ELECTRONIC SUPPLEMENTARY INFORMATION

"Design and Synthesis of Novel Pyrrole Coupled Tryptamine Derivatives as Contenders against *Staphylococcus aureus*."

1.1 Spectroscopic data of the synthesized compounds

1.1.1.(Z)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-N-phenyl-1H-indole-1-carboxamide (5a)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.2.(Z)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(p-tolyl)-1H-indole-1-carboxamide (5b)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.82 (t, 2H, CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{24}H_{24}N_4O$:384.47 IR Vmax (cm-1) 2245 (O=CNH), 1645 (C=N), 1630(C=C), 1245(C-N) Elemental Analysis: Calculated: C, 74.97; H, 6.29; N, 14.57; O, 4.16 Experimental: C, 74.97; H, 6.29; N, 14.57; O, 4.16.

1.1.3. (Z)-N-(4-methoxyphenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5c)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{24}H_{24}N_4O_2$: 400.47 IR Vmax (cm^{-1}) 2255 (O=CNH), 1660 (C=N), 1625(C=C), 1230 (C-N) 2810 (O-CH_3) Elemental Analysis: Calculated: C, 71.98; H, 6.04; N, 13.99; O, 7.99; Experimental: C, 71.98; H, 6.04; N, 13.99; O, 7.99.

1.1.4. (Z)-N-(4-hydroxyphenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5d)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O_2$:386.45 IR Vmax (cm-1) 3250 (OH) 2260 (O=CNH), 1660 (C=N), 1620(C=C), 1270(C-N) Elemental Analysis: Calculated: C, 71.48; H, 5.74; N, 14.50; O, 8.28; Experimental: C, 71.48; H, 5.74; N, 14.50; O, 8.28.

1.1.5. (Z)-N-(4-chlorophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5e)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{19}H_{24}ClN_5O$: 373.17 IR Vmax (cm-1) 2270 (O=CNH), 1650 (C=N), 1630(C=C), 1260(C-N) 750 (C-Cl) Elemental Analysis: Calculated: C, 68.23; H, 5.23; Cl, 8.76; N, 13.84; O, 3.95; Experimental: C, 68.23; H, 5.23; Cl, 8.76; N, 13.84; O, 3.95.

1.1.6. (Z)-N-(3-chlorophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5f)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.7. (Z)-N-(2-chlorophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5g)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.8. (Z)-N-(2,5-dichlorophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5h)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.9. (Z)-N-(4-fluorophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5i)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.10. (Z)-N-(4-bromophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5j)

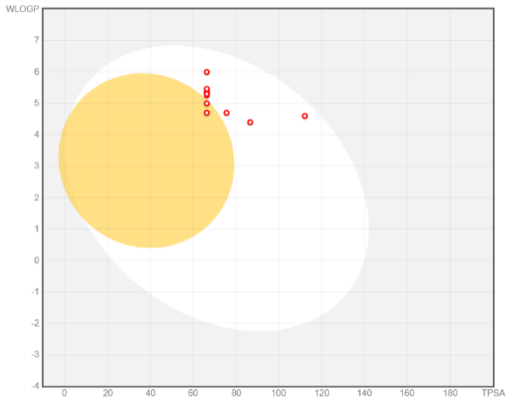
^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

1.1.11. (Z)-N-(4-iodophenyl)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-1H-indole-1-carboxamide (5k)

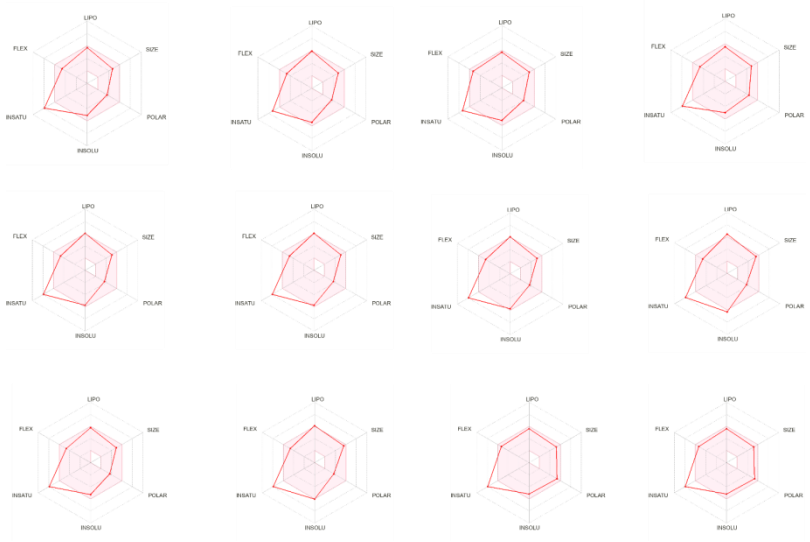
^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

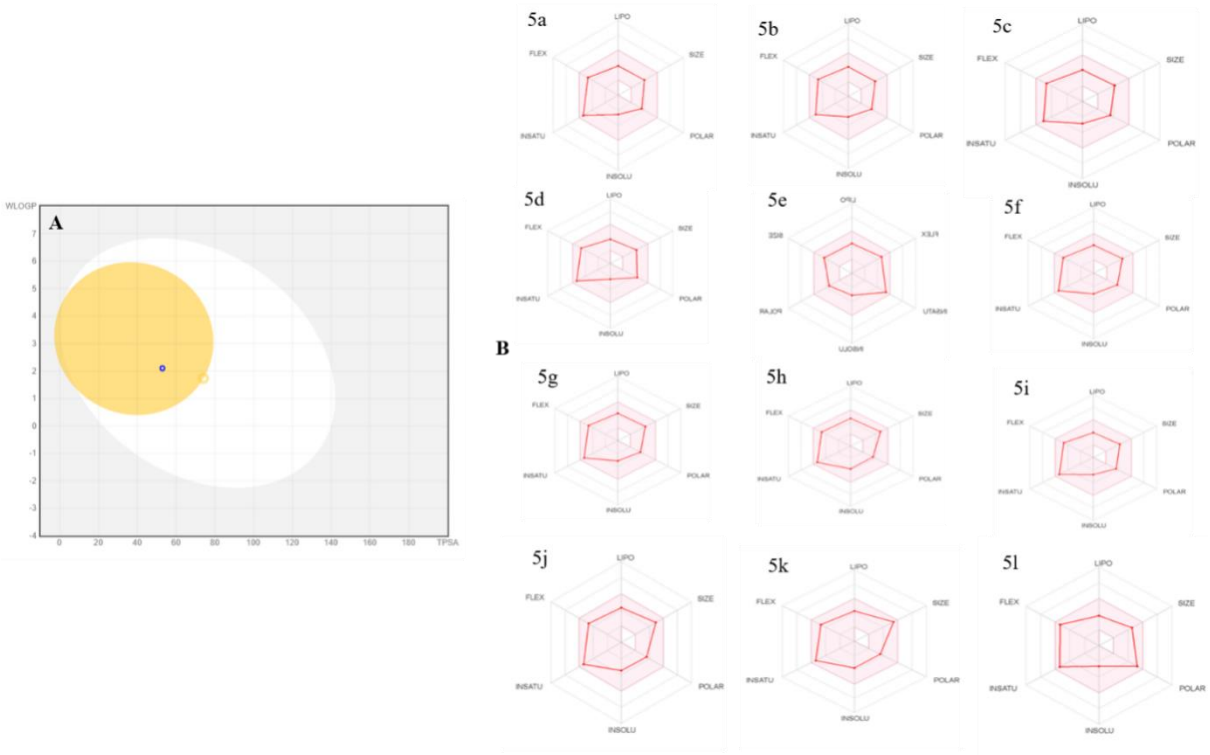
1.1.12. (Z)-2-(2-(((1-methyl-1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(4-nitrophenyl)-1H-indole-1-carboxamide (5l)

^{1}H NMR (400 MHz, $CDCl_3$), 9.39 (s, 1H, NH-C) 8.23 (s, 1H,CH=N) 7.92 (d,1H, Ind-H) 7.78 (t, 2H, Ar-H) 7.45 (d, 1H, Py-H) 7.42 (q, 2H, Ar-H) 7.37 (t, 1H, Ind-H) 7.23 (d,1H, Py-H) 7.13 (t,1H,Ar-H) 6.79 (t,1H,Ind-H) 6.41 (d,1H,Py-H) 6.23 (s,1H, Ind-H) 6.10 (t,1H,Py-H) 3.86 (s,3H,CH_3) 2.63 (t,.2H,CH_2) 1.81 (t,2H,CH_2) ^{13}C NMR: (400Hz, $CDCl_3$) 156 (C=N) 149 (C=O) 139 (C-N) 136(Py-CH) 133 (Py-CH) 132 (Py-CH) 128.5(Ar-CH) 128 (Ar-CH) 127 (Ar-CH) 126 (Ar-CH) 122 (Ind-CH) 121.5 (Ind-CH) 104 (Ind-CH) 54.5 (CH_2-CH_2) 38.5 (CH_3) 32(CH_2) LCMS m/z Calculated for $C_{23}H_{22}N_4O$: 370.45 IR Vmax (cm-1) 2250 (O=CNH), 1655 (C=N), 1560(C=C), 1340(C-N) Elemental Analysis: Calculated: C, 74.57; H, 5.99; N, 15.12; O, 4.32; Experimental: C, 74.56; H, 5.98; N, 15.12; O, 4.33;

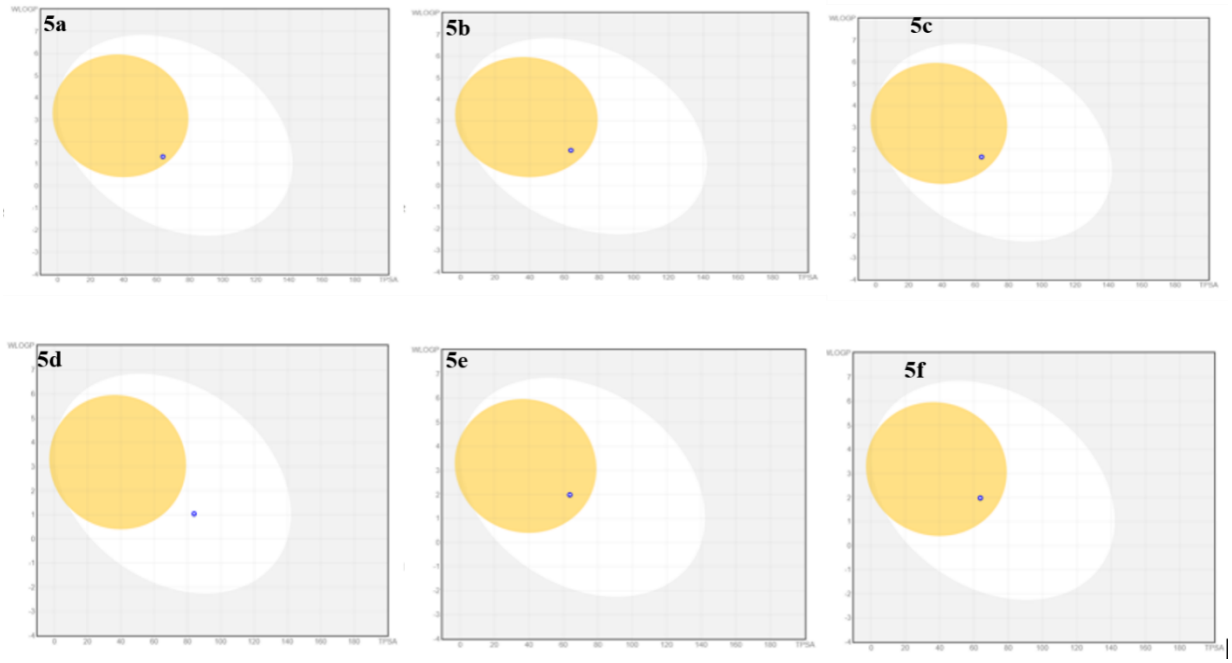


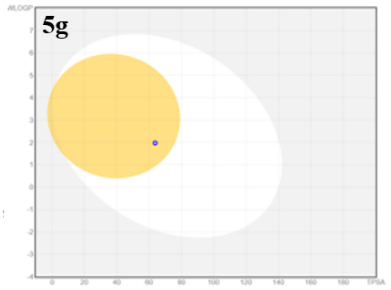
Supplementary Fig S1. Structure of synthesized compounds 5(a-l): (A) The BOILED-Egg representation of GI and BBB properties of the Compound 5j. (B) Bioavailability radar graph of 5(a-l) (pink area reflects the allowed values of drug likeness properties of the mole





Supplementary Fig S2: The BOILED-Egg representation of GI and BBB properties of the Compounds 5(a-l)

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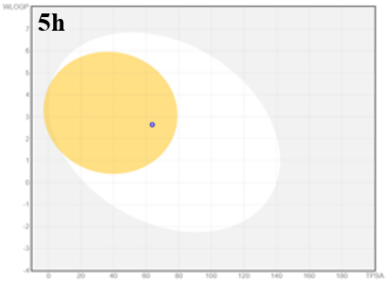
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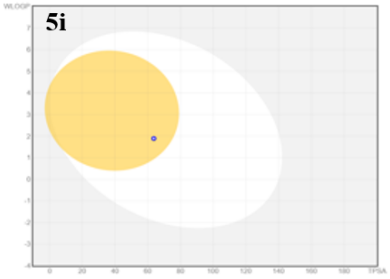
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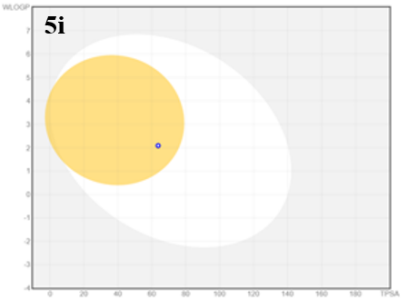
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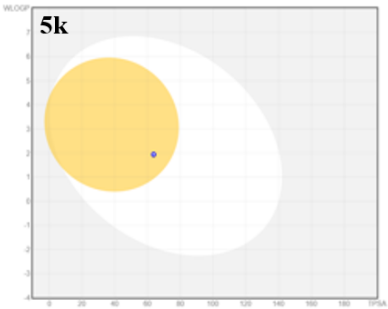
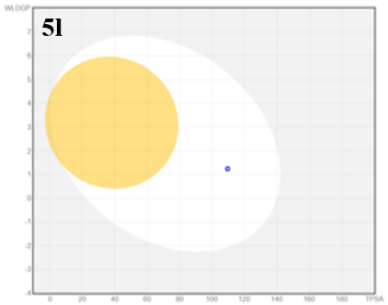
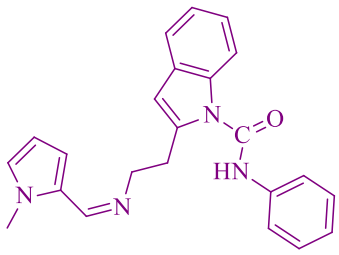
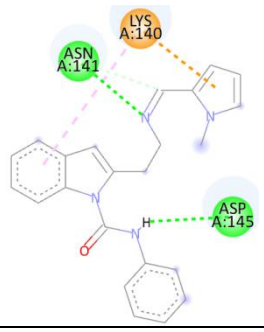
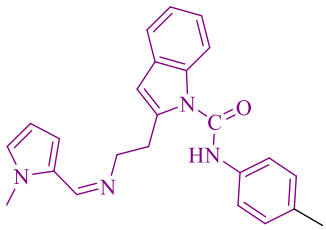
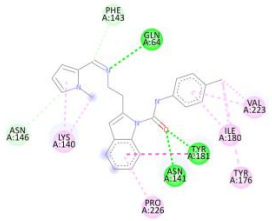
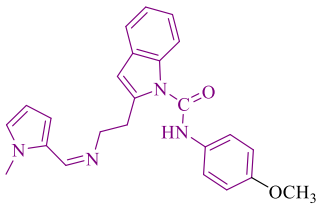
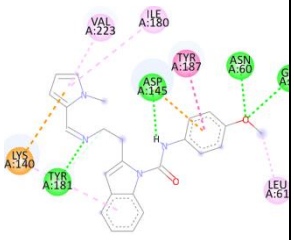
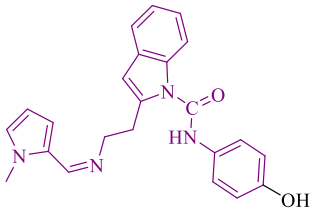
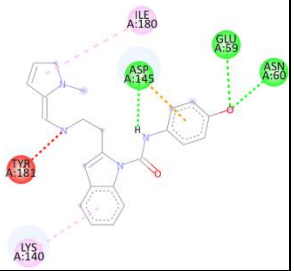
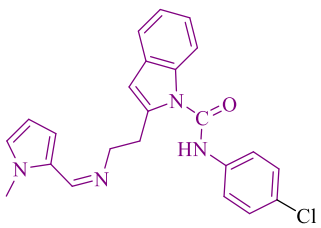
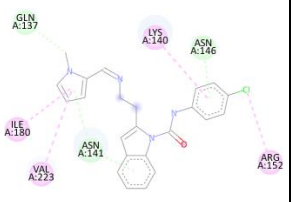
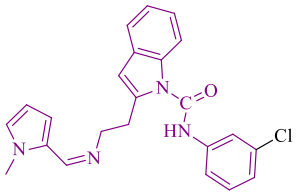
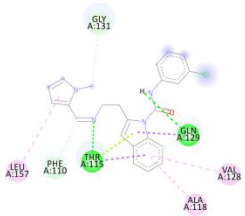
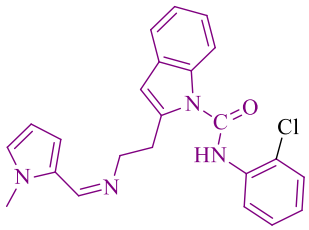
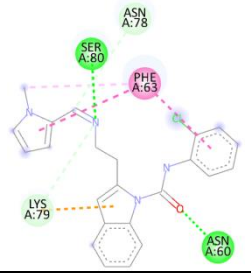
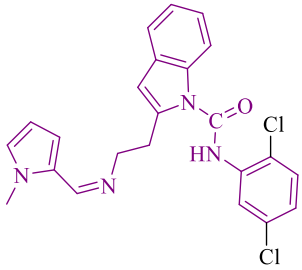
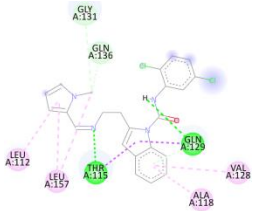
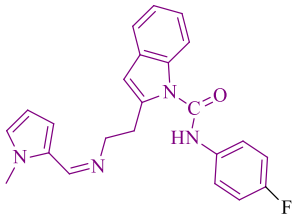
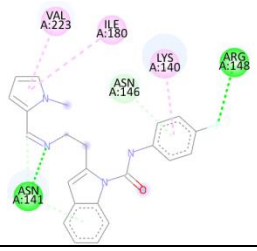
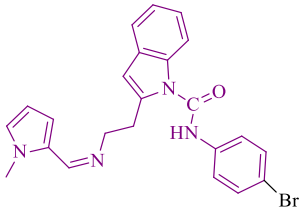
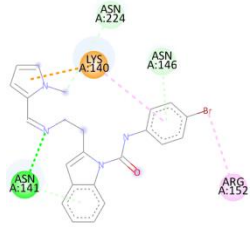
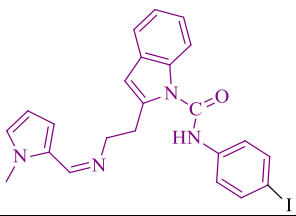
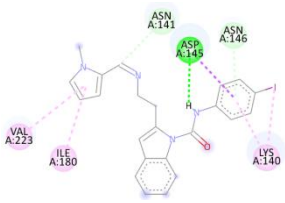
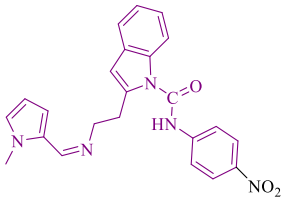
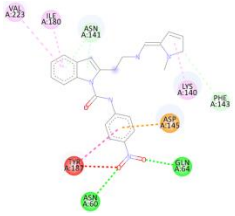
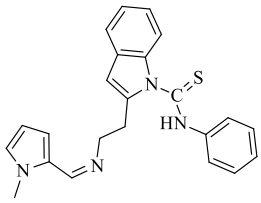
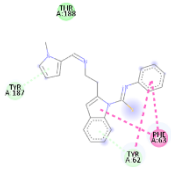
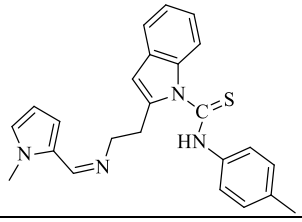
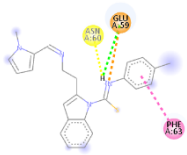
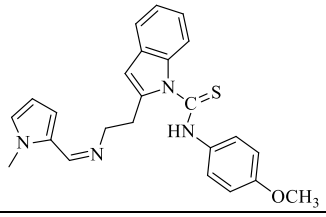
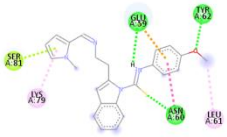
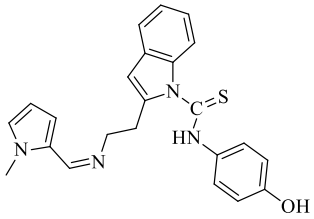
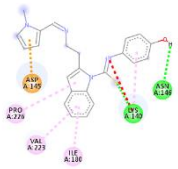
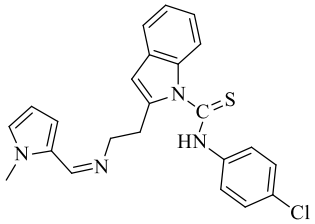
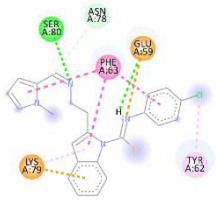

5k

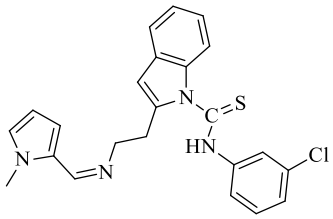
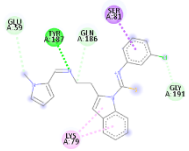
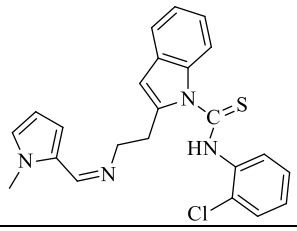
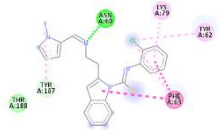
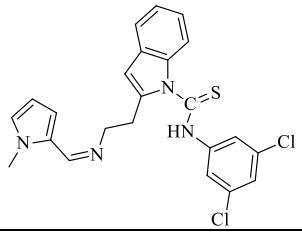
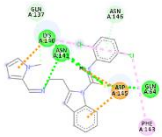
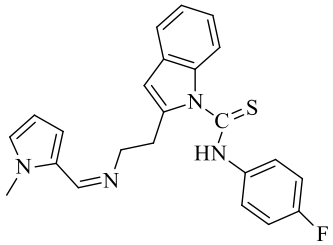
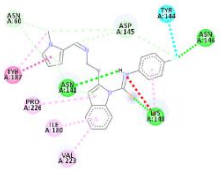
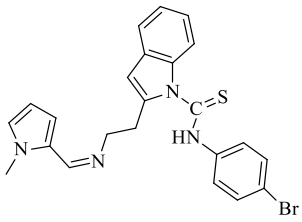
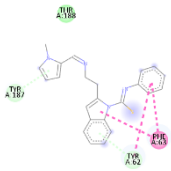
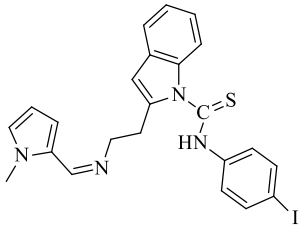
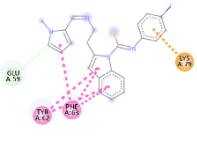

5l

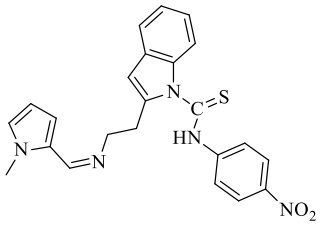
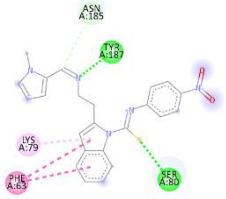
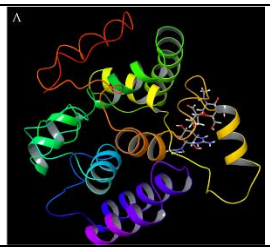
Supplementary table S1: Molecular docking proof for standard streptomycin against proteins 6FTB

Sl no	Molecule	Lowest Binding Energy	Hydrogen Bonding Interaction	Other Interaction	Unfavourable Bond	2D interaction
1		-8.00	ASN141, ASP145	LYS140	–	
2		-8.05	GLN64, ASN141, PHE143, ASN146, TYR181	LYS140, TYR176, ILE180, VAL223, PRO226	–	
3		-8.79	GLU59, ASN60, ASP145, TYR181	LEU61, LYS140, ILE180, TYR187, VAL223	–	
4		-8.46	GLU59, ASN60, ASP145	LYS140, ILE180	TYR181	
5		-8.21	GLN137, ASN141, ASN146	LYS140, ARG152, ILE180, VAL223	–	

6		-7.83	PHE110, THR115, GLN129, GLY131	ALA118, VAL128, LEU157	–	
7		-7.78	ASN60, ASN78, LYS79, SER80	PHE63	–	
8		-8.42	THR115, GLN129, GLY131, GLN136	LEU112, ALA118, VAL128, LEU157	–	
9		-7.94	ASN141, ASN146, ARG148	LYS140, ILE180, VAL223	–	
10		-7.99	ASN141, ASN146, ASN224	LYS140, ARG152	–	
11		-8.31	ASN141, ASP145, ASN146	LYS140, ILE180, VAL223	–	

12		-10.20	ASN60, GLN64, ASN141, PHE143	LYS140, ASP145, ILE180, VAL223	TYR187	
13		-6.20	PHE 63	TYR 62,	THR 188, TYR 187,	
14		-6.58	PHE 63,	ASN 60	GLU 59,	
15		-6.40	LYS 79, LEU 61	SER 81,	GLU 59, TYR 62, ASN 60,	
16		-7.03	PRO 226,	VAL 223 ILE 180	LYS 140, ASN 146, ASP 145,	
17		-6.96	LYS 79, TYR 62	GLU 59,	SER 80, ASN 78, PHE 63,	

18		-7.35	GLYY 191, LYS 79	SER 81,	TYR 187, GLU 59, GLN 186,	
19		-6.61	TYR 62 LYS 79	PHE 63,	ASN 60, TYR 187 THR 188	
20		-7.96	ASP 145, PHE 143,	GLN 137, ASN 146	LYS 140, ASN 141, GLN 64,	
21		-7.60	PRO 226, ILE 180,	VAL 223, ASP 145, TYR 144,	ASN 60, ASN 141, LYS 140, ASN 146, TYR 187,	
22		-6.20	TYR 62, PHE 63	TYR 187,	THR 188,	
23		-6.41	PHE 63, LYS 79	TYR 62,	GLU 59,	

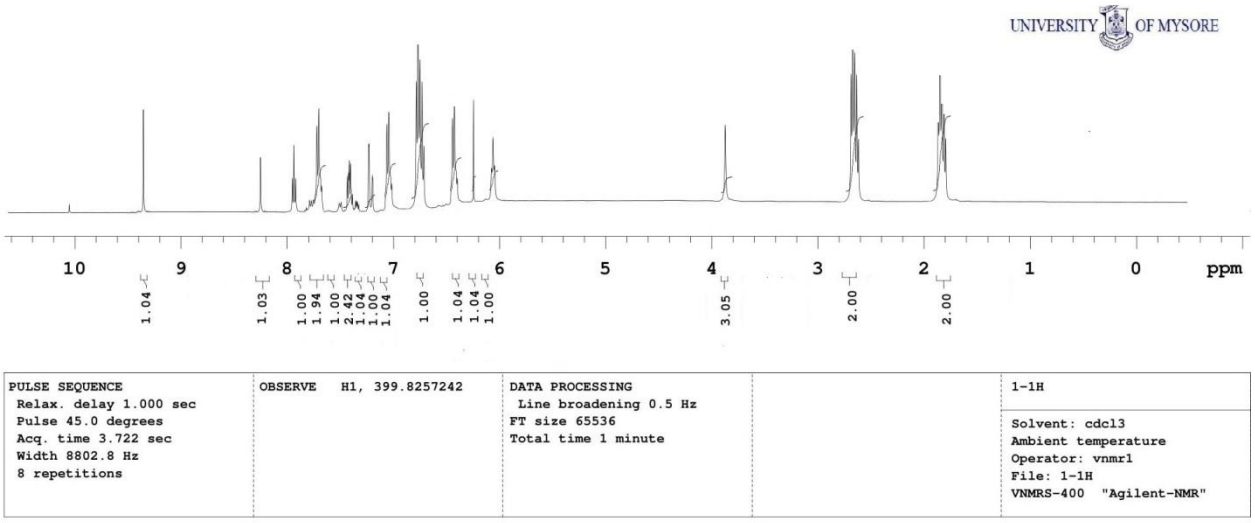
24		-7.90	TYR 187,	LYS 79, PHE 63, SER 80	ASN 185,	
25	Streptomycin	-10.65	TYR 62, PHE 63, PHE 63, LYS 79	LYS140, ILE180		

NMR and LC-MS data of new compounds

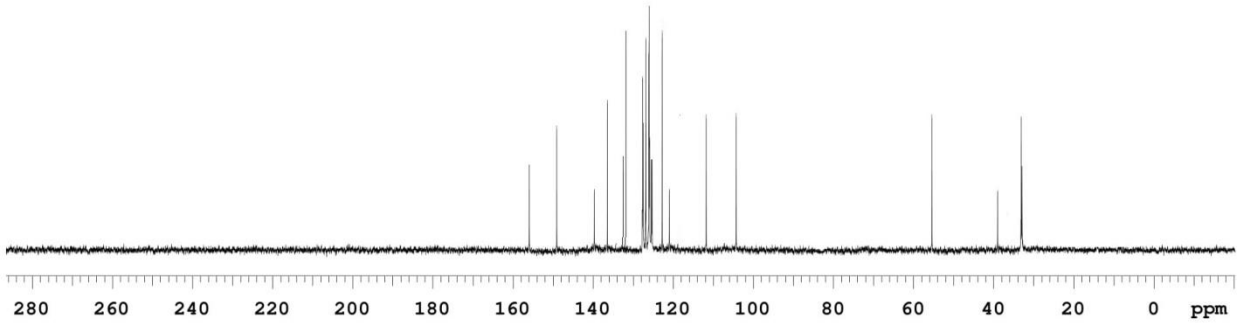
[NOTE: A. ^{1}H NMR spectra, B.^{13}C NMR spectra, C. FTIR and D.LC-MS]

Supplementary Fig S3: Compound (5a)

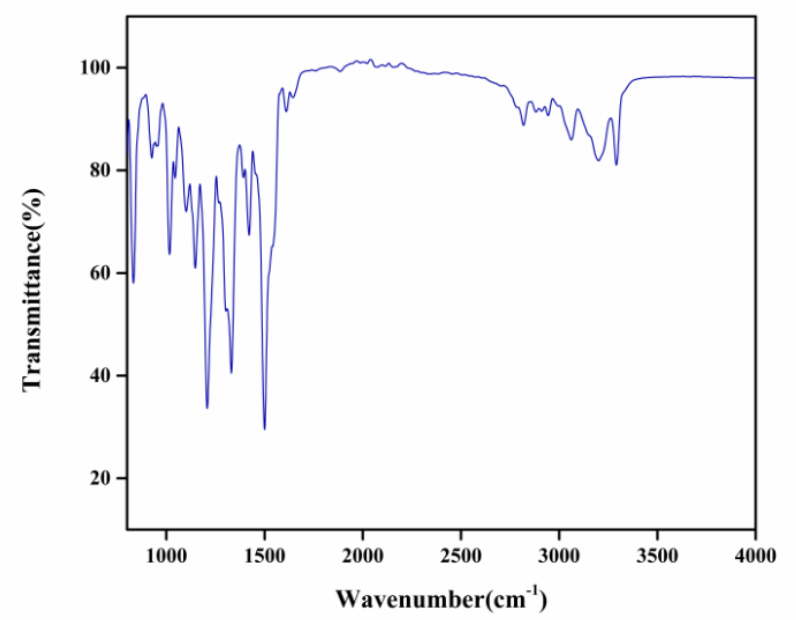
(A)



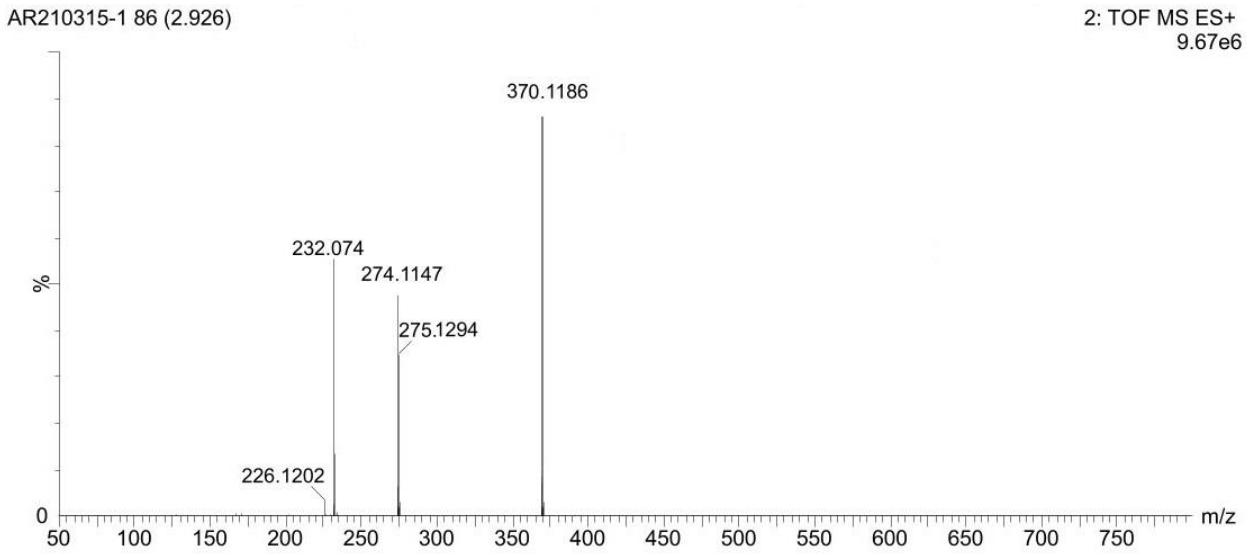
(B)


280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm

(C)

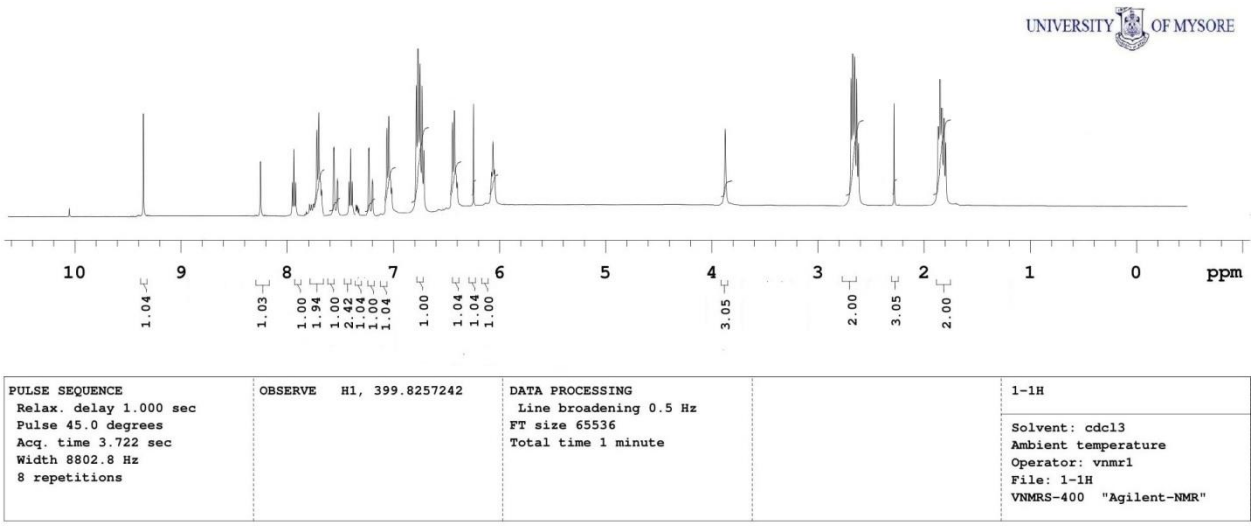

Transmittance(%)
100
80
60
40
20
1000
1500
2000
2500
3000
3500
4000
Wavenumber(cm-1)

(D)

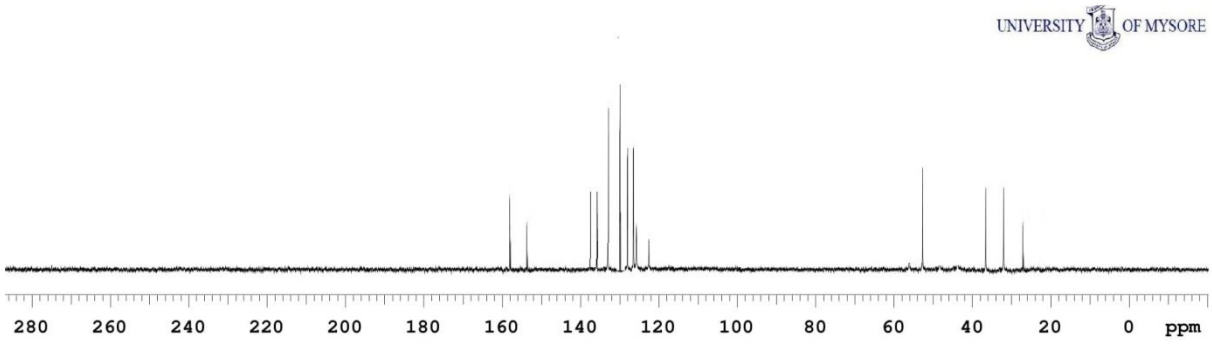


Supplementary Fig S4: Compound (5b)

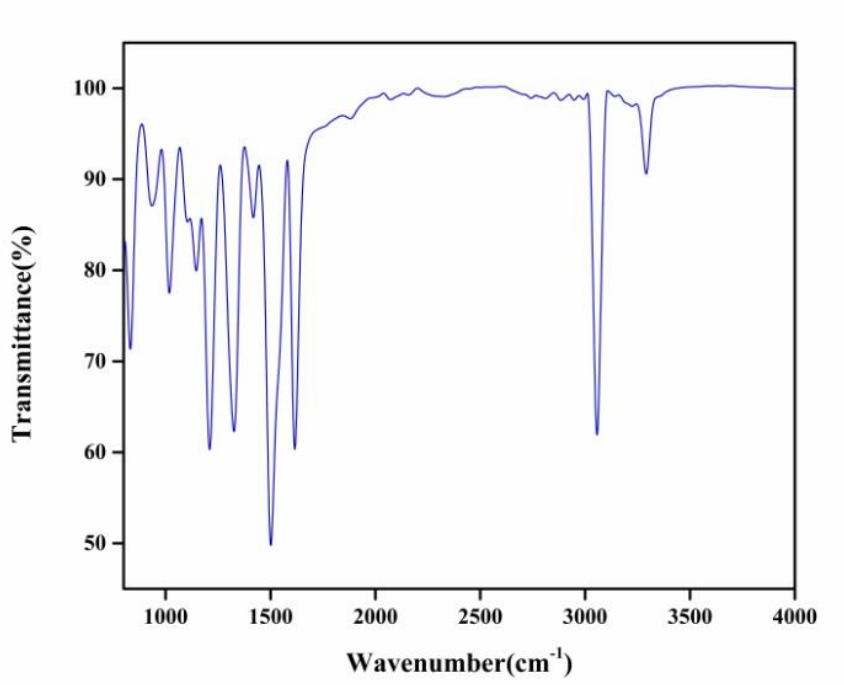
(A)



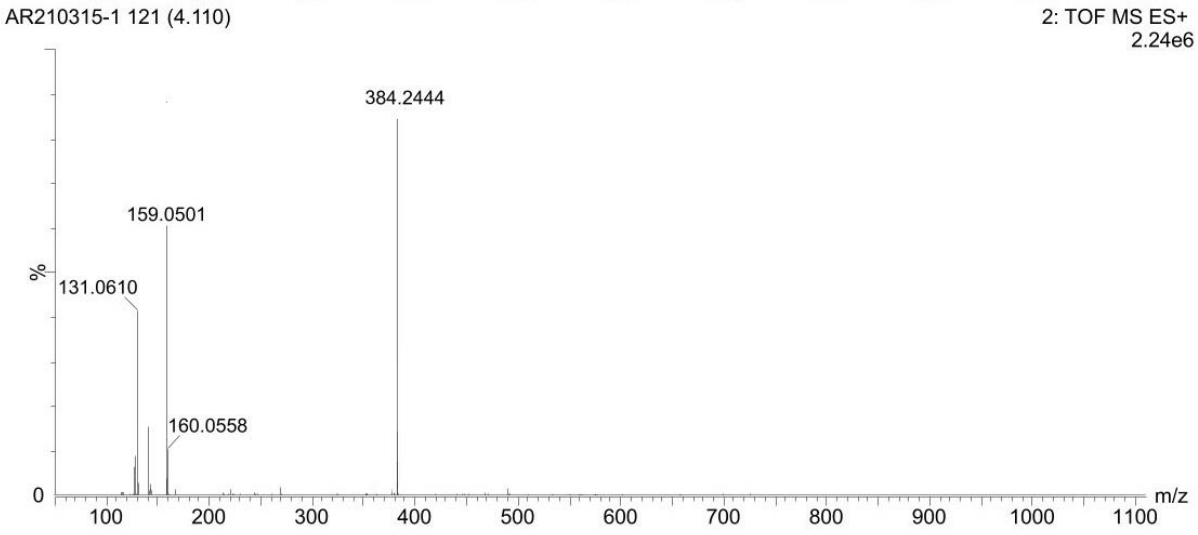
(B)


UNIVERSITY OF MYSORE
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm

(C)

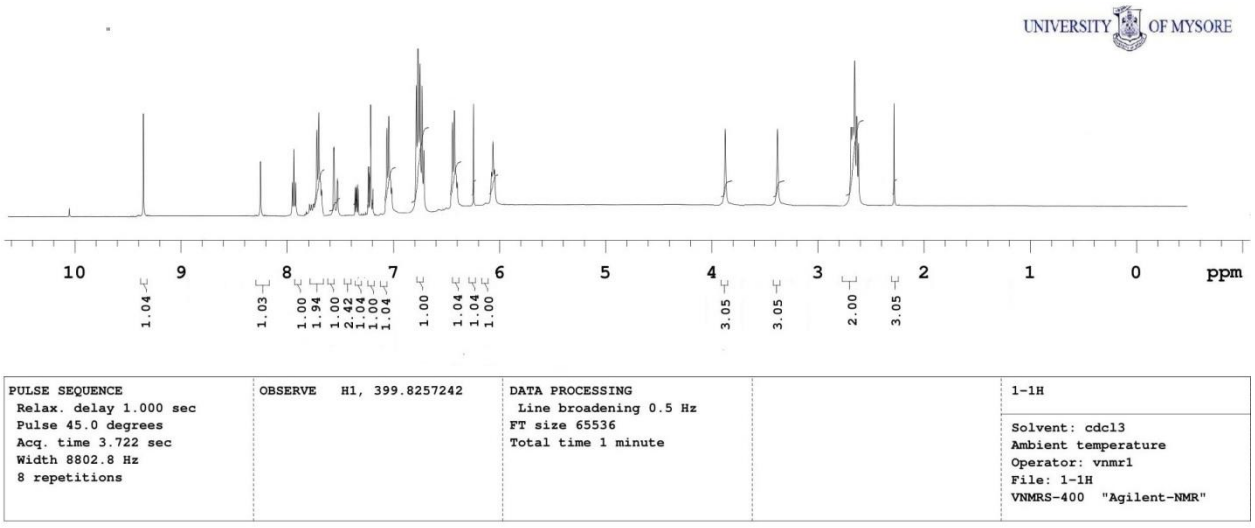

Transmittance(%)
100
90
80
70
60
50
1000
1500
2000
2500
3000
3500
4000
Wavenumber(cm-1)

(D)

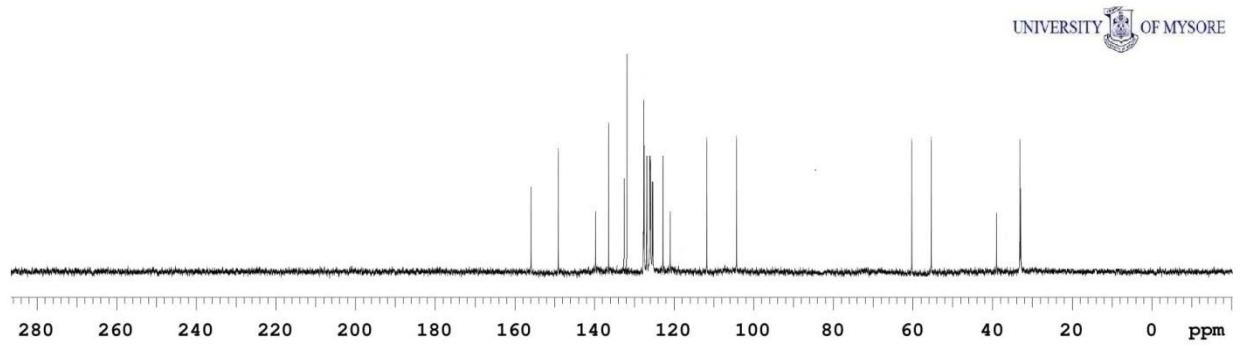


Supplementary Fig S5:Compound (5c)

(A)

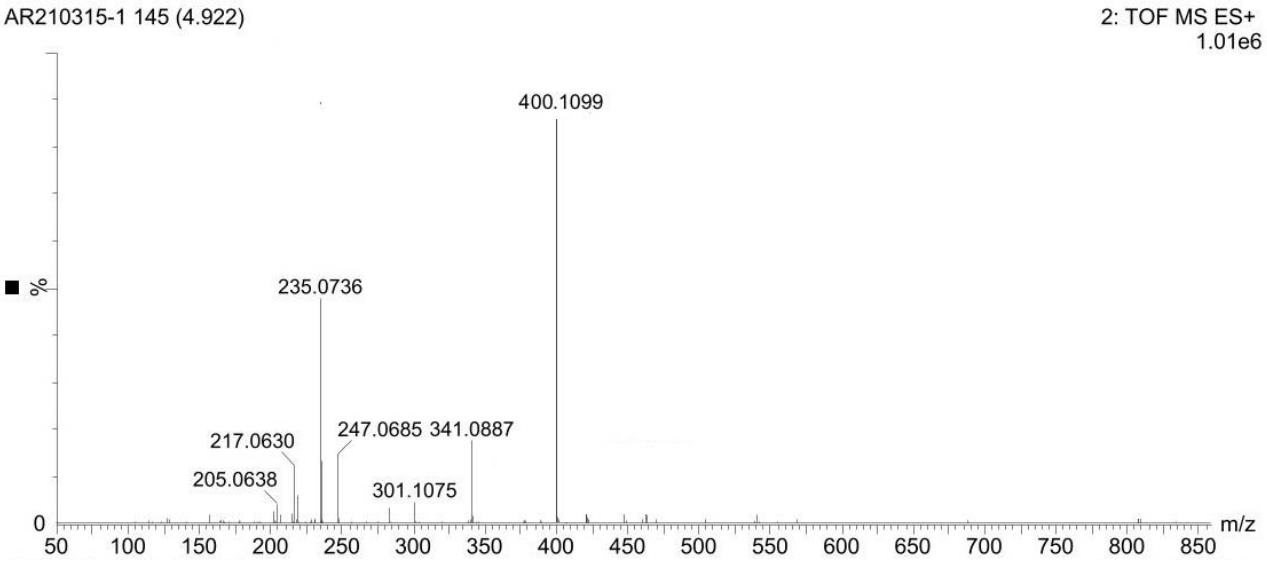


(B)



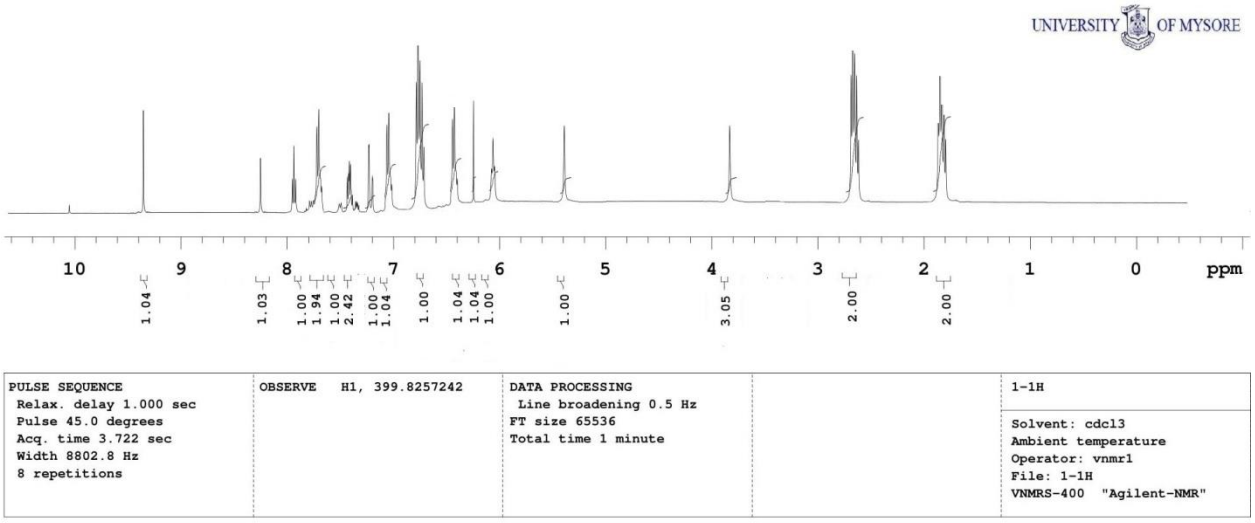
(C)

(D)

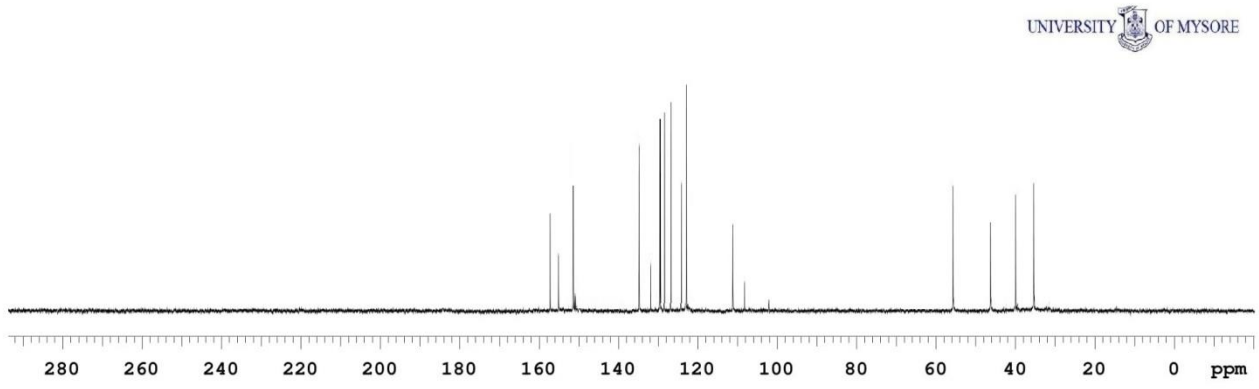


Supplementary Fig S6: Compound (5d)

(A)

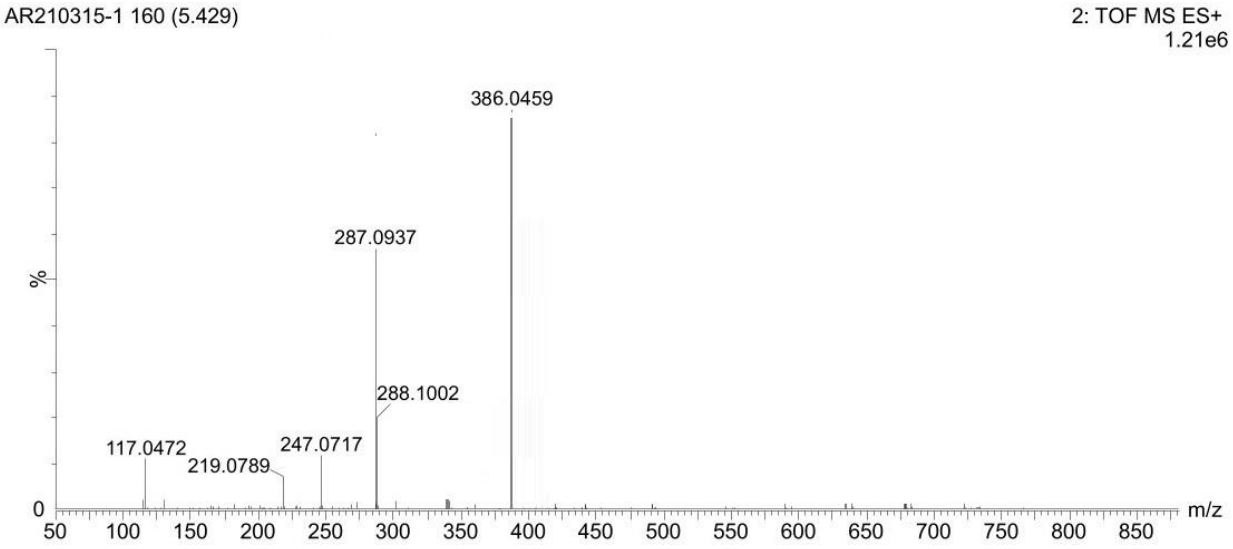

UNIVERSITY OF MYSORE
10 9 8 7 6 5 4 3 2 1 0 ppm
1.04 1.03 1.00 1.94 1.00 2.42 1.00 1.04 1.00 1.04 1.04 1.00 1.00 3.05 2.00 2.00
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.722 sec
Width 8802.8 Hz
8 repetitions
OBSERVE H1, 399.8257242
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 minute
1-1H
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
File: 1-1H
VNMRS-400 "Agilent-NMR"

(B)


UNIVERSITY OF MYSORE
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm

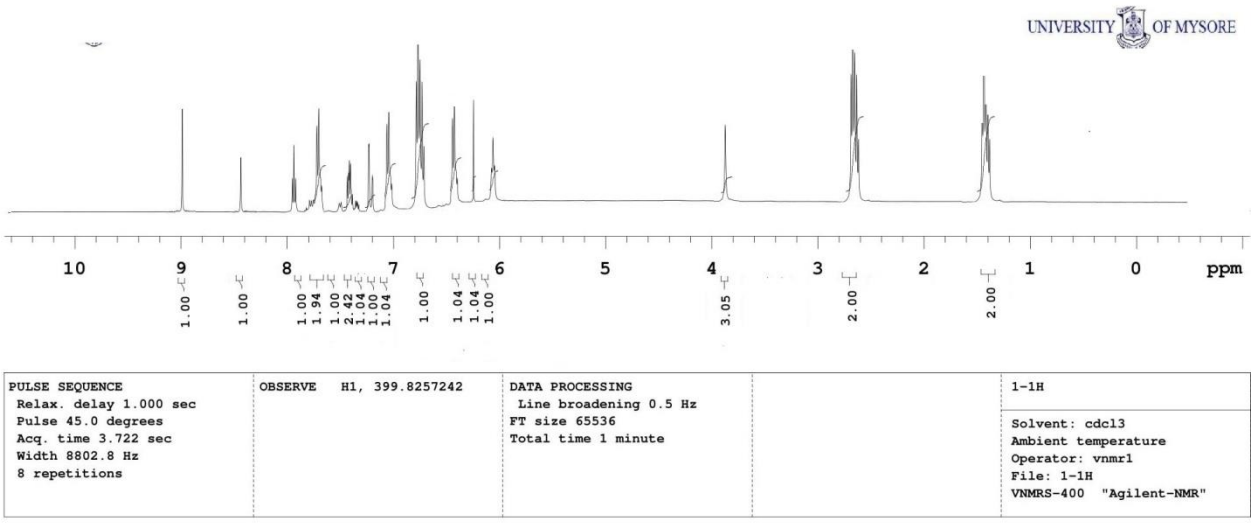
(C)

(D)

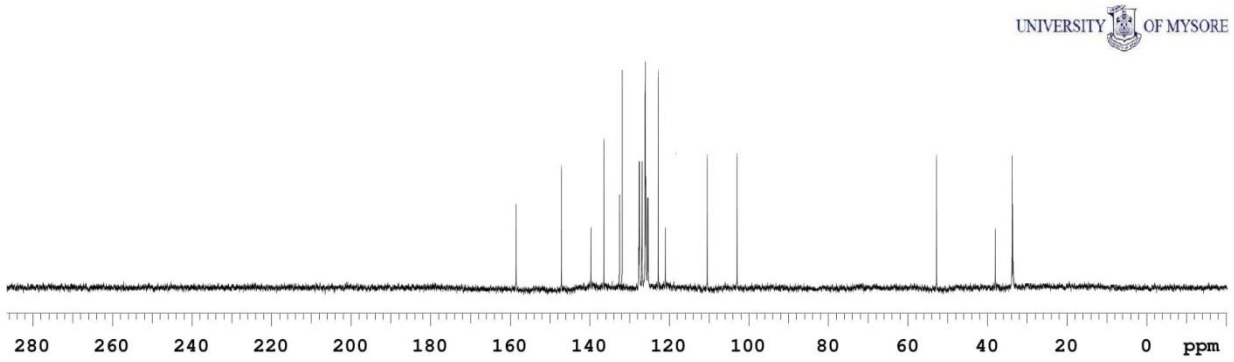


Supplementary Fig S7: Compound (5e)

(A)

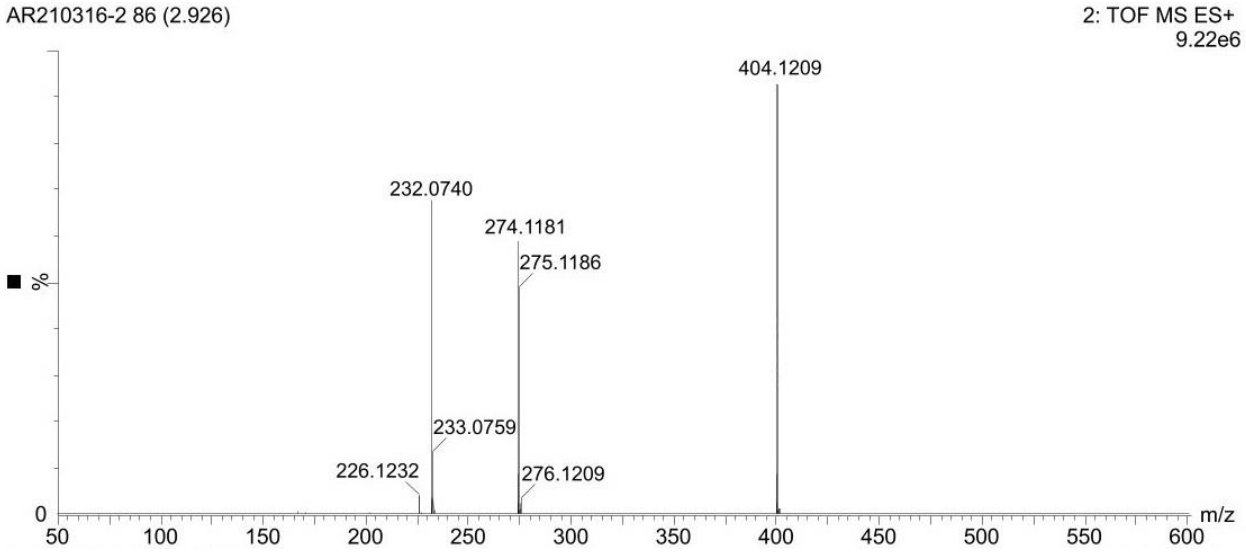


(B)



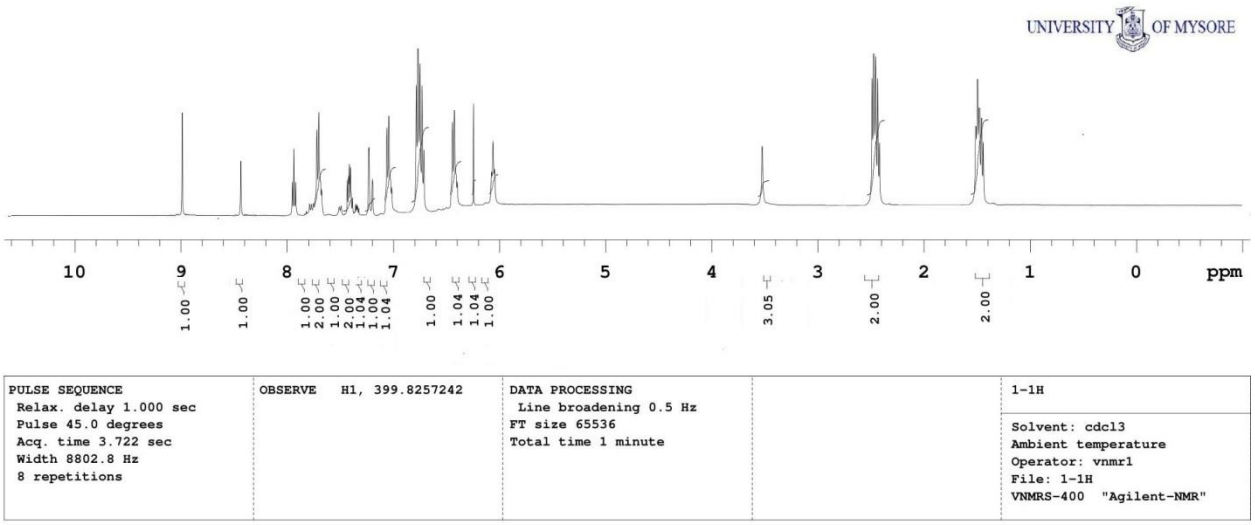
(C)

(D)

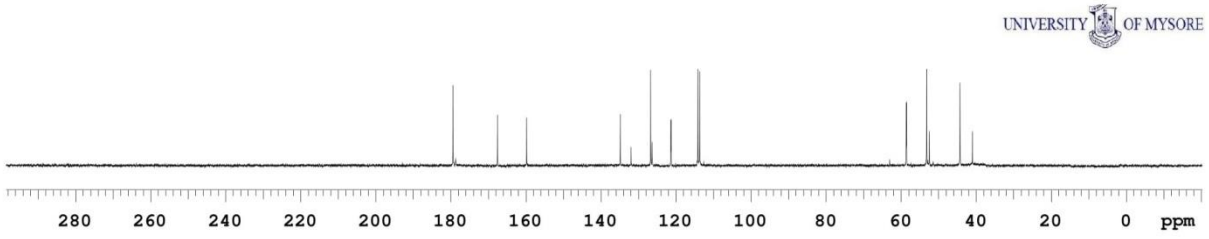


Supplementary Fig S8: Compound (5f)

(A)

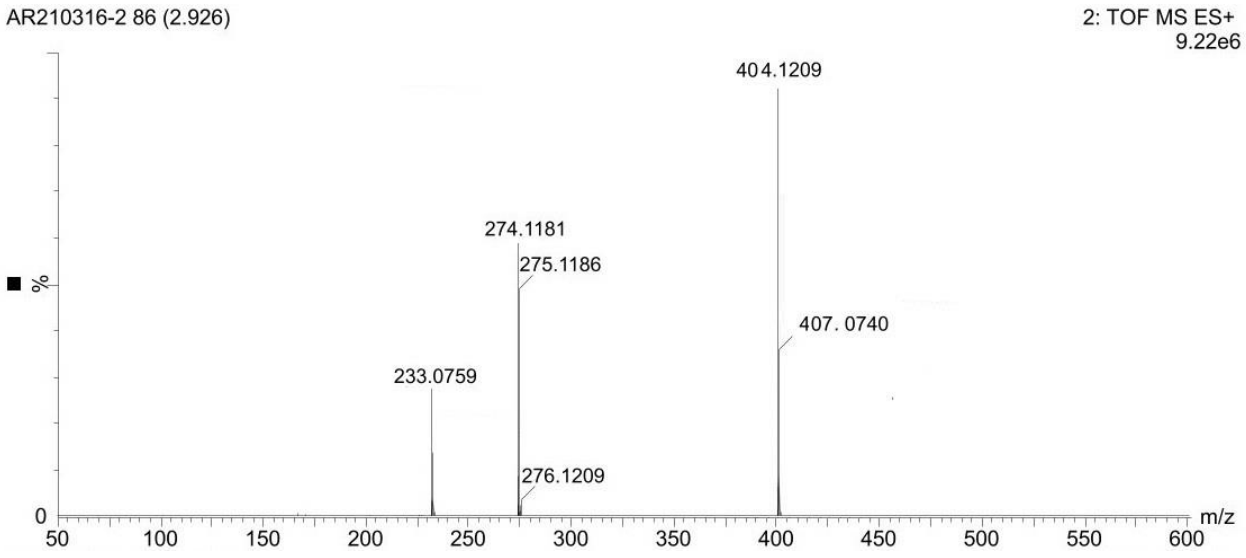

UNIVERSITY OF MYSORE
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.00 1.00 2.00 1.00 2.00 1.00 1.04 1.00 1.04 1.04 1.00 3.05 2.00 2.00
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.722 sec
Width 8802.8 Hz
8 repetitions
OBSERVE H1, 399.8257242
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 minute
1-1H
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
File: 1-1H
VNMRS-400 "Agilent-NMR"

(B)


UNIVERSITY OF MYSORE
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm

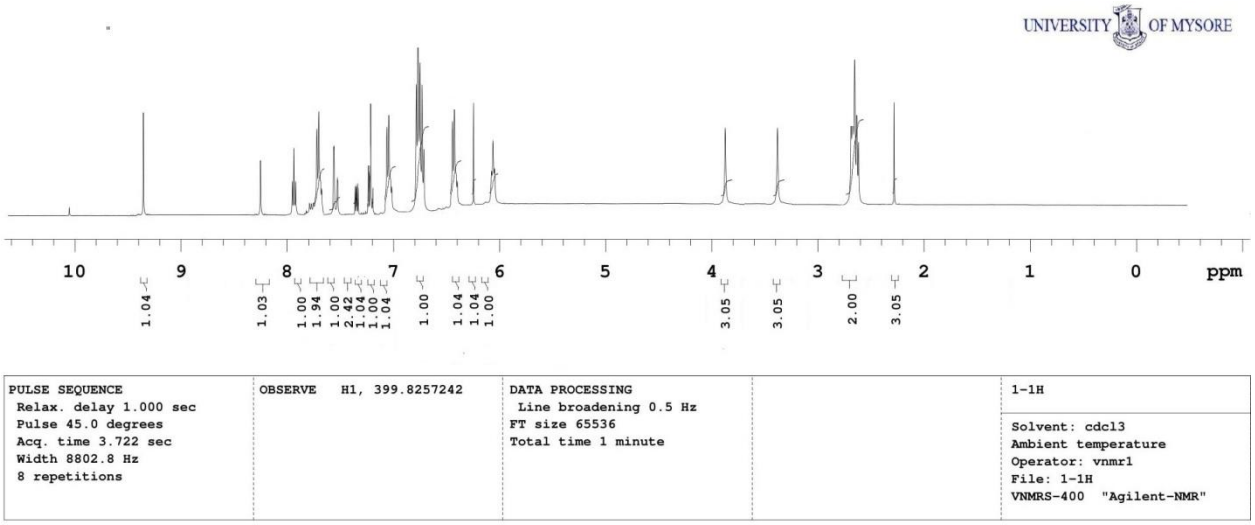
(C)

(D)

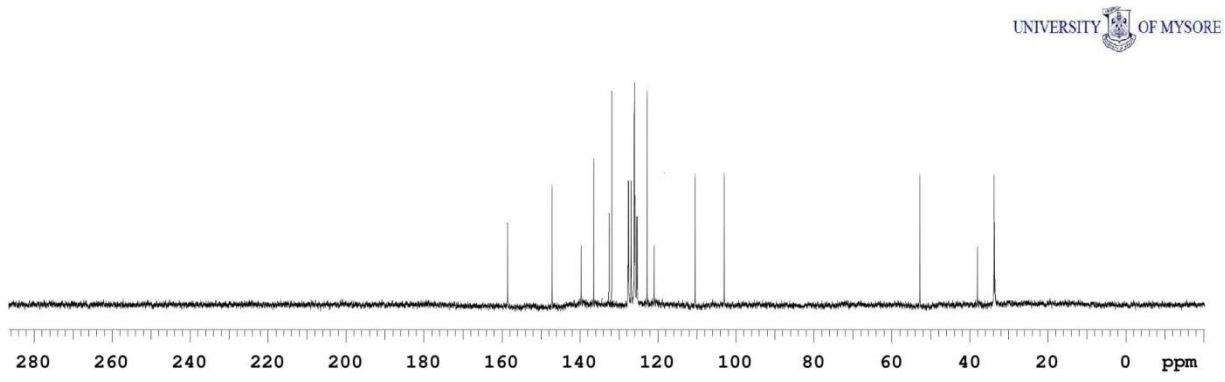

AR210316-2 86 (2.926)
2: TOF MS ES+
9.22e6
404.1209
274.1181
275.1186
407. 0740
233.0759
276.1209
%
0
50 100 150 200 250 300 350 400 450 500 550 600
m/z

Supplementary Fig S9: Compound (5g)

(A)

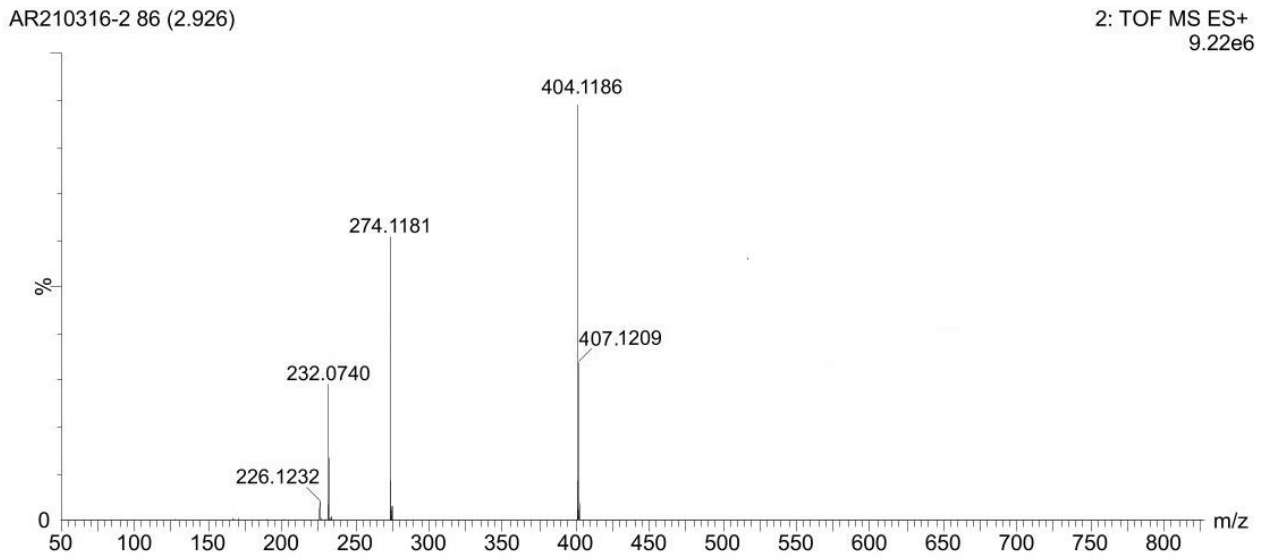


(B)



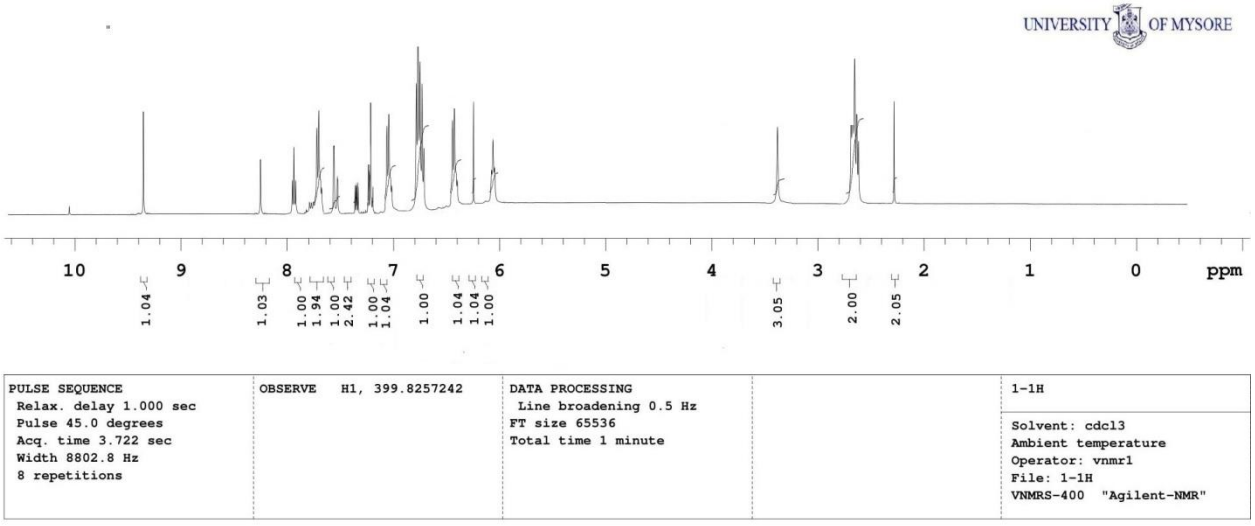
(C)

(D)

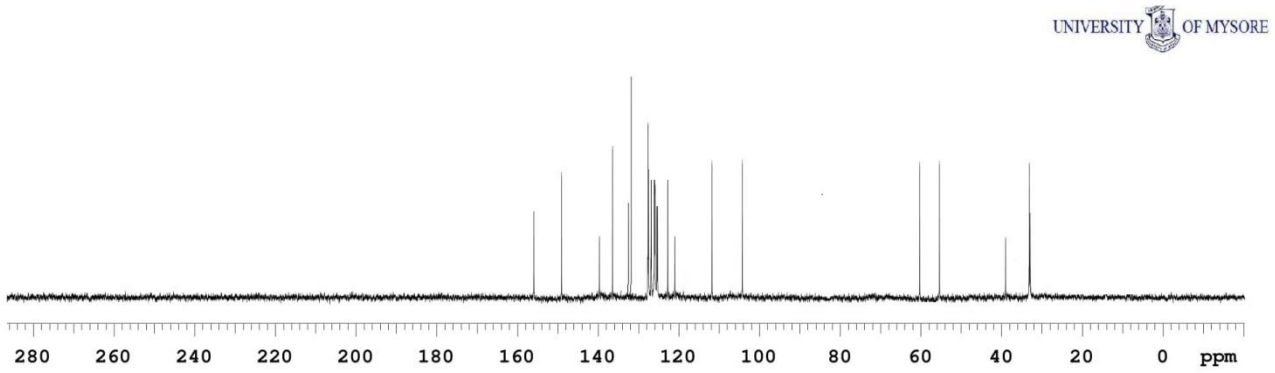


Supplementary Fig S10: compound 5h

(A)

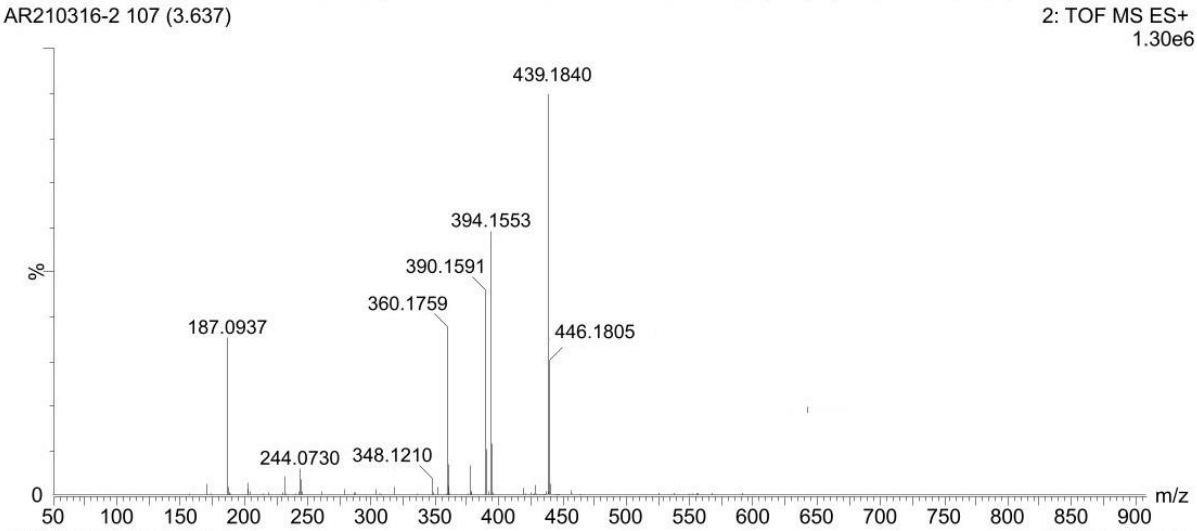


(B)



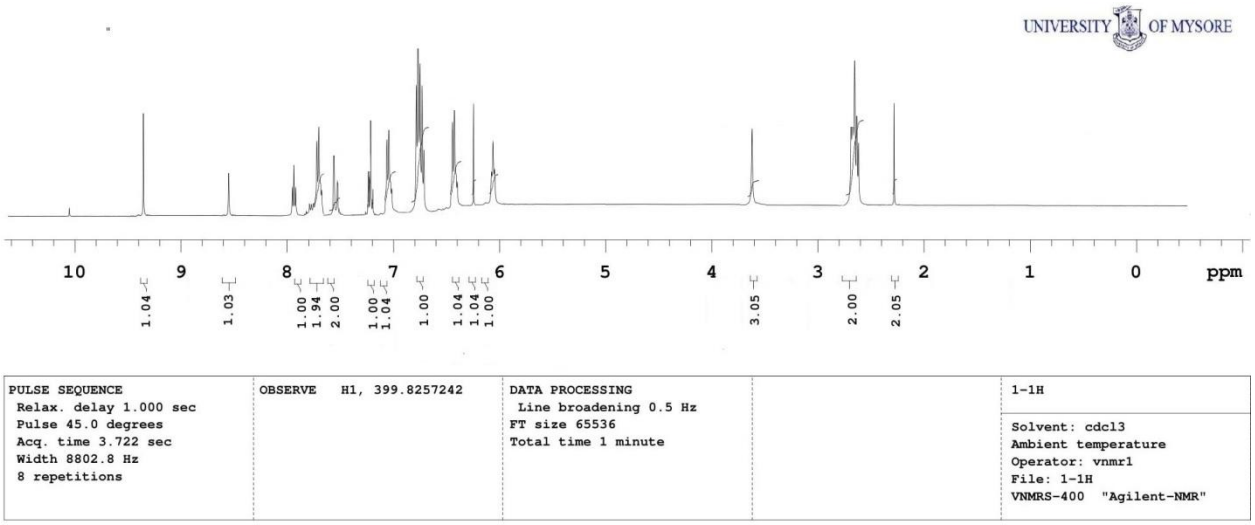
(C)

(D)

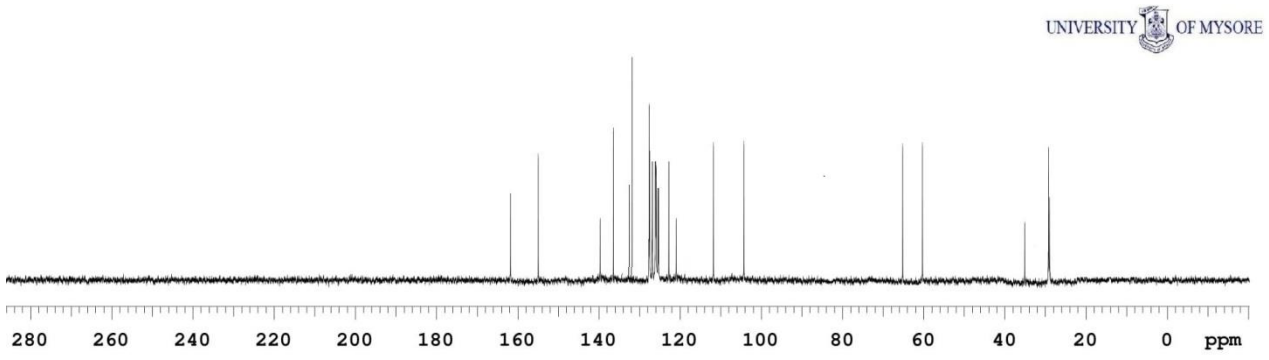


Supplementary Fig S11: compound 5i

(A)

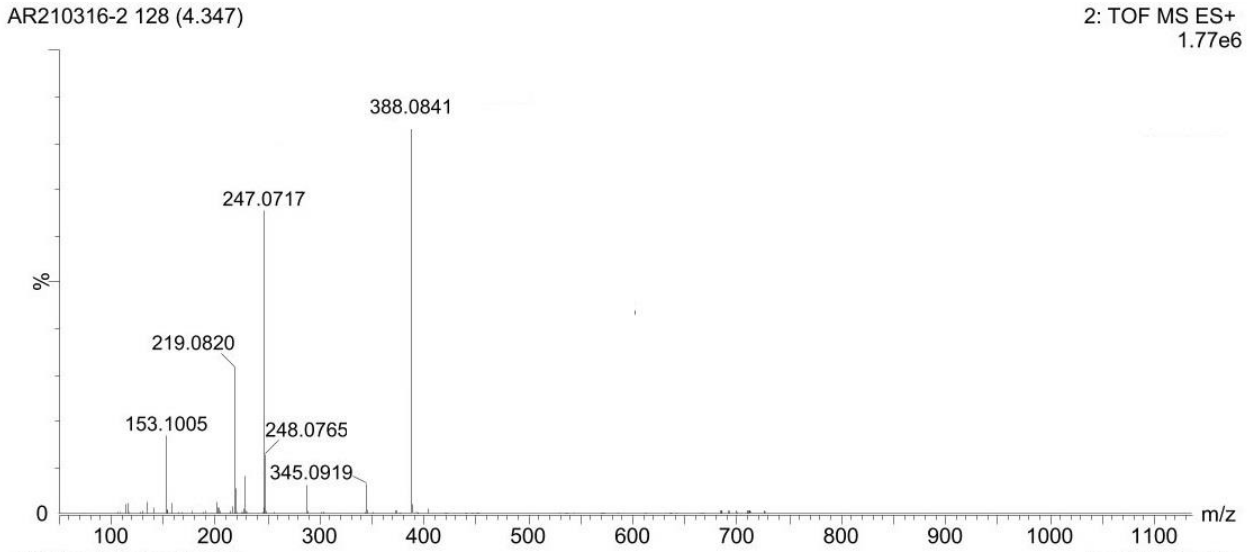

UNIVERSITY OF MYSORE
10 9 8 7 6 5 4 3 2 1 0 ppm
1.04 1.03 1.00 1.94 2.00 1.00 1.04 1.00 1.04 1.04 1.00 3.05 2.00 2.05
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.722 sec
Width 8802.8 Hz
8 repetitions
OBSERVE H1, 399.8257242
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 minute
1-1H
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
File: 1-1H
VNMRS-400 "Agilent-NMR"

(B)


UNIVERSITY OF MYSORE
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm

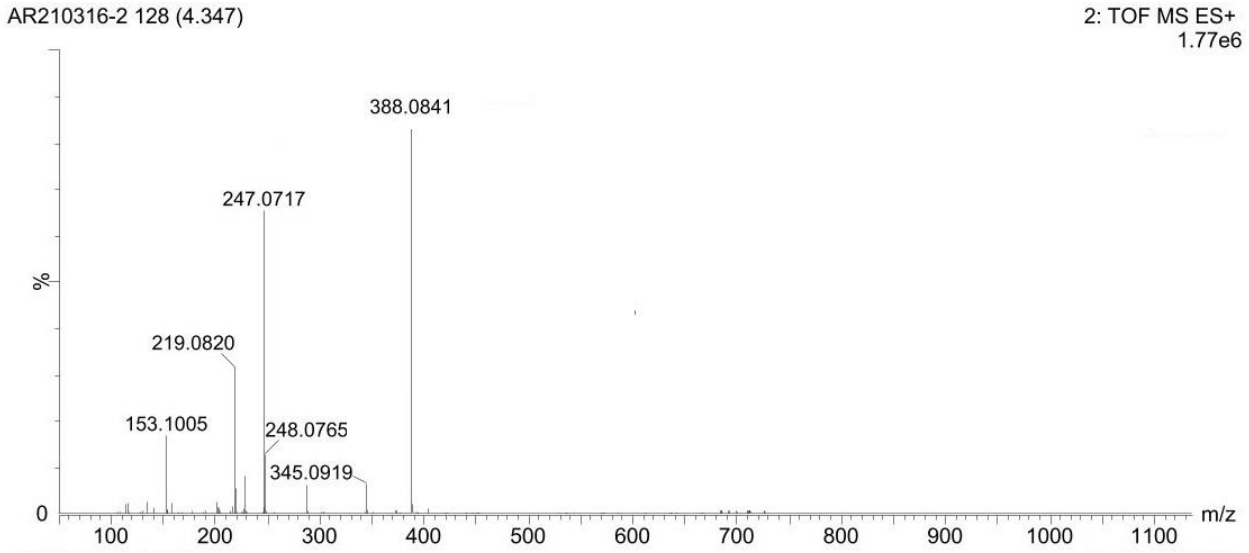
(C)

(D)

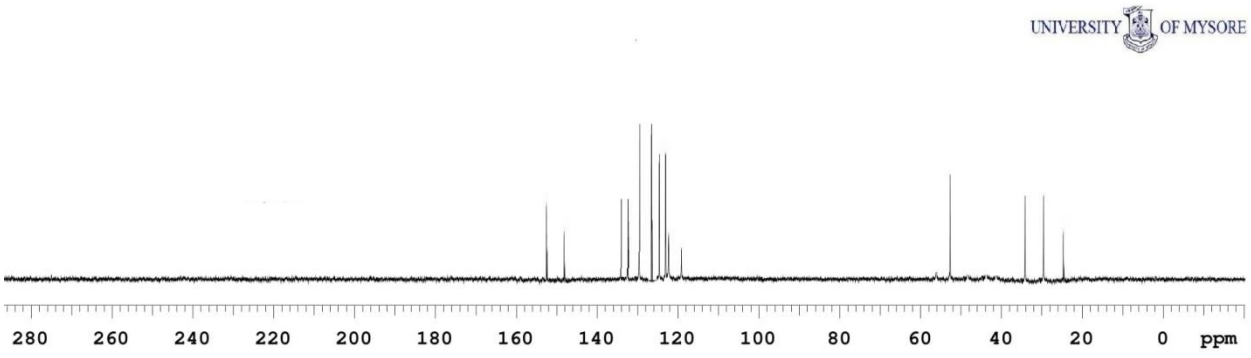


Supplementary Fig S12: compound 5j

(A)

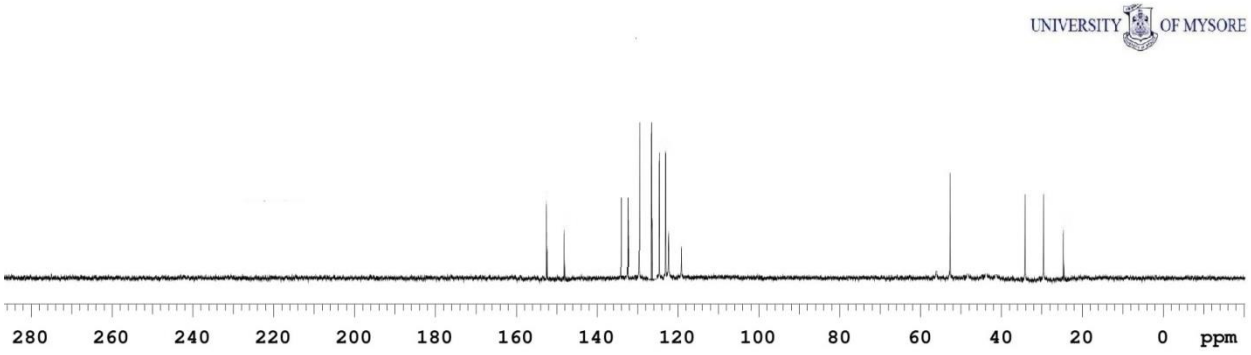


(B)



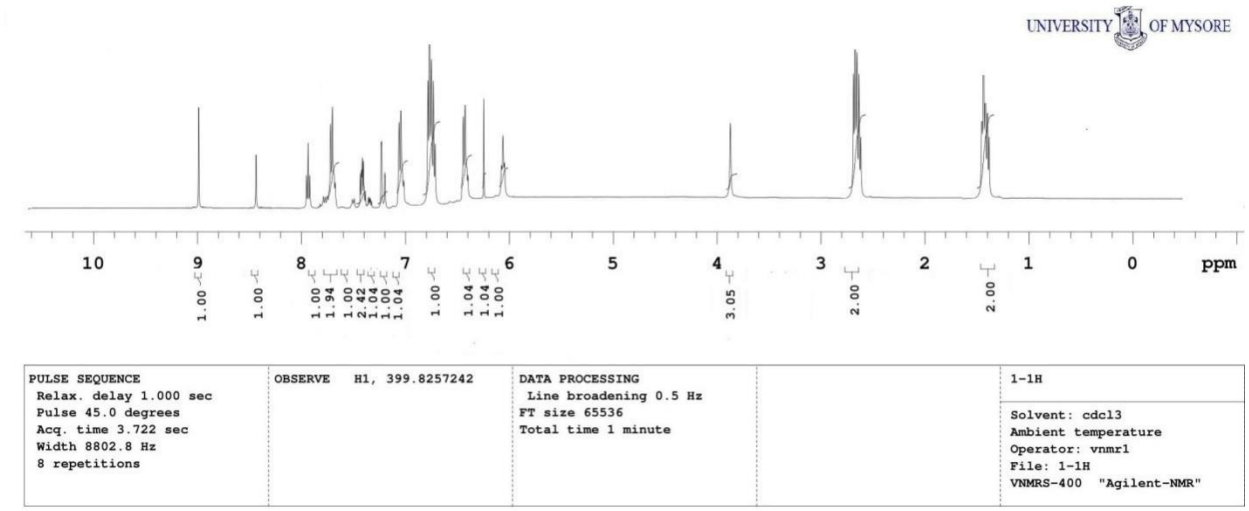
(C)

(D)

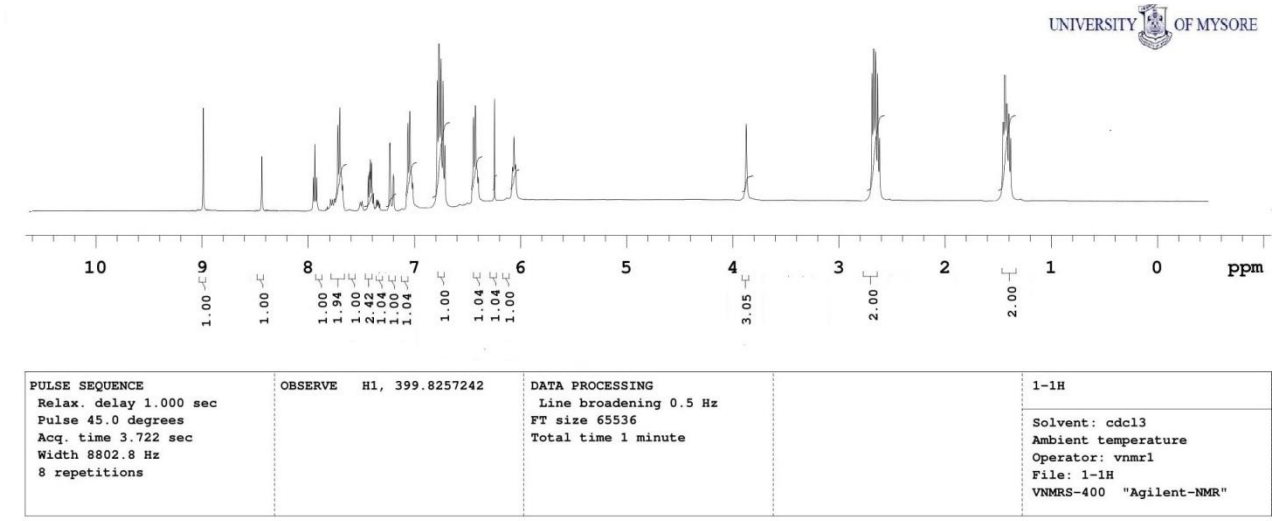


Supplementary Fig S13: compound 5k

A)

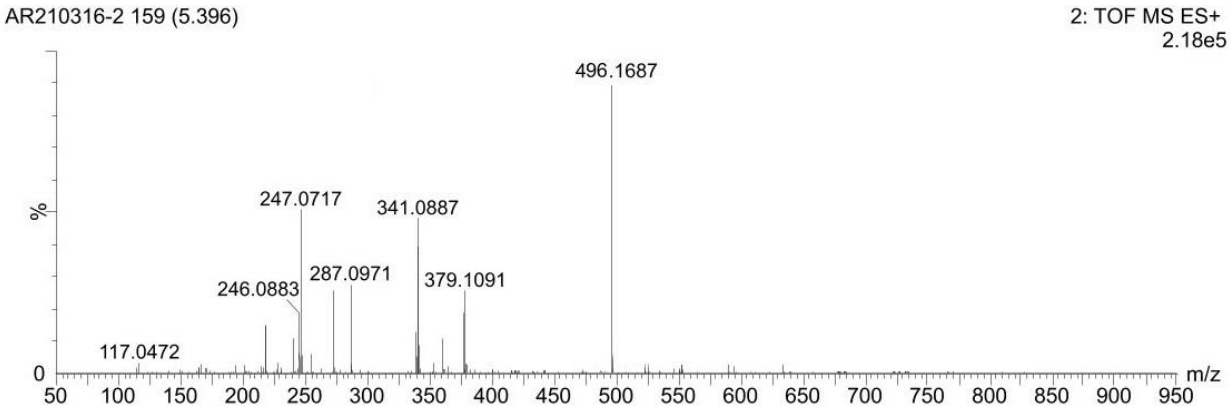


B)



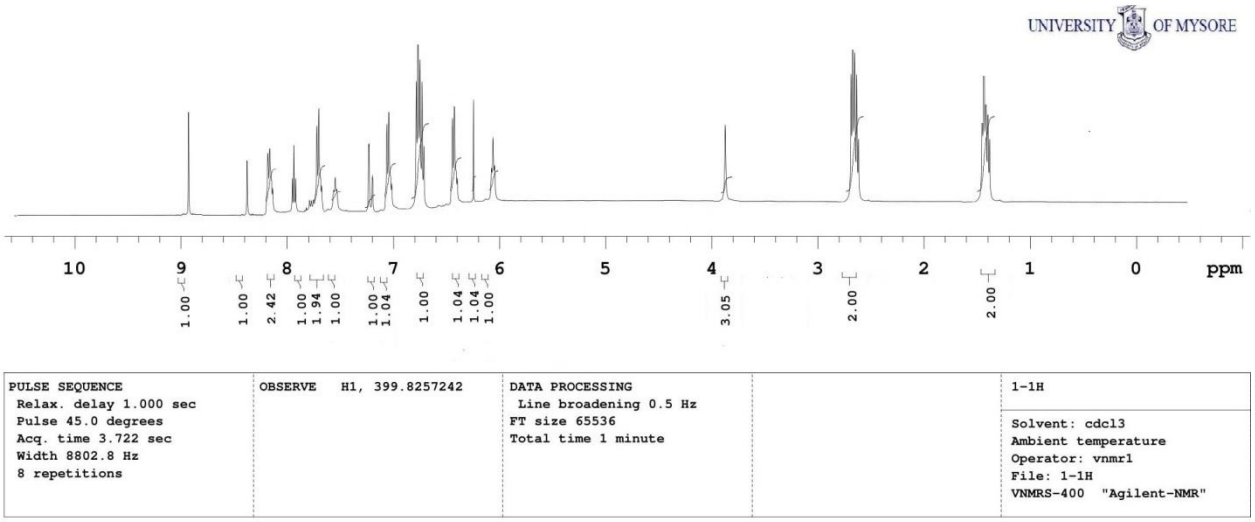
C)

D)

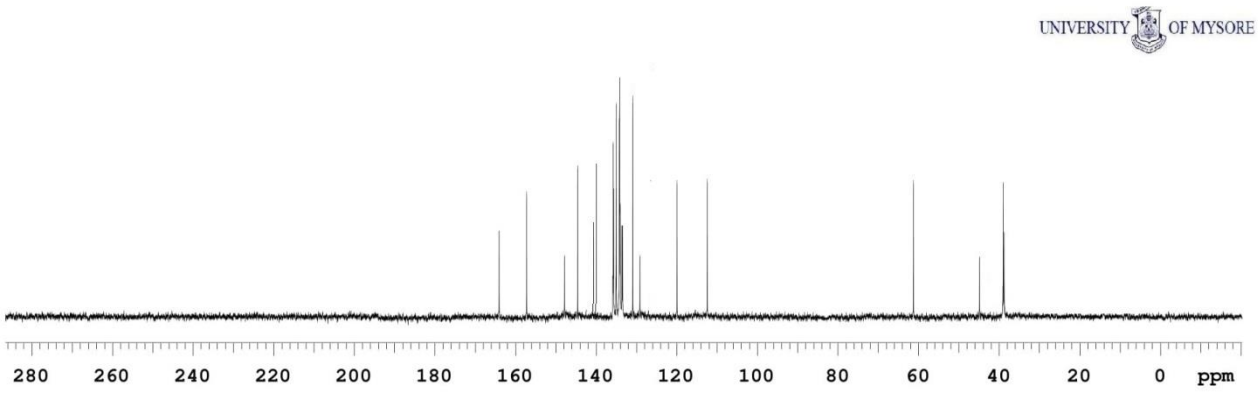


Supplementary Fig S14: compound 5l

A)

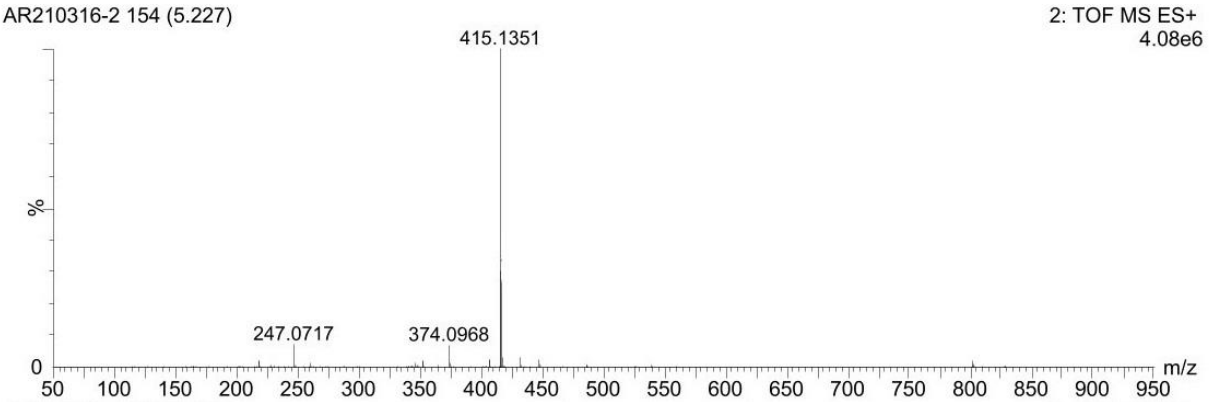


B)



C)

D)



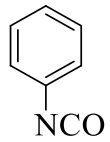
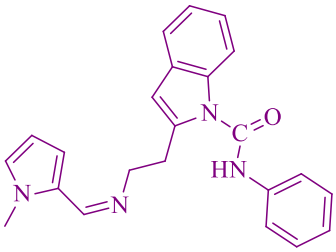
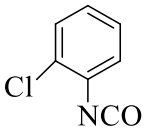
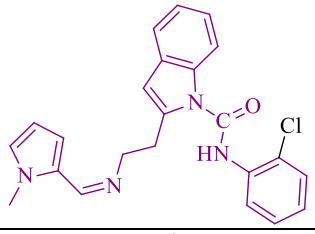
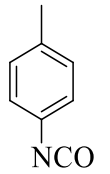
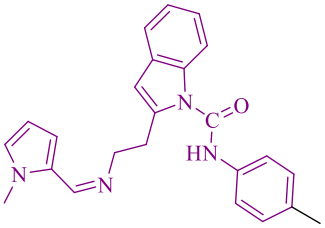
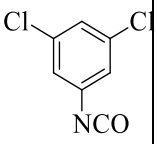
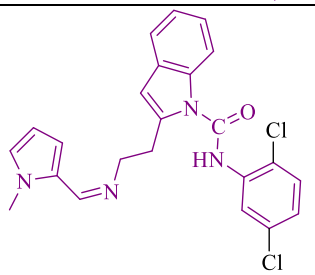
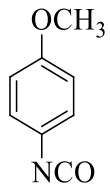
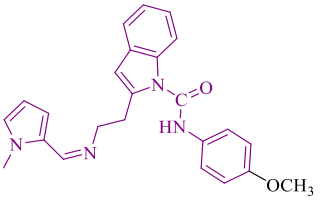
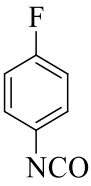
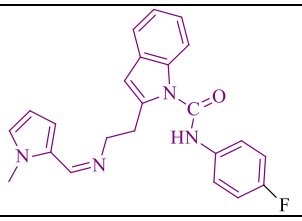
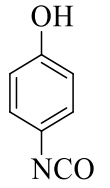
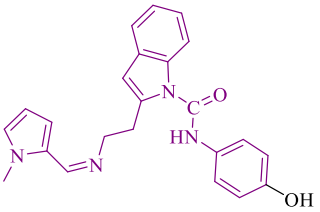
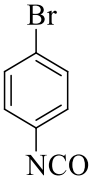
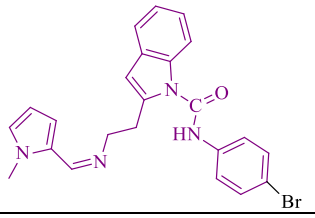
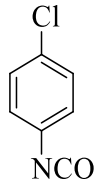
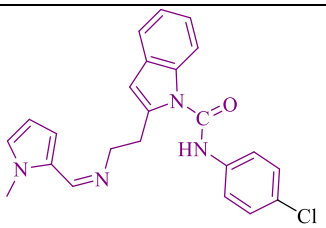
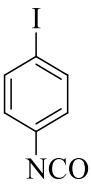
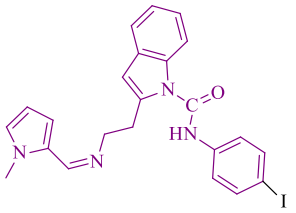
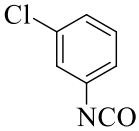
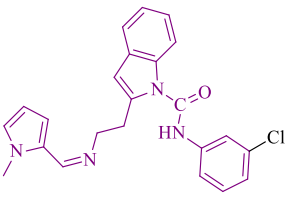
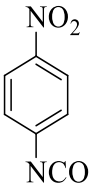
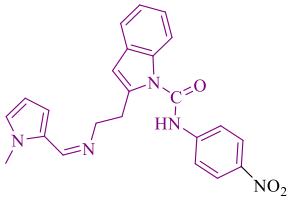
Supplementary Table S1: Synthesized analogues 5(a-1) and their bio-activity score

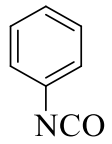
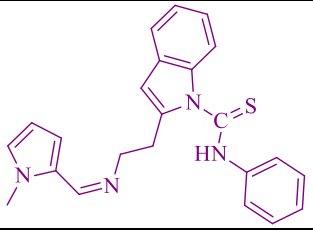
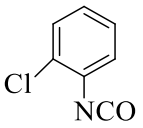
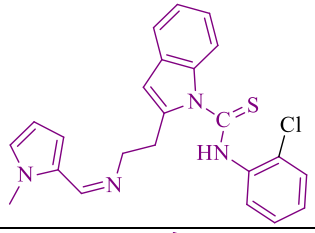
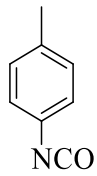
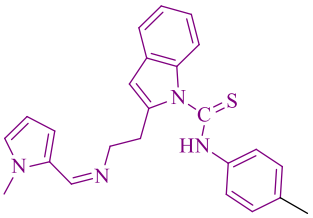
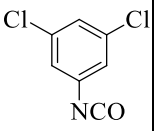
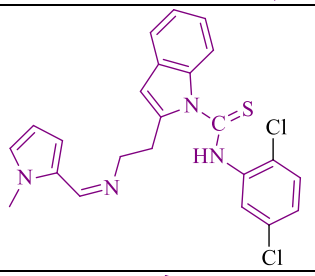
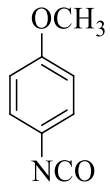
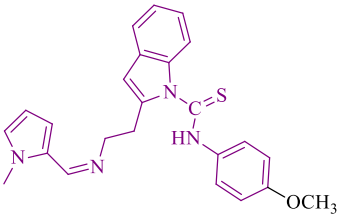
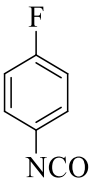
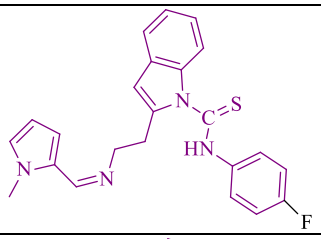
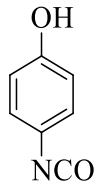
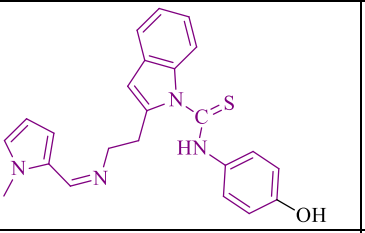
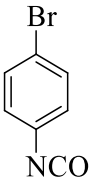
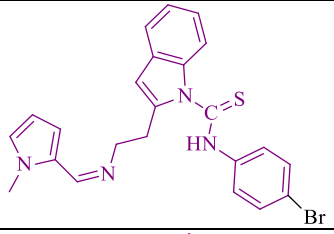
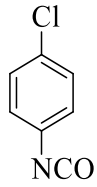
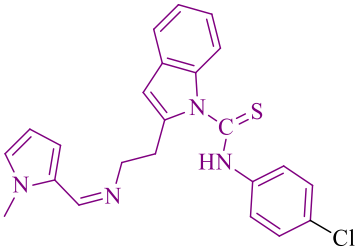
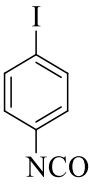
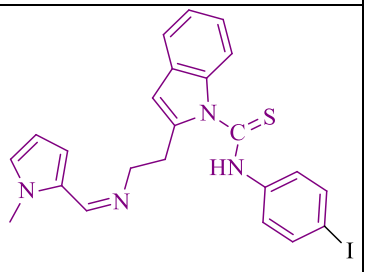
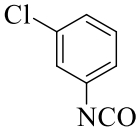
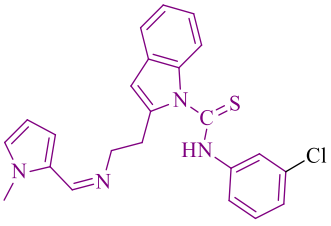
Compound	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
5(a)	0.12	-0.05	0.18	-0.39	-0.24	0.12
5(b)	0.07	-0.13	0.13	-0.40	-0.29	0.05
5(c)	0.06	-0.13	0.13	-0.38	-0.28	0.06
5(d)	0.15	-0.01	0.22	-0.24	-0.22	0.16
5(e)	0.11	-0.06	0.16	-0.40	-0.27	0.08
5(f)	0.10	-0.06	0.16	-0.41	-0.30	0.06
5(g)	0.08	-0.07	0.19	-0.45	-0.33	0.04
5(h)	0.11	-0.04	0.16	-0.38	-0.28	0.06
5(i)	0.12	-0.07	0.21	-0.36	-0.25	0.10
5(j)	0.01	-0.13	0.13	-0.49	-0.34	0.04
5(k)	0.11	-0.06	0.19	-0.35	-0.30	0.06
5(l)	-0.04	-0.09	0.02	-0.43	-0.34	0.01

Supplementary table S2 - Predicted biological activities of compounds 5(a-l), Pa (probability "to be active"), Pi (probability "to be inactive").

Activity	5a		5b		5c		5d		5e		5f	
	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi
Antineoplastic	0.651	0.035	0.603	0.044	0.642	0.036	0.648	0.035	0.538	0.060	0.539	0.060
Protein kinase inhibitor	0.150	0.092	0.130	0.107	0.125	0.113	0.123	0.115	0.142	0.097	0.154	0.088
Antineoplastic (lymphoticleukemia)	0.209	0.036	0.189	0.041	0.187	0.042	0.174	0.047	0.164	0.050	0.160	0.052
Antineoplastic(melanoma)	0.183	0.065	0.195	0.058	0.201	0.055	0.178	0.069	0.153	0.097	0,157	0.093
Antineoplastic (multiple myeloma)	0.504	0.010	0.460	0.014	0.444	0.015	0.467	0.013	0.502	0.010	0.502	0,010
Anxiolytic	0.227	0.103	0.192	0.128	0.192	0.129	0.173	0.047	0.237	0.097	0,220	0.108
Aurora-c-kinase inhibitor	0.168	0.061	0.161	0.066	0.137	0.082	0.143	0.079	0.137	0.084	0.125	0.095
chemosensitizer	0.588	0.008	0.563	0.010	0.568	0.010	0.578	0.009	0.569	0.009	0.556	0.001

Activity	5g		5h		5i		5j		5k		5l	
	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi
antineoplastic	0.492	0.074	0.533	0.062	0.579	0.050	0.636	0.038	0.664	0,032	0.591	0.047
Protein kinase inhibitor	0.179	0.076	0.149	0.092	0.168	0.081	0.158	0.086	0.156	0.087	0.157	0.083
Antineoplastic (lymphoticleukemia)	0.146	0.058	0.144	0.060	0,157	0.053	0.188	0.041	0.203	0.037	0.216	0.034
Antineoplastic (melanoma)	0.129	0.128	0.148	0.104	0.155	0.095	0.188	0.062	0.193	0.059	0,169	0.078
Antineoplastic (multiple myeloma)	0.500	0.010	0.501	0.010	0.483	0.011	0.432	0.017	0,380	0.030	0.443	0.016
Anxiolytic	0.214	0.112	0.227	0.103	0.278	0.077	0.215	0.111	0.278	0.075	0.214	0.143
Aurora-c-kinase inhibitor	0.116	0.104	0.157	0.068	0.159	0.069	0.248	0.018	0.210	0.036	0.159	0.069
chemosensitizer	0.600	0.006	0.569	0.009	0.548	0.012	0.558	0.011	0.602	0.006	0.631	0.005

Supplementary table S5: Structure of synthesized compounds 5(a-l)					
Compound name	R	Structure	Compound name	R	Structure
5a			5g		
5b			5h		
5c			5i		
5d			5j		
5e			5k		
5f			5l		

6a			6g		
6b			6h		
6c			6i		
6d			6j		
6e			6k		
6f			6l