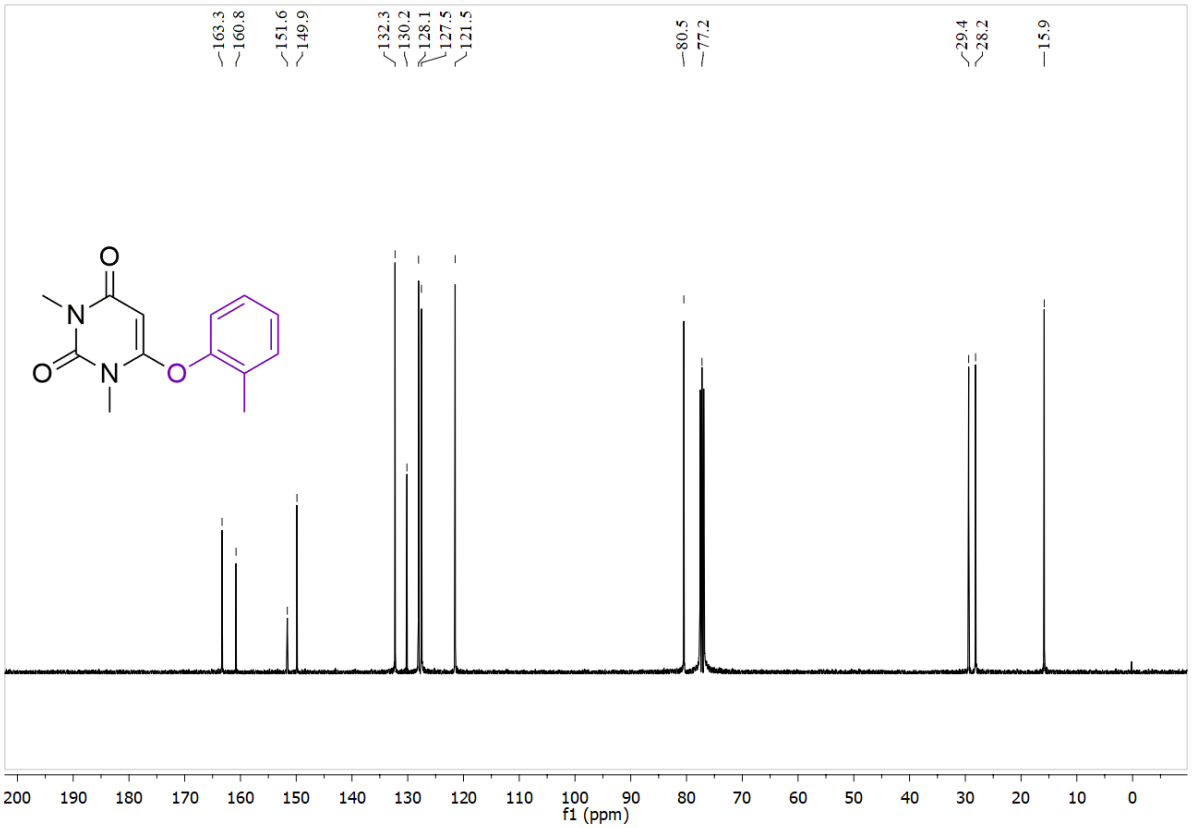


Fig. S27: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3j**

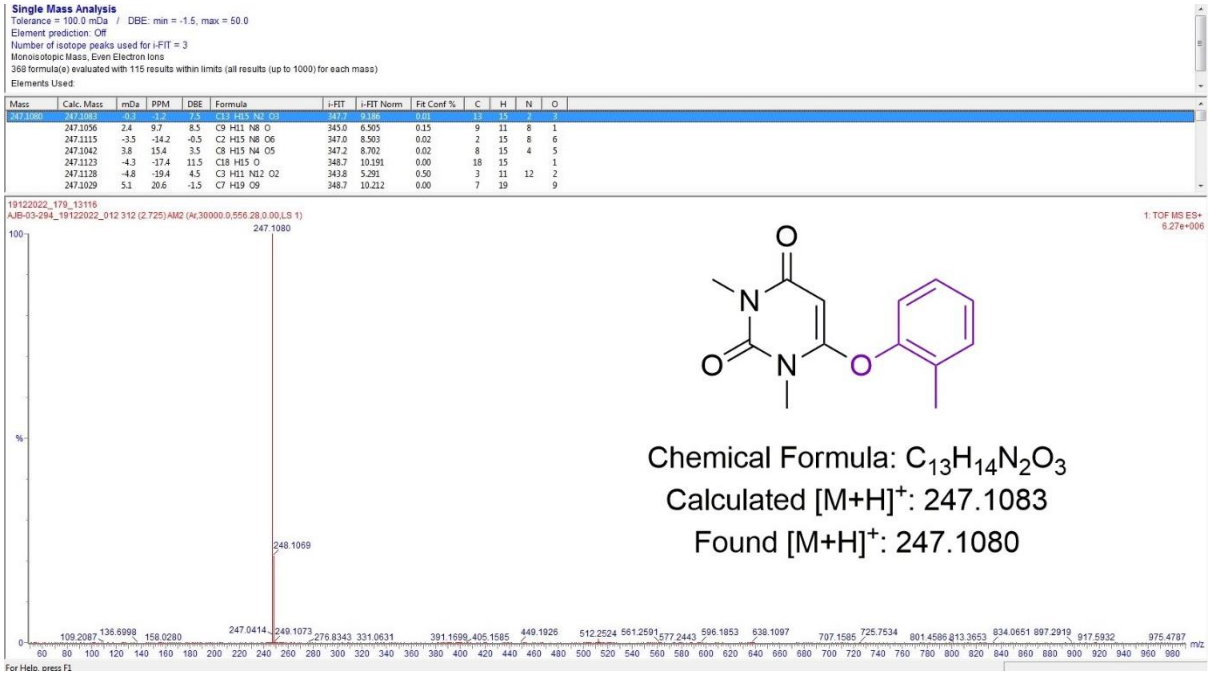


Fig. S28: HRMS spectra of **3j**

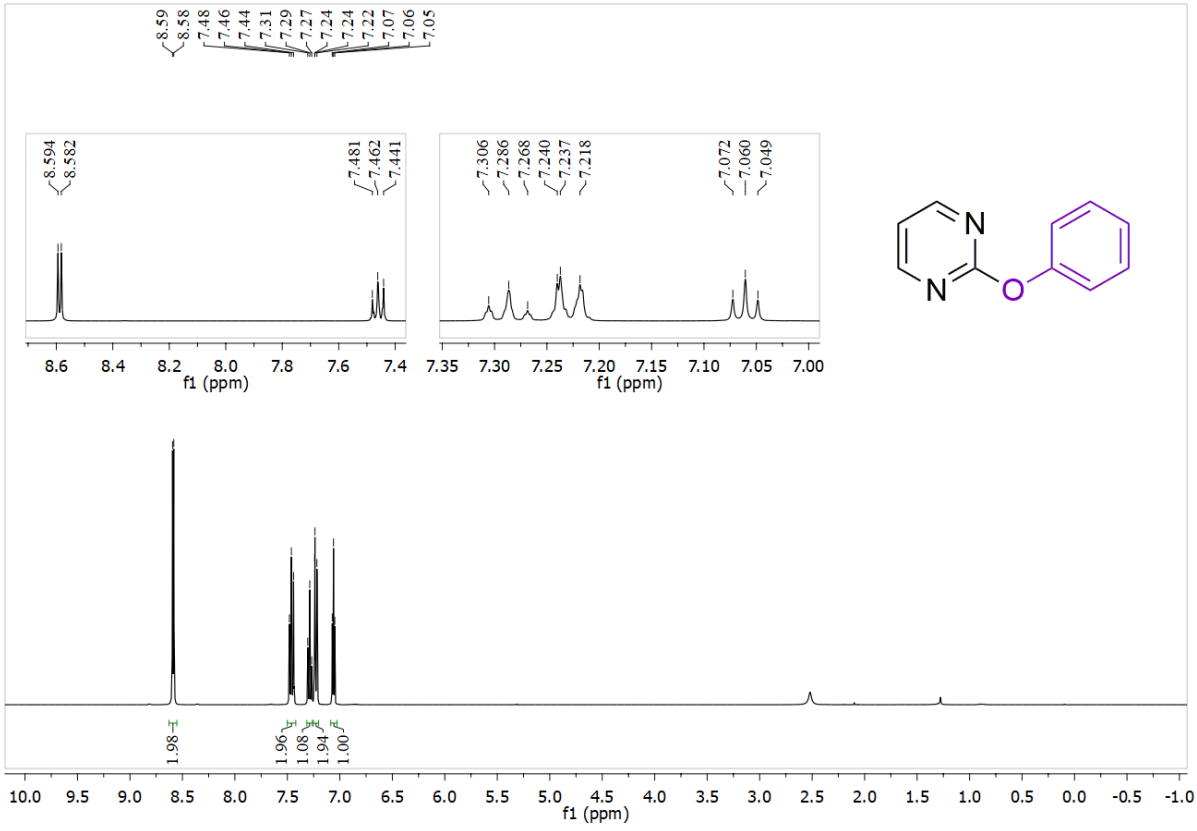


Fig. S29: ^{1}H NMR (400 MHz) spectra **3k**

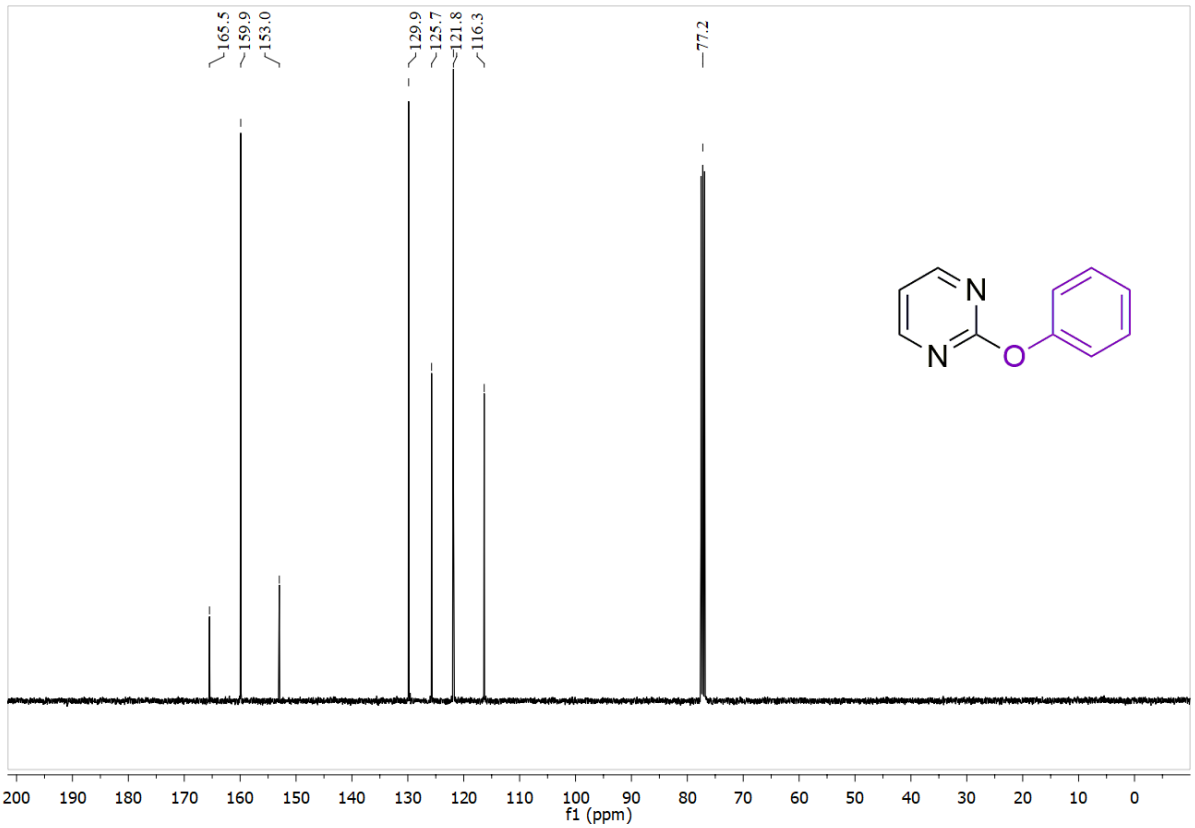


Fig. S30: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3k**

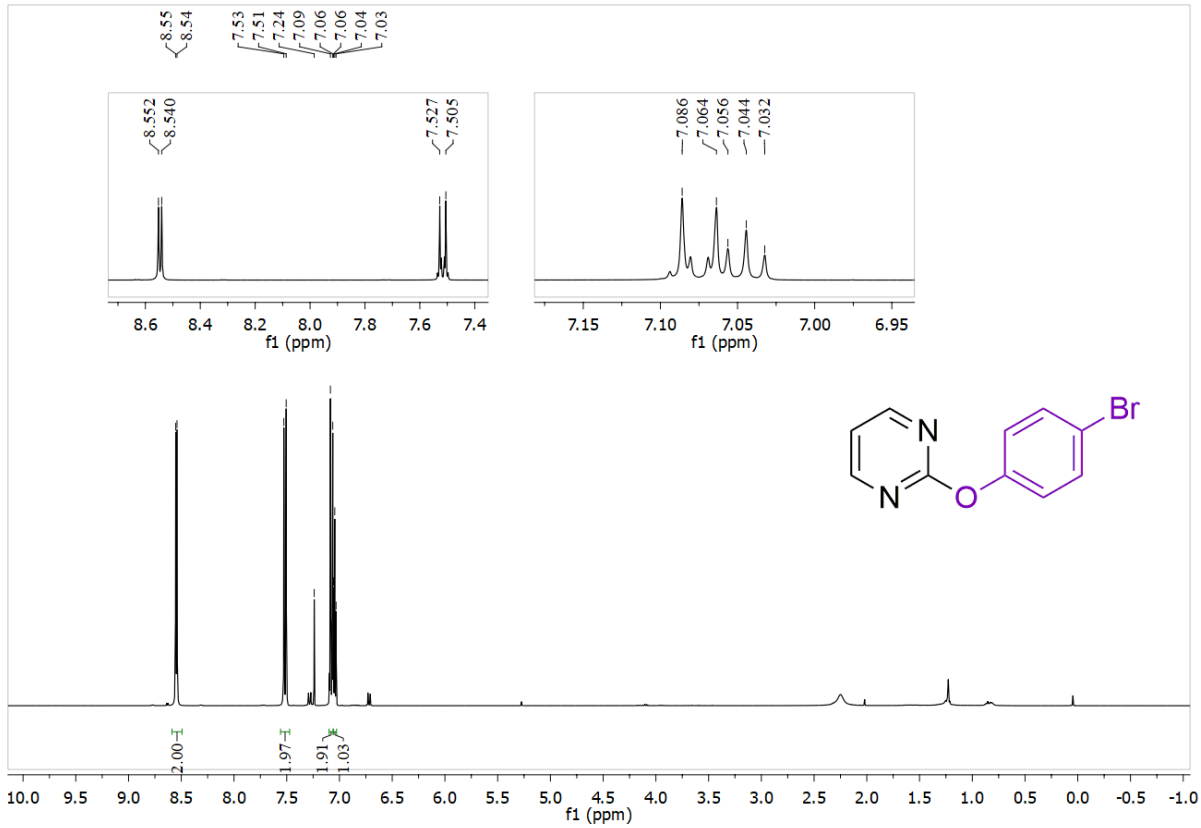


Fig. S31: ^{1}H NMR (400 MHz) spectra **3l**

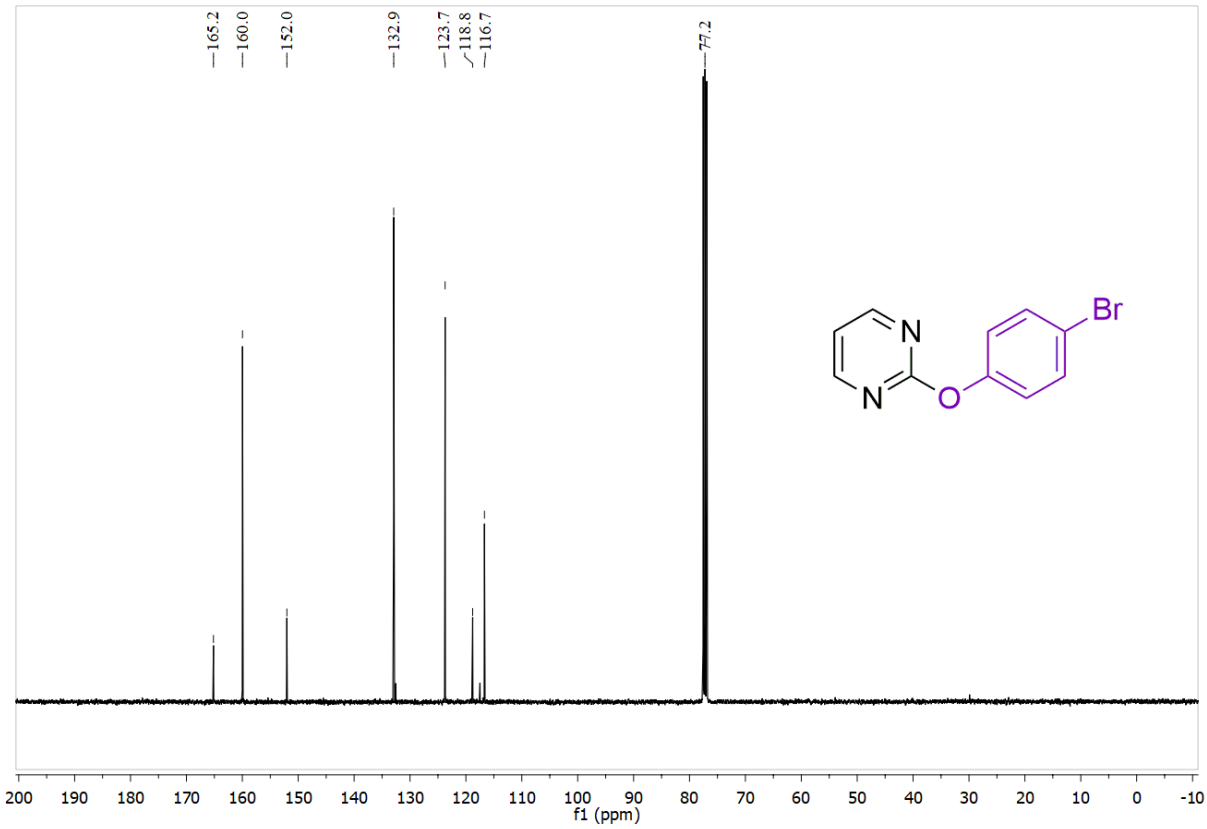


Fig. S32: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3l**

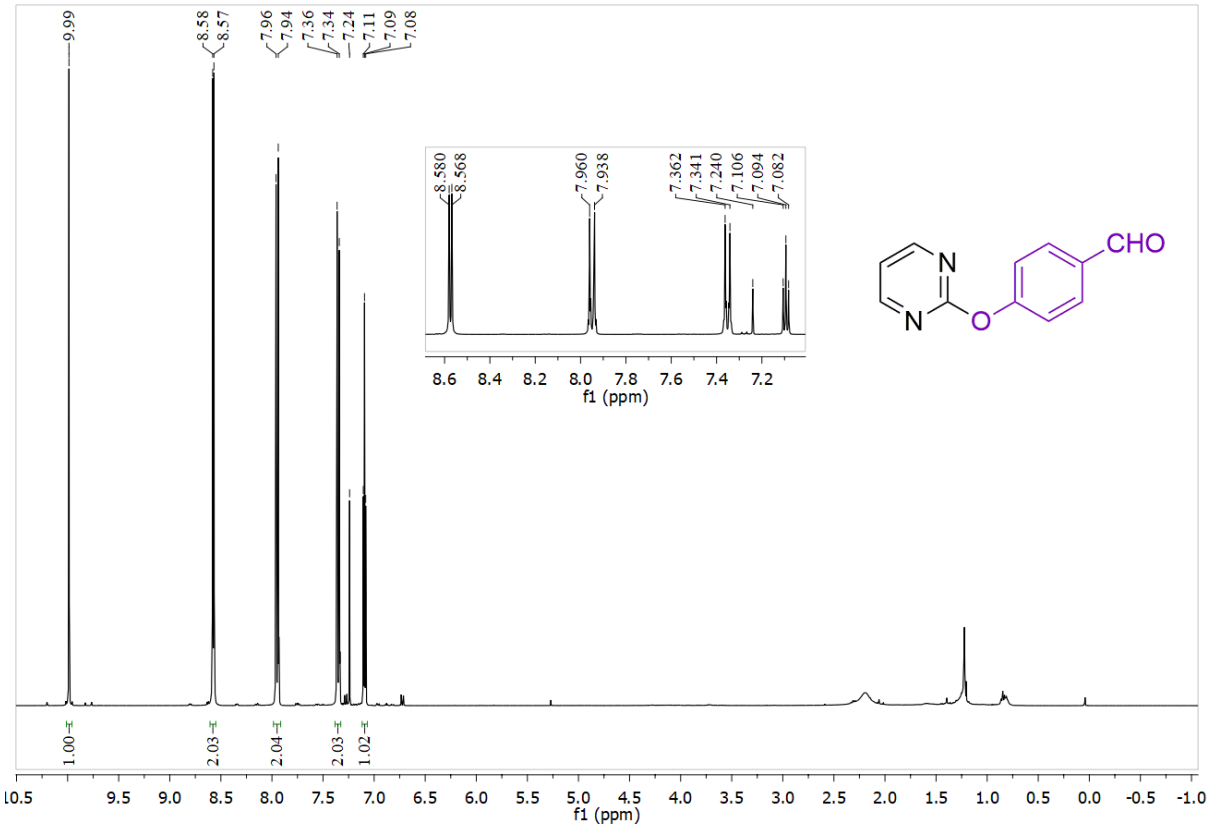


Fig. S33: ^{1}H NMR (400 MHz) spectra **3m**

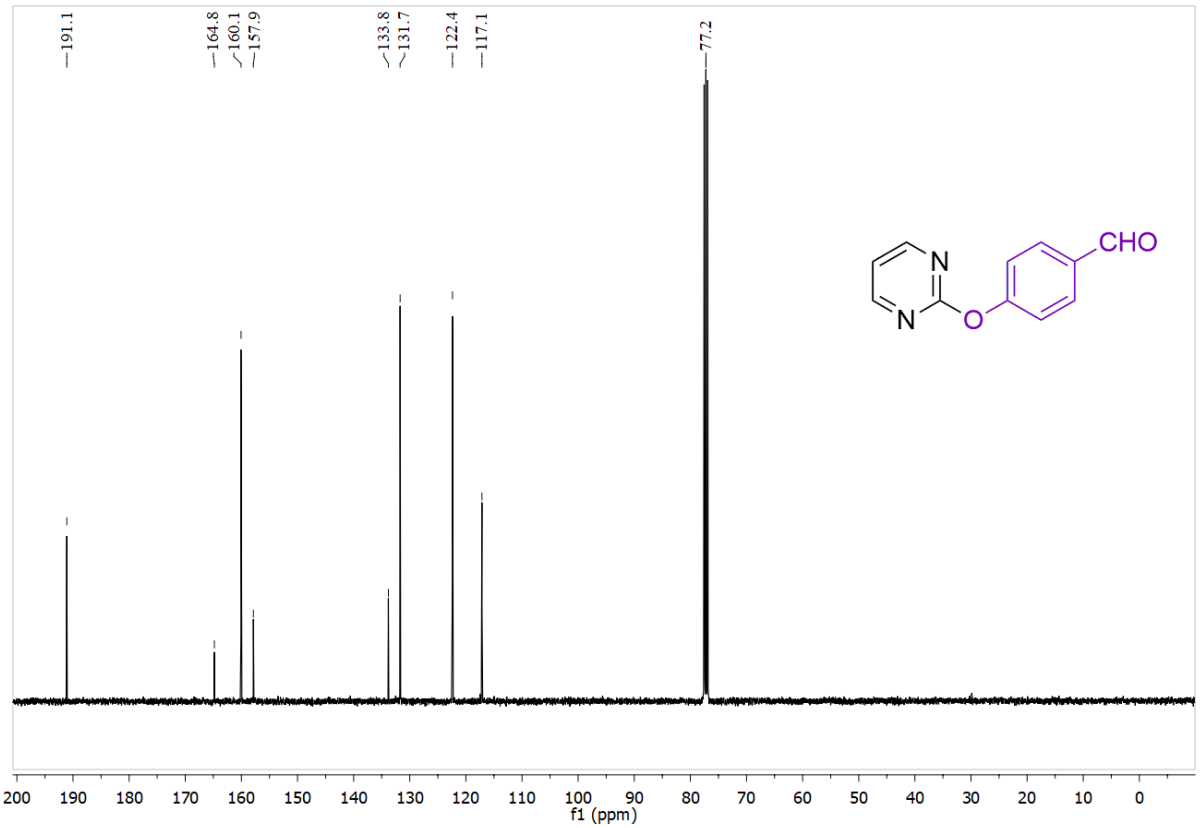


Fig. S34: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3m**

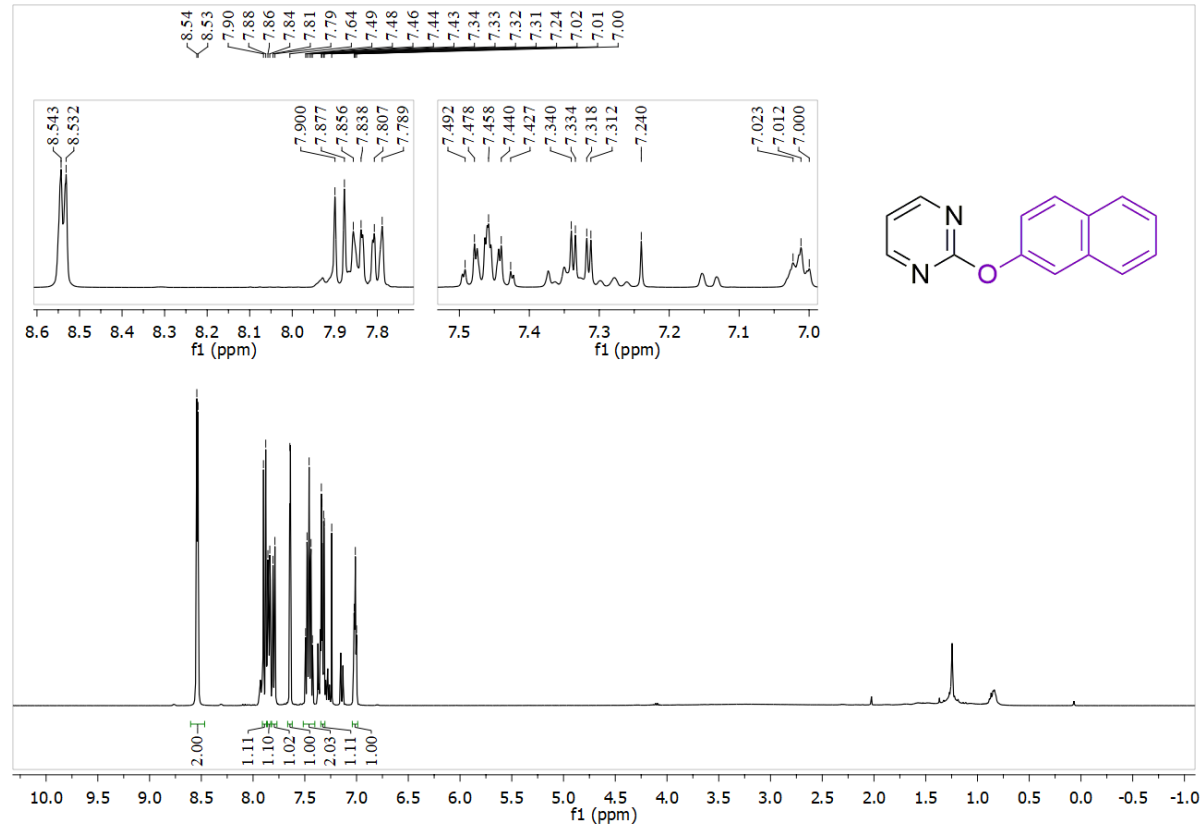


Fig. S35: ^{1}H NMR (400 MHz) spectra **3n**

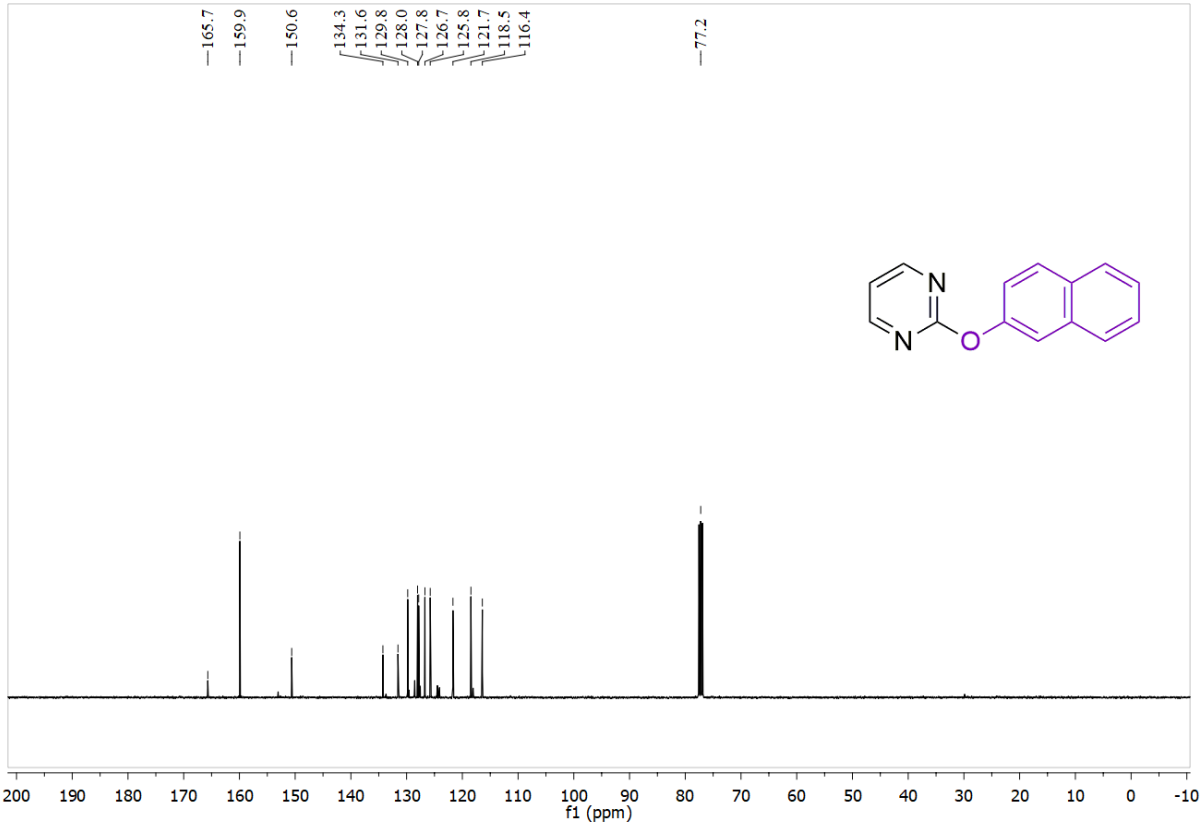


Fig. S36: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3n**

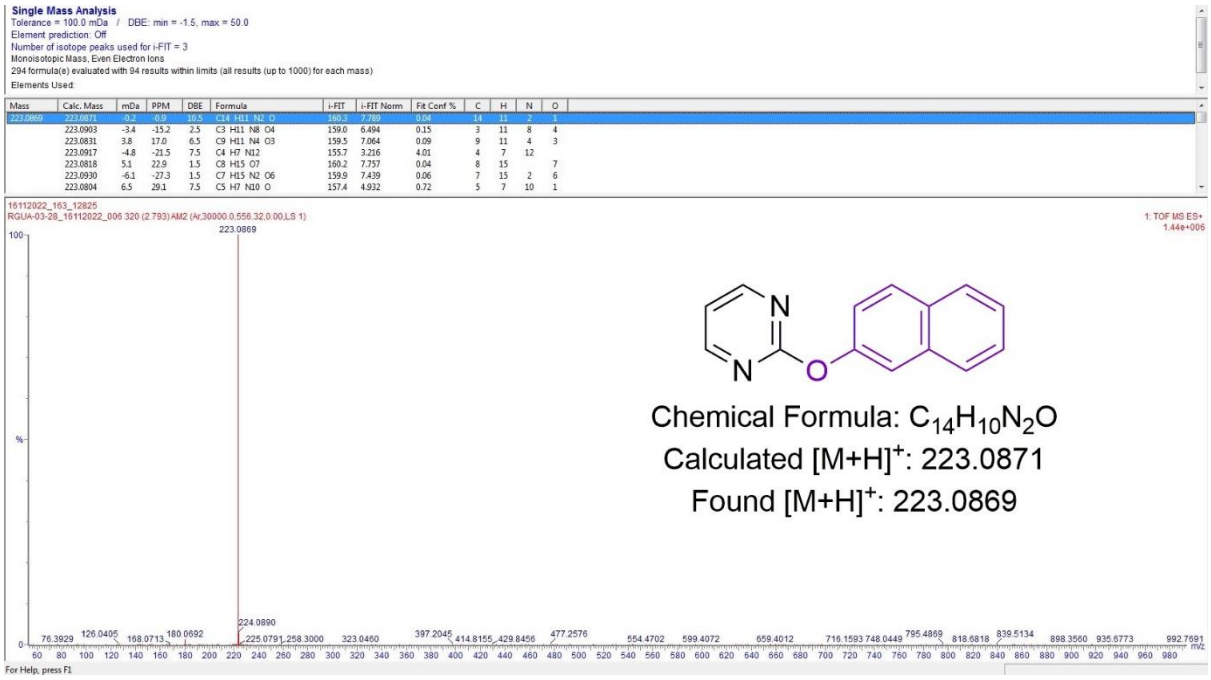


Fig. S37: HRMS spectra of **3n**

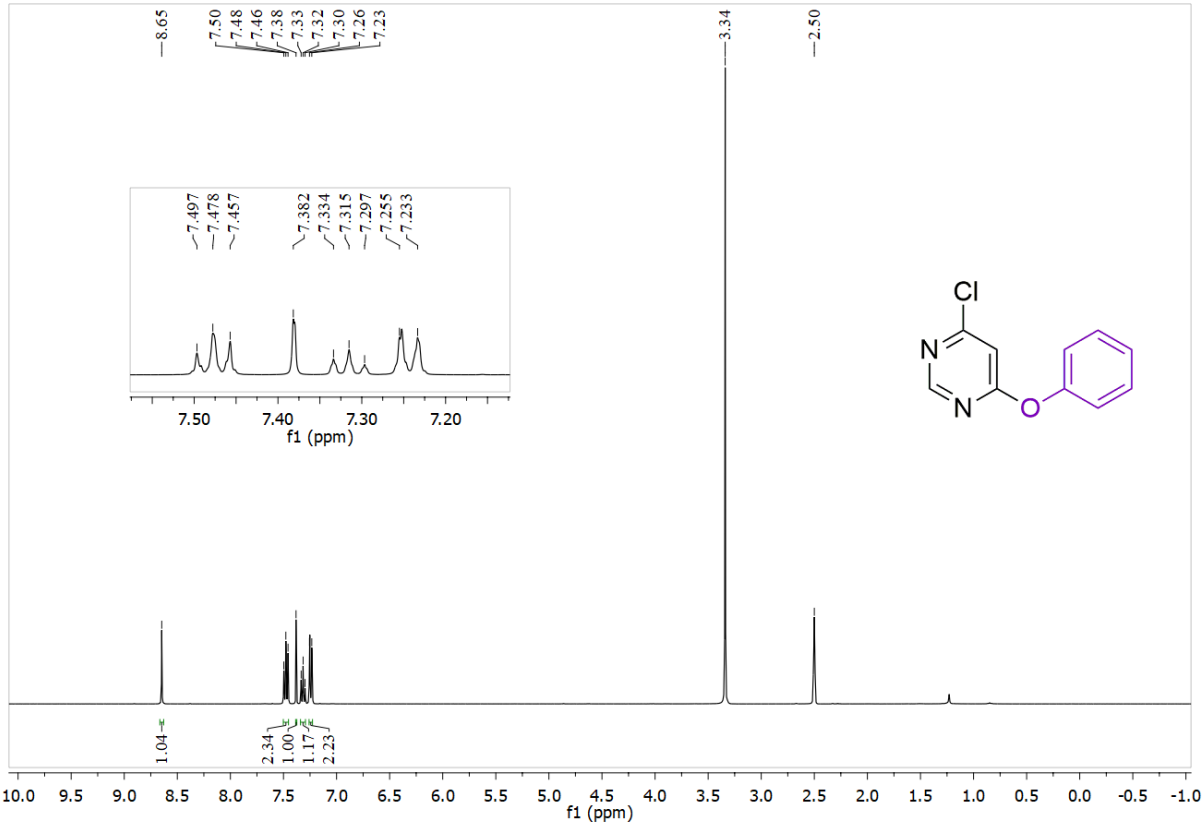


Fig. S38: ^{1}H NMR (400 MHz) spectra **3o**

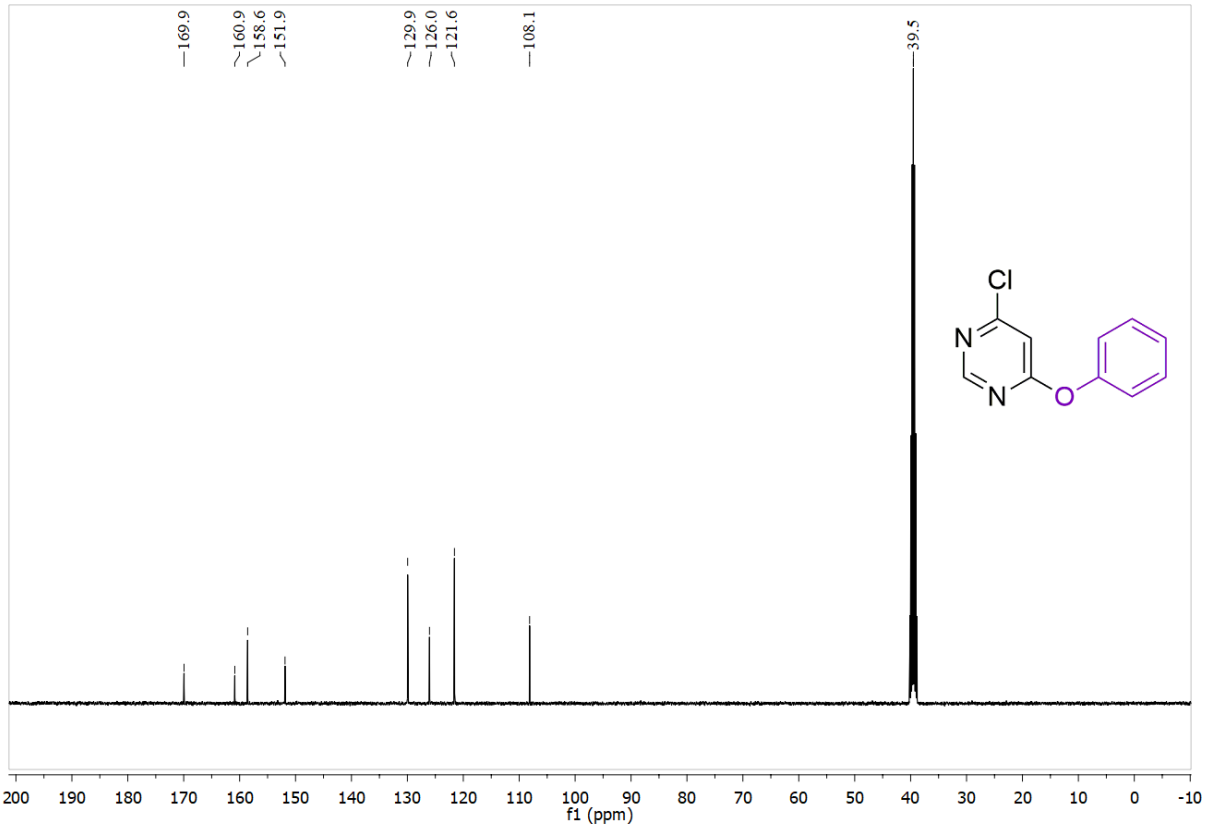


Fig. S39: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3o**

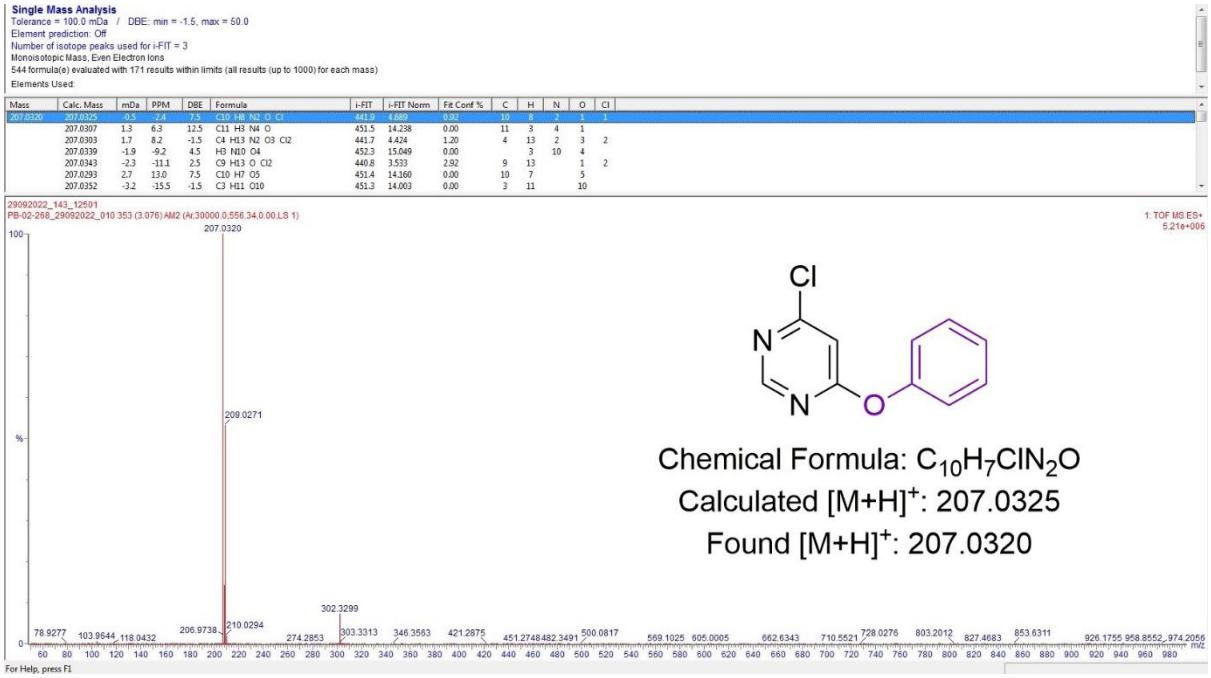


Fig. S40: HRMS spectra of **3o**

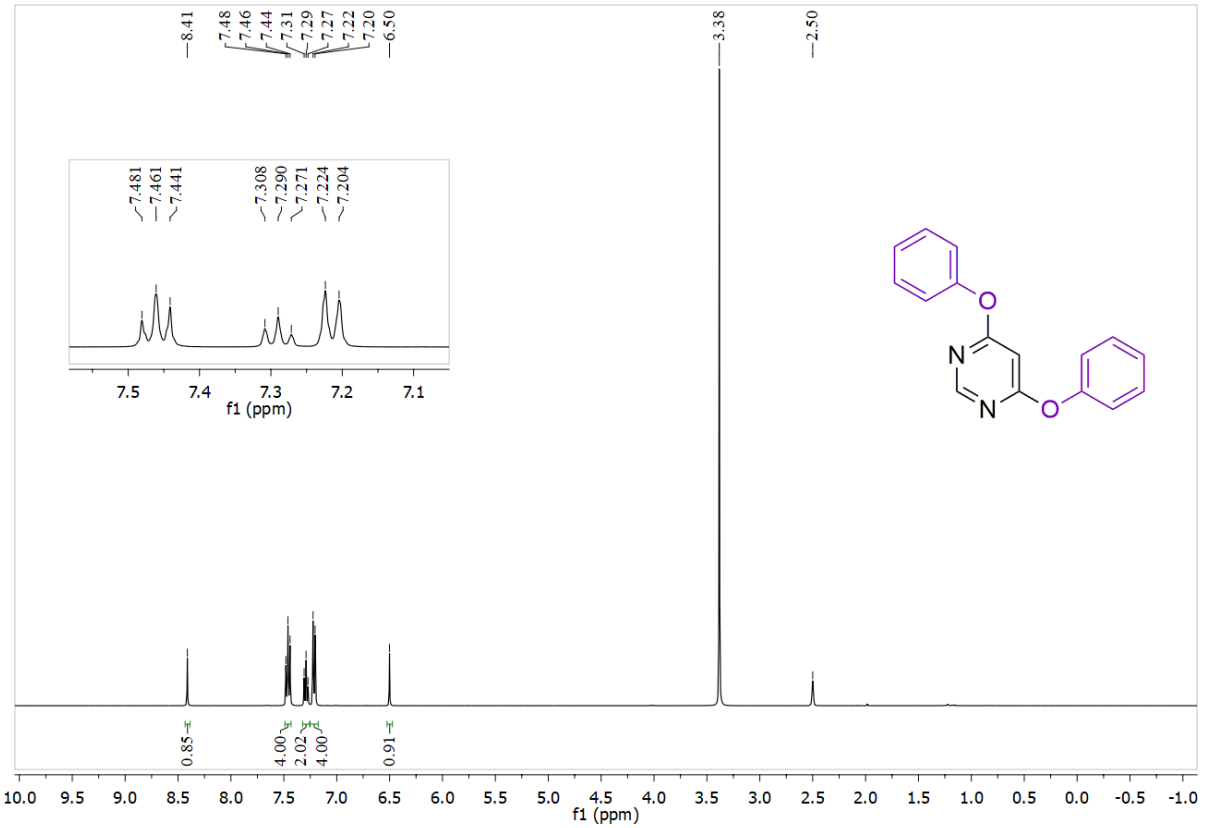


Fig. S41: ^{1}H NMR (400 MHz) spectra **3p**

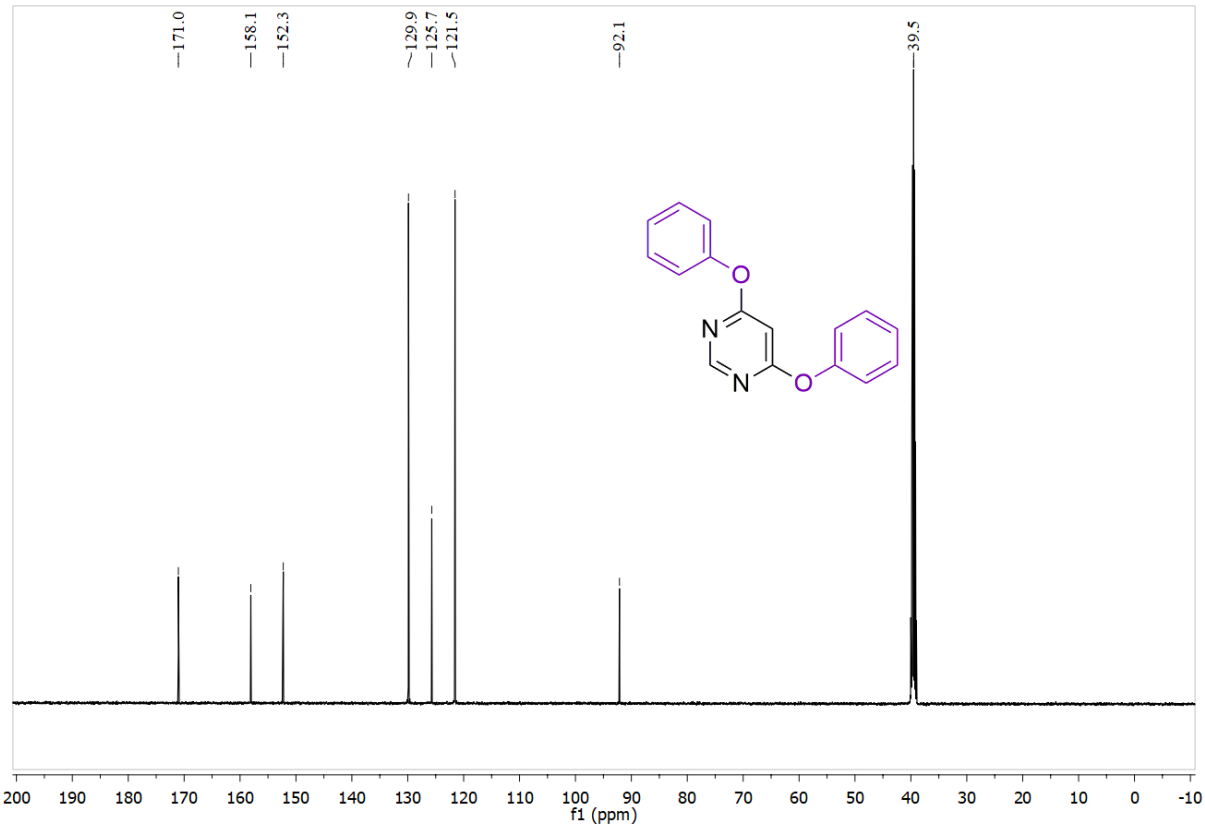


Fig. S42: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3p**

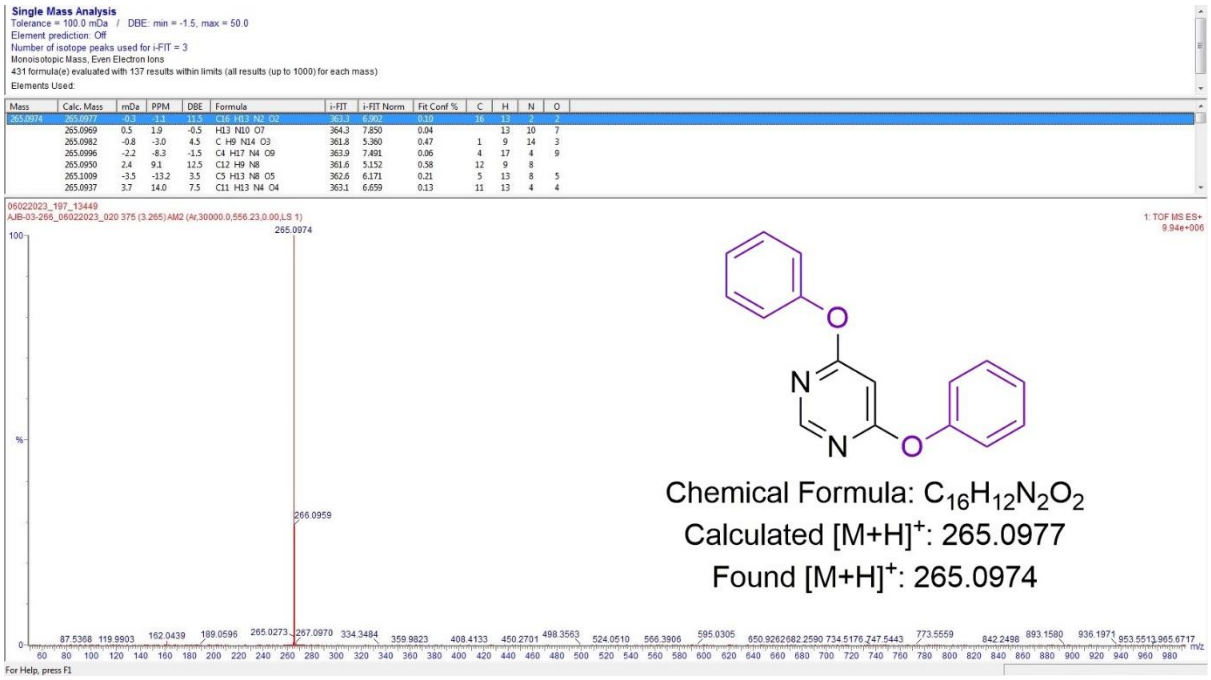


Fig. S43: HRMS spectra of **3p**

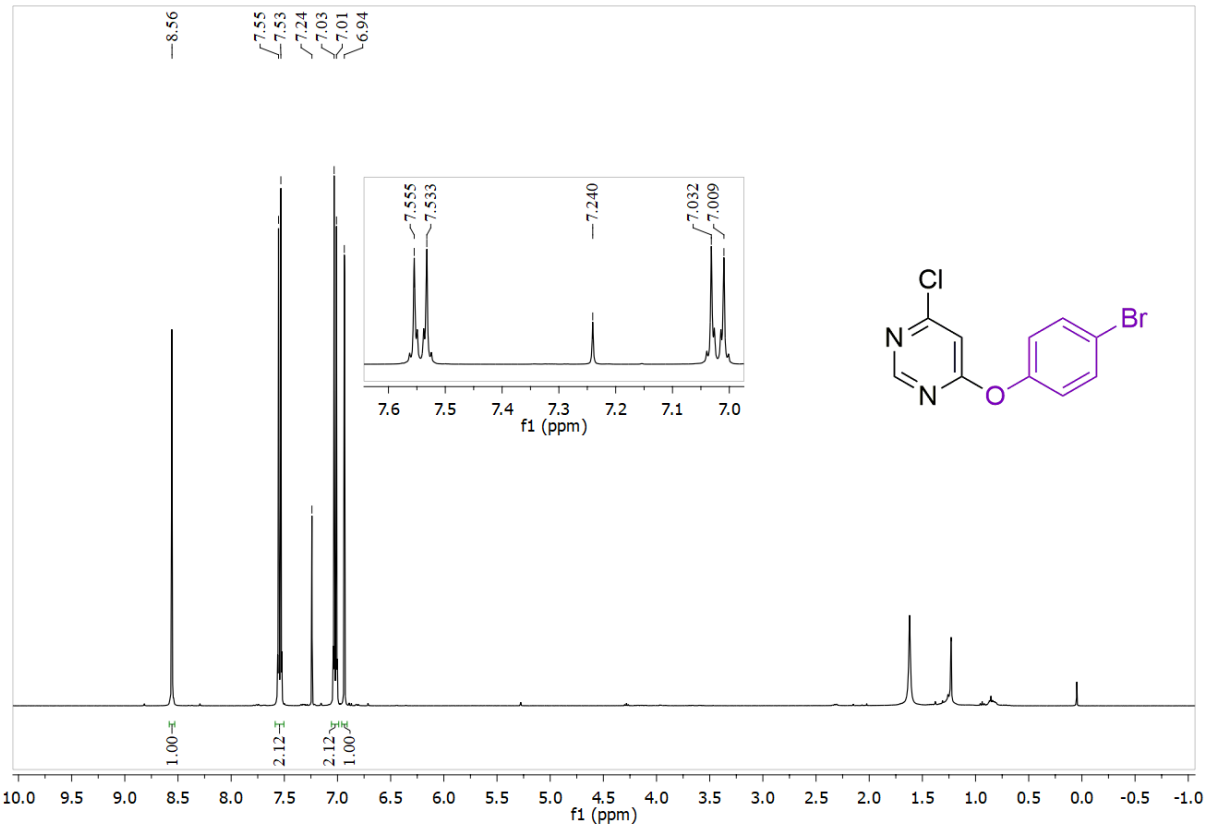


Fig. S44: ^{1}H NMR (400 MHz) spectra **3q**

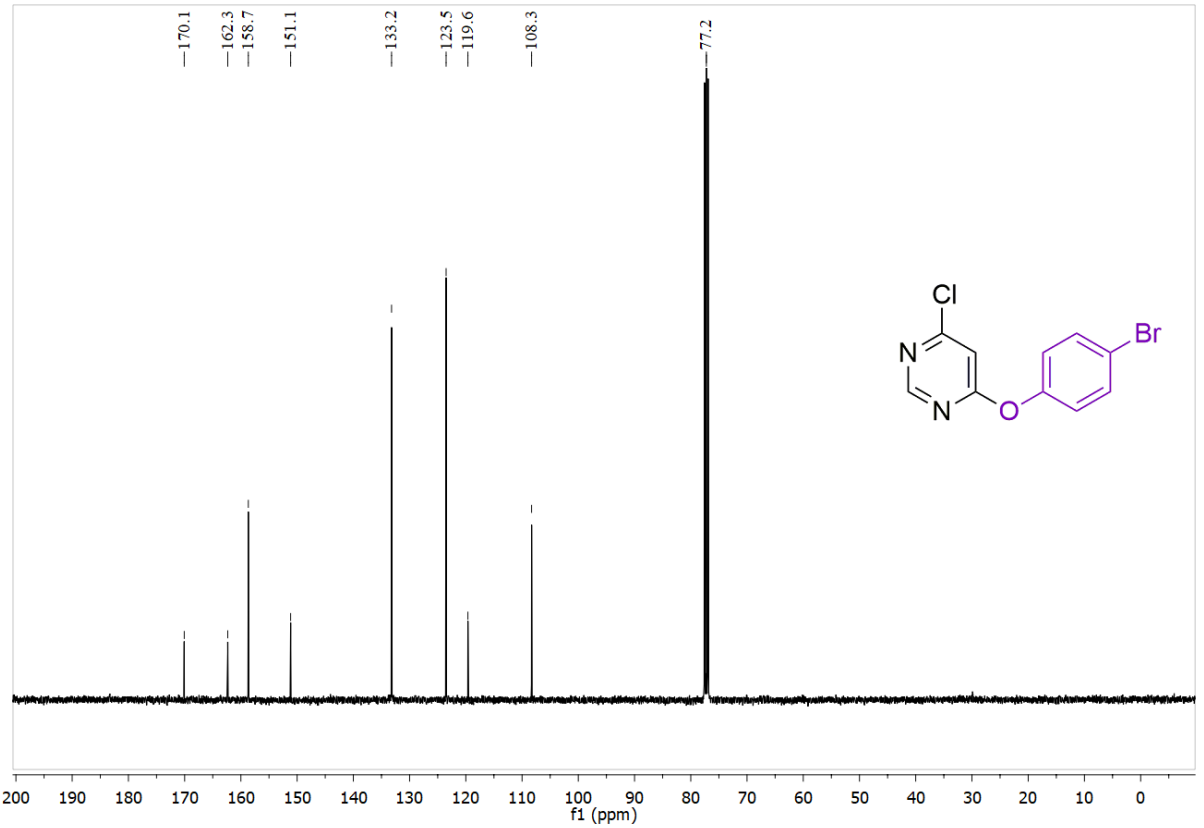


Fig. S45: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3q**

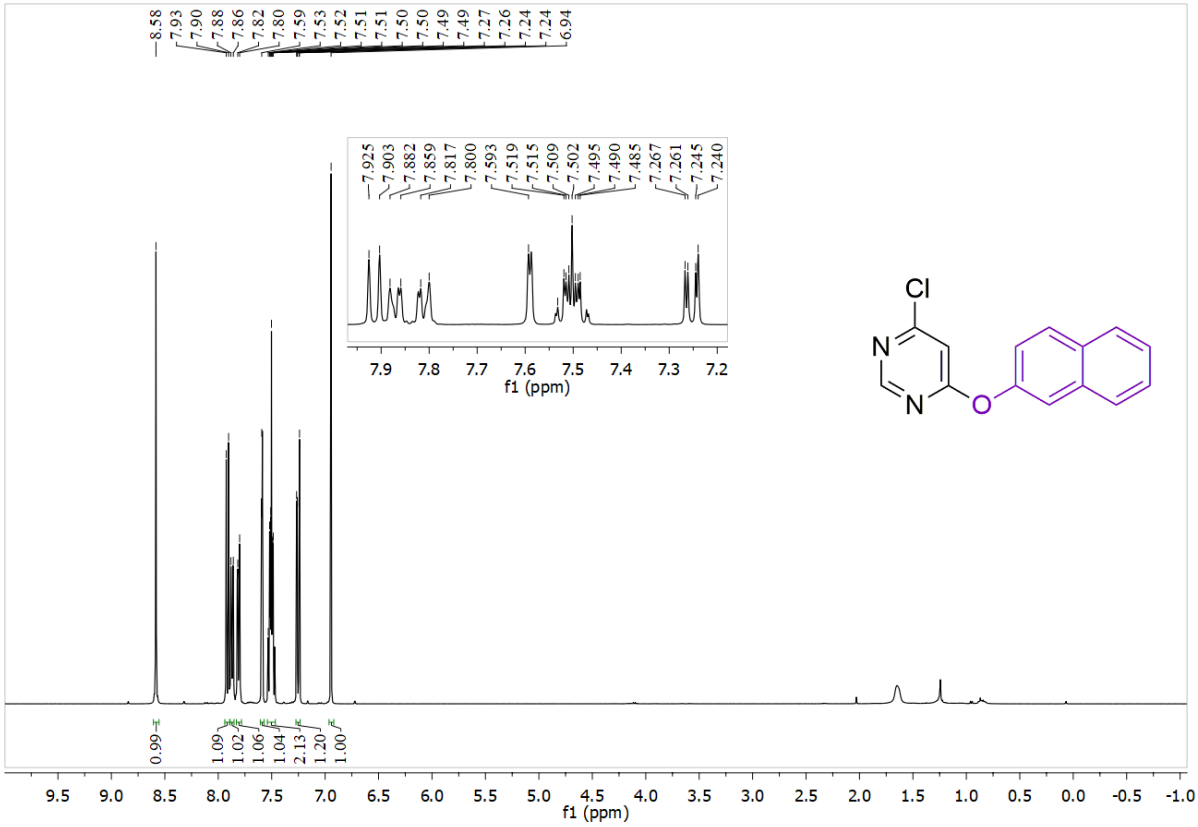


Fig. S46: ^{1}H NMR (400 MHz) spectra **3r**

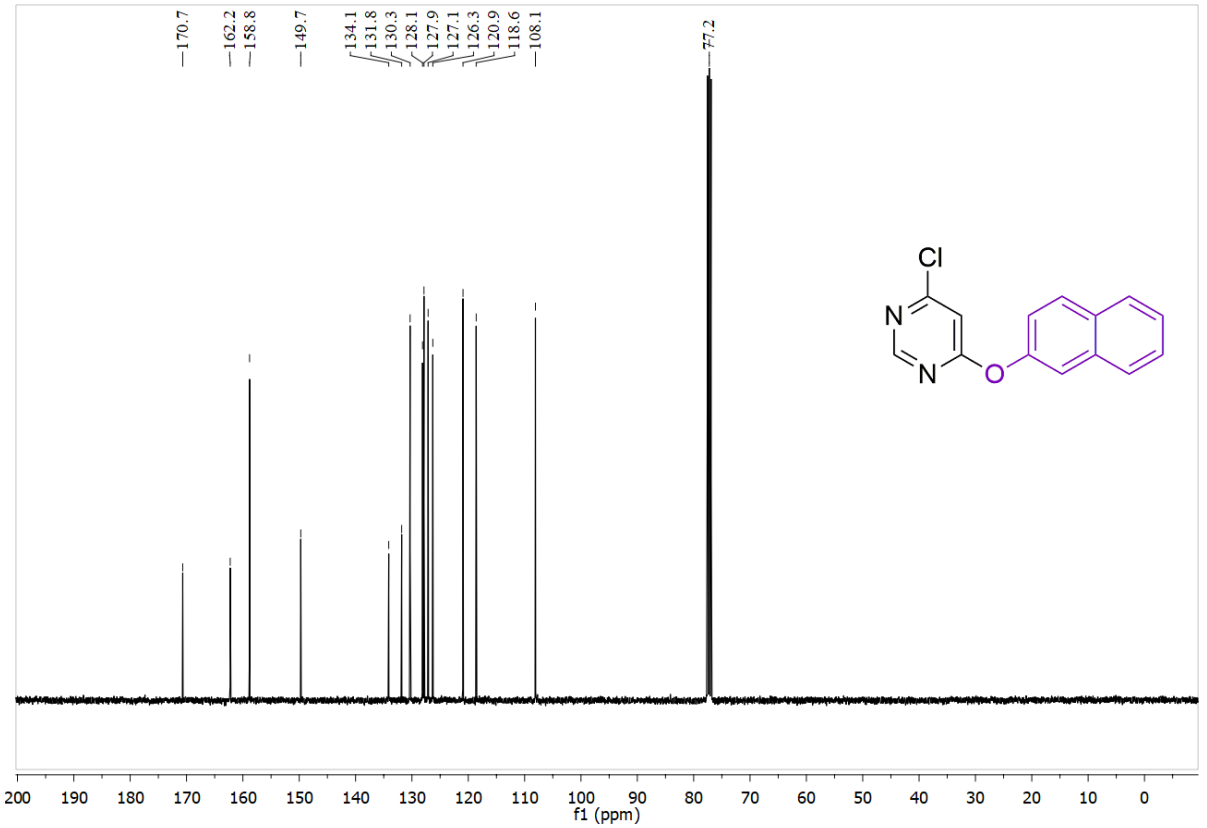


Fig. S47: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3r**

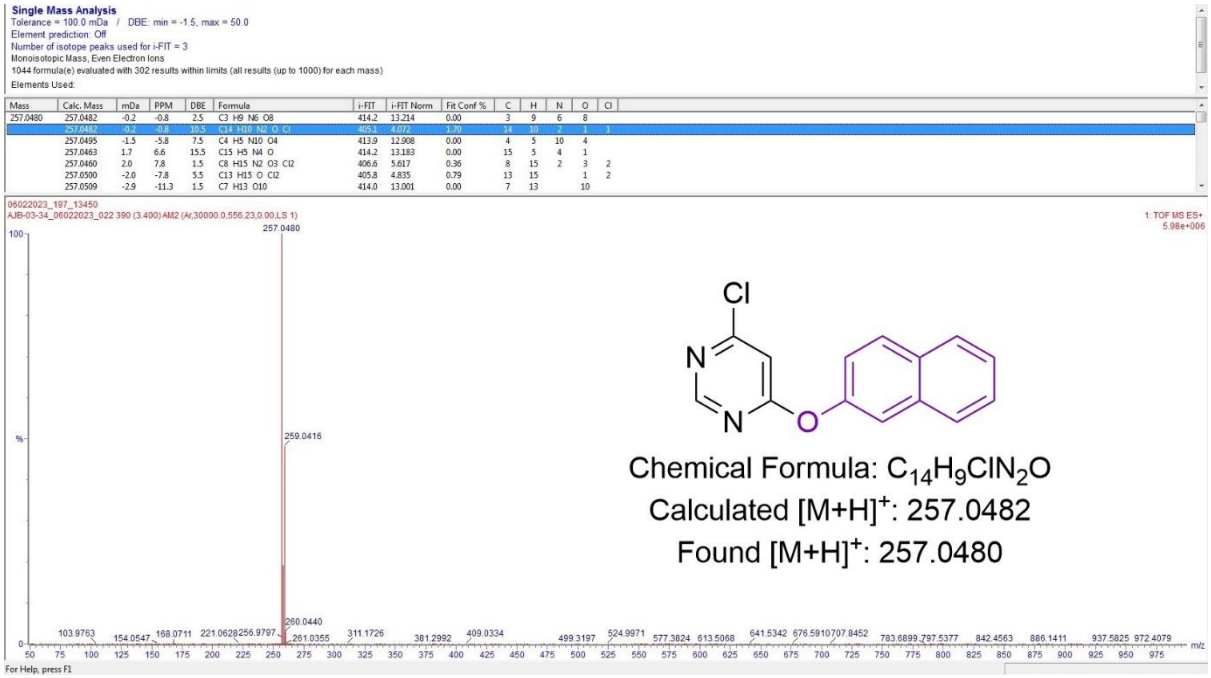


Fig. S48: HRMS spectra of **3r**

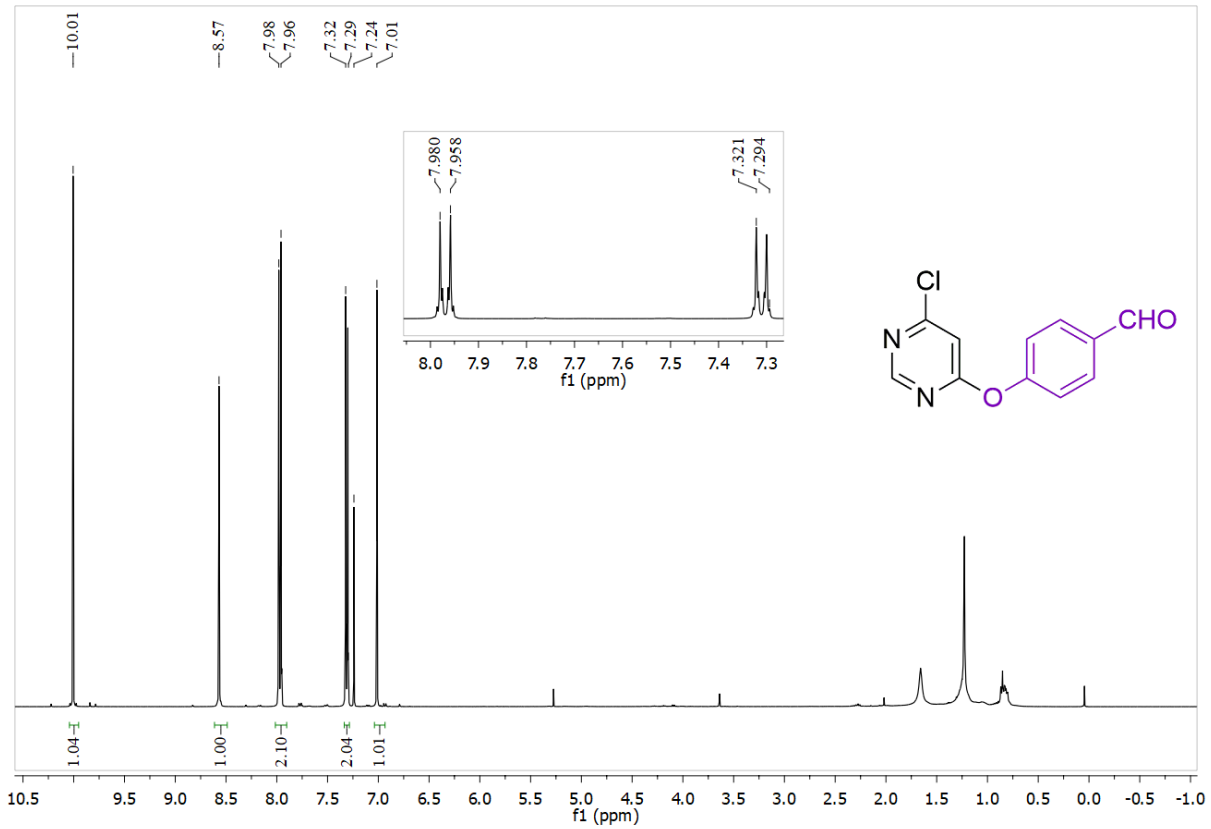


Fig. S49: ^{1}H NMR (400 MHz) spectra **3s**

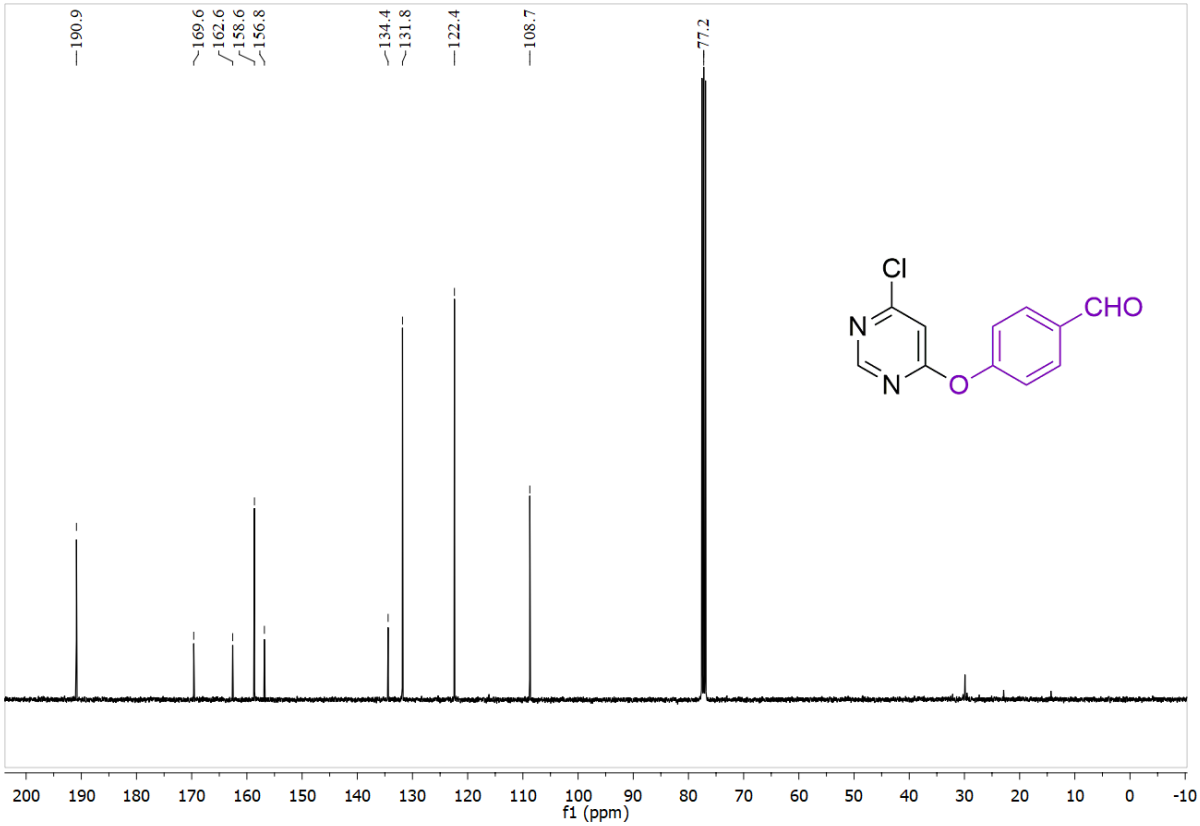


Fig. S50: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3s**

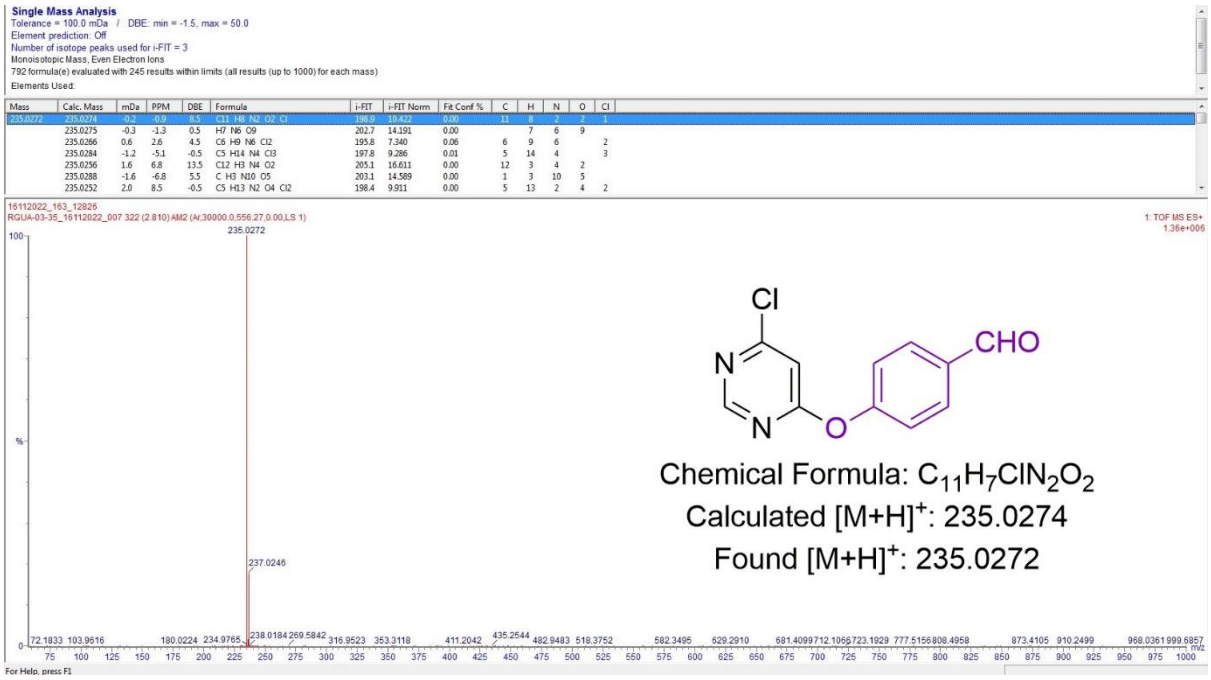


Fig. S51: HRMS spectra of **3s**

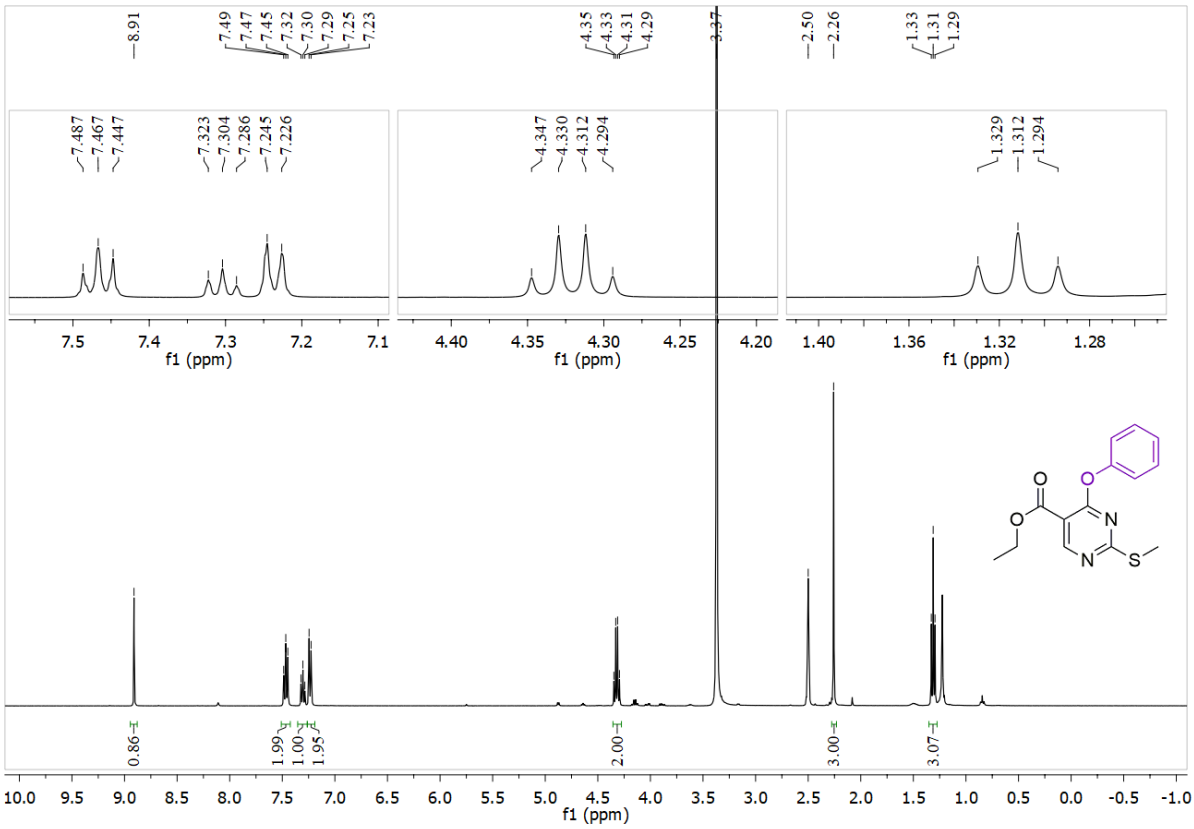


Fig. S52: ^{1}H NMR (400 MHz) spectra **3t**

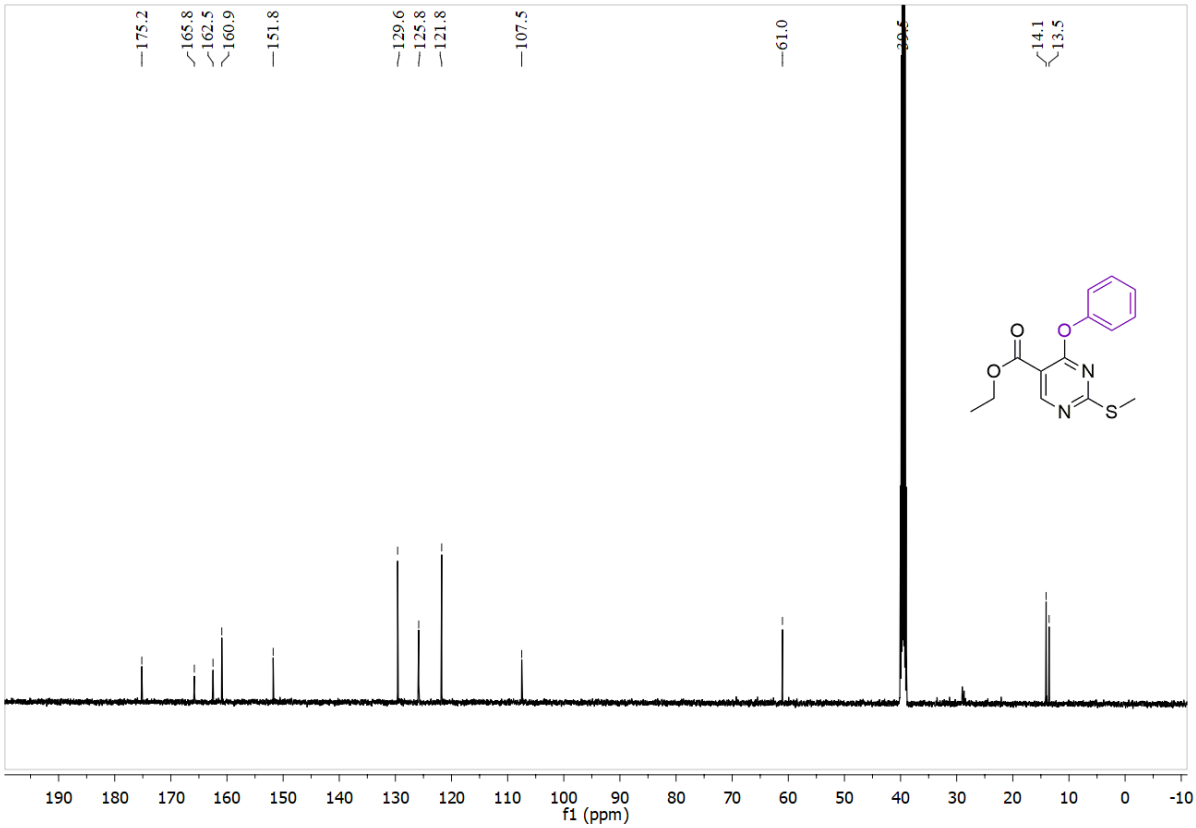


Fig. S53: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3t**

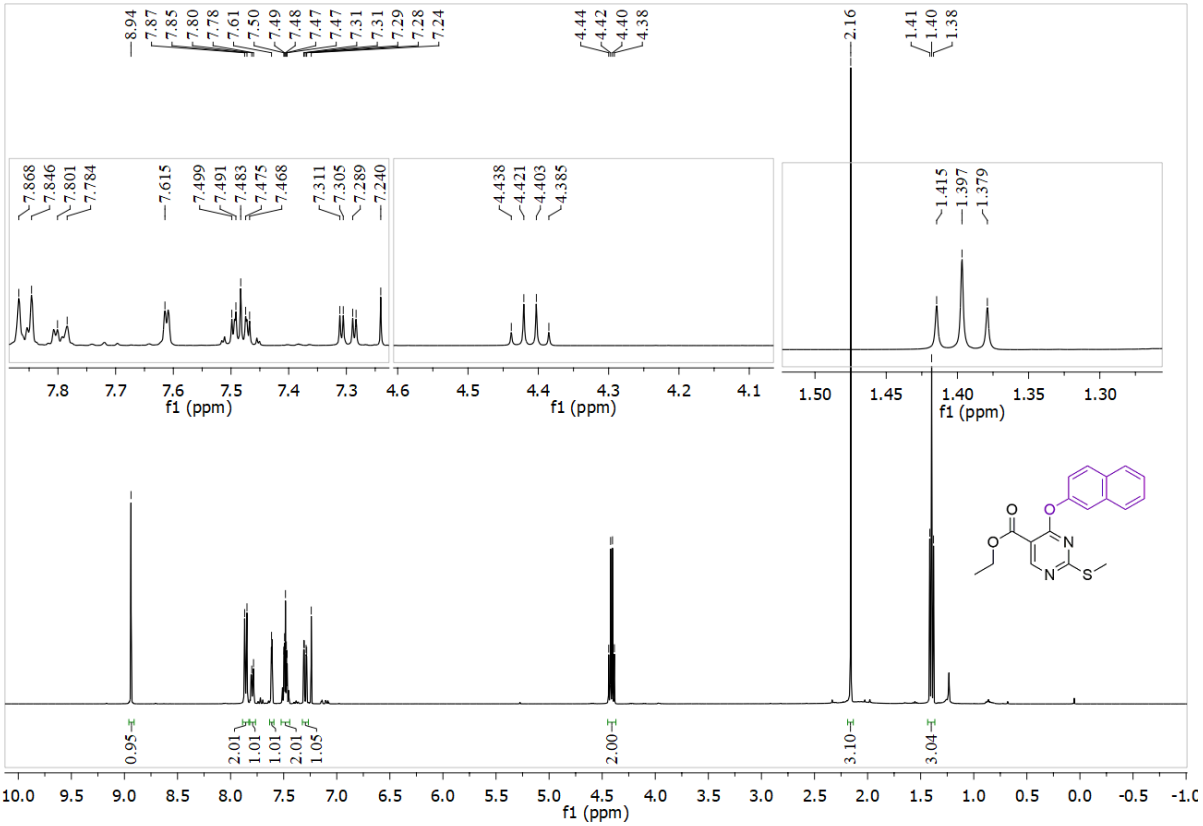


Fig. S54: ^{1}H NMR (400 MHz) spectra **3u**

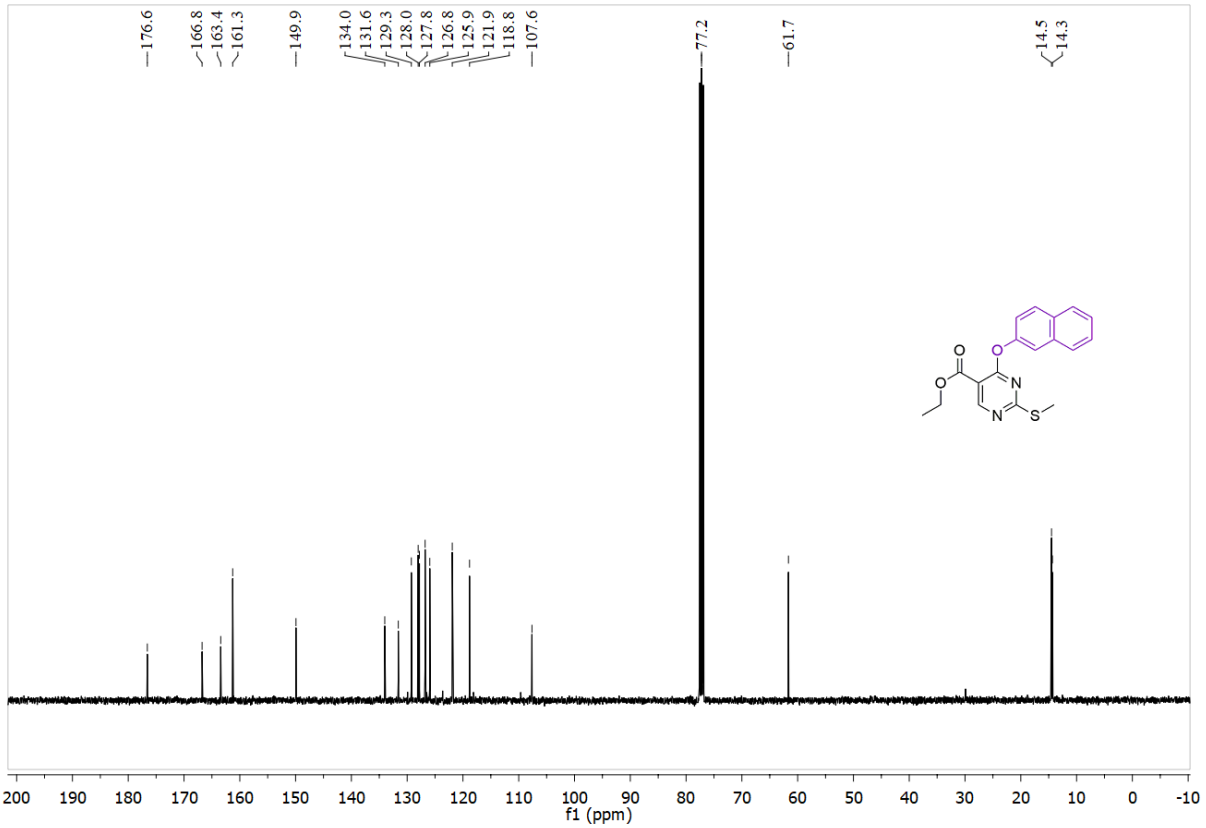


Fig. S55: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3u**

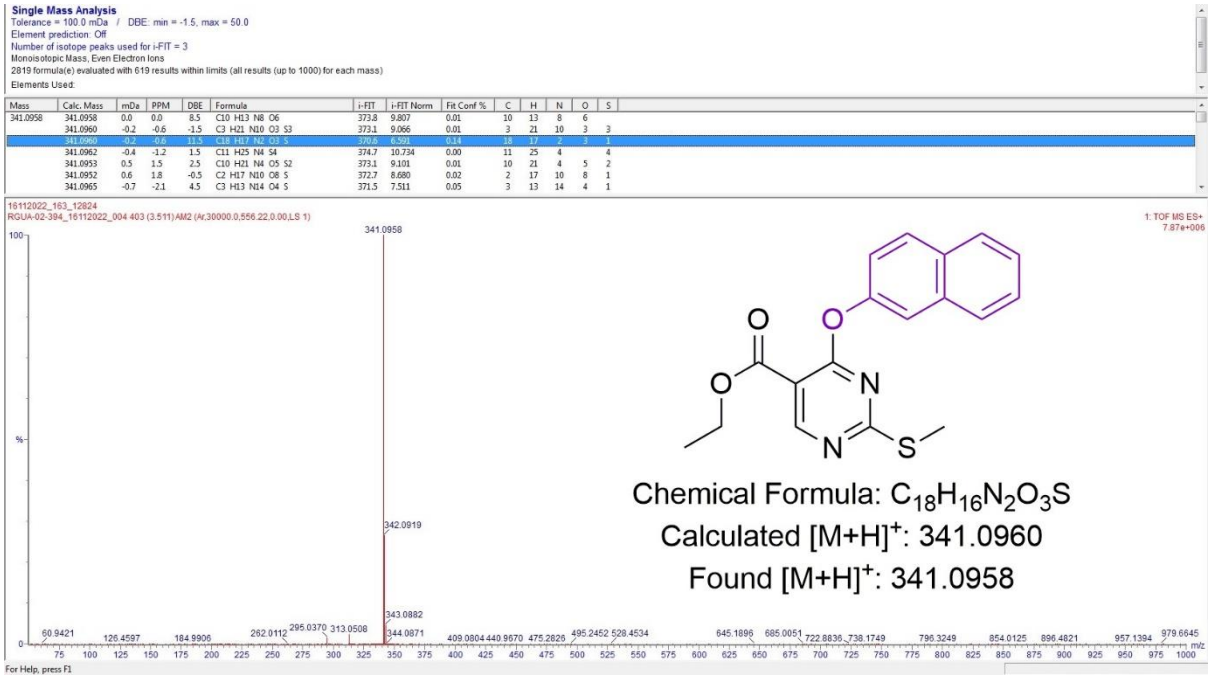


Fig. S56: HRMS spectra of **3u**

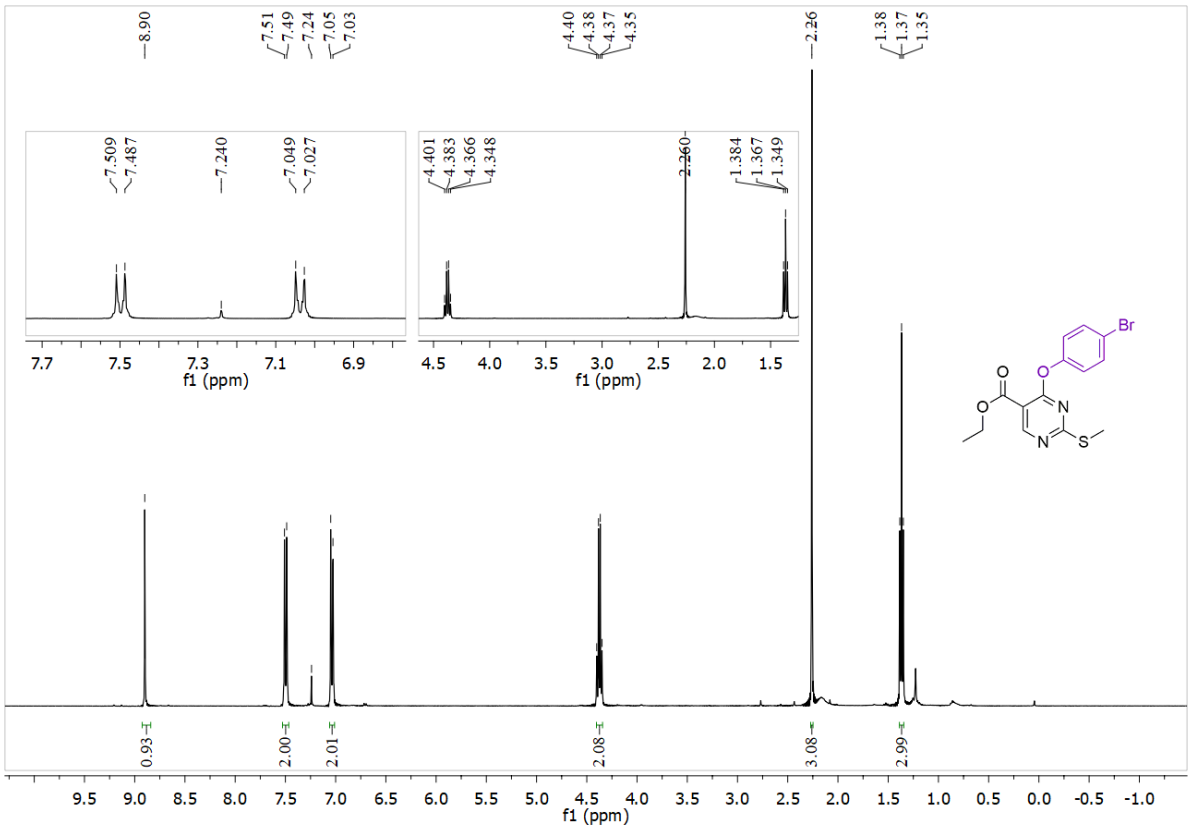


Fig. S57: ^{1}H NMR (400 MHz) spectra **3v**

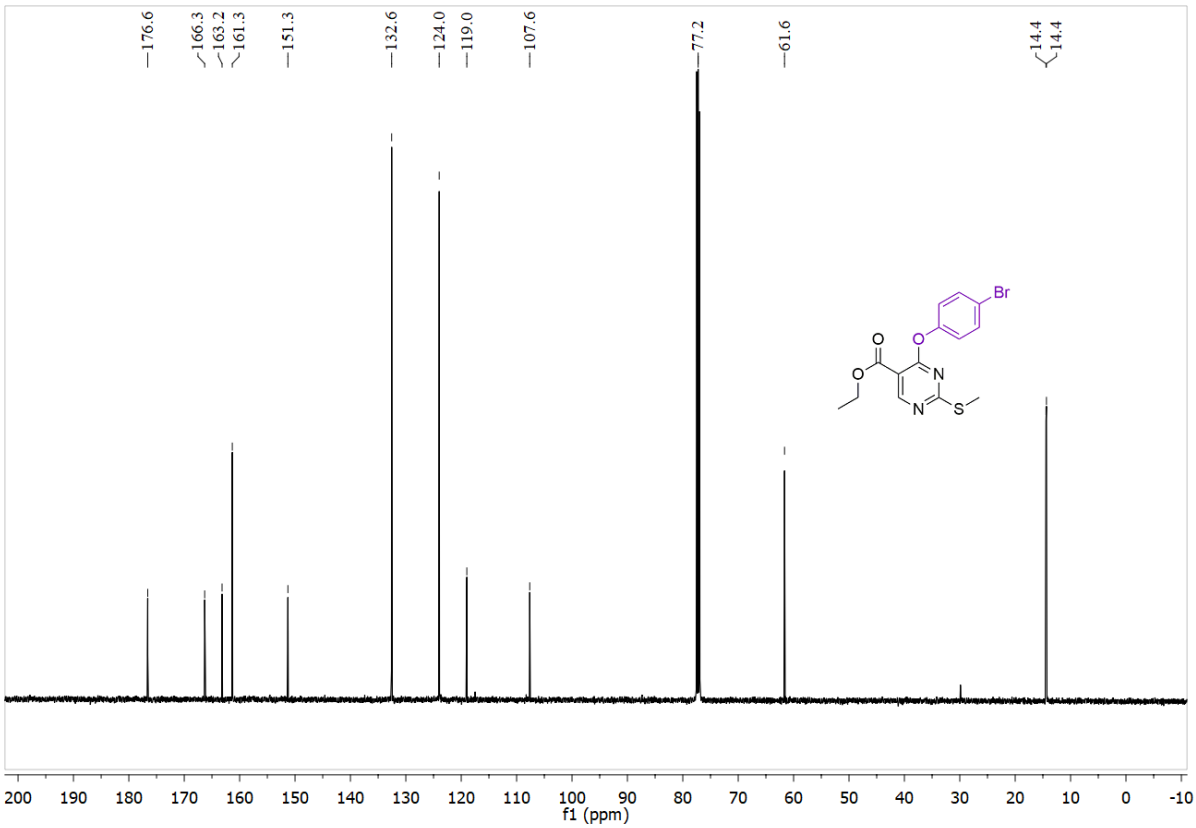


Fig. S58: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3v**

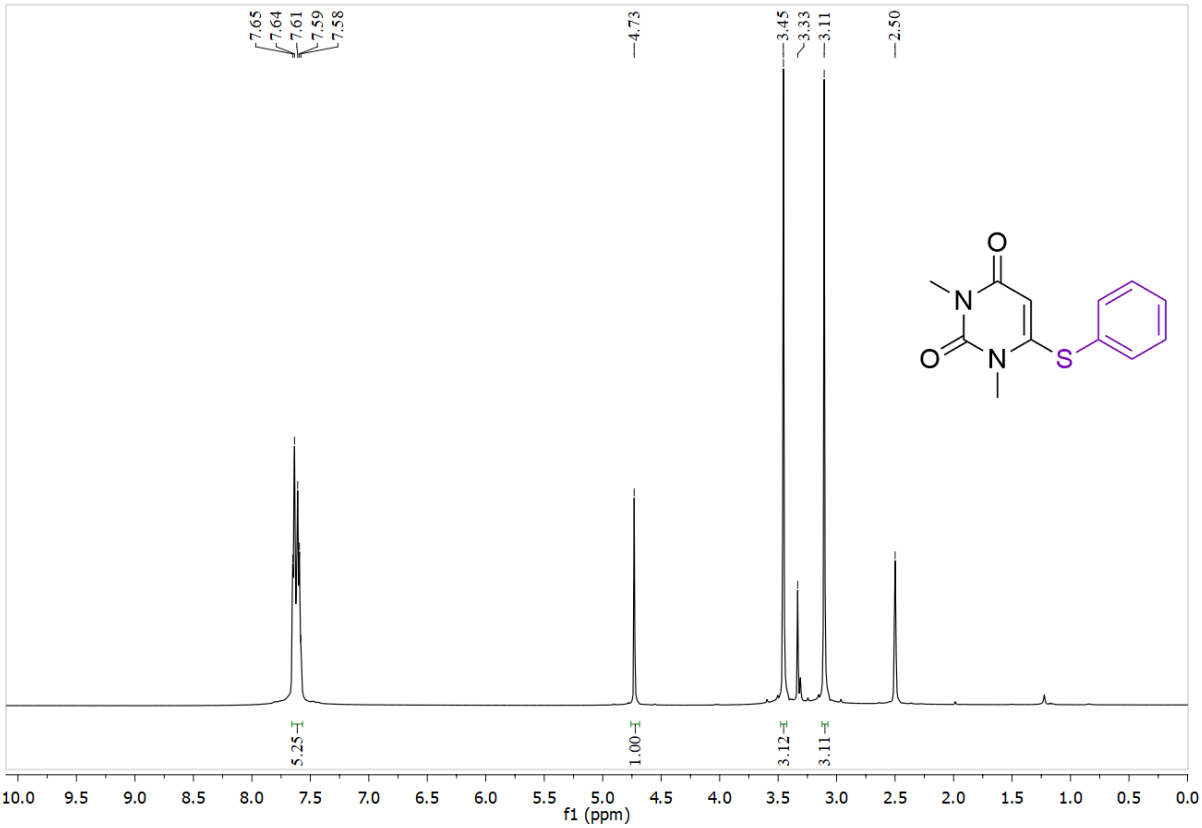


Fig. S59: ^{1}H NMR (400 MHz) spectra **3w**

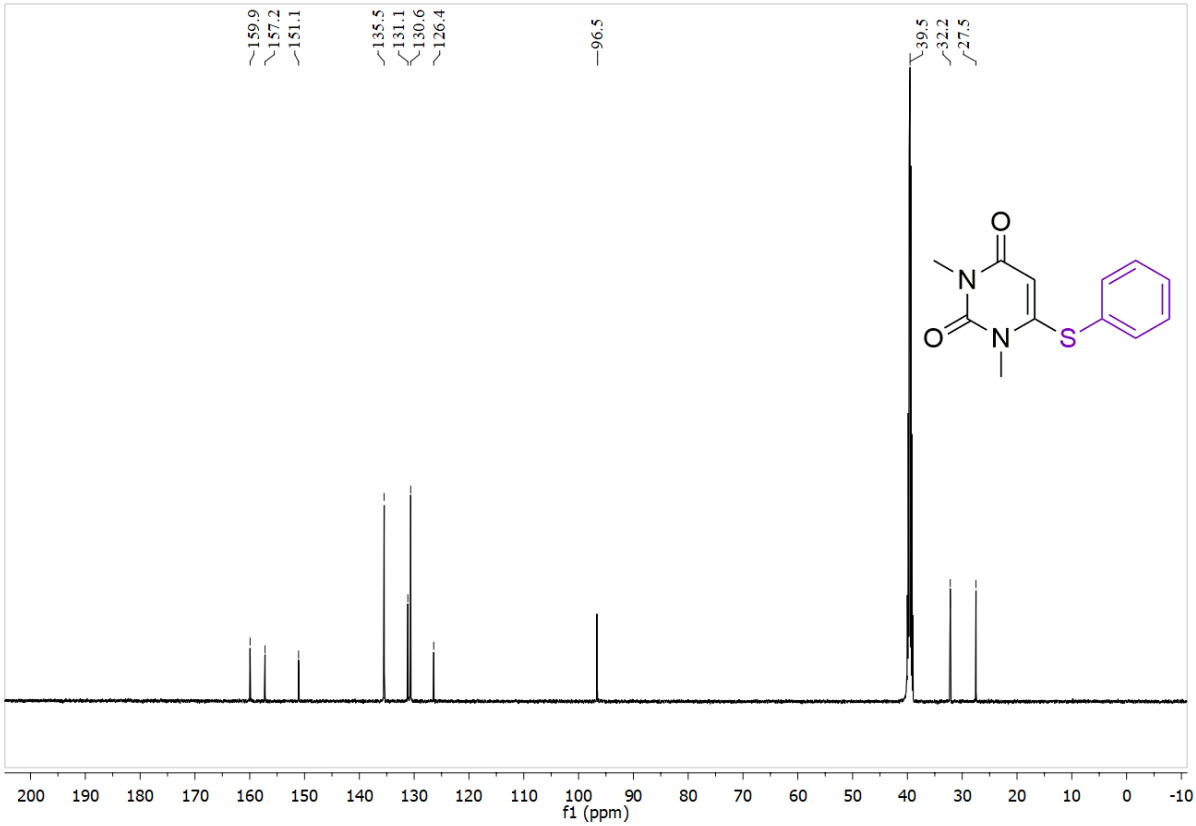


Fig. S60: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3w**

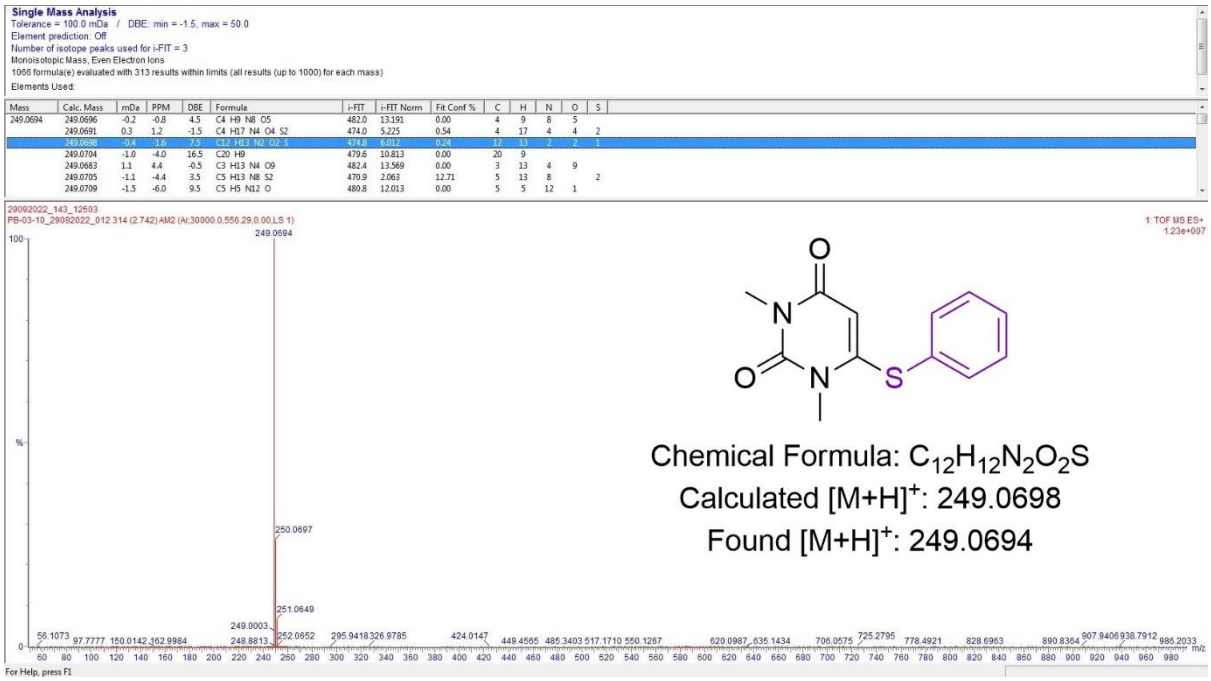


Fig. S61: HRMS spectra of **3w**

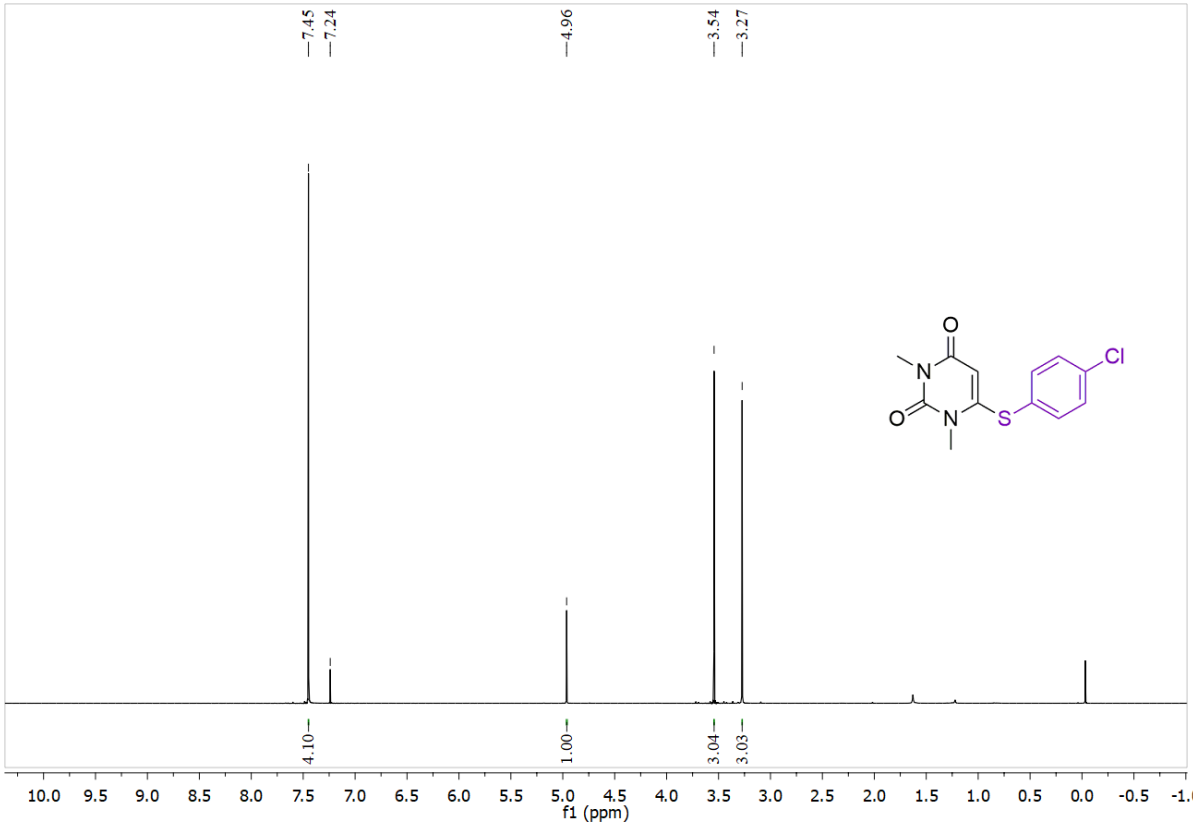


Fig. S62: ^{1}H NMR (400 MHz) spectra **3x**

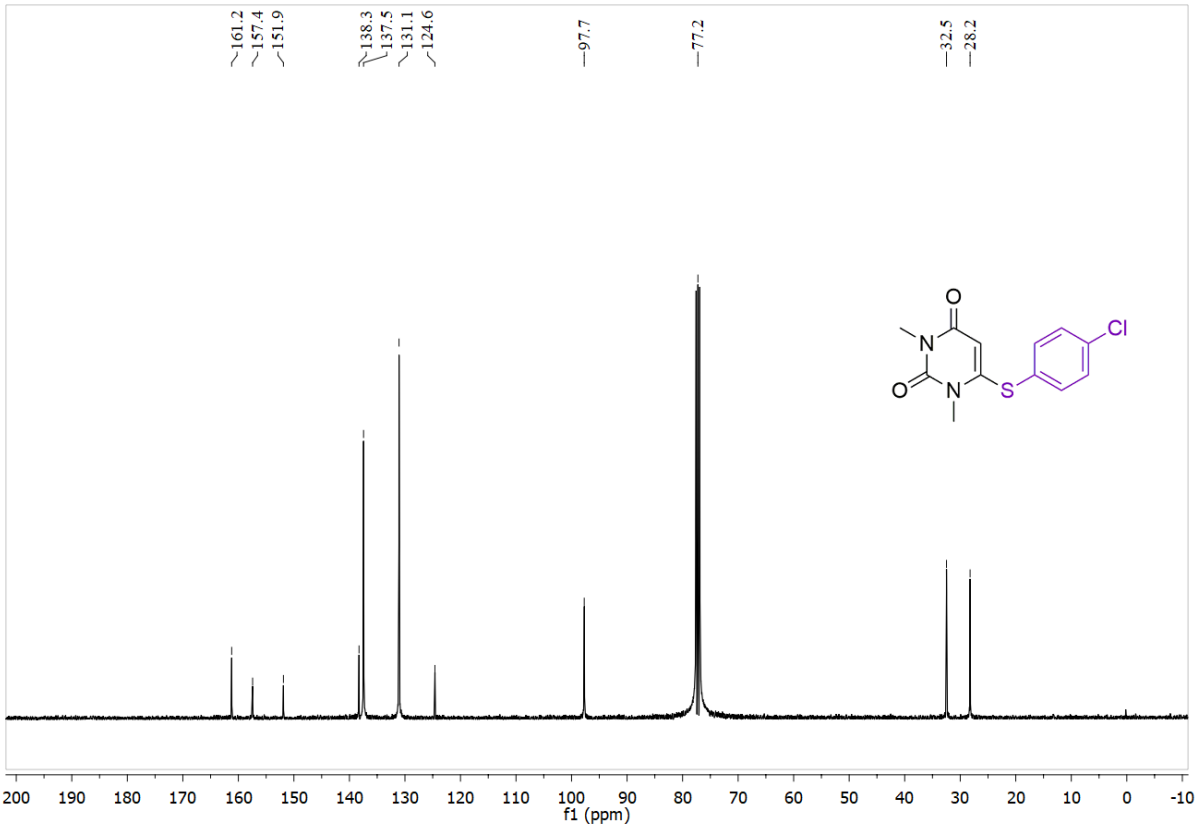


Fig. S63: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3x**

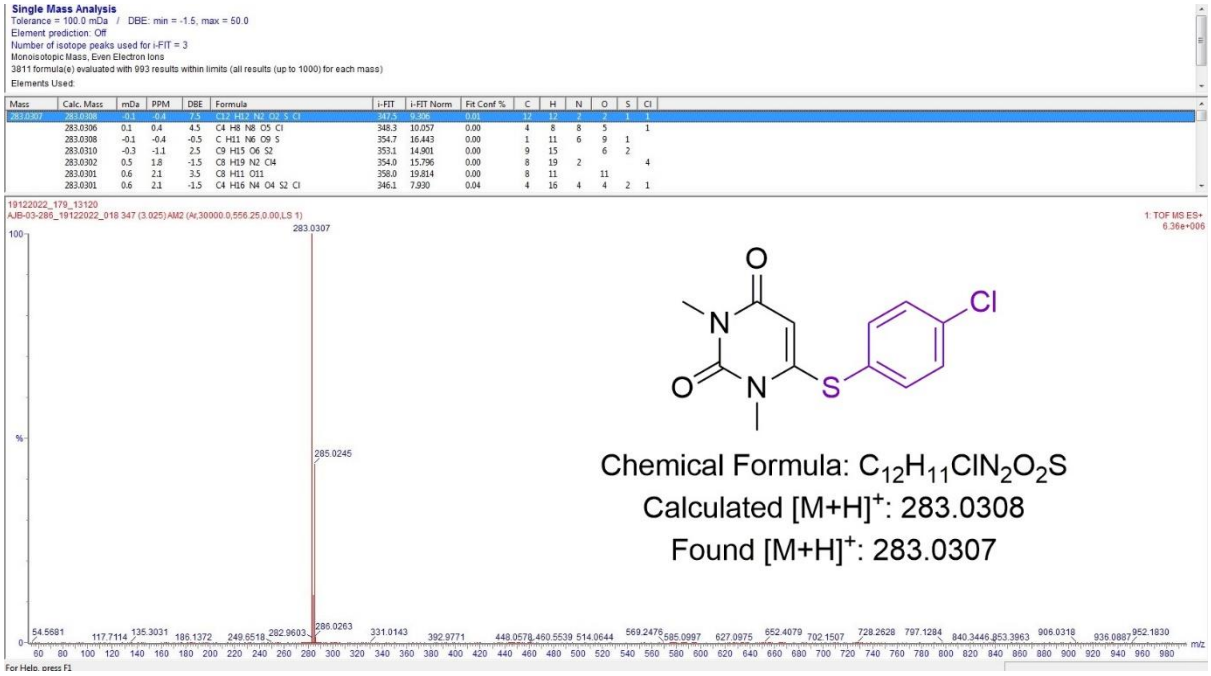


Fig. S64: HRMS spectra of **3x**

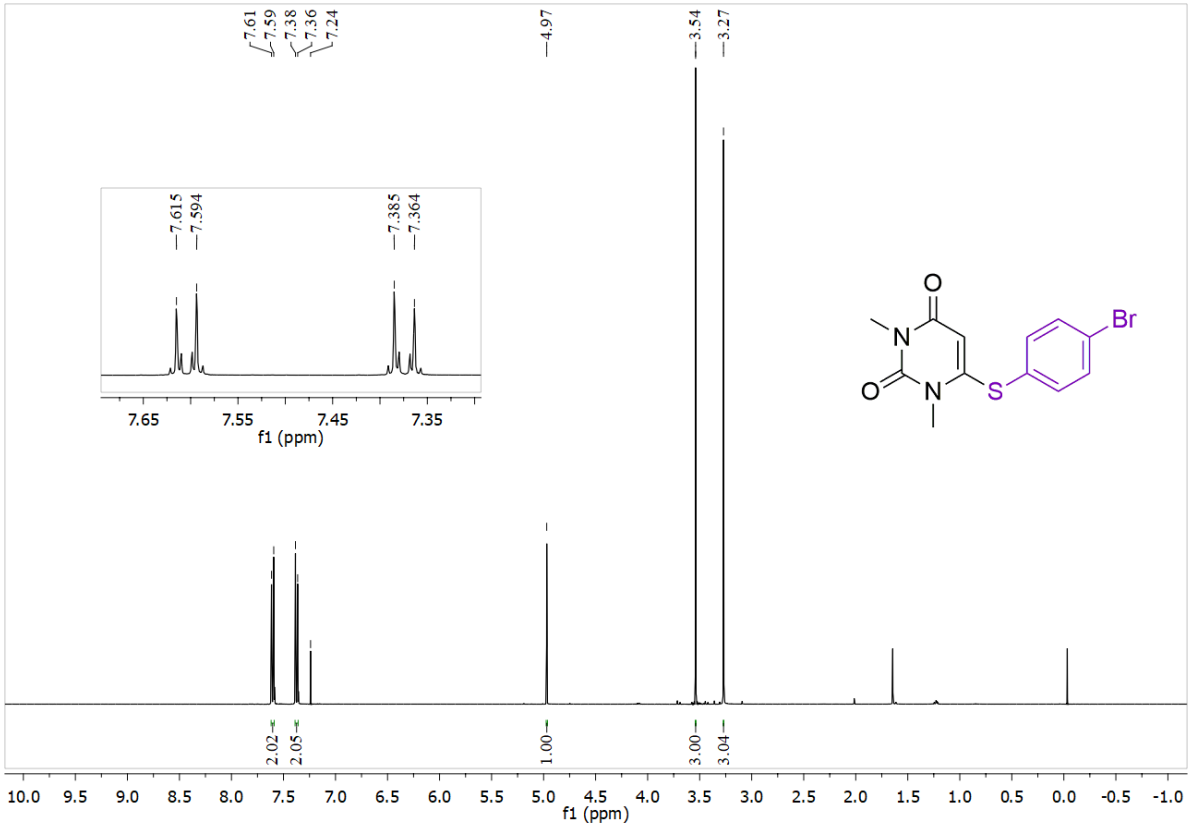


Fig. S65: ^{1}H NMR (400 MHz) spectra **3y**

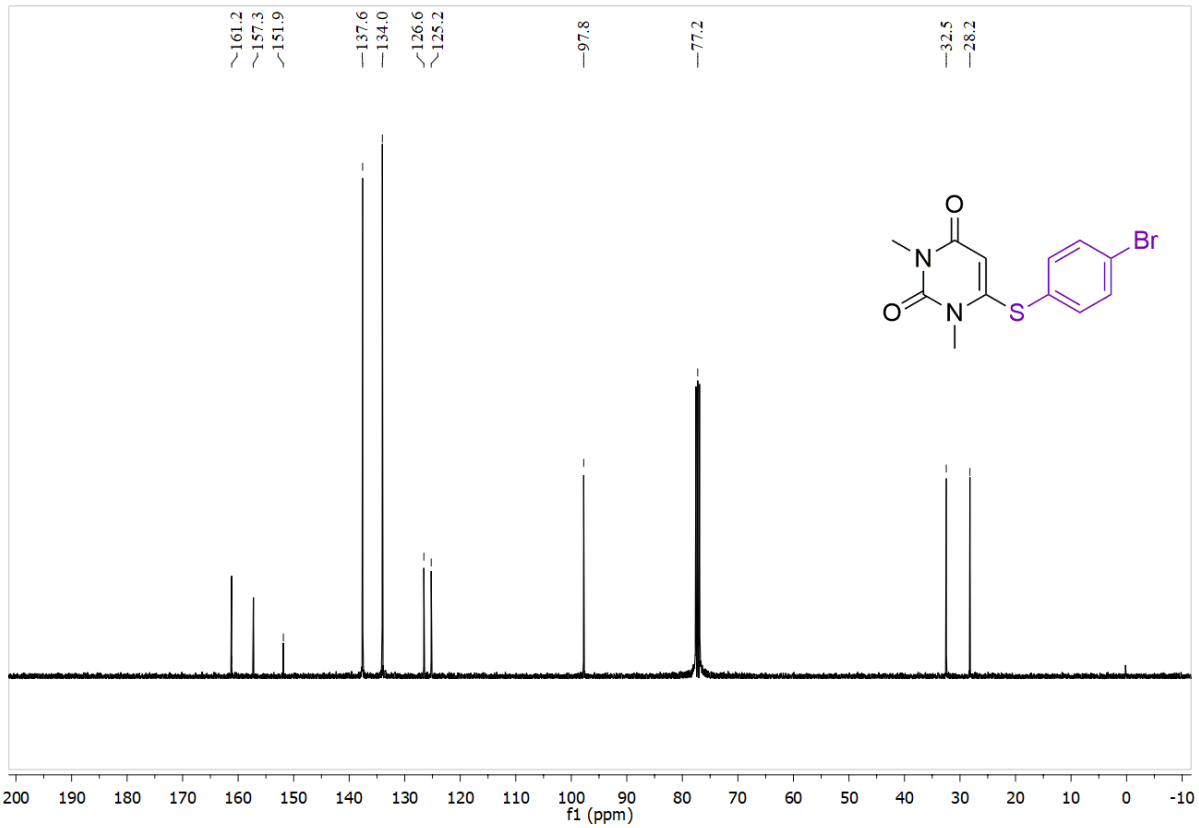


Fig. S66: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3y**

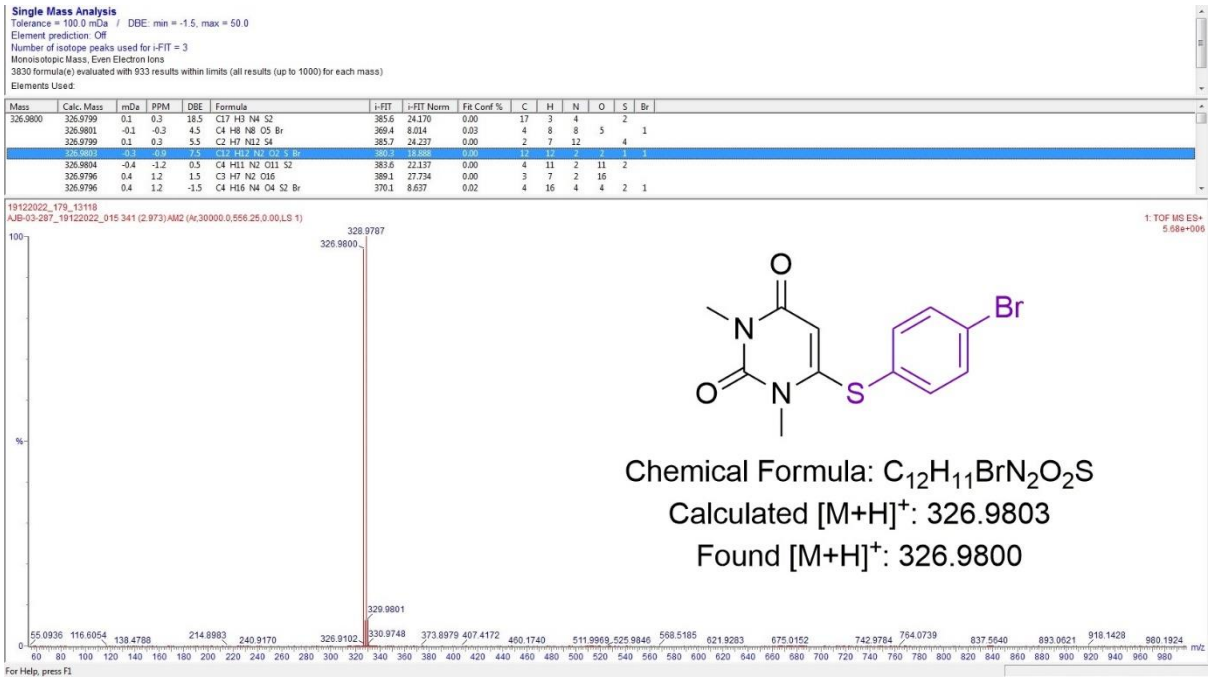


Fig. S67: HRMS spectra of **3y**

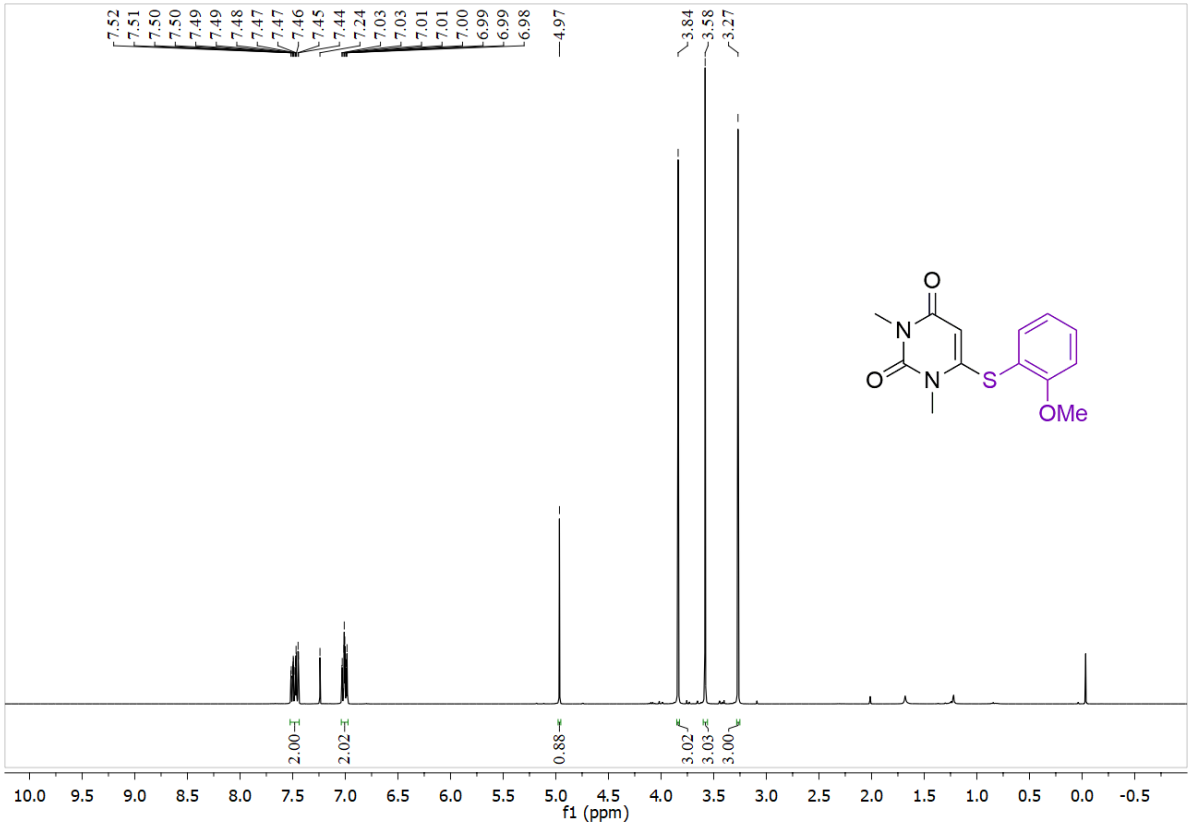


Fig. S68: ^{1}H NMR (400 MHz) spectra **3z**

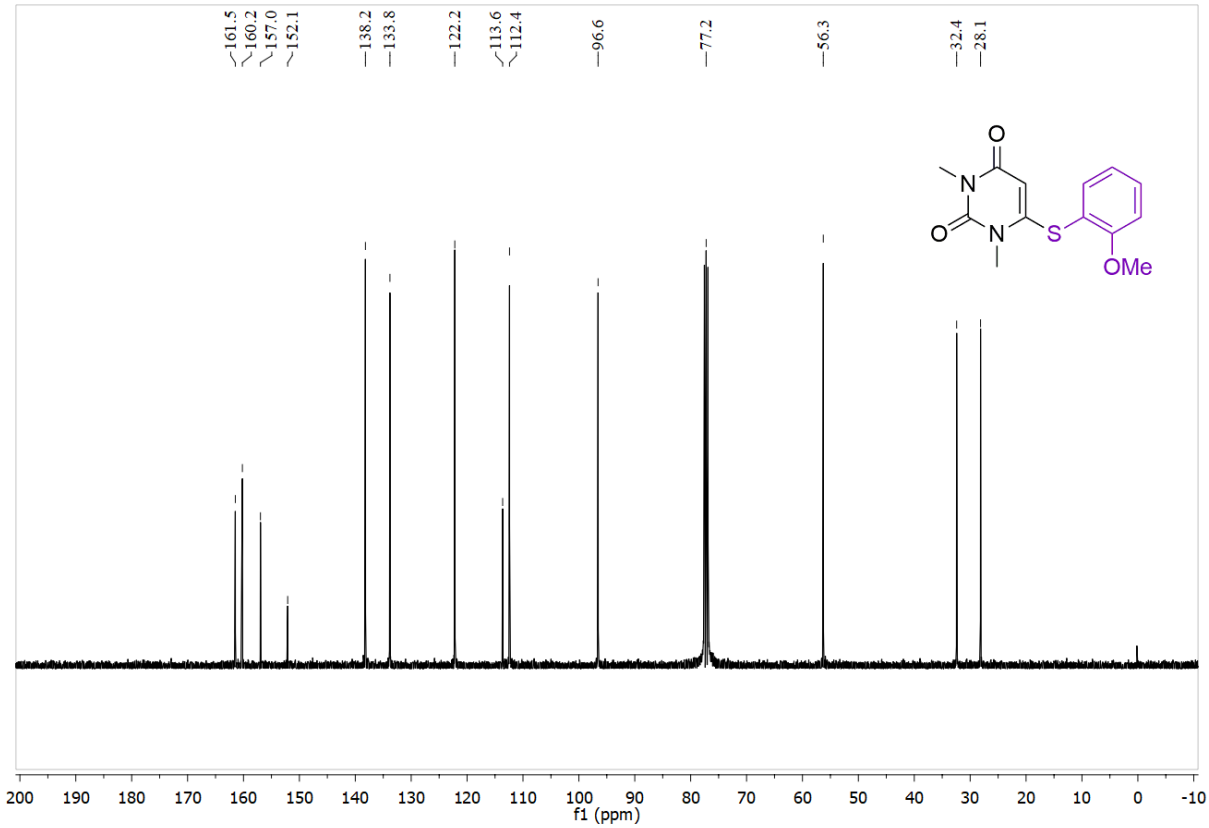


Fig. S69: ^{13}C{^{1}H} NMR (100 MHz) spectra of **3z**

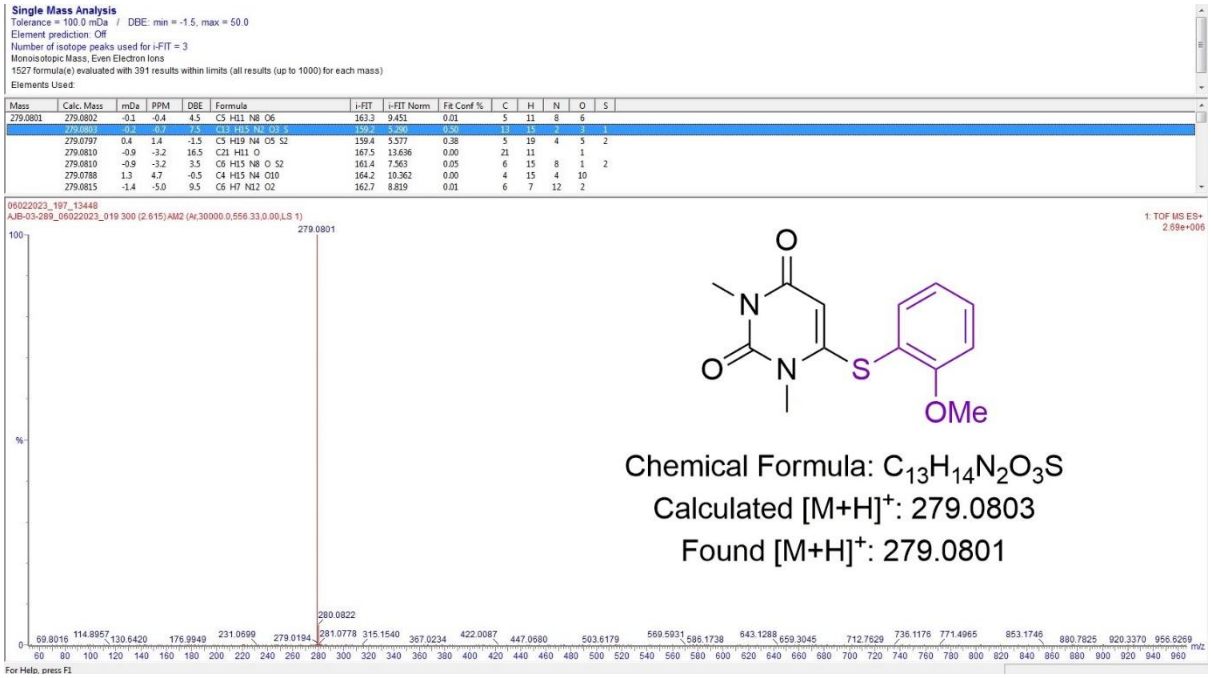


Fig. S70: HRMS spectra of **3z**

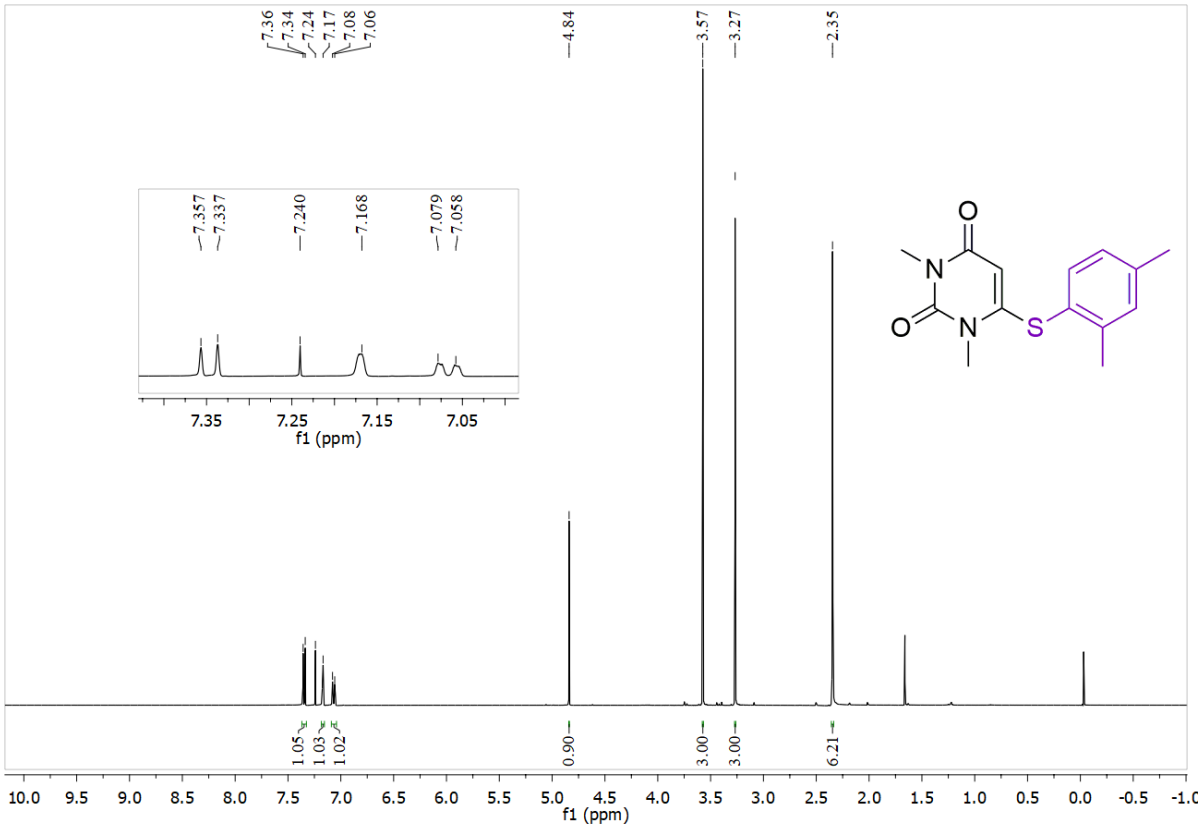


Fig. S71: ^{1}H NMR (400 MHz) spectra **3aa**

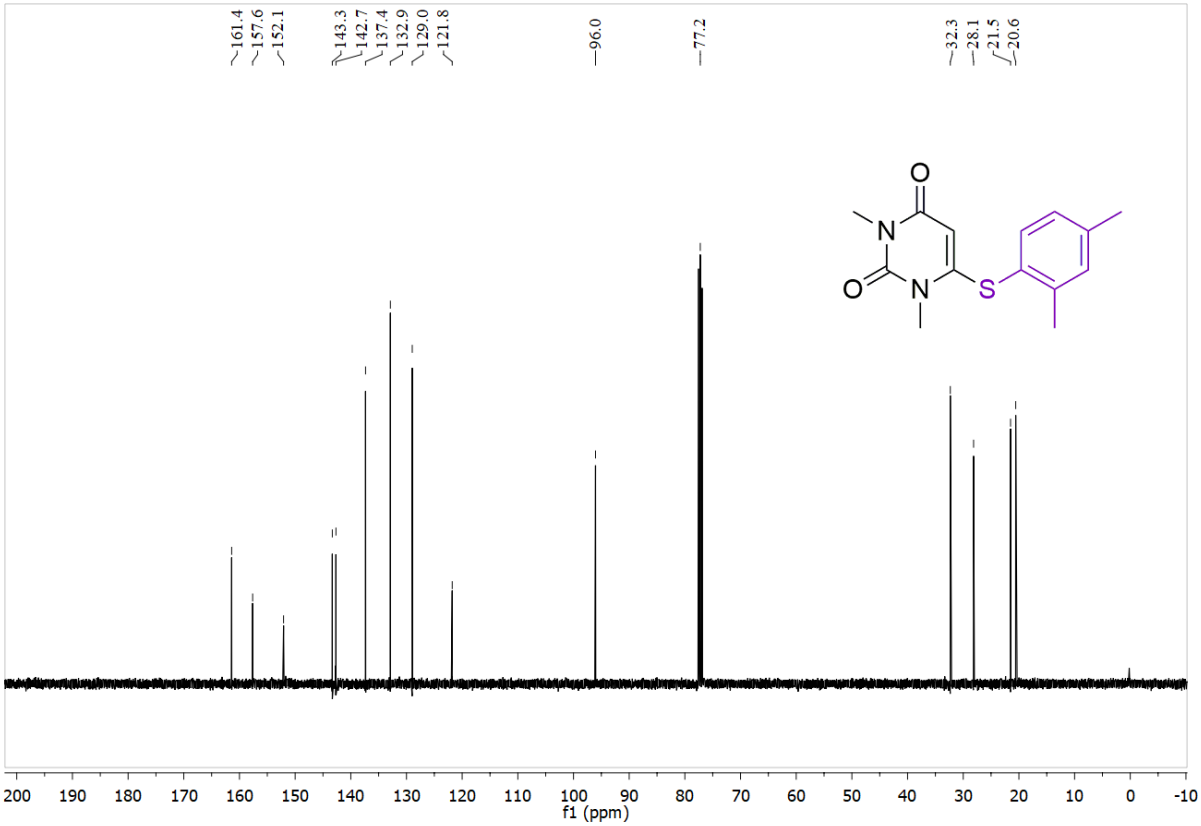


Fig. S72: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3aa**

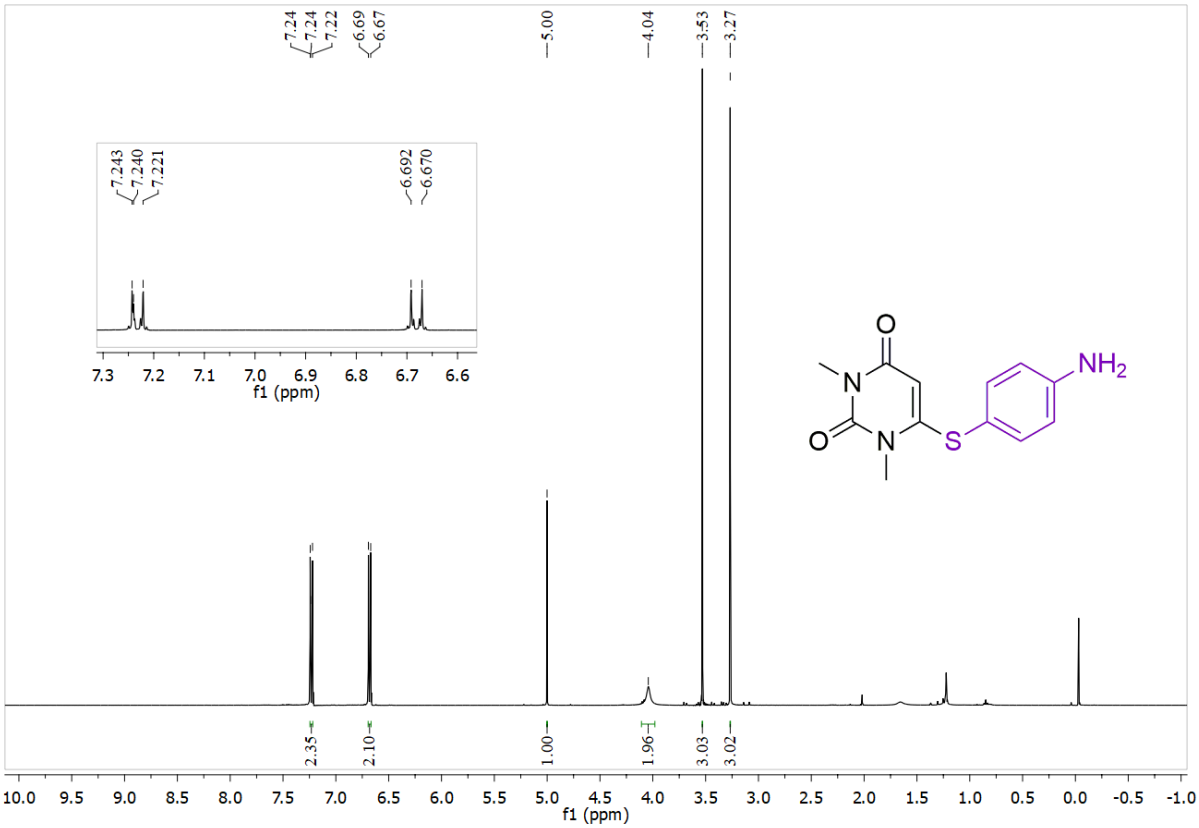


Fig. S73: ^{1}H NMR (400 MHz) spectra **3ab**

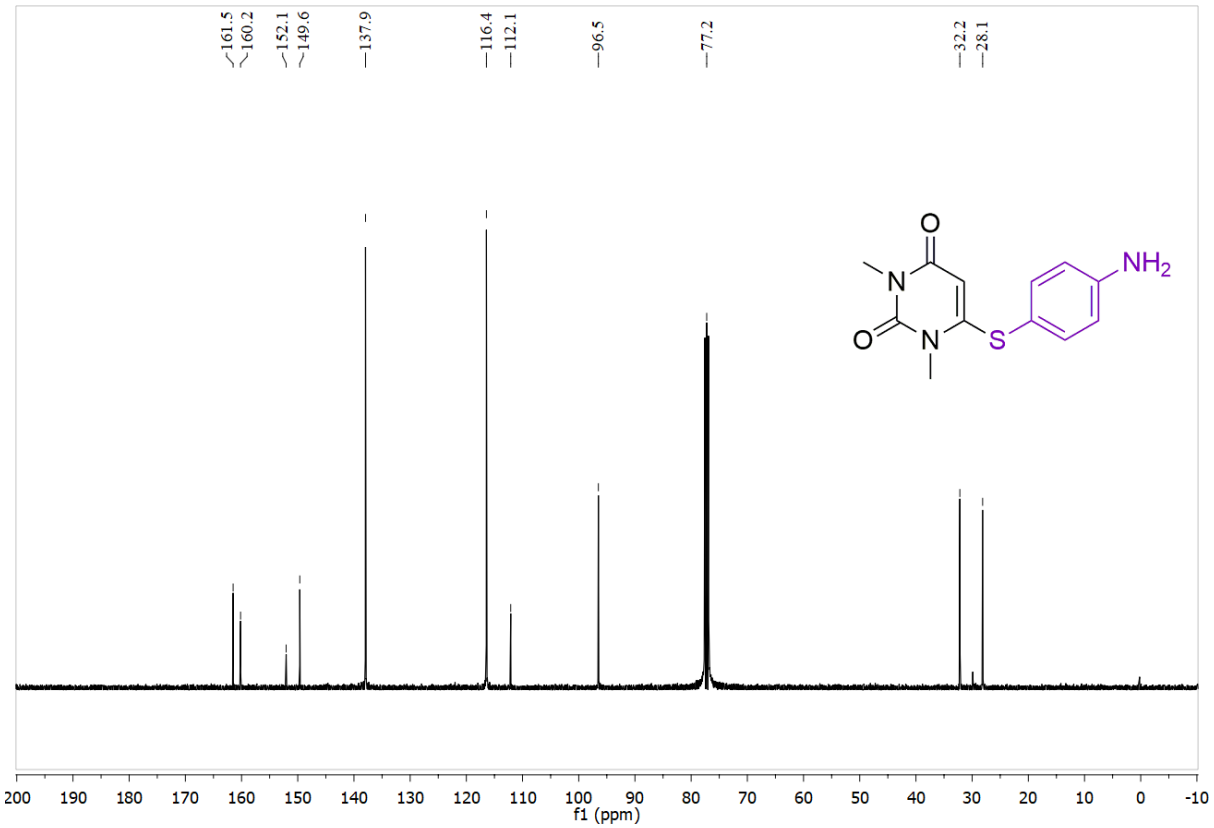


Fig. S74: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectra of **3ab**

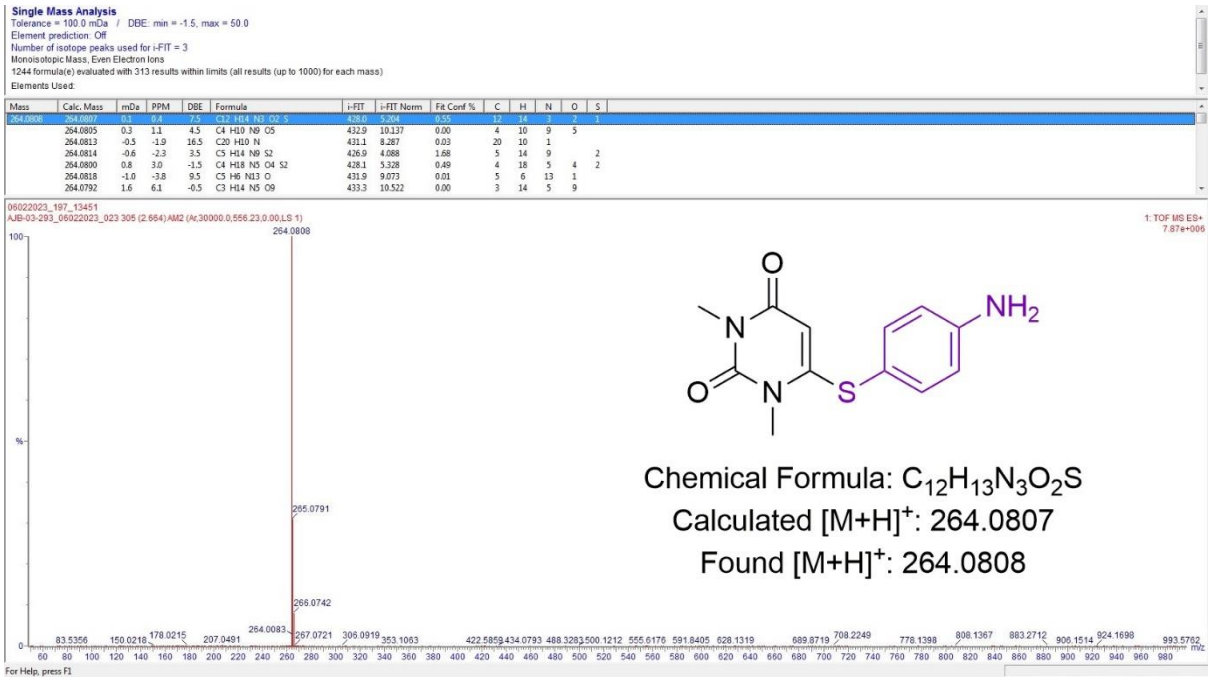


Fig. S75: HRMS spectra of **3ab**

3. X-ray crystallographic information

Table S1: Crystal data and structure refinement for compound 1

Identification code	**Compound 1**
Empirical formula	$C_{29}H_{44}Cu_{1.5}IN_8O_5$
Formula weight	806.93
Temperature/K	293(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	10.2357(4)
b/Å	12.1215(5)
c/Å	14.9718(6)
α/°	76.079(2)
β/°	80.501(2)
γ/°	79.118(2)
Volume/Å^3	1756.60(12)
Z	2
ρ_{calc}g/cm^3	1.526
μ/mm^{-1}	1.842
F(000)	821.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.824 to 56.982
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19
Reflections collected	63410
Independent reflections	8771 [R_{int} = 0.0608, R_{sigma} = 0.0433]
Data/restraints/parameters	8771/0/380
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1110
Final R indexes [all data]	R_1 = 0.0732, wR_2 = 0.1243
Largest diff. peak/hole / eÅ^{-3}	1.02/-1.01

$^{\dagger}wR2 = +^{½}$; $R1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, $^{*}GooF = S = \{\Sigma[w(F_o^2-F_c^2)^2] / (n-p)\}^{½}$

Table S2. Bond Lengths for compound 1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	N1	2.0289(15)	C2	C1	1.3900
Cu1	N1^1	2.0290(15)	N5	C15	1.3900
Cu1	O3^1	1.951(2)	N5	C19	1.3900
Cu1	O3	1.951(2)	C15	C16	1.3900
Cu2	N7	2.0320(14)	C16	C17	1.3900
Cu2	N5	2.0453(15)	C17	C18	1.3900
Cu2	O1^2	2.273(2)	C17	N6	1.408(3)
Cu2	O1	1.985(2)	C18	C19	1.3900
Cu2	N3	2.015(3)	O1	C29^2	1.299(3)
N7	C22	1.3900	O2	C29	1.265(4)

Table S2. Bond Lengths for compound 1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N7	C26	1.3900	O3	C29	1.284(4)
C22	C23	1.3900	N3	C8	1.344(4)
C23	C24	1.3900	N3	C12	1.353(4)
C24	C25	1.3900	C9	C8	1.374(5)
C24	N8	1.401(3)	C9	C10	1.413(5)
C25	C26	1.3900	C10	C11	1.406(5)
N8	C28	1.450(5)	C10	N4	1.355(5)
N8	C27	1.454(5)	C12	C11	1.374(5)
N1	C5	1.3900	N4	C14	1.455(5)
N1	C1	1.3900	N4	C13	1.460(6)
C5	C4	1.3900	N6	C21	1.451(5)
C4	C3	1.3900	N6	C20	1.444(5)
C3	C2	1.3900	N2	C7	1.460(7)
C3	N2	1.401(4)	N2	C6	1.448(7)

[1]3-X,-Y,-Z; [2]2-X,-Y,-Z

Table S3. Bond Angles for compound 1

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Cu1	N1[1]	180.0	C2	C1	N1	120.0
O3[1]	Cu1	N1	90.78(9)	C15	N5	Cu2	120.77(10)
O3	Cu1	N1[1]	90.78(9)	C15	N5	C19	120.0
O3[1]	Cu1	N1[1]	89.22(9)	C19	N5	Cu2	119.03(10)
O3	Cu1	N1	89.22(9)	C16	C15	N5	120.0
O3[1]	Cu1	O3	180.0	C15	C16	C17	120.0
N7	Cu2	N5	172.19(8)	C16	C17	N6	119.64(19)
N7	Cu2	O1[2]	91.59(8)	C18	C17	C16	120.0
N5	Cu2	O1[2]	96.22(8)	C18	C17	N6	120.35(19)
O1	Cu2	N7	89.71(8)	C19	C18	C17	120.0
O1	Cu2	N5	91.98(8)	C18	C19	N5	120.0
O1	Cu2	O1[2]	74.52(8)	Cu2	O1	Cu2[2]	105.48(8)
O1	Cu2	N3	174.36(9)	C29[2]	O1	Cu2	110.79(18)
N3	Cu2	N7	90.93(10)	C29[2]	O1	Cu2[2]	143.30(19)
N3	Cu2	N5	86.65(10)	C29	O3	Cu1	102.32(17)
N3	Cu2	O1[2]	111.06(9)	C8	N3	Cu2	124.2(2)
C22	N7	Cu2	118.55(10)	C8	N3	C12	116.1(3)
C22	N7	C26	120.0	C12	N3	Cu2	119.6(2)
C26	N7	Cu2	121.21(10)	C8	C9	C10	120.3(3)
N7	C22	C23	120.0	N3	C8	C9	123.9(3)
C24	C23	C22	120.0	C11	C10	C9	115.5(3)
C23	C24	N8	119.99(18)	N4	C10	C9	121.7(3)
C25	C24	C23	120.0	N4	C10	C11	122.7(3)

Table S3. Bond Angles for compound 1

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C25	C24	N8	119.94(18)	N3	C12	C11	124.0(3)
C24	C25	C26	120.0	C12	C11	C10	120.1(3)
C25	C26	N7	120.0	C10	N4	C14	121.6(3)
C24	N8	C28	120.4(3)	C10	N4	C13	121.3(3)
C24	N8	C27	121.1(3)	C14	N4	C13	117.1(3)
C28	N8	C27	118.0(3)	C17	N6	C21	120.8(3)
C5	N1	Cu1	119.46(11)	C17	N6	C20	120.8(3)
C5	N1	C1	120.0	C20	N6	C21	118.1(3)
C1	N1	Cu1	120.43(11)	C3	N2	C7	120.4(4)
N1	C5	C4	120.0	C3	N2	C6	121.9(4)
C3	C4	C5	120.0	C6	N2	C7	117.7(4)
C4	C3	N2	119.6(3)	O2	C29	O1[2]	119.9(3)
C2	C3	C4	120.0	O2	C29	O3	122.0(2)
C2	C3	N2	120.4(3)	O3	C29	O1[2]	118.1(3)
C3	C2	C1	120.0				

[1]3-X,-Y,-Z; [2]2-X,-Y,-Z

Table S4. Torsion Angles for compound 1

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	N1	C5	C4	176.20(15)	C3	C2	C1	N1	0.0
Cu1	N1	C1	C2	−176.16(15)	C2	C3	N2	C7	-175.8(4)
Cu1	O3	C29	O1[1]	177.1(2)	C2	C3	N2	C6	2.3(6)
Cu1	O3	C29	O2	-3.6(3)	C1	N1	C5	C4	0.0
Cu2	N7	C22	C23	174.47(14)	N5	C15	C16	C17	0.0
Cu2	N7	C26	C25	−174.32(14)	C15	N5	C19	C18	0.0
Cu2	N5	C15	C16	−174.82(14)	C15	C16	C17	C18	0.0
Cu2	N5	C19	C18	174.91(14)	C15	C16	C17	N6	-179.4(2)
Cu2	N3	C8	C9	-174.3(3)	C16	C17	C18	C19	0.0
Cu2	N3	C12	C11	175.2(3)	C16	C17	N6	C21	177.7(3)
N7	C22	C23	C24	0.0	C16	C17	N6	C20	3.8(5)
C22	N7	C26	C25	0.0	C17	C18	C19	N5	0.0
C22	C23	C24	C25	0.0	C18	C17	N6	C21	-1.7(4)
C22	C23	C24	N8	-176.9(2)	C18	C17	N6	C20	-175.6(3)
C23	C24	C25	C26	0.0	C19	N5	C15	C16	0.0
C23	C24	N8	C28	-3.9(4)	N3	C12	C11	C10	-0.5(6)
C23	C24	N8	C27	-175.9(3)	C9	C10	C11	C12	0.4(5)
C24	C25	C26	N7	0.0	C9	C10	N4	C14	-178.9(4)
C25	C24	N8	C28	179.2(3)	C9	C10	N4	C13	1.1(6)
C25	C24	N8	C27	7.2(4)	C8	N3	C12	C11	0.0(5)
C26	N7	C22	C23	0.0	C8	C9	C10	C11	0.2(5)

Table S4. Torsion Angles for compound 1

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N8	C24	C25	C26	176.9(2)	C8	C9	C10	N4	180.0(3)
N1	C5	C4	C3	0.0	C10	C9	C8	N3	-0.8(6)
C5	N1	C1	C2	0.0	C12	N3	C8	C9	0.7(5)
C5	C4	C3	C2	0.0	C11	C10	N4	C14	0.9(6)
C5	C4	C3	N2	179.5(3)	C11	C10	N4	C13	-179.2(4)
C4	C3	C2	C1	0.0	N4	C10	C11	C12	-179.3(4)
C4	C3	N2	C7	4.7(5)	N6	C17	C18	C19	179.4(2)
C4	C3	N2	C6	-177.2(4)	N2	C3	C2	C1	-179.5(3)

[1]2-X,-Y,-Z

Table S5. Bond valence calculation of compound 1

>>>> Bond valence calculation for central atom : Cu2

>>>

Atoms within bonding distance - bondrad(1) + bondrad(2) + 0.50 Angstroms :

	ato1	ato2	dist	x1	y1	z1	x2	y2	z2	NS
1	Cu2	- N3	2.0290	1.5000	0.0000	0.0000	1.5088	-0.1594	0.0837	1
2	Cu2	- N3	2.0290	1.5000	0.0000	0.0000	1.4912	0.1594	-0.0837	2
3	Cu2	- O4	1.9509	1.5000	0.0000	0.0000	1.3096	0.0316	0.0449	1
4	Cu2	- O4	1.9509	1.5000	0.0000	0.0000	1.6904	-0.0316	-0.0449	2

Assuming a valence of 1 for Cu2, the atomic BVS contributions are :

atom		distance	rho	B	Bval	sum
N3	-	2.0290	1.520	0.370	0.253	0.253
N3	-	2.0290	1.520	0.370	0.253	0.505
O4	-	1.9509	1.610	0.370	0.398	0.903
O4	-	1.9509	1.610	0.370	0.398	1.301

Bond valence sum = 1.301 : discrepancy = 0.301

Assuming a valence of 2 for Cu2, the atomic BVS contributions are :

atom distance rho B Bval sum

N3 - 2.0290 1.751 0.370 0.472 0.472

N3 - 2.0290 1.751 0.370 0.472 0.943

O4 - 1.9509 1.679 0.360 0.470 1.413

O4 - 1.9509 1.679 0.360 0.470 1.883

Bond valence sum = 1.883 : discrepancy = 0.117

Assuming a valence of 3 for Cu2, the atomic BVS contributions are :

atom distance rho B Bval sum

N3 - 2.0290 1.768 0.370 0.494 0.494

N3 - 2.0290 1.768 0.370 0.494 0.988

O4 - 1.9509 1.735 0.370 0.558 1.546

O4 - 1.9509 1.735 0.370 0.558 2.104

Bond valence sum = 2.104 : discrepancy = 0.896

>>

>>>> Bond valence calculation for central atom : Cu1

>>

Atoms within bonding distance - bondrad(1) + bondrad(2) + 0.50 Angstroms :

	ato1	ato2	dist	x1	y1	z1	x2	y2	z2	NS
1	Cu1	- N1	2.0319	0.9382	0.0461	0.0993	0.9255	0.2128	0.0292	1
2	Cu1	- N5	2.0454	0.9382	0.0461	0.0993	0.9270	-0.1147	0.1804	1
3	Cu1	- O1	1.9848	0.9382	0.0461	0.0993	0.8738	0.0062	-0.0052	1
4	Cu1	- O1	2.2730	0.9382	0.0461	0.0993	1.1262	-0.0062	0.0052	2
5	Cu1	- N0AA	2.0147	0.9382	0.0461	0.0993	0.9847	0.0876	0.2114	1

Assuming a valence of 1 for Cu1, the atomic BVS contributions are :

atom distance rho B Bval sum

N1 - 2.0319 1.520 0.370 0.251 0.251

N5 - 2.0454 1.520 0.370 0.242 0.492

O1 - 1.9848 1.610 0.370 0.363 0.856

O1 - 2.2730 1.610 0.370 0.167 1.022

N0AA - 2.0147 1.520 0.370 0.263 1.285

Bond valence sum = 1.285 : discrepancy = 0.285

Assuming a valence of 2 for Cu1, the atomic BVS contributions are :

atom		distance	rho	B	Bval	sum
N1	-	2.0319	1.751	0.370	0.468	0.468
N5	-	2.0454	1.751	0.370	0.451	0.919
O1	-	1.9848	1.679	0.360	0.428	1.347
O1	-	2.2730	1.679	0.360	0.192	1.539
N0AA	-	2.0147	1.751	0.370	0.490	2.029

Bond valence sum = 2.029 : discrepancy = 0.029

Assuming a valence of 3 for Cu1, the atomic BVS contributions are :

atom		distance	rho	B	Bval	sum
N1	-	2.0319	1.768	0.370	0.490	0.490
N5	-	2.0454	1.768	0.370	0.473	0.963
O1	-	1.9848	1.735	0.370	0.509	1.472
O1	-	2.2730	1.735	0.370	0.234	1.705
N0AA	-	2.0147	1.768	0.370	0.513	2.219

Bond valence sum = 2.219 : discrepancy = 0.781

>>>> The BVS calculations suggest the following central atom valencies :

Cu2 +2 (0.117) Cu1 +2 (0.029)

4. Retrieved data from SwissADME

Table S6: Physicochemical data of synthesized aryloxypyrimidines

Molecule	Code	Canonical SMILES	Formula	MW
Molecule 1	3a	O=c1cc(Oc2ccccc2)n(c(=O)n1C)C	$C_{12}H_{12}N_2O_3$	232.24
Molecule 2	3b	Brc1ccc(cc1)Oc1cc(=O)n(c(=O)n1C)C	$C_{12}H_{11}BrN_2O_3$	311.13
Molecule 3	3c	O=c1cc(Oc2ccc3c(c2)cccc3)n(c(=O)n1C)C	$C_{16}H_{14}N_2O_3$	282.29
Molecule 4	3d	Cc1ccc(cc1)Oc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{14}N_2O_3$	246.26
Molecule 5	3e	O=Cc1ccc(cc1)Oc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{12}N_2O_4$	260.25
Molecule 6	3f	O=c1cc(Oc2ccc(cc2)[N+](=O)[O-])n(c(=O)n1C)C	$C_{12}H_{11}N_3O_5$	277.23
Molecule 7	3g	COc1ccccc1Oc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{14}N_2O_4$	262.26
Molecule 8	3h	O=Cc1ccc(c(c1)OC)Oc1cc(=O)n(c(=O)n1C)C	$C_{14}H_{14}N_2O_5$	290.27
Molecule 9	3i	COc1ccc(cc1)Oc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{14}N_2O_4$	262.26
Molecule 10	3j	Cc1ccccc1Oc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{14}N_2O_3$	246.26
Molecule 11	3k	c1ccc(cc1)Oc1ncccn1	$C_{10}H_8N_2O$	172.18
Molecule 12	3l	Brc1ccc(cc1)Oc1ncccn1	$C_{10}H_7BrN_2O$	251.08
Molecule 13	3m	O=Cc1ccc(cc1)Oc1ncccn1	$C_{11}H_8N_2O_2$	200.19
Molecule 14	3n	c1cnc(nc1)Oc1ccc2c(c1)cccc2	$C_{14}H_{10}N_2O$	222.24
Molecule 15	3o	Clc1ncnc(c1)Oc1ccccc1	$C_{10}H_7ClN_2O$	206.63
Molecule 16	3p	c1ccc(cc1)Oc1ncnc(c1)Oc1ccccc1	$C_{16}H_{12}N_2O_2$	264.28
Molecule 17	3q	Brc1ccc(cc1)Oc1ncnc(c1)Cl	$C_{10}H_6BrClN_2O$	285.52
Molecule 18	3r	Clc1ncnc(c1)Oc1ccc2c(c1)cccc2	$C_{14}H_9ClN_2O$	256.69
Molecule 19	3s	O=Cc1ccc(cc1)Oc1ncnc(c1)Cl	$C_{11}H_7ClN_2O_2$	234.64
Molecule 20	3t	CCOC(=O)c1cnc(nc1Oc1ccccc1)SC	$C_{14}H_{14}N_2O_3S$	290.34
Molecule 21	3u	CCOC(=O)c1cnc(nc1Oc1ccc2c(c1)cccc2)SC	$C_{18}H_{16}N_2O_3S$	340.4
Molecule 22	3v	CCOC(=O)c1cnc(nc1Oc1ccc(cc1)Br)SC	$C_{14}H_{13}BrN_2O_3S$	369.23

Table S7: Physicochemical data of synthesized aryloxypyrimidines

Code	HA	AHA	F-Csp3	RB	HBA	HBD	MR	TPSA
3a	17	12	0.17	2	3	0	64	53.23
3b	18	12	0.17	2	3	0	71.7	53.23
3c	21	16	0.12	2	3	0	81.51	53.23
3d	18	12	0.23	2	3	0	68.97	53.23
3e	19	12	0.15	3	4	0	69.39	70.3
3f	20	12	0.17	3	5	0	72.82	99.05
3g	19	12	0.23	3	4	0	70.49	62.46
3h	21	12	0.21	4	5	0	75.88	79.53
3i	19	12	0.23	3	4	0	70.49	62.46
3j	18	12	0.23	2	3	0	68.97	53.23
3k	13	12	0	2	3	0	48.55	35.01
3l	14	12	0	2	3	0	56.25	35.01
3m	15	12	0	3	4	0	53.94	52.08
3n	17	16	0	2	3	0	66.05	35.01

3o	14	12	0	2	3	0	53.56	35.01
3p	20	18	0	4	4	0	75.06	44.24
3q	15	12	0	2	3	0	61.26	35.01
3r	18	16	0	2	3	0	71.06	35.01
3s	16	12	0	3	4	0	58.95	52.08
3t	20	12	0.21	6	5	0	76.36	86.61
3u	24	16	0.17	6	5	0	93.86	86.61
3v	21	12	0.21	6	5	0	84.06	86.61

Table S8: Lipophilicity data of aryloxypyrimidines

Code	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos -IT Log P	Consensus Log P
3a	2.47	1.13	0.88	1.33	1.1	1.38
3b	2.86	1.82	1.64	2.01	1.77	2.02
3c	2.77	2.38	2.03	2.19	2.13	2.3
3d	2.73	1.5	1.18	1.61	1.59	1.72
3e	2.17	0.59	0.69	1.12	1.29	1.17
3f	2.03	0.96	0.78	0.41	-1.06	0.63
3g	2.65	1.1	0.88	1.47	1.13	1.45
3h	2.44	0.56	0.7	0.86	1.33	1.18
3i	2.72	1.1	0.88	1.47	1.13	1.46
3j	2.59	1.5	1.18	1.61	1.59	1.69
3k	2.02	2.06	2.27	1.38	2.03	1.95
3l	2.41	2.76	3.03	2.08	2.66	2.59
3m	1.81	1.53	2.08	0.74	2.14	1.66
3n	2.43	3.64	3.42	2.29	3	2.96
3o	2.3	3.03	2.92	1.94	2.63	2.56
3p	3.06	3.93	4.06	2.85	3.04	3.39
3q	2.73	3.72	3.68	2.63	3.28	3.21
3r	2.74	4.28	4.08	2.82	3.61	3.5
3s	2.05	2.49	2.73	1.29	2.76	2.26
3t	3.04	3.13	3.17	2.08	2.81	2.84
3u	3.43	4.38	4.32	2.87	3.86	3.77
3v	3.46	3.82	3.93	2.73	3.49	3.49

Table S9: Water solubility data of aryloxypyrimidines

Code	ESOL				Ali				Silicos-IT			
	Log S	Solubility (mg/ml)	Solubility (mol/l)	Class	Log S	Solubility (mg/ml)	Solubility (mol/l)	Class	LogSw	Solubility (mg/ml)	Solubility (mol/l)	Class
3a	-2.38	9.63E-01	4.15E-03	S	-1.84	3.34E+00	1.44E-02	VS	-2.86	3.24E-01	1.39E-03	S
3b	-3.28	1.64E-01	5.29E-04	S	-2.56	8.62E-01	2.77E-03	S	-3.68	6.44E-02	2.07E-04	S

3c	-3.52	8.50E-02	3.01E-04	S	-3.14	2.05E-01	7.27E-04	S	-4.52	8.53E-03	3.02E-05	MS
3d	-2.67	5.23E-01	2.12E-03	S	-2.23	1.46E+00	5.95E-03	S	-3.24	1.41E-01	5.73E-04	S
3e	-2.09	2.09E+00	8.04E-03	S	-1.64	5.97E+00	2.29E-02	VS	-2.8	4.12E-01	1.58E-03	S
3f	-2.41	1.08E+00	3.89E-03	S	-2.63	6.54E-01	2.36E-03	S	-2.23	1.64E+00	5.93E-03	S
3g	-2.43	9.78E-01	3.73E-03	S	-2	2.60E+00	9.90E-03	S	-2.98	2.75E-01	1.05E-03	S
3h	-2.15	2.05E+00	7.06E-03	S	-1.8	4.57E+00	1.58E-02	VS	-2.92	3.51E-01	1.21E-03	S
3i	-2.43	9.78E-01	3.73E-03	S	-2	2.60E+00	9.90E-03	S	-2.98	2.75E-01	1.05E-03	S
3j	-2.67	5.23E-01	2.12E-03	S	-2.23	1.46E+00	5.95E-03	S	-3.24	1.41E-01	5.73E-04	S
3k	-2.76	3.02E-01	1.75E-03	S	-2.42	6.49E-01	3.77E-03	S	-3.9	2.14E-02	1.24E-04	S
3l	-3.64	5.78E-02	2.30E-04	S	-3.15	1.78E-01	7.07E-04	S	-4.77	4.29E-03	1.71E-05	MS
3m	-2.44	7.28E-01	3.64E-03	S	-2.23	1.17E+00	5.85E-03	S	-3.86	2.74E-02	1.37E-04	S
3n	-4.08	1.87E-02	8.40E-05	MS	-4.06	1.92E-02	8.64E-05	MS	-5.59	5.67E-04	2.55E-06	MS
3o	-3.53	6.07E-02	2.94E-04	S	-3.43	7.67E-02	3.71E-04	S	-4.53	6.07E-03	2.94E-05	MS
3p	-4.36	1.16E-02	4.40E-05	MS	-4.56	7.31E-03	2.76E-05	MS	-6.17	1.79E-04	6.78E-07	PS
3q	-4.41	1.10E-02	3.86E-05	MS	-4.15	2.04E-02	7.13E-05	MS	-5.37	1.21E-03	4.24E-06	MS
3r	-4.65	5.70E-03	2.22E-05	MS	-4.73	4.80E-03	1.87E-05	MS	-6.21	1.60E-04	6.24E-07	PS
3s	-3.22	1.41E-01	6.02E-04	S	-3.23	1.39E-01	5.91E-04	S	-4.48	7.73E-03	3.30E-05	MS
3t	-3.66	6.35E-02	2.19E-04	S	-4.62	7.00E-03	2.41E-05	MS	-4.88	3.80E-03	1.31E-05	MS
3u	-4.81	5.31E-03	1.56E-05	MS	-5.92	4.14E-04	1.22E-06	MS	-6.53	1.00E-04	2.94E-07	PS
3v	-4.56	1.01E-02	2.74E-05	MS	-5.33	1.71E-03	4.63E-06	MS	-5.69	7.57E-04	2.05E-06	MS

Table S10: Pharmacokinetic properties of aryloxypyrimidines

Code	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)
3a	High	Yes	No	Yes	No	No	No	No	-6.91
3b	High	Yes	No	Yes	No	No	No	No	-6.91
3c	High	Yes	No	Yes	Yes	Yes	No	No	-6.33
3d	High	Yes	No	Yes	No	No	No	No	-6.74
3e	High	No	No	No	No	No	No	No	-7.47
3f	High	No	No	No	No	No	No	No	-7.31
3g	High	Yes	No	Yes	No	No	No	No	-7.12
3h	High	No	No	No	No	No	No	No	-7.67
3i	High	Yes	No	Yes	No	No	No	No	-7.12
3j	High	Yes	No	Yes	No	No	No	No	-6.74
3k	High	Yes	No	Yes	No	No	No	No	-5.89
3l	High	Yes	No	Yes	Yes	No	No	No	-5.87
3	High	Yes	No	Yes	No	No	No	No	-6.43
3n	High	Yes	No	Yes	Yes	No	Yes	No	-5.07
3o	High	Yes	No	Yes	Yes	No	No	No	-5.41
3p	High	Yes	No	Yes	Yes	Yes	Yes	No	-5.12
3q	High	Yes	No	Yes	Yes	Yes	No	No	-5.4
3r	High	Yes	No	Yes	Yes	No	Yes	No	-4.83
3s	High	Yes	No	Yes	Yes	No	No	No	-5.96

3t	High	No	No	Yes	Yes	Yes	No	No	-5.85
3u	High	No	No	Yes	Yes	Yes	No	Yes	-5.27
3v	High	No	No	Yes	Yes	Yes	No	No	-5.84

Table S11: Druglikeliness for synthesized aryloxypyrimidines

Code	Lipinski violations	Ghose violations	Veber violations	Egan violations	Muegge violations	Bioavail-ability Score	PAINS alerts	Brenk alerts	Leadlike-ness violations	Synthetic Accessib-ility
3a	0	0	0	0	0	0.55	0	0	1	2.45
3b	0	0	0	0	0	0.55	0	0	0	2.5
3c	0	0	0	0	0	0.55	0	0	0	2.66
3d	0	0	0	0	0	0.55	0	0	1	2.47
3e	0	0	0	0	0	0.55	0	1	0	2.41
3f	0	0	0	0	0	0.55	0	2	0	2.57
3g	0	0	0	0	0	0.55	0	0	0	2.56
3h	0	0	0	0	0	0.55	0	1	0	2.6
3i	0	0	0	0	0	0.55	0	0	0	2.59
3j	0	0	0	0	0	0.55	0	0	1	2.52
3k	0	0	0	0	1	0.55	0	0	1	1.74
3l	0	0	0	0	0	0.55	0	0	0	1.87
3m	0	0	0	0	0	0.55	0	1	1	1.63
3n	0	0	0	0	0	0.55	0	0	2	1.95
3o	0	0	0	0	0	0.55	0	0	1	2.06
3p	0	0	0	0	0	0.55	0	0	1	2.32
3q	0	0	0	0	0	0.55	0	0	1	2.14
3r	0	0	0	0	0	0.55	0	0	1	2.26
3s	0	0	0	0	0	0.55	0	1	1	1.94
3t	0	0	0	0	0	0.55	0	0	0	2.56
3u	0	0	0	0	0	0.55	0	0	1	2.77
3v	0	0	0	0	0	0.55	0	0	2	2.61

Table S12: Physicochemical properties of arylthiopyrimidines

Molecule	Code	Canonical SMILES	Formula	MW
Molecule 1	3w	O=c1cc(Sc2ccccc2)n(c(=O)n1C)C	$C_{12}H_{12}N_2O_2S$	248.3
Molecule 2	3x	Clc1ccc(cc1)Sc1cc(=O)n(c(=O)n1C)C	$C_{12}H_{11}ClN_2O_2S$	282.75
Molecule 3	3y	Brc1ccc(cc1)Sc1cc(=O)n(c(=O)n1C)C	$C_{12}H_{11}BrN_2O_2S$	327.2
Molecule 4	3z	COc1ccccc1Sc1cc(=O)n(c(=O)n1C)C	$C_{13}H_{14}N_2O_3S$	278.33
Molecule 5	3aa	Cc1ccc(c(c1)C)Sc1cc(=O)n(c(=O)n1C)C	$C_{14}H_{16}N_2O_2S$	276.35

Molecule 6	3ab	Nc1ccc(cc1)Sc1cc(=O)n(c(=O)n1C)C	$C_{12}H_{13}N_3O_2S$	263.32

Table S13: Physicochemical properties of arylthiopyrimidines

Code	HA	AHA	F-Csp3	RB	HBA	HBD	MR	TPSA
3w	17	12	0.17	2	2	0	68.05	69.3
3x	18	12	0.17	2	2	0	73.06	69.3
3y	18	12	0.17	2	2	0	75.75	69.3
3z	19	12	0.23	3	3	0	74.54	78.53
3aa	19	12	0.29	2	2	0	77.98	69.3
3ab	18	12	0.17	2	2	1	72.46	95.32

Table S14: Lipophilicity data of arylthiopyrimidines

Code	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos -IT Log P	Consensus Log P
3w	2.47	1.67	1.24	2.16	1.66	1.84
3x	2.67	2.3	1.89	2.7	2.3	2.37
3y	2.79	2.36	2	2.84	2.33	2.46
3z	2.71	1.64	1.24	1.87	1.69	1.83
3aa	2.94	2.4	1.85	2.7	2.65	2.51
3ab	2.1	0.99	0.83	1.6	0.94	1.29

Table S15: Water solubility data of arylthiopyrimidines

Code	ESOL				Ali				Silicos-IT			
	Log S	Solubility (mg/ml)	Solubility (mol/l)	Class	Log S	Solubility (mg/ml)	Solubility (mol/l)	Class	LogSw	Solubility (mg/ml)	Solubility (mol/l)	Class
3w	-2.82	3.74E-01	1.51E-03	S	-2.74	4.52E-01	1.82E-03	S	-3.22	1.48E-01	5.97E-04	S
3x	-3.4	1.12E-01	3.95E-04	S	-3.39	1.14E-01	4.04E-04	S	-3.83	4.17E-02	1.48E-04	S
3y	-3.72	6.28E-02	1.92E-04	S	-3.46	1.15E-01	3.50E-04	S	-4.05	2.94E-02	8.99E-05	MS
3z	-2.87	3.77E-01	1.35E-03	S	-2.9	3.49E-01	1.25E-03	S	-3.34	1.26E-01	4.53E-04	S
3aa	-3.4	1.10E-01	3.97E-04	S	-3.5	8.80E-02	3.18E-04	S	-3.99	2.81E-02	1.02E-04	S
3ab	-2.46	9.18E-01	3.49E-03	S	-2.58	6.92E-01	2.63E-03	S	-2.86	3.62E-01	1.37E-03	S

Table S16: Pharmacokinetic properties of arylthiopyrimidines

Code	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)
3w	High	No	No	Yes	No	No	No	No	-6.63
3x	High	Yes	No	Yes	Yes	Yes	No	No	-6.39
3y	High	Yes	No	Yes	Yes	Yes	No	No	-6.62
3z	High	No	No	Yes	No	No	No	No	-6.83
3aa	High	Yes	No	Yes	Yes	Yes	No	No	-6.28
3ab	High	No	No	Yes	No	No	No	No	-7.2

Table S17: Druglikeliness for synthesized arylthiopyrimidines

Code	Lipinski violations	Ghose violations	Veber violations	Egan violations	Muegge violations	Bioavail-ability Score	PAINS alerts	Brenk alerts	Leadlike ness violations	Synthetic Accessib ility
3w	0	0	0	0	0	0.55	0	0	1	2.31
3x	0	0	0	0	0	0.55	0	0	0	2.34
3y	0	0	0	0	0	0.55	0	0	0	2.37
3z	0	0	0	0	0	0.55	0	0	0	2.64
3aa	0	0	0	0	0	0.55	0	0	0	2.53
3ab	0	0	0	0	0	0.55	0	1	0	2.36

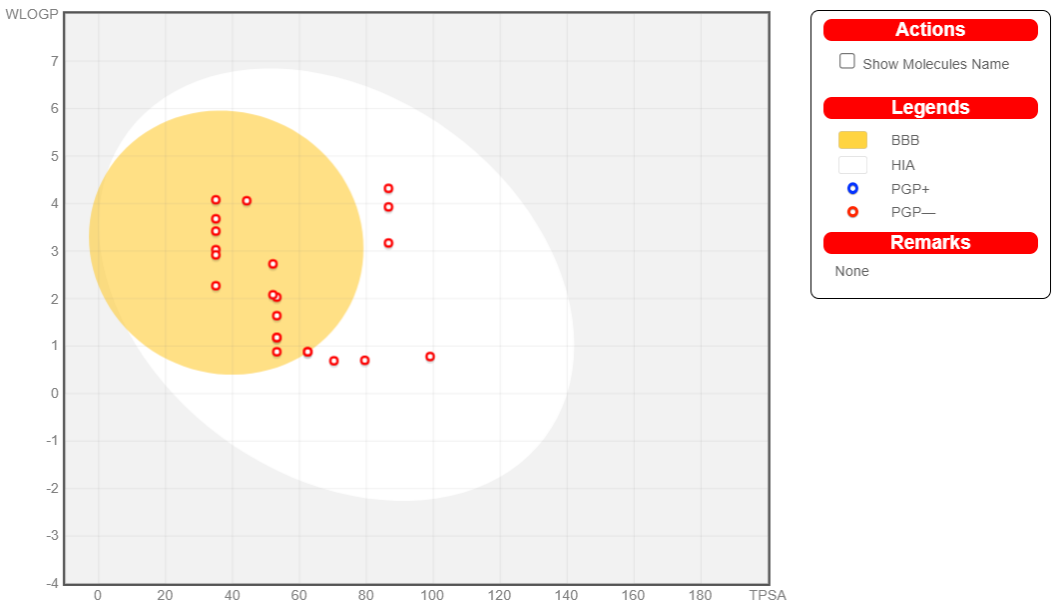


Fig. S76: BOILED-Egg model of aryloxypyrimidines

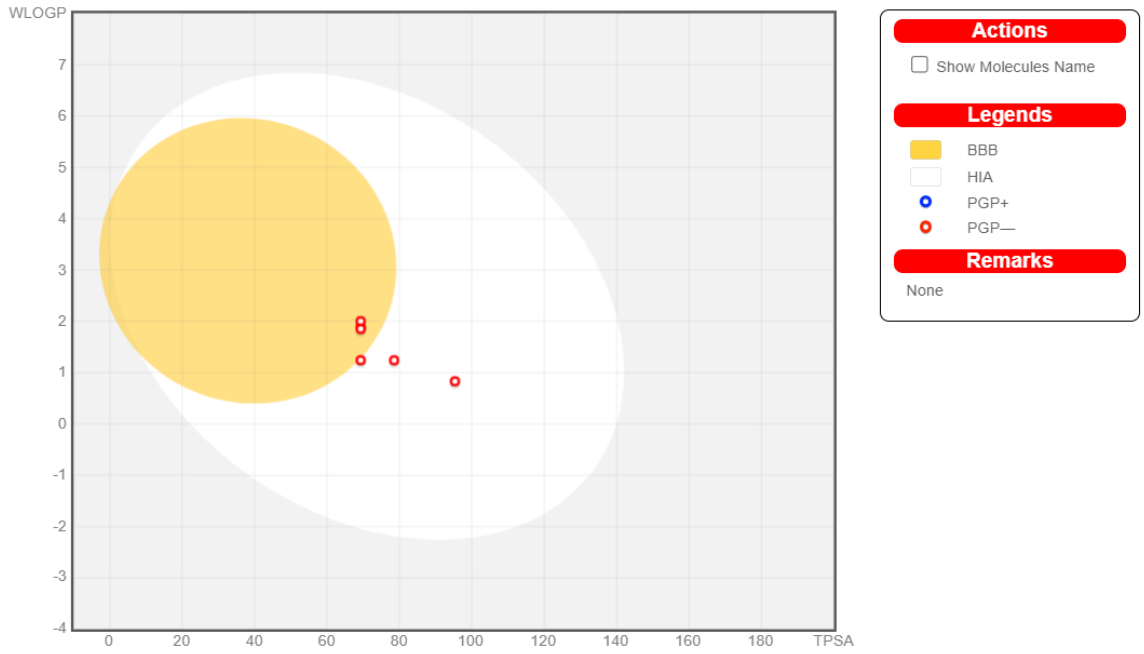


Fig. S77: BOILED-Egg model of arylthiopyrimidines