ELECTRONIC SUPPLEMENTARY INFORMATION

Design and Synthesis of Potential Pyrrole-Coupled Carboxamide Derivatives as an Anti-superbug MRSA Agent

1.1 Spectroscopic data of the synthesized compounds

1.1.1(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-phenylpiperazine-1-carboxamide (5a)

^{1}H NMR (400 MHz, $CDCl_3$), 8.52 (d, 2H, Ar-H) 7.79 (d, 2H,Ar-H) 7.42 (d,2H,Py-H) 7.23 (t, 1H, Ar-H) 6.83 (t, 1H, Py-H) 6.81 (s, 1H, CH=N) 6.11 (s, 1H, NH) 4.19,2.9and 2.52 (d, 4H, CH2CH2) 3.81 (s, 3H, CH_3-Py) 3.42 (d,4H, pip-H) 2.21 (d,4H,pip-H) ^{13}C NMR: (400Hz, $CDCl_3$) 181.0(C=N) 161 (CONH)150 (Py-C) 147 (PyC) 139 (Py-C) 134 (Ar-C) 131 (Ar-C) 128 (Ar-C) 125 (Ar-C) 121(Ar-C) 63 (Pip-C) 56 (Pip-C) 52 (Pip-C) LCMS m/z Calculated for $C_{19}H_{25}N_5O$: 339.21 IR Vmax (cm-1) 2250 (O=CNH), 1650 (C=N), 1640(C=C), 1250(C-N)Elemental Analysis: Calculated: C,67.23 ; H,7.42 ; N,20.63 ; O,4.71; Experimental: C,67.21 ; H,7.41 ; N,20.62 ; O,4.70.

1.1.2.(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(p-tolyl)piperazine-1-carboxamide (5b)

.^{1}H NMR (400 MHz, $CDCl_3$) 8.21 (1H,s,CH=N) 8.19 (2H,d,Ar-H) 7.42 (2H,d,Ar-H) 7.21 (1H,t, py-H) 6.84 (2H,d, Py-H) 6.31 (1H,s,NH) 4.19 (3H,s,Py-CH_3) 3.81 (2H,d, CH2) 3.6 (2H,t,CH_2) 3.21 (4H,d,Pip-H) 2.52 (3H,s,CH_3) 2.23 (4H,d,Pip-H) ^{13}C NMR: (400Hz, $CDCl_3$) 184.0 (C=N) 161 (CONH) 152 (Py-C) 150 (PyC) 138 (Py-C) 136 (Ar-C) 128 (Ar-C) 126 (Ar-C) 64(Pip-C) 56 (Pip-C) 52 (Pip-C) LCMS m/z Calculated for $C_{20}H_{27}N_5O$:353.22IR Vmax (cm-1) 2245 (O=CNH), 1645 (C=N), 1630(C=C), 1245(C-N) Elemental Analysis: Calculated: C,67.96 ; H,7.70; N,19.81 ; O,4.53; Experimental: C,67.93 ; H,7.69 ; N,19.78 ; O,4.51.

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

^{1}H NMR (400 MHz, $CDCl_3$), 8.39 (1H, s, CH=N) 7.89 (1H,t,Py-H) 7.78 (1H,d,Py-H) 7.62 (2H,d,Ar-H) 7.43 (2H,d,Pip-H) 7.21 (1H,d,Py-H) 5.85 (1H,s,NH) 3.92 (4H,dd,CH_2-CH_2) 3.79 (4H, dd, Pip-H)

3.5 (3H,s,O-CH_3) 3.21 (4H,dd,Pip-H) 2.63 (3H,s,Py-CH_3) ^{13}C NMR: (400Hz, $CDCl_3$)184.0 (C=N) 160 (CONH) 152 (Py-C) 150 (PyC) 138 (Py-C) 136 (Ar-C) 128 (Ar-C) 126 (Ar-C)64 (Pip-C) 60 (Pip-C) 56 (CH_2) 52 (CH_2)LCMS m/z Calculated for $C_{20}H_{27}N_5O_2$:369.22IR Vmax (cm^{-1}) 2255 (O=CNH), 1660 (C=N), 1625(C=C), 1230 (C-N) 2810 (O-CH_3) Elemental Analysis: Calculated: C,65.02 ; H,7.37 ; N, 18.96 ; O,8.66; Experimental: C,65.00 ; H,7.36; N,18.92; O,8.65.

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

^{1}H NMR (400 MHz, $CDCl_3$), 7.72 (1H,s,CH=N) 7.43 (2H,d,Ar-H) 7.14 (2H,d,Ar-H) 6.75 (1H, t, Py-H) 6.48 (1H, d,Py-H) 6.21 (1H,d,Py-H) 4.98 ((1H, s,NH) 4.31 (1H,s,OH) 3.39 (4H,d,Pip-H) 3.05 (4H,d, pip-H) 2.61 (2H,d,CH_2) 2.22(2H,d,CH_2) 2.40(3H,s,Py-CH_3)^{13}C NMR: (400Hz, $CDCl_3$) 184.0 (C=N) 160 (CONH) 152 (Py-C) 150 (PyC) 138 (Py-C) 136 (Ar-C) 128 (Ar-C) 126 (Ar-C) 64 (Pip-C) 56 (Pip-C) 52 (CH_2) LCMS m/z Calculated for $C_{19}H_{25}N_5O_2$:355.20IR Vmax (cm-1) 3250 (OH) 2260 (O=CNH), 1660 (C=N), 1620(C=C), 1270(C-N) Elemental Analysis: Calculated: C,64.20; H,7.09 ; N, 19.70 ; O,9.00; Experimental: C,64.19 ; H,7.06; N,19.69; O,9.01.

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

^{1}H NMR (400 MHz, $CDCl_3$),8.45 (2H, d,ar-H) 7.79(1H,t,Py-H) 7.44(2H, d,Ar-H) 7.21 (1H,s,CH=N) 6.89 (2H, d, Py-H) 6.17 (1H,s,NH) 4.18 (3H,s,Py-CH3) 3.80(2H, d, CH2) 3.40 (4H,dd,Pip-H) 2.91 (2H, d, CH2) 2.21(4H,d, Pip-H) ^{13}C NMR: (400Hz, $CDCl_3$)187.0 (C=N) 164 (CONH) 155 (Py-C) 153 (PyC) 141 (Py-C) 139 (Ar-C) 131 (Ar-C) 129 (Ar-C) 67 (Pip-C) 59 (Pip-C) 55 (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,61.04; H,6.47; Cl,9.48; N,18.73; O,4.28; Experimental: C,61.00; H,6.46; Cl,9.44; N,18.71; O,4.27.

1.1.6.(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(3-chlorophenyl)piperazine-1-carboxamide(5f)

^{1}H NMR (400 MHz, $CDCl_3$),8.45 (2H, d,ar-H) 7.79(1H,t,Py-H) 7.44(2H, d,Ar-H) 7.21 (1H,s,CH=N) 6.89 (2H, d, Py-H) 6.17 (1H,s,NH) 4.18 (3H,s,Py-CH3) 3.80(2H, d, CH2) 3.40 (4H,dd,Pip-H) 2.91 (2H, d, CH2) 2.21(4H,d, Pip-H)^{13}C NMR: (400Hz, $CDCl_3$)181.0 (C=N) 160 (CONH) 150 (Py-C) 147 (PyC) 139 (Py-C) 133 (Ar-C) 131 (Ar-C) 128 (Ar-C) 125 (Ar-C) 121(Ar-C) 63 (Pip-C) 56 (Pip-C) 52 (CH_2) LCMS m/z Calculated for $C_{19}H_{24}ClN_5O$: 373.17 IR Vmax (cm-1)2280 (O=CNH), 1660 (C=N), 1635(C=C), 1260(C-N) 740 (C-Cl) Elemental Analysis: Calculated: C,61.04; H,6.47; Cl,9.48; N,18.73; O,4.28; Experimental: C,61.00; H,6.46; Cl,9.44; N,18.71; O,4.27.

1.1.7.(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(2-chlorophenyl)piperazine-1-carboxamide(5g)

^{1}H NMR (400 MHz, $CDCl_3$), 7.57 (d, 1H, Ar-H) 8.04(d, 1H,Ar-H) 7.24 (t,1H,Ar-H) 7.41 (t,1H,Ar-H) 8.90 (s, 1H, N-H) 3.39 (t, 4H, Pip-H) 2.48 (t, 4H, Pip-H) 2.4 (t, 2H, CH_2) 1.61 (t, 2H, CH_2) 8.35(s, 1H, C=N) 6.51 (d, 1H, Pyr-H) 6.15 (t,1H, Pyr-H) 6.95 (d, 1H, Pyr-H) 3.91(s,3H, CH_3)^{13}C NMR: (400Hz, $CDCl_3$)181.0 (C=N) 161 (CONH) 149 (Py-C) 147 (PyC) 139 (Py-C) 133 (Py-C) 131 (Ar-C) 128 (Ar-C)125 (Ar-C)121 (Ar-C) 63 (Pip-C) 56 (Pip-C) 52 (CH_2)LCMS m/z Calculated for $C_{19}H_{24}ClN_5O$:373.17 IR Vmax (cm-1))2280 (O=CNH), 1660 (C=N), 1635(C=C), 1260(C-N) 740 (C-Cl) Elemental Analysis: Calculated: C,61.04; H,6.47; Cl,9.48; N,18.73; O,4.28; Experimental: C,61.00; H,6.46; Cl,9.44; N,18.71; O,4.27.

1.1.8.(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(3,5-dichlorophenyl)piperazine-1-carboxamide(5h)

^{1}H NMR (400 MHz, $CDCl_3$), 9.52 (1H,s,CH=N) 7.40(9.52 (1H,s,CH=N) 7.40(H,dd, Py-H) 6.82 (3H,dd,Ar-H) 5.32 (1H,s,NH) 3.60(4H,dd,CH2-CH2) 3.35 (8H,dd,Pip-H) 1.82 (3H,s,Py-H) ^{13}C

NMR: (400Hz, $CDCl_3$)188.0 (C=N) 164 (CONH) 155 (Py-C) 153 (PyC) 141 (Py-C) 139 (Py-C) 131 (Ar-C) 128 (Ar-C)67 (Pip-C) 59 (Pip-C) 56 (CH_2)LCMS m/z Calculated for $C_{19}H_{23}Cl_2N_5O$:407.13 IR Vmax (cm-1)2290 (O=CNH), 1660 (C=N), 1635(C=C), 1260(C-N) 750 (C-Cl) Elemental Analysis: Calculated: C,55.89; H,5.68; N,17.15; Cl,17.36; O,3.92; Experimental: C,55.87; H,5.65; N,17.14; Cl,17.33; O,3.91.

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

^1H NMR (400 MHz, $CDCl_3$), 9.80 (1H,s,CH=N) 8.21 (1H,d,Py-H) 7.22 (2H, d,Py-H) 6.98 (4H,dd,Ar-H) 5.29 (1H,s,NH) 3.82 (6H,d,Pip-H) 3.39 (2H,d,Pip-H) 3.75 (1H,d, CH2) 2.80 (3H,s, Py-CH3) 2.52 (3H,d,CH2-CH2 ^{13}C NMR: (400Hz, $CDCl_3$)186.0 (C=N) 164 (CONH) 155 (Py-C) 152 (PyC) 141 (Py-C) 139 (Py-C) 131 (Ar-C) 129(Ar-C)67(Pip-C) 59 (Pip-C) 56 (CH_2) LCMS m/z Calculated for $C_{19}H_{24}FN_5O$:357.43 IR Vmax (cm-1) 2250 (O=CNH), 1680 (C=N), 1635(C=C), 1250 (C-N) 650 (C-F) Elemental Analysis: Calculated: C,63.85; H,6.77; N,19.59; O,4.48; F,5.32 ; Experimental: C,63.81; H,6.75; N,19.57; O,4.47; F,5.30.

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

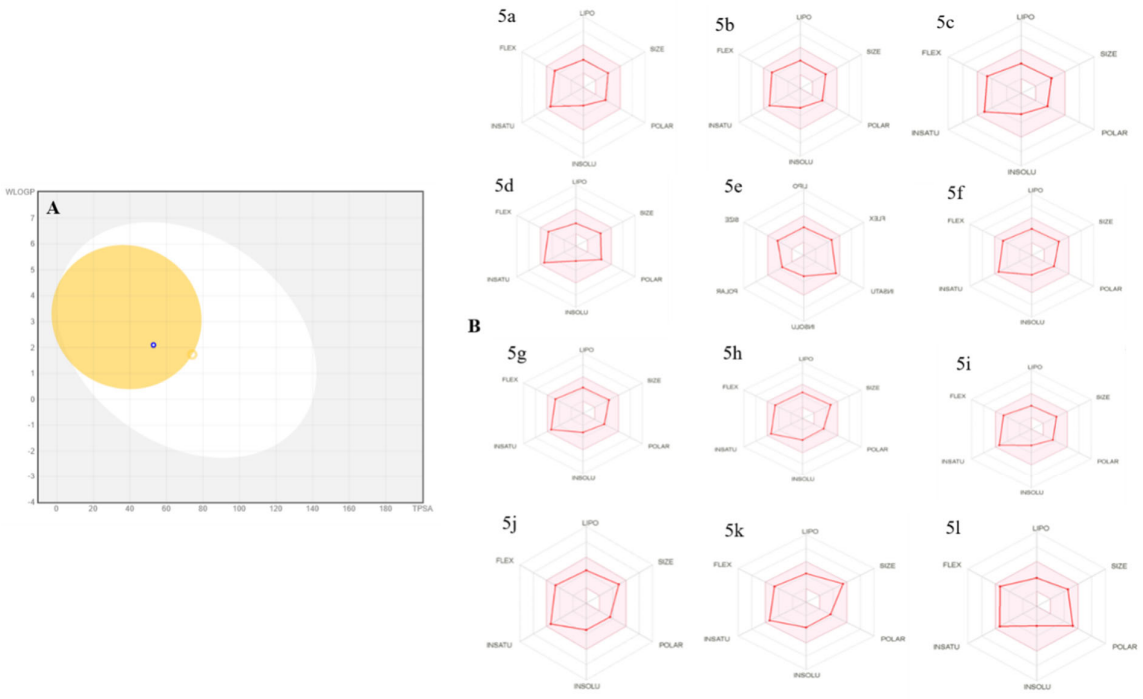
^1H NMR (400 MHz, $CDCl_3$), 8.21 (1H,d,Py-H) 7.21 (4H, d,Ar-H) 7.01(2H,d,Py-H) 6.45 (1H,s,CH=N) 5.24 (1H,s,NH) 3.75(8H,dd,Pp-H) 3.65(1H,d,CH2-CH2) 3.30(3H,s,Py-CH3) 3.22(3H,d,CH2-CH2) ^{13}C NMR: (400Hz, $CDCl_3$)191.0 (C=N) 167 (CONH) 158 (Py-C) 157 (PyC) 143 (Py-C) 145 (Py-C) 134 (Ar-C) 133 (Ar-C) 71 (Pip-C) 62 (Pip-C) 60 (CH_2)LCMS m/z Calculated for $C_{19}H_{24}BrN_5O$:418.33 IR Vmax (cm-1) 2270 (O=CNH), 1665 (C=N), 1640(C=C), 1260(C-N) 580 (C-Br) Elemental Analysis: Calculated: C,54.55; H,5.78; N,16.74; O,3.82; Br,19.10 Experimental: C,54.52; H,5.77; N,16.71; O,3.81; Br,19.06.

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

^{1}H NMR (400 MHz, $CDCl_3$), 7.83 (2H, d,Ar-H) 7.59(1H,s,CH=N) 7.32(2H,d,Ar-H) 7.14 (3H,d,Py-H) 5.32 (1H,s,NH) 2.91(8H,dd,Pip-H) 2.25 (4H,dd,CH2-CH2) 2.95 (3H,s,Py-CH3) ^{13}C NMR: (400Hz, $CDCl_3$)181.0 (C=N) 161 (CONH) 150 (Py-C) 147 (PyC) 138 (Py-C) 134 (Py-C) 131 (Ar-C) 128 (Ar-C)125 (Ar-C)121 (Ar-C) 63 (Pip-C) 58 (Pip-C) 52 (CH_2)LCMS m/z Calculated for $C_{19}H_{24}IN_5O$:465.33 IR Vmax (cm-1) 2290 (O=CNH), 1685 (C=N), 1620(C=C), 1270 (C-N) 560 (C-Br) Elemental Analysis: Calculated:C, 49.04; H, 5.20; I, 27.27; N, 15.05; O, 3.44; Experimental: C, 49.02; H, 5.17; I, 27.24; N, 15.04; O, 3.43.

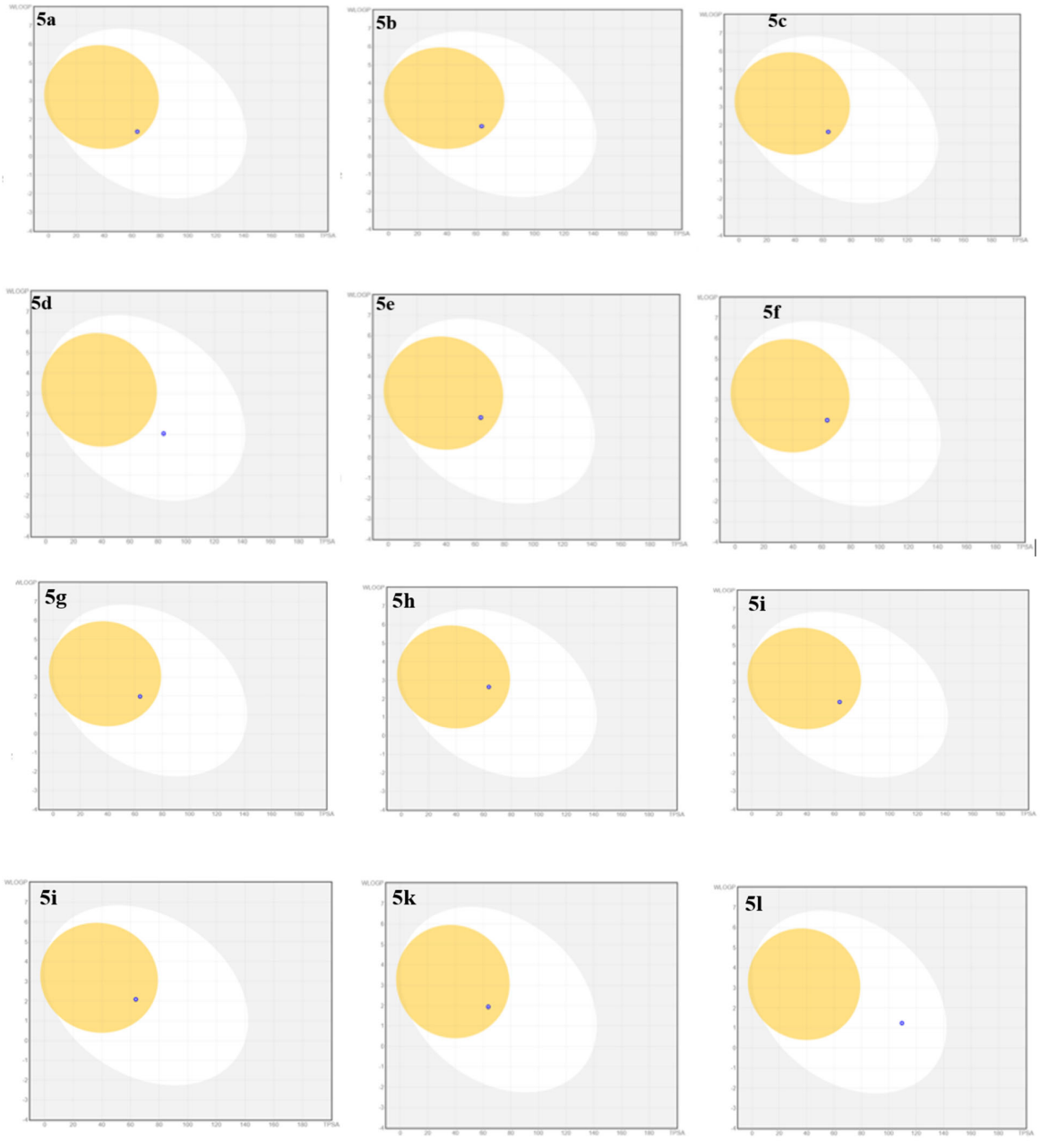
1.1.12.(Z)-4-(2-(((1H-pyrrol-2-yl)methylene)amino)ethyl)-N-(4-nitrophenyl)piperazine-1-carboxamide(5l)

^{1}H NMR (400 MHz, $CDCl_3$), 8.92 (1H,s,CH=N) 8.45 (2H,d, Ar-H) 7.80 (1H, d, Py-H) 7.45 (2H,d,Ar-H) 7.21 (1H,s,NH) 6.90 (2H, d,Py-H) 4.19 (3H,s,Py-CH3) 3.81 (2H,d,CH2-CH2) 3.42(4H,d,Pip-H) 2.92 (2H,d,CH2-CH2) 2.20 (4H,d,Pip-H)^{13}C NMR: (400Hz, $CDCl_3$)182.0 (C=N) 161 (CONH) 150 (Py-C) 147 (PyC) 139 (Py-C) 134 (Py-C) 131 (Ar-C) 128 (Ar-C)125 (Ar-C)121 (Ar-C) 63 (Pip-C) 52 (Pip-C) LCMS m/z Calculated for $C_{19}H_{24}N_6O_3$:384.13IR Vmax (cm-1) 2280(O=CNH), 1670 (C=N), 1635 (C=C), 1260(C-N) 1580 (C-NO_2) Elemental Analysis: Calculated:C, 59.36; H, 6.29; N, 21.86; O, 12.48; Experimental: C, 59.35; H, 6.28; N, 21.85; O, 12.4

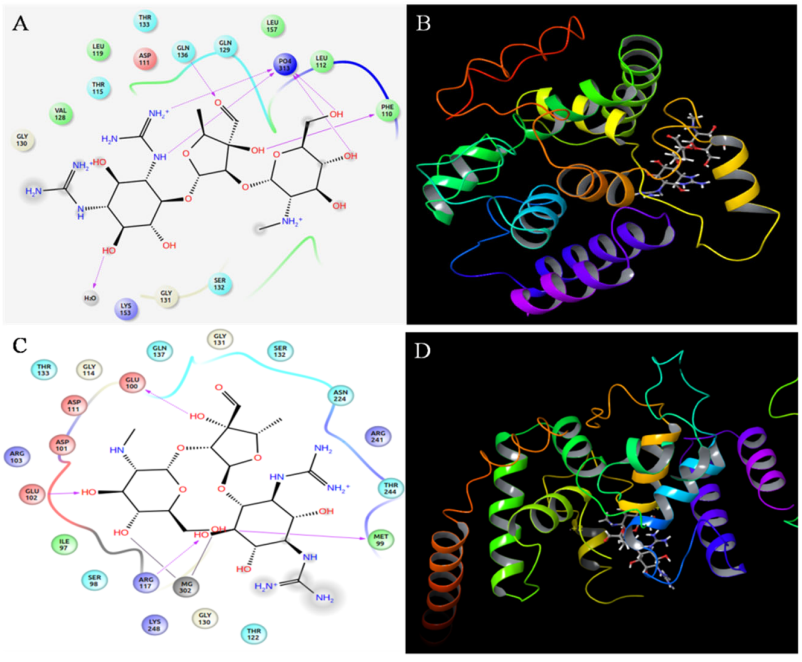


Supplementary Fig S1. Structure of synthesized compounds 5(a-l): (A) The BOILED-Egg representation of GI and BBB properties of the Compound 5j. (B) Bioavailability radar graph of 5(a-l) (pink area reflects the allowed values of drug likeness properties of the molecule

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



Supplementary Fig S3: Molecular docking proof for standard streptomycin against proteins6FTB (A&B), 3VMT (C&D) of MRSA.

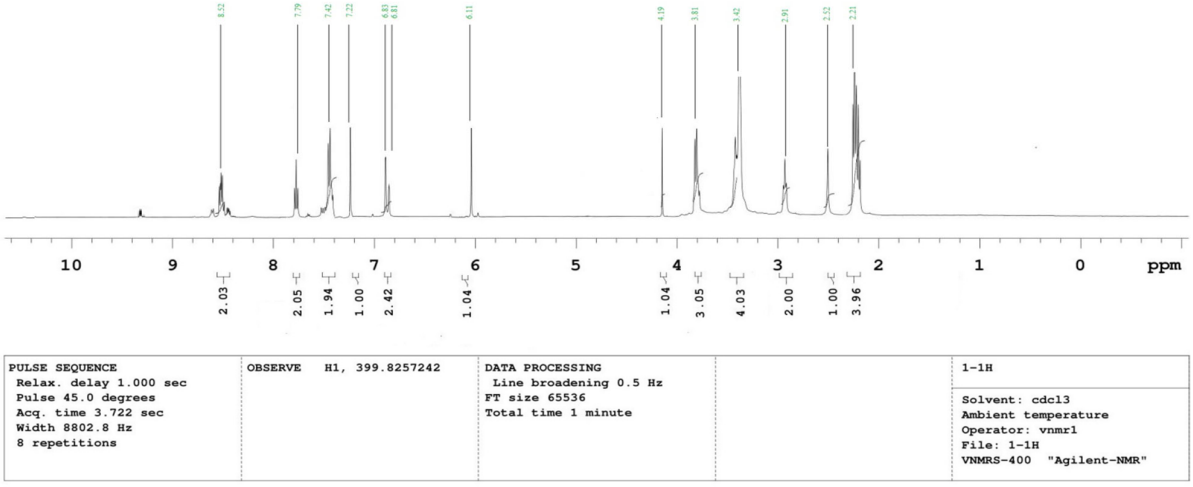


NMRand LC-MS data of new compounds

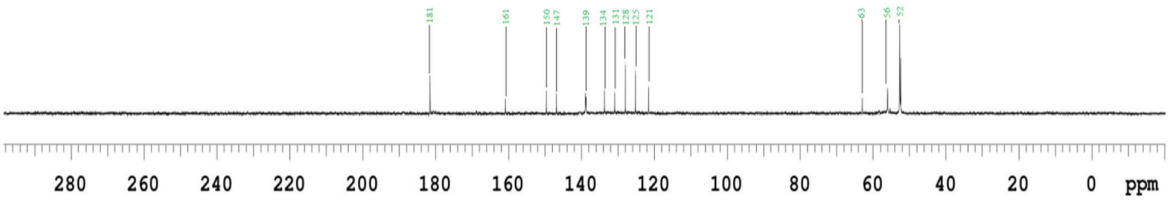
[NOTE:A. ^{1}H NMR spectra, B.^{13}C NMR spectra, C. FTIR and D.LC-MS]

Supplementary Fig S4: Compound (5a)

(A)

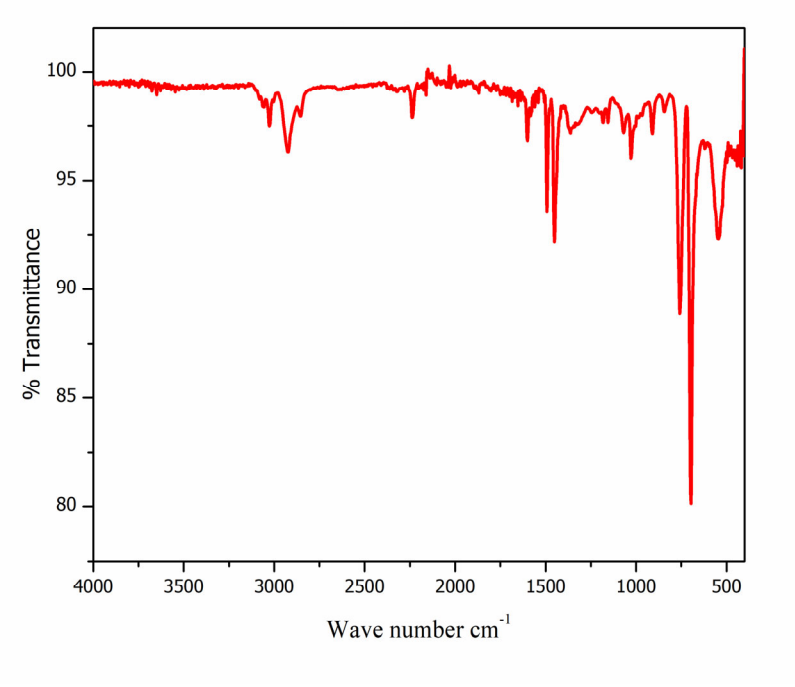


(B)

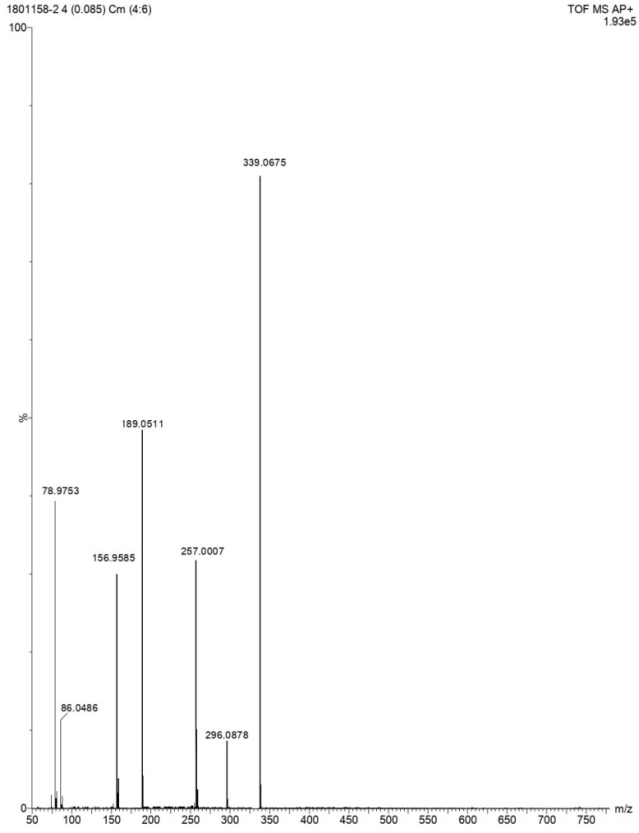


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 2722 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 91 minutes		7-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 7-13C VNMRS-400 "Agilent-NMR"

(C)

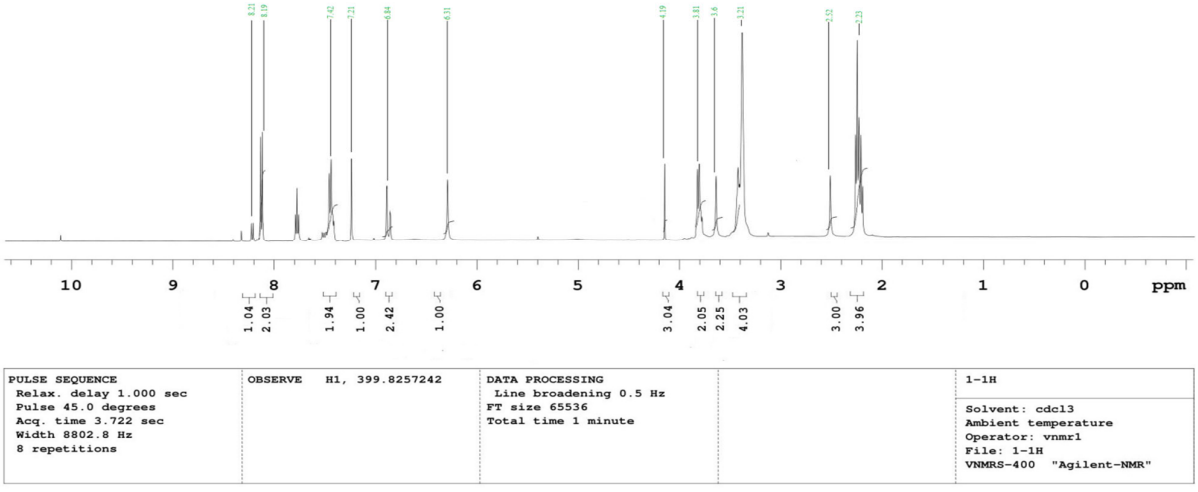


(D)

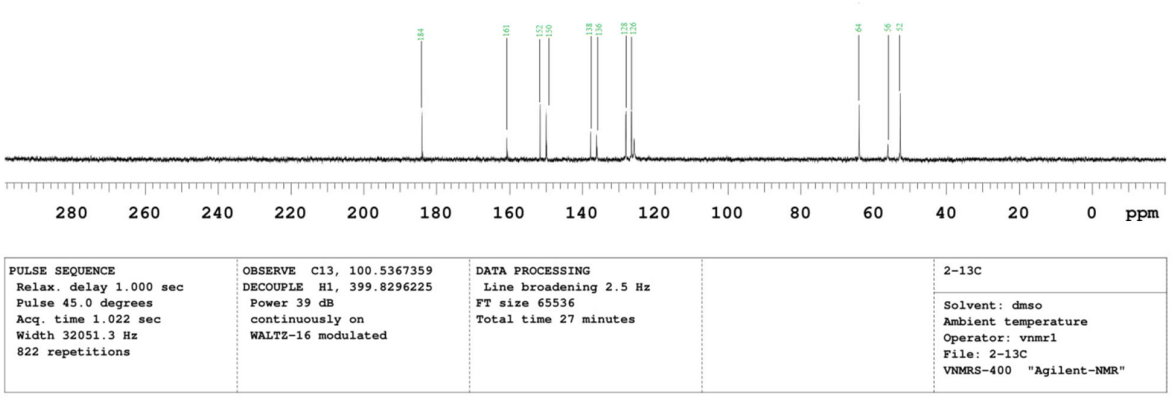


Supplementary Fig S5: Compound (5b)

(A)

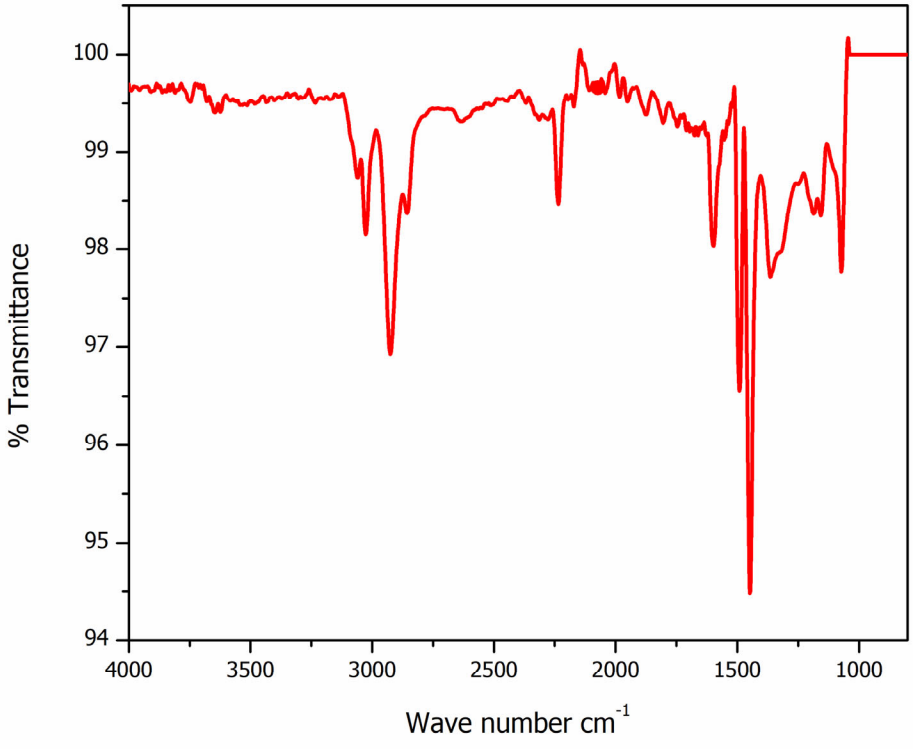


(B)

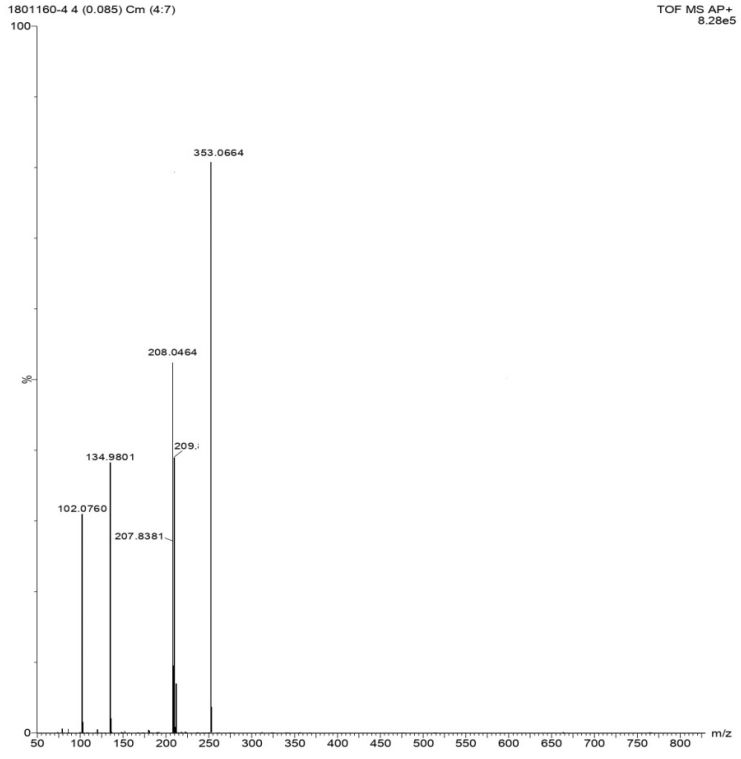


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 822 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 27 minutes		2-13C Solvent: dmso Ambient temperature Operator: vnmrl File: 2-13C VNMRS-400 "Agilent-NMR"

(C)

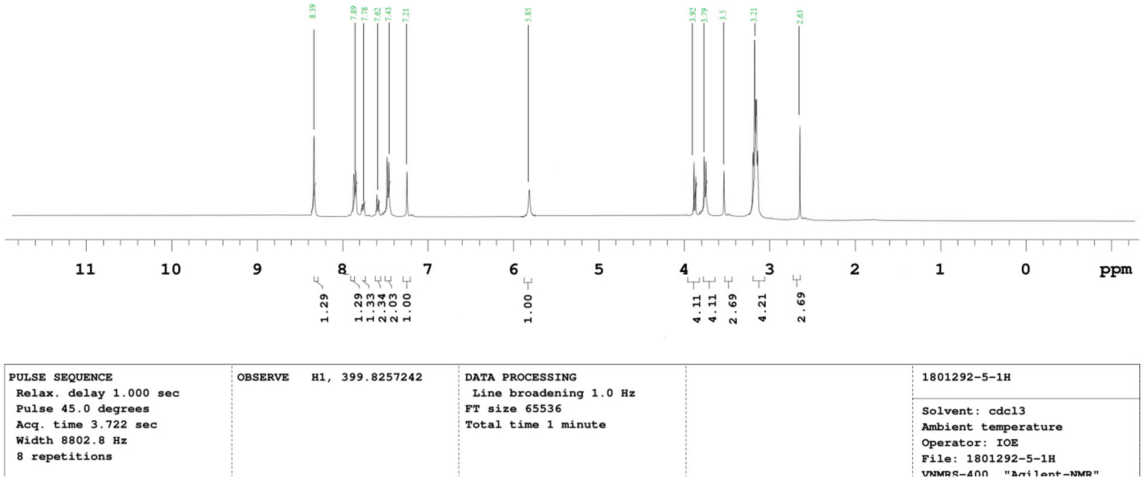


(D)

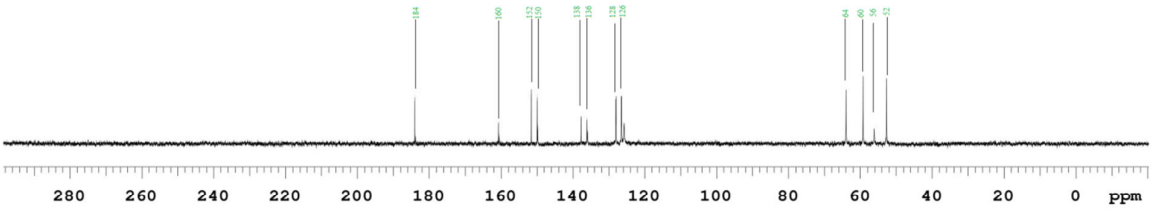


Supplementary Fig S6: Compound (5c)

(A)

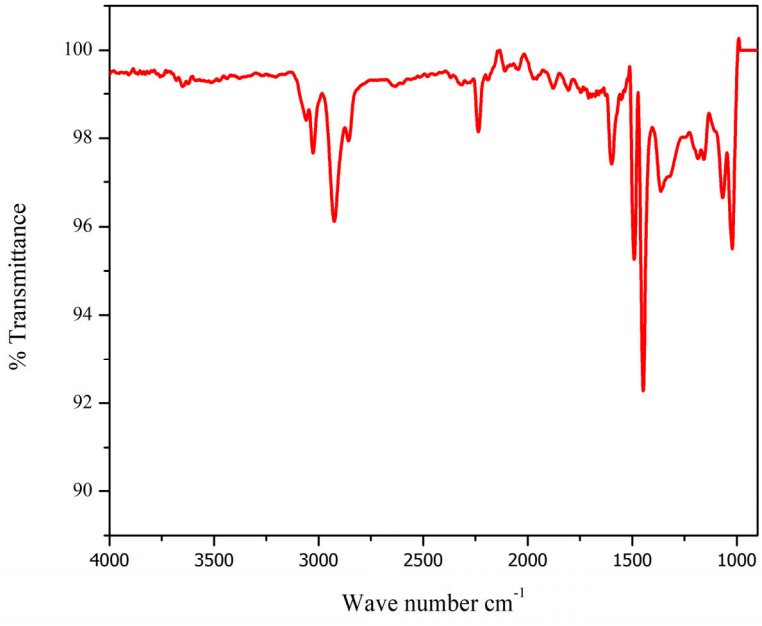


(B)

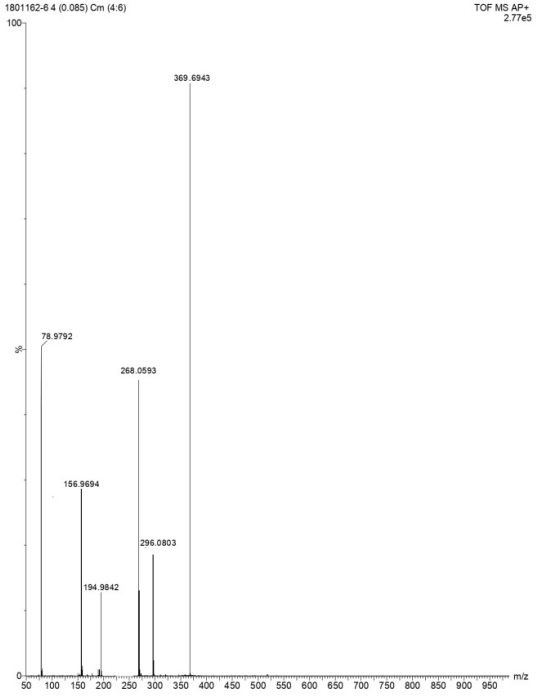


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 822 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 27 minutes		2-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 2-13C VNMRS-400 "Agilent-NMR"

(C)

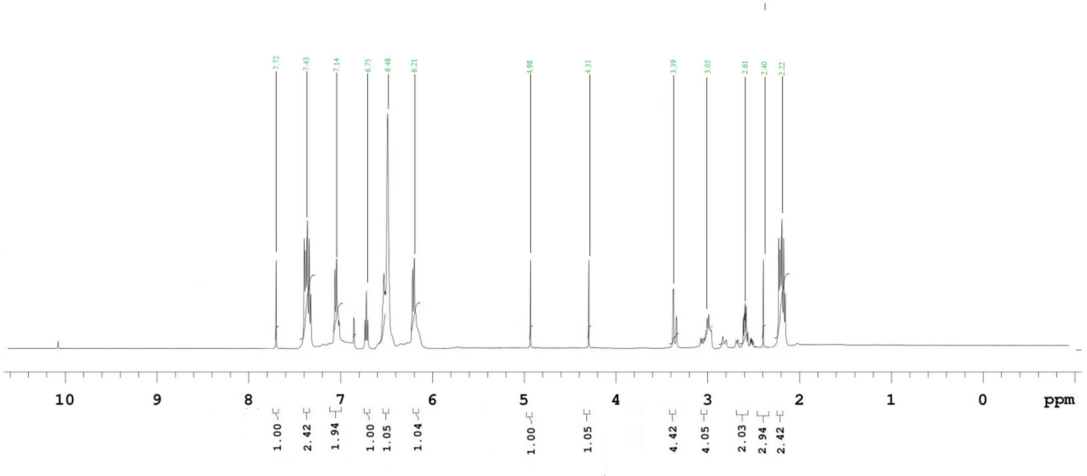


(D)

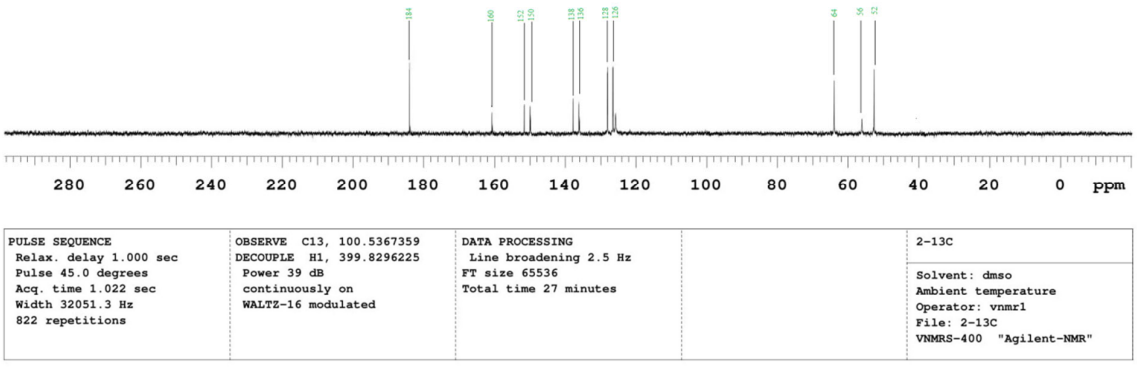


Supplementary Fig S7: Compound (5d)

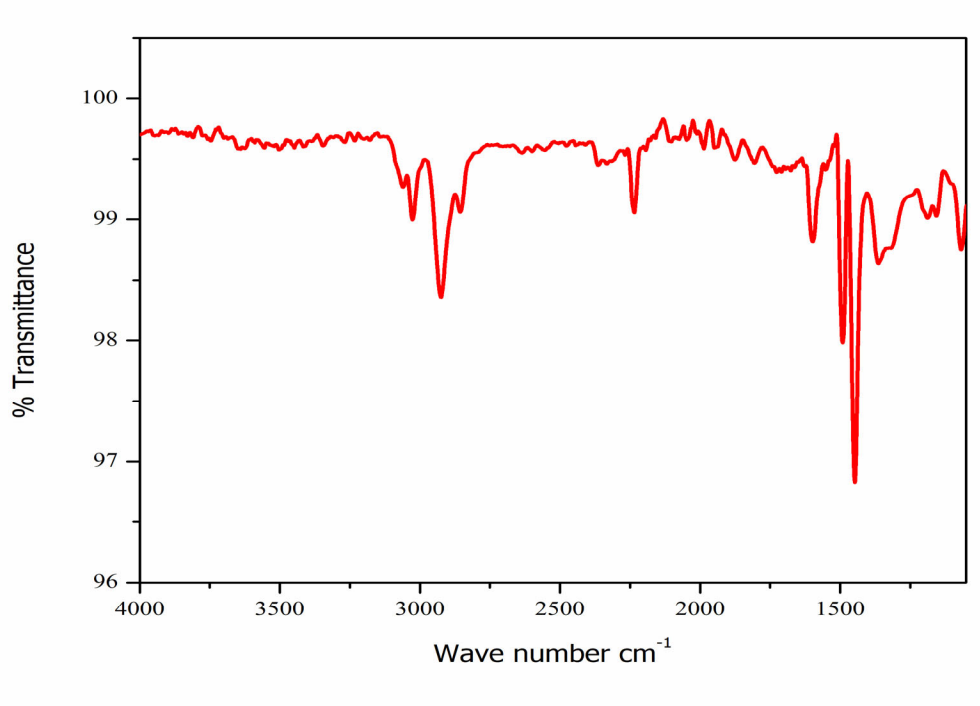
(A)



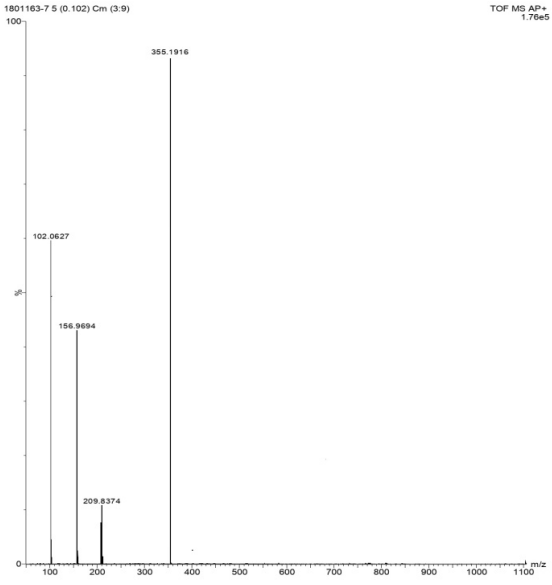
(B)


184
160
152
150
138
136
128
126
64
56
52
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
822 repetitions
OBSERVE C13, 100.5367359
DECOUPLE H1, 399.8296225
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 65536
Total time 27 minutes
2-13C
Solvent: dmso
Ambient temperature
Operator: vnmr1
File: 2-13C
VNMRS-400 "Agilent-NMR"

(C)

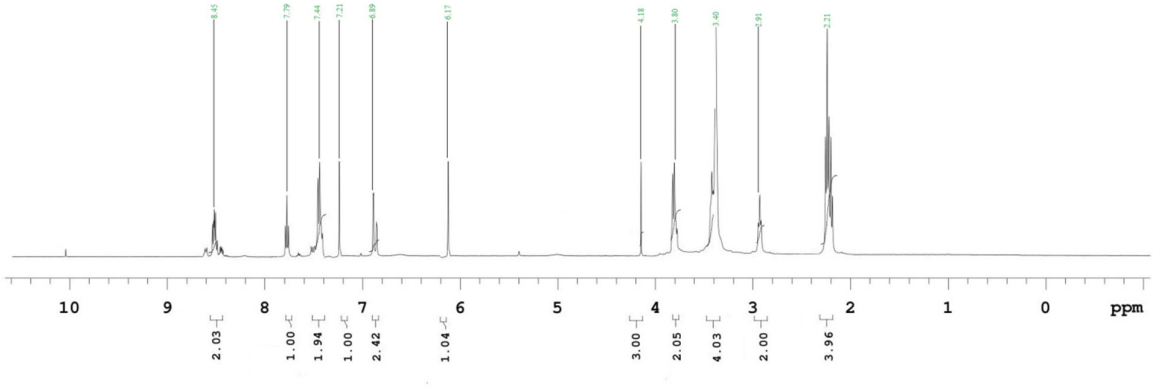

100
99
98
97
96
% Transmittance
4000
3500
3000
2500
2000
1500
Wave number cm-1

(D)



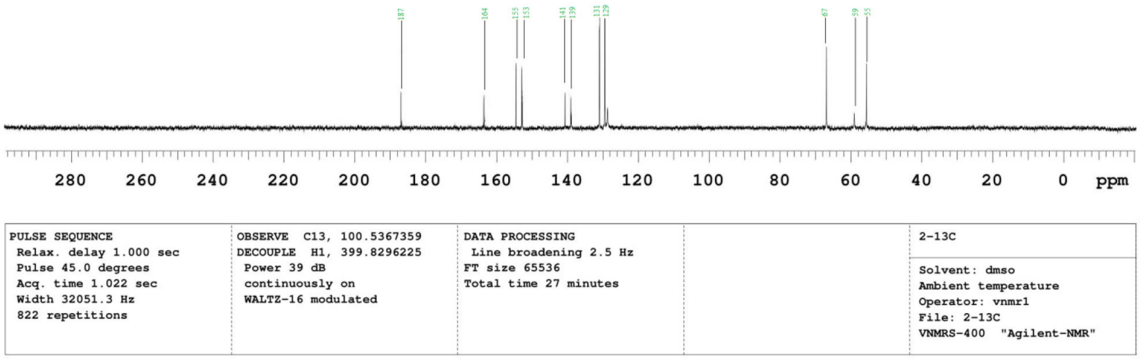
Supplementary Fig S8: Compound (5e)

(A)

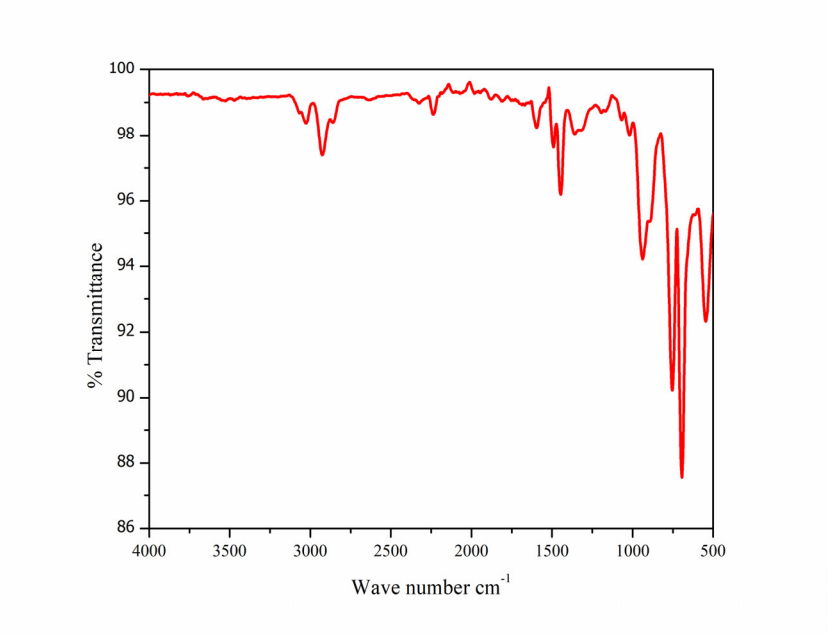


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 3.722 sec Width 8802.8 Hz 8 repetitions	OBSERVE H1, 399.8257242	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 1 minute		1-1H Solvent: cdcl3 Ambient temperature Operator: vnmr1 File: 1-1H VNMRS-400 "Agilent-NMR"

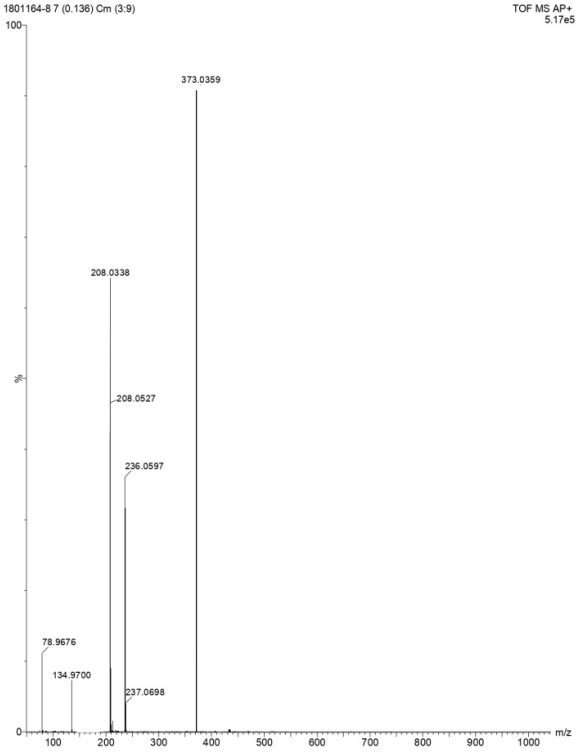
(B)


187
164
155
153
141
139
131
129
67
59
55
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
822 repetitions
OBSERVE C13, 100.5367359
DECOUPLE H1, 399.8296225
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 65536
Total time 27 minutes
2-13C
Solvent: dmso
Ambient temperature
Operator: vnmr1
File: 2-13C
VNMRS-400 "Agilent-NMR"

(C)

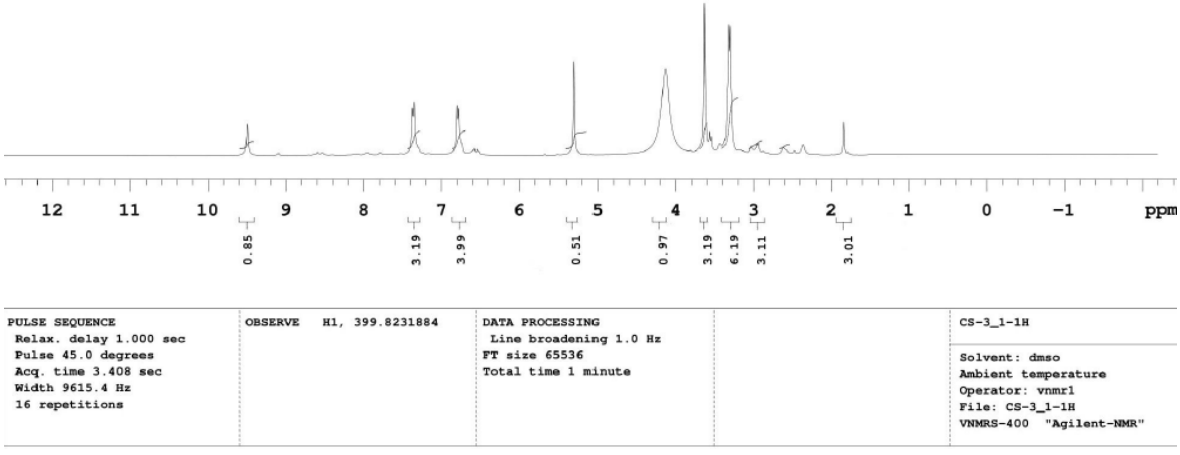

100
98
96
94
92
90
88
86
% Transmittance
4000 3500 3000 2500 2000 1500 1000 500
Wave number cm-1

(D)

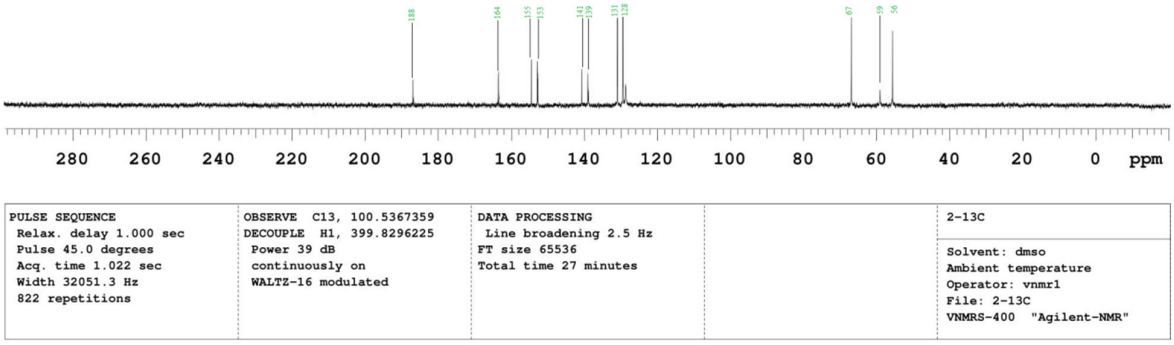


Supplementary Fig S9: Compound (5h)

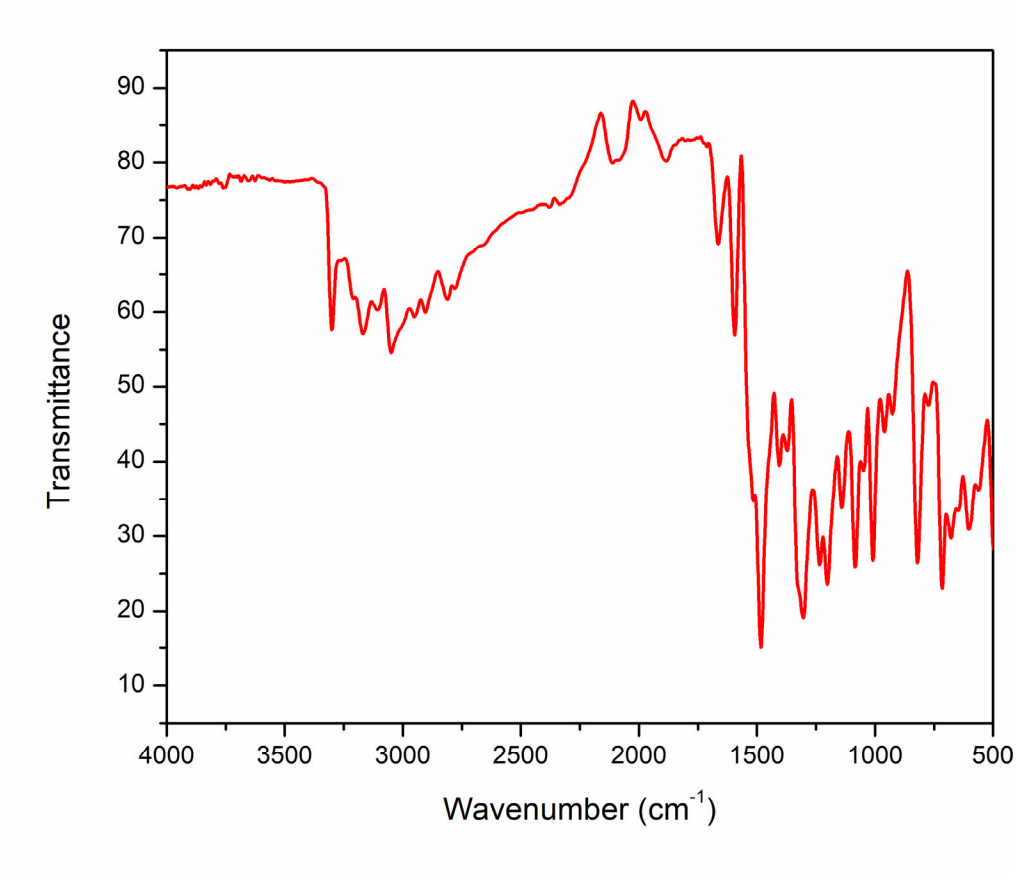
(A)



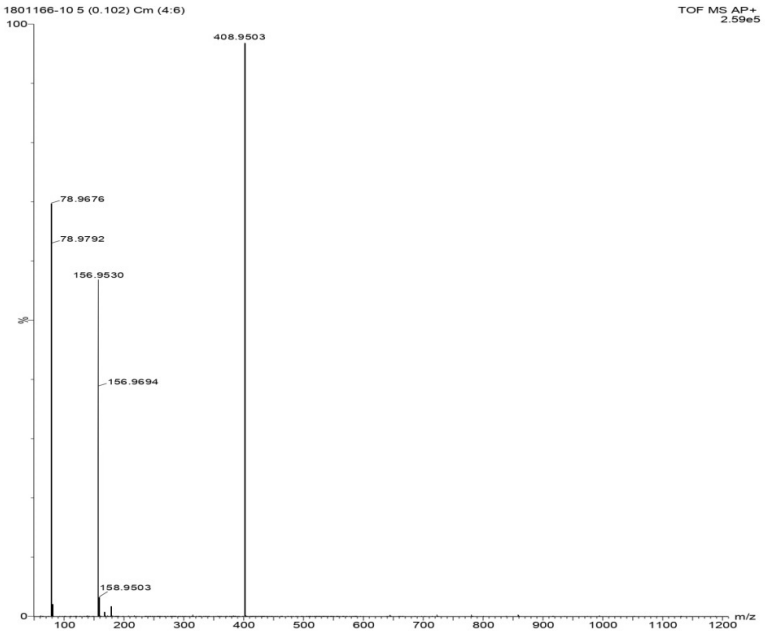
(B)


188
164
155
153
141
139
131
128
67
59
56
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
822 repetitions
OBSERVE C13, 100.5367359
DECOUPLE H1, 399.8296225
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 65536
Total time 27 minutes
2-13C
Solvent: dmso
Ambient temperature
Operator: vnmr1
File: 2-13C
VNMRS-400 "Agilent-NMR"

(C)

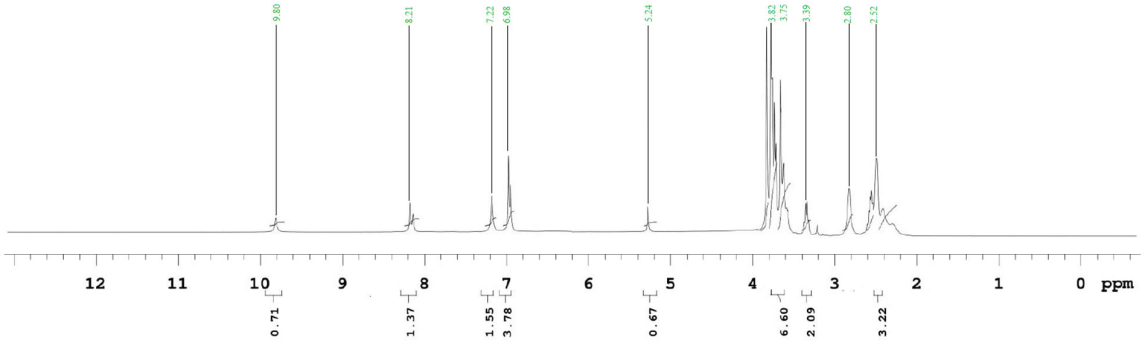

Transmittance
90
80
70
60
50
40
30
20
10
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

(D)



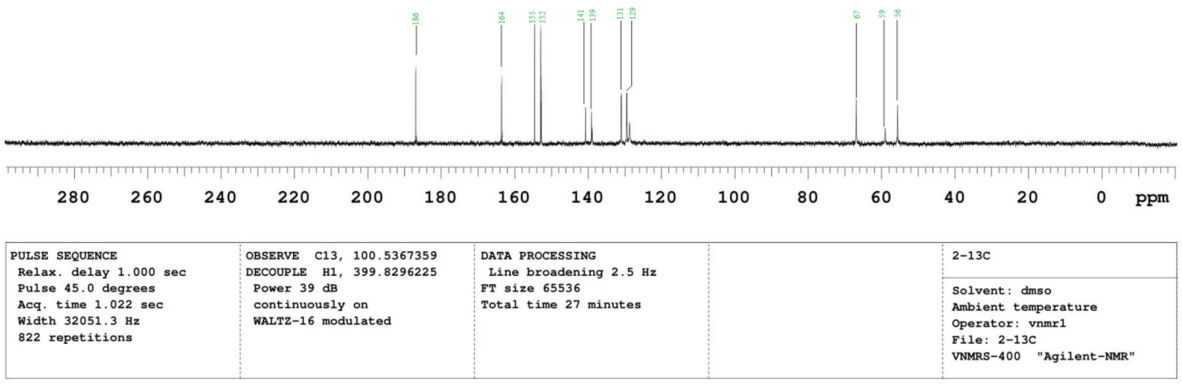
Supplementary Fig S10: Compound (5i)

(A)

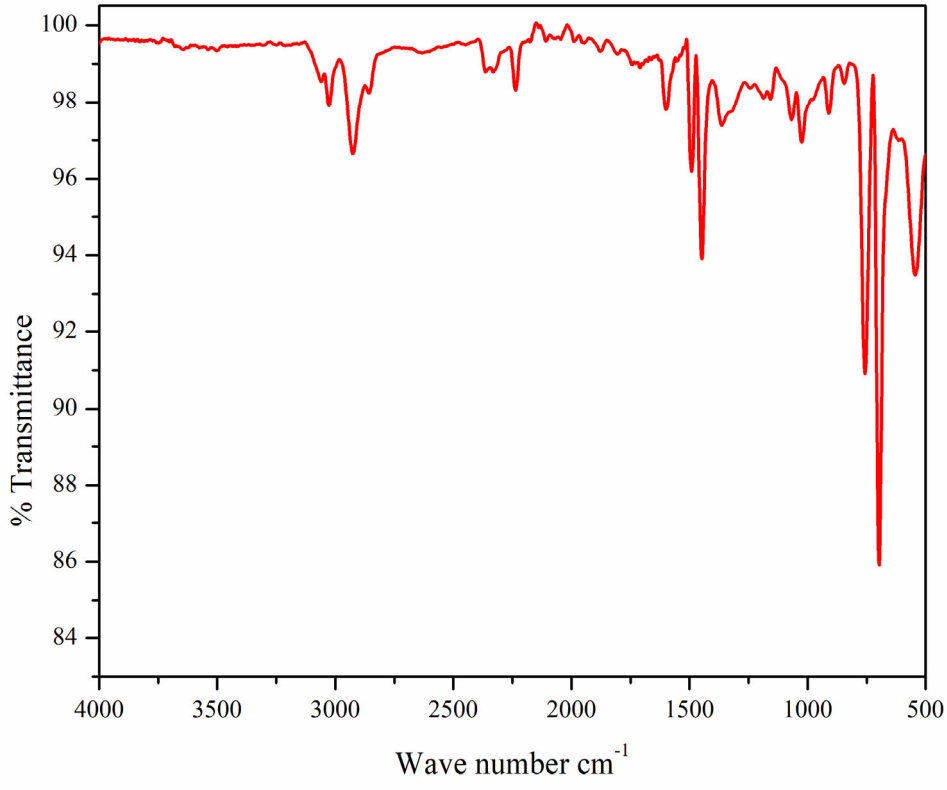


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 3.408 sec Width 9615.4 Hz 16 repetitions	OBSERVE H1, 399.8231884	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 1 minute		NS-1_1-1H Solvent: dmso Ambient temperature Operator: vnmr1 File: NS-1_1-1H VNMRS-400 "Agilent-NMR"

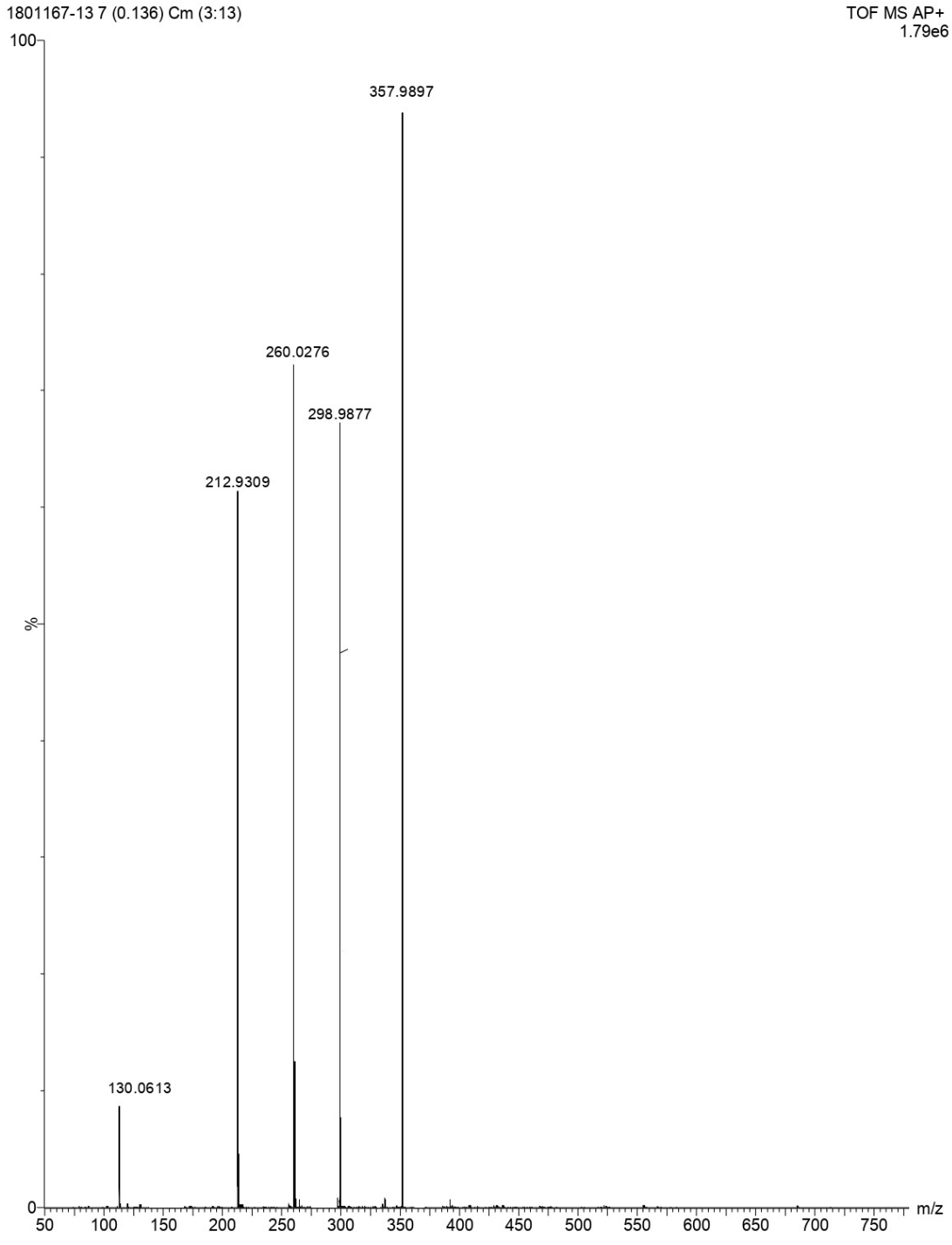
(B)


186
164
155
152
141
139
131
129
67
59
56
280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
822 repetitions
OBSERVE C13, 100.5367359
DECOUPLE H1, 399.8296225
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 65536
Total time 27 minutes
2-13C
Solvent: dmso
Ambient temperature
Operator: vnmr1
File: 2-13C
VNMRS-400 "Agilent-NMR"

(C)

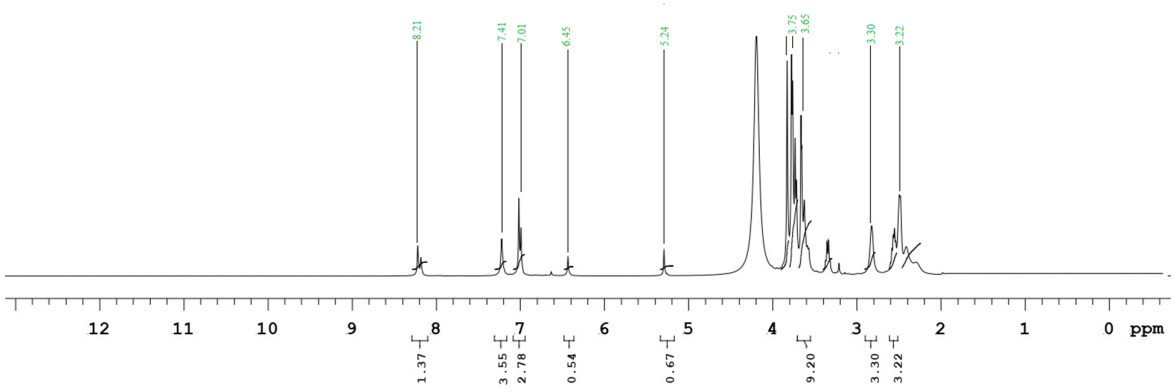

% Transmittance
100
98
96
94
92
90
88
86
84
4000 3500 3000 2500 2000 1500 1000 500
Wave number cm-1

(D)


1801167-13 7 (0.136) Cm (3:13)
TOF MS AP+
1.79e6
100
%
0
357.9897
260.0276
298.9877
212.9309
130.0613
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
m/z

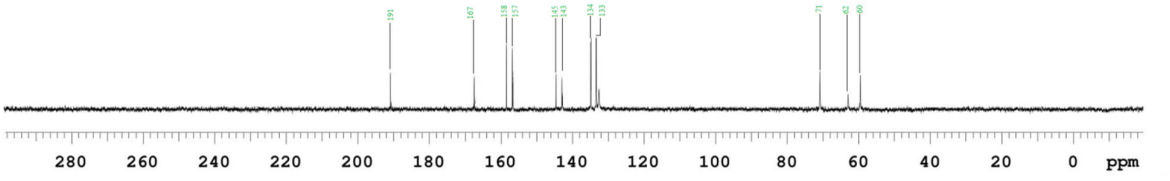
Supplementary Fig S11: compound 5j

(A)



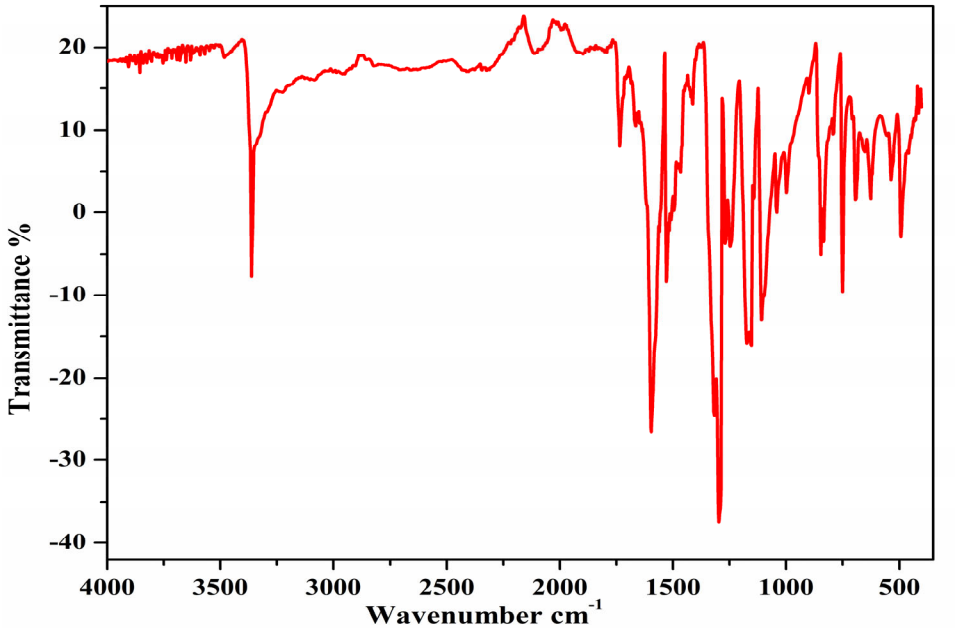
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 3.408 sec Width 9615.4 Hz 16 repetitions	OBSERVE H1, 399.8231884	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 1 minute		NS-1_1-1H Solvent: dmso Ambient temperature Operator: vnmr1 File: NS-1_1-1H VNMRS-400 "Agilent-NMR"

(B)

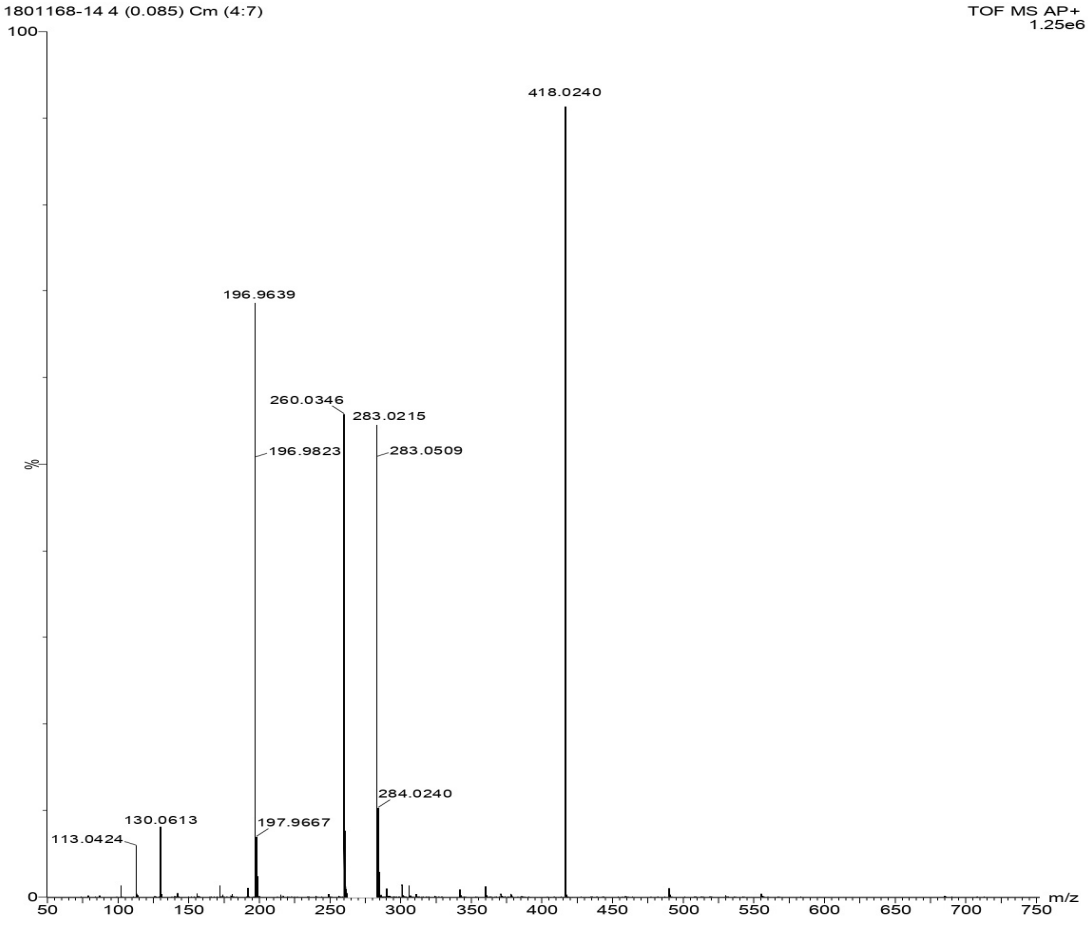


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 822 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 27 minutes		2-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 2-13C VNMRS-400 "Agilent-NMR"

(C)

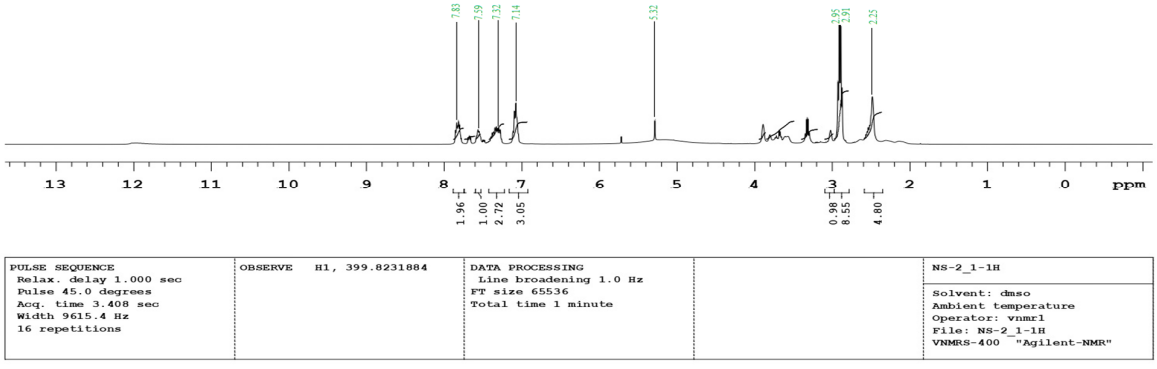

Transmittance %
20
10
0
-10
-20
-30
-40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(D)



Supplementary Fig S12: compound 5k

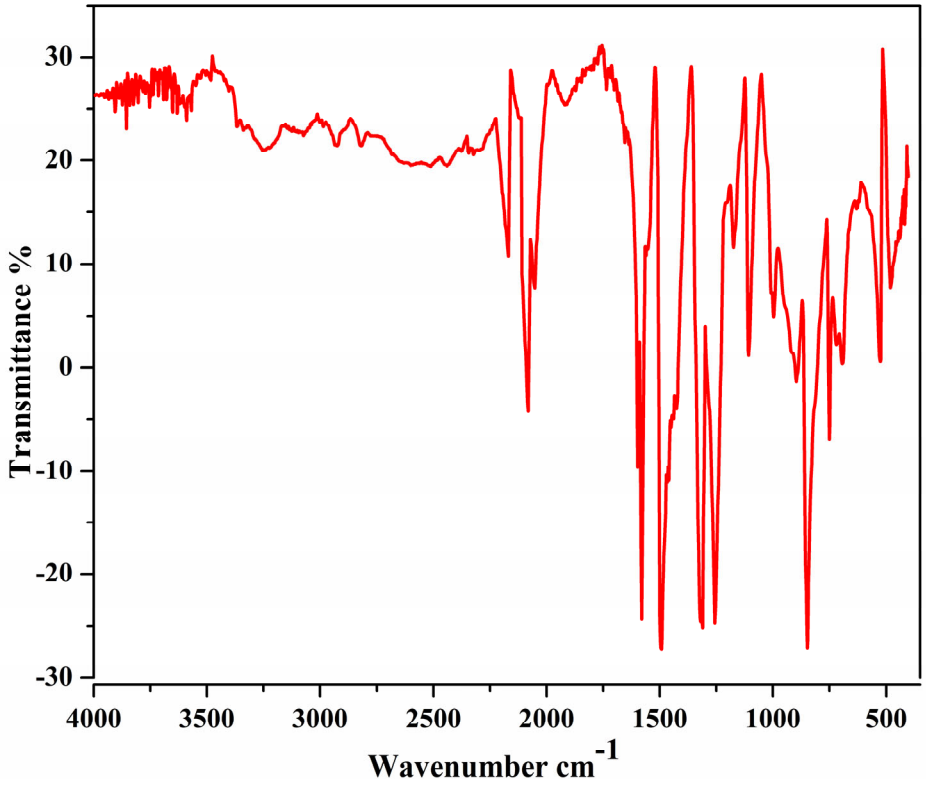
(A)



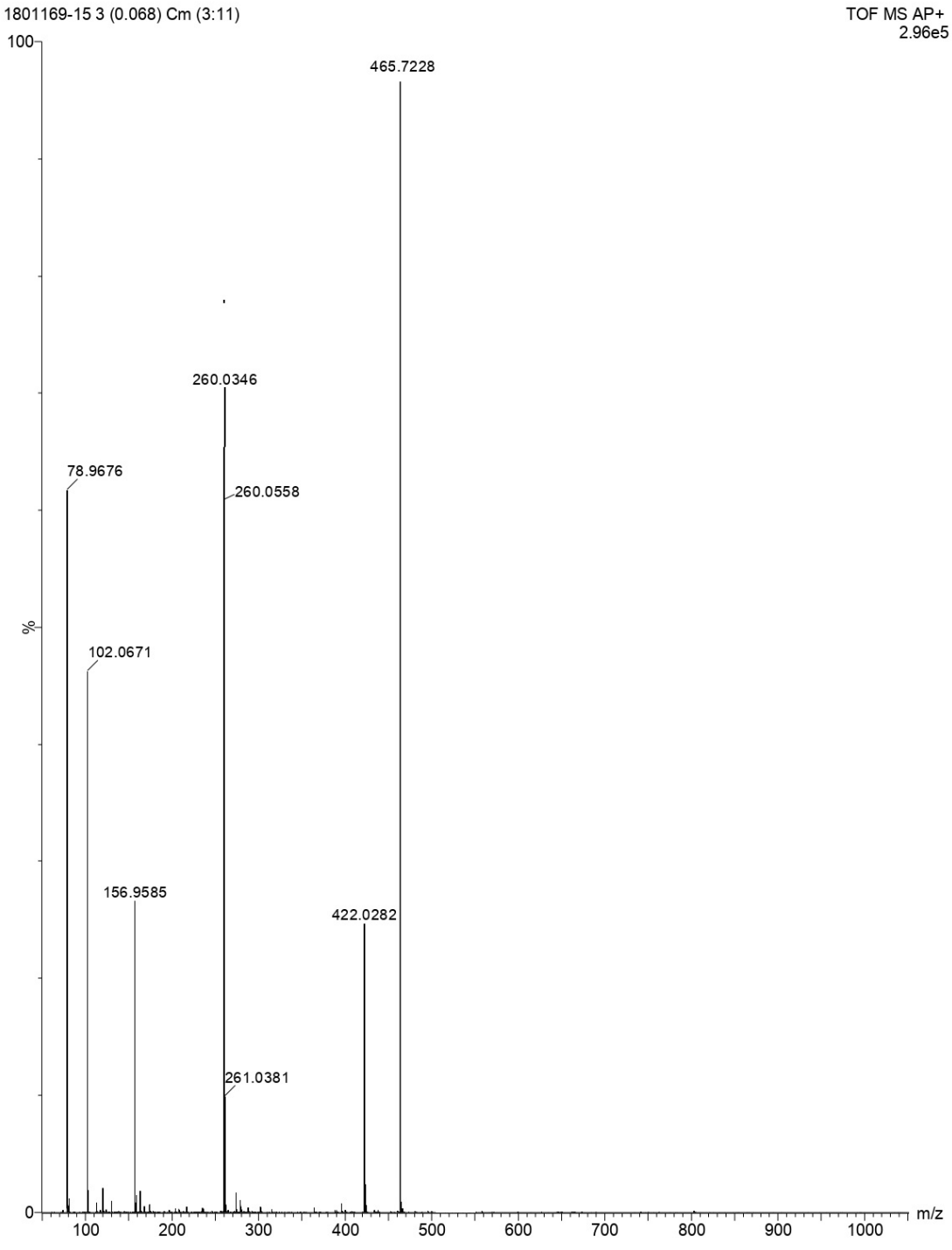
(B)


181
161
150
147
138
134
131
128
125
121
63
58
52
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
2722 repetitions
OBSERVE C13, 100.5367359
DECOUPLE H1, 399.8296225
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 65536
Total time 91 minutes
7-13C
Solvent: dmso
Ambient temperature
Operator: vnmr1
File: 7-13C
VNMRS-400 "Agilent-NMR"

(C)

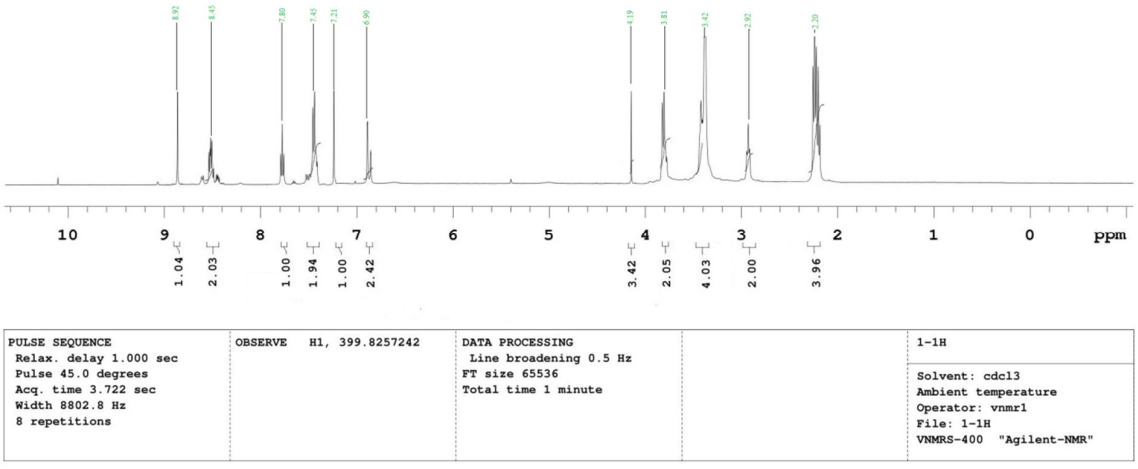

Transmittance %
30
20
10
0
-10
-20
-30
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(D)


1801169-15 3 (0.068) Cm (3:11)
TOF MS AP+
2.96e5
100
%
0
465.7228
260.0346
260.0558
78.9676
102.0671
156.9585
422.0282
261.0381
100
200
300
400
500
600
700
800
900
1000
m/z

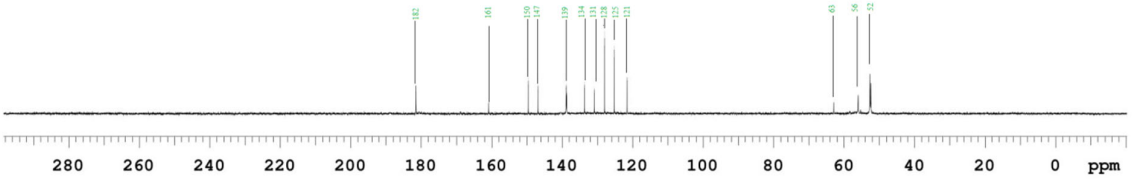
Supplementary Fig S13: compound 5l

(A)



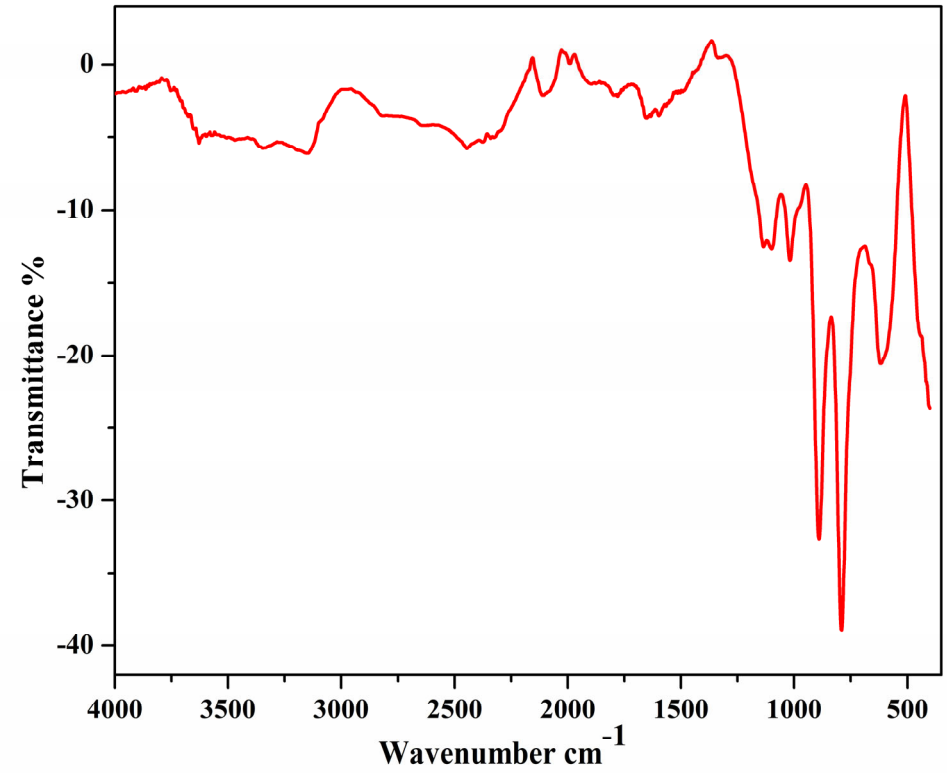
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 3.722 sec Width 8802.8 Hz 8 repetitions	OBSERVE H1, 399.8257242	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 1 minute		1-1H Solvent: cdcl3 Ambient temperature Operator: vnmr1 File: 1-1H VNMRS-400 "Agilent-NMR"

(B)

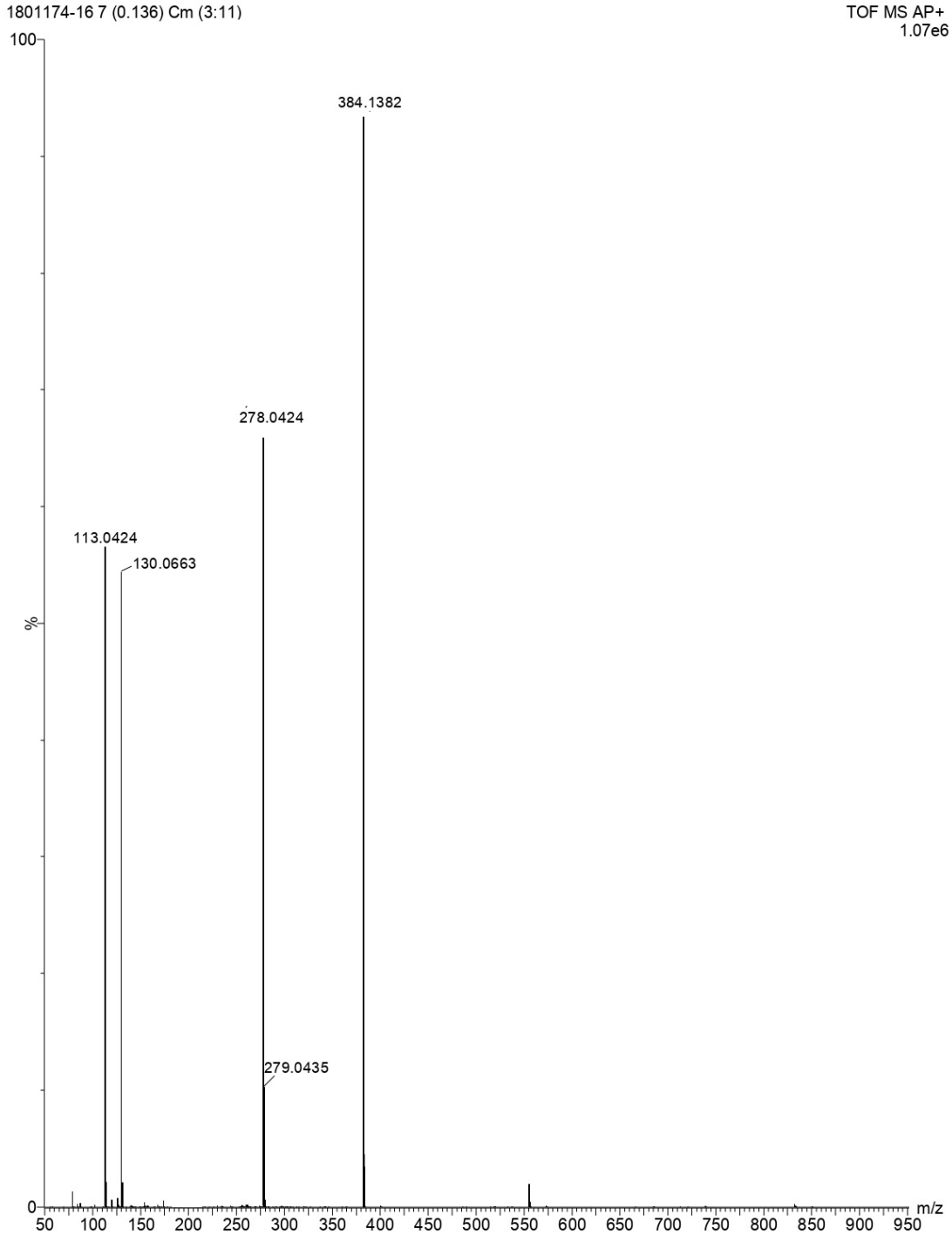


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 2722 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 91 minutes		7-13C Solvent: dmso Ambient temperature Operator: vnmr1 File: 7-13C VNMRS-400 "Agilent-NMR"

(C)


0
-10
-20
-30
-40
Transmittance %
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(D)


1801174-16 7 (0.136) Cm (3:11)
TOF MS AP+
1.07e6
100
%
0
384.1382
278.0424
113.0424
130.0663
279.0435
m/z
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950

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

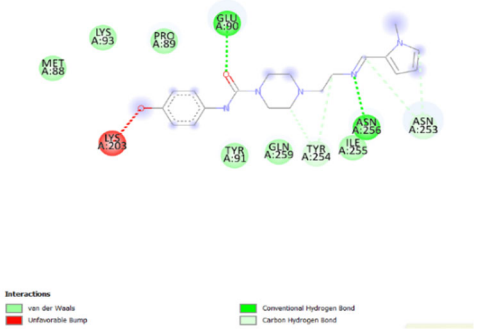
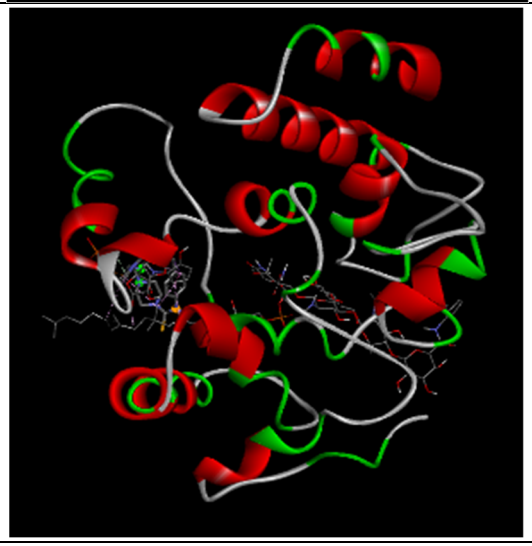
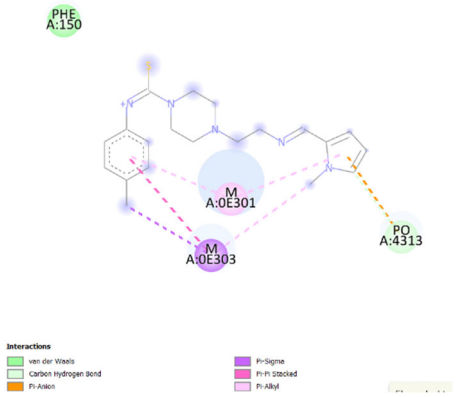
Compound	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
5(a)	0.12	-0.05	0.18	-0.39	-0.24	0.12
5(b)	0.07	-0.13	0.13	-0.40	-0.29	0.05
5(c)	0.06	-0.13	0.13	-0.38	-0.28	0.06
5(d)	0.15	-0.01	0.22	-0.24	-0.22	0.16
5(e)	0.11	-0.06	0.16	-0.40	-0.27	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

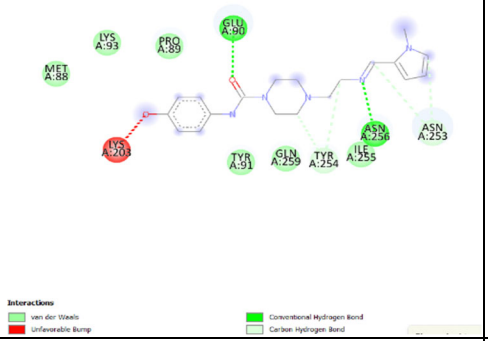
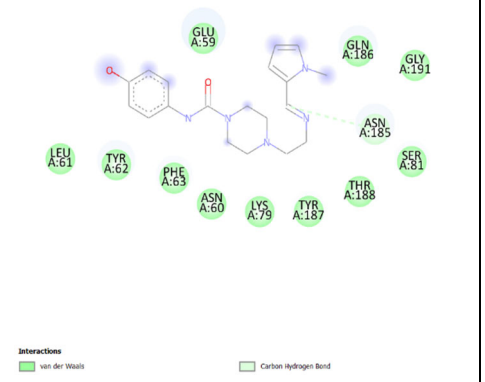
Supplementary table S2 - Predicted biological activities of compounds 5(a-l), Pa (probability "to be active"), Pi (probability "to be inactive").

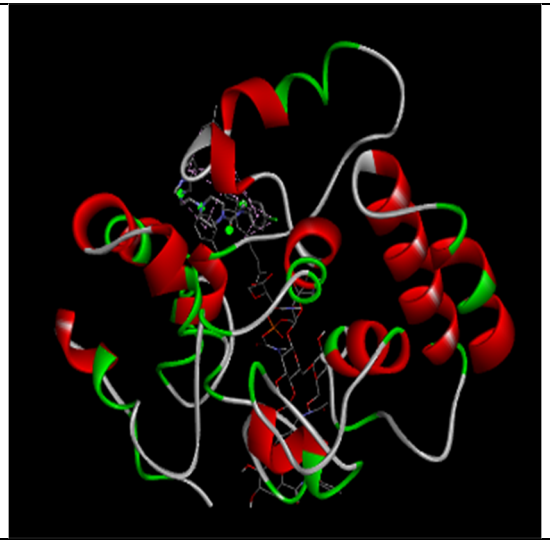
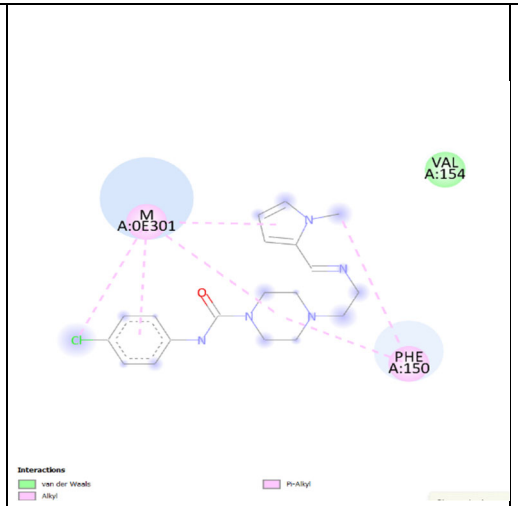
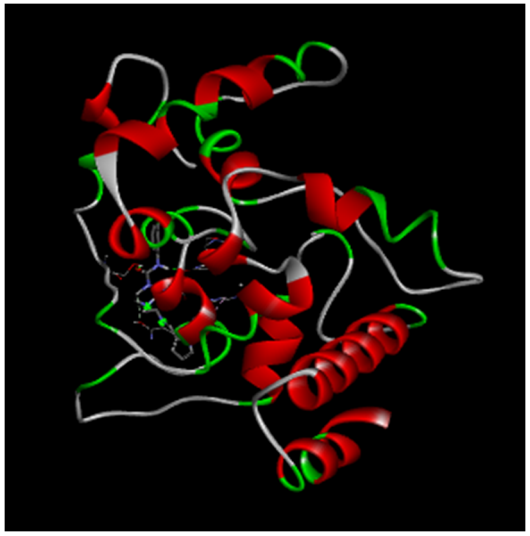
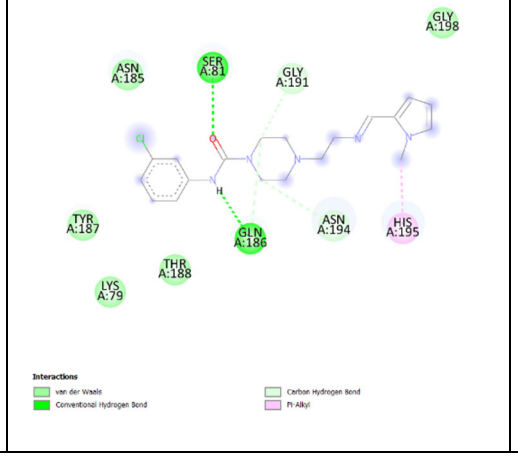
Activity	5a		5b		5c		5d		5e		5f	
	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi
Antineoplastic	0.651	0.035	0.603	0.044	0.642	0.036	0.648	0.035	0.538	0.060	0.539	0.060
Protein kinase inhibitor	0.150	0.092	0.130	0.107	0.125	0.113	0.123	0.115	0.142	0.097	0.154	0.088
Antineoplastic (lymphoticleukemia)	0.209	0.036	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
chemo sensitizer	0.588	0.008	0.563	0.010	0.568	0.010	0.578	0.009	0.569	0.009	0.556	0.001

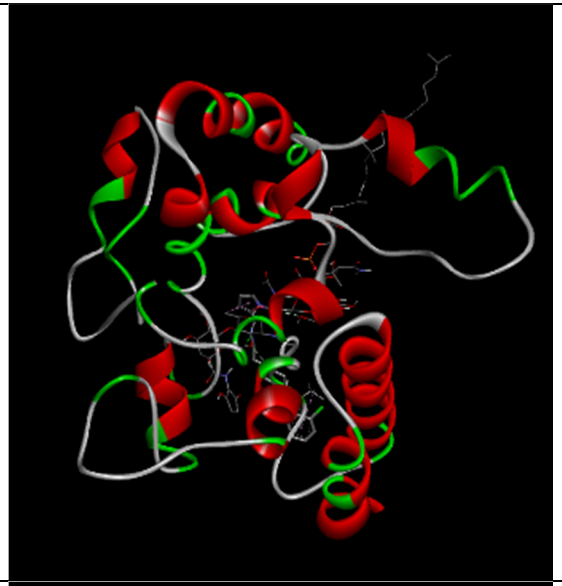
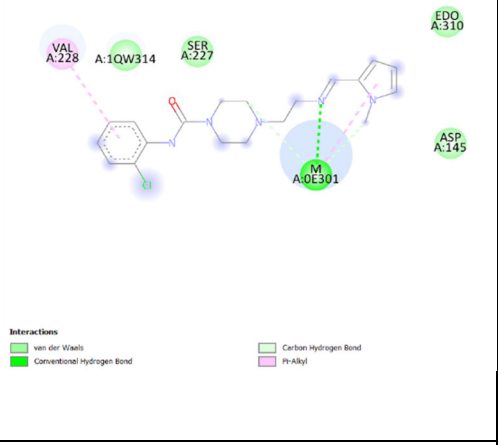
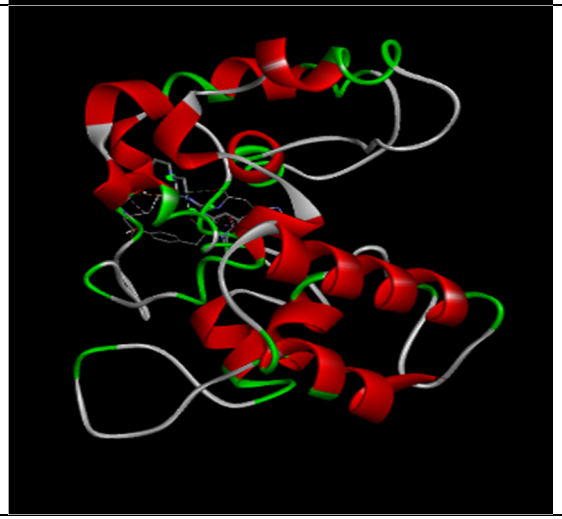
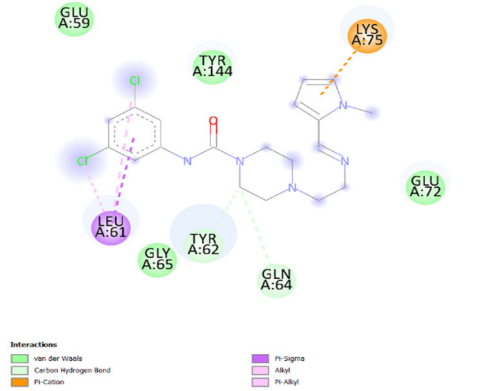
Activity	5g		5h		5i		5j		5k		5l	
	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi
antineoplastic	0.492	0.074	0.533	0.062	0.579	0.050	0.636	0.038	0.664	0,032	0.591	0.047
Protein kinase inhibitor	0.179	0.076	0.149	0.092	0.168	0.081	0.158	0.086	0.156	0.087	0.157	0.083
Antineoplastic (lymphatic leukaemia)	0.146	0.058	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
chemo sensitizer	0.600	0.006	0.569	0.009	0.548	0.012	0.558	0.011	0.602	0.006	0.631	0.005

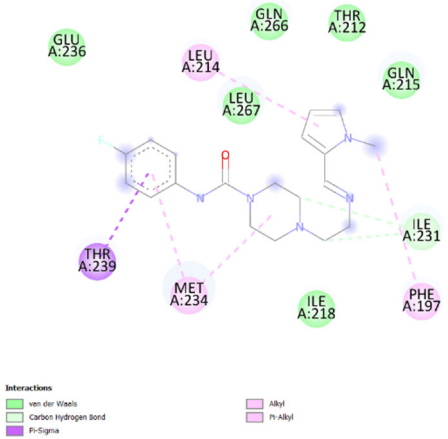
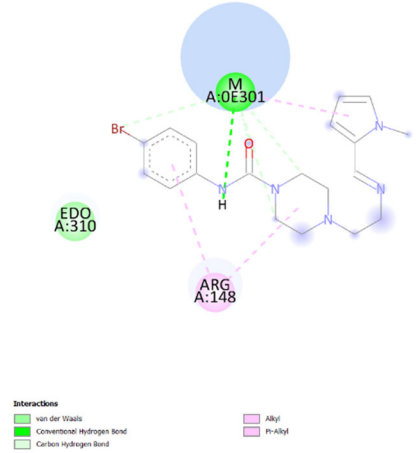
Supplementary table S3: Molecular docking interactive map of ligands **5(a-l)** and antibiotic streptomycin for **6FTB**of binding deep inside the active site, depicting the best docking pose showing 2D respectively.

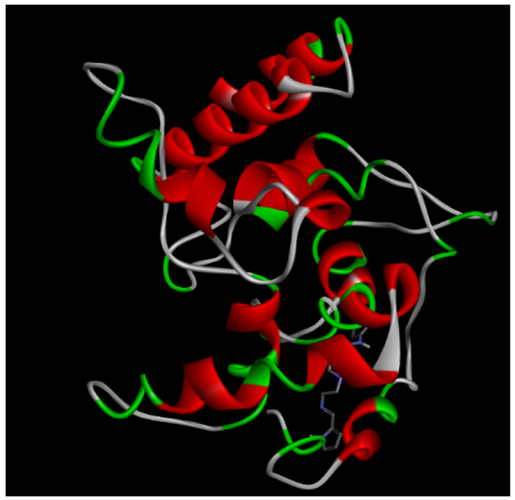
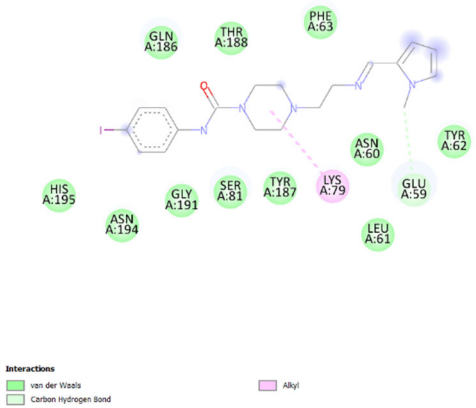
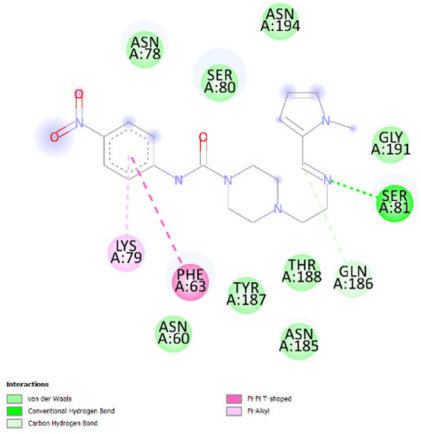
5a				-8.25
5b				- 8.51

5c			 GLU A:90 LYS A:93 PRO A:89 MET A:88 LYS A:203 TYR A:91 GLN A:259 TYR A:254 ILE A:255 ASN A:256 ASN A:253 Interactions van der Waals Unfavorable Bump Conventional Hydrogen Bond Carbon Hydrogen Bond	-8.50
5d			 GLU A:59 GLN A:186 GLY A:191 ASN A:185 LEU A:61 TYR A:62 PHE A:63 SER A:81 THR A:188 ASN A:60 LYS A:79 TYR A:187 Interactions van der Waals Carbon Hydrogen Bond	-8.00

5e			 VAL A:154 M A:0E301 PHE A:150 Interactions van der Waals Alkyl Pi-Alkyl	-8.62
5f			 GLY A:198 ASN A:185 SER A:81 GLY A:191 TYR A:187 GLN A:186 ASN A:194 HIS A:195 THR A:188 LYS A:79 Interactions van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Alkyl	-8.09

5g			 VAL A:228 A:1QW314 SER A:227 EDO A:310 ASP A:145 M A:DE301 Cl Interactions van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Alkyl	-8.48
5h			 GLU A:59 LYS A:75 TYR A:144 Cl Cl O N N N N GLU A:72 LEU A:61 TYR A:62 GLY A:65 GLN A:64 Interactions van der Waals Carbon Hydrogen Bond Pi-Cation Pi-Sigma Alkyl Pi-Alkyl	-8.95

5i			 GLN A:266 THR A:212 GLU A:236 LEU A:214 GLN A:215 LEU A:267 ILE A:231 THR A:239 MET A:234 ILE A:218 PHE A:197 Interactions van der Waals Carbon Hydrogen Bond Pi-Sigma Alkyl Pi-Alkyl	-9.11
5j			 M A:0E301 Br EDO A:310 ARG A:148 Interactions van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Alkyl Pi-Alkyl	-8.48

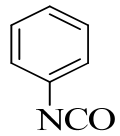
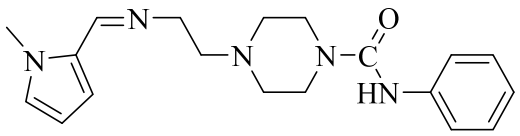
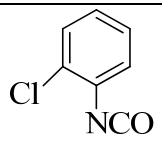
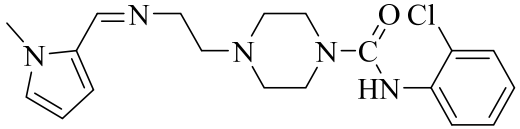
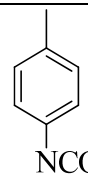
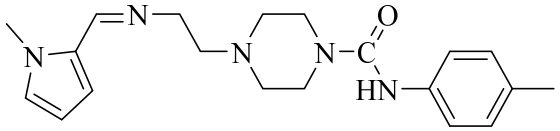
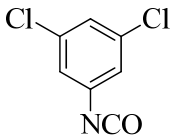
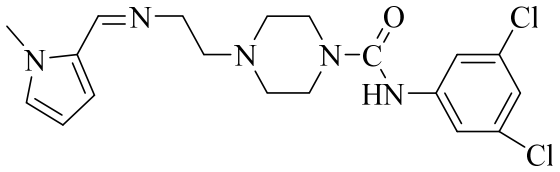
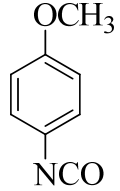
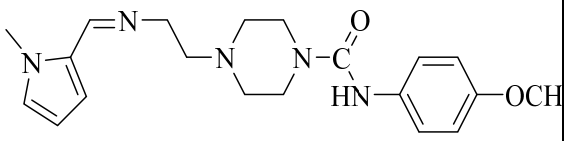
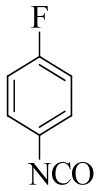
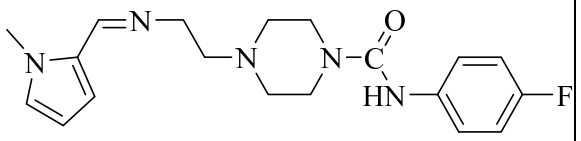
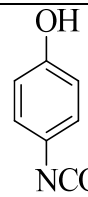
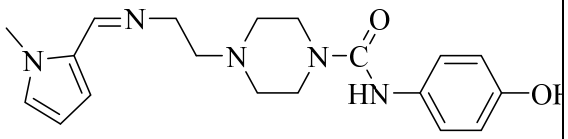
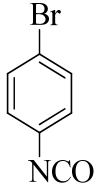
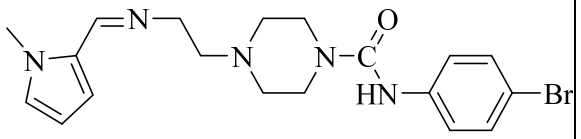
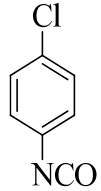
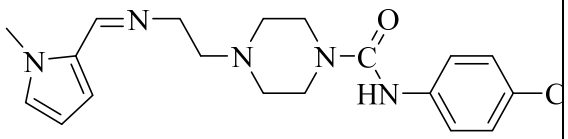
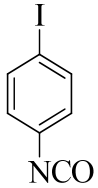
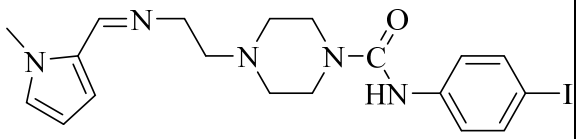
5k			 PHE A:63 GLN A:186 THR A:188 TYR A:62 ASN A:60 HIS A:195 GLY A:191 SER A:81 TYR A:187 LYS A:79 GLU A:59 ASN A:194 LEU A:61 Interactions van der Waals Alkyl Carbon Hydrogen Bond	-8.75
5l			 ASN A:194 ASN A:78 SER A:80 GLY A:191 SER A:81 LYS A:79 PHE A:63 TYR A:187 THR A:188 GLN A:186 ASN A:60 ASN A:185 Interactions van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Pi T-shaped Pi-Alkyl	-8.15

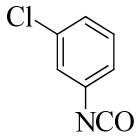
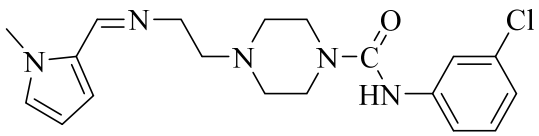
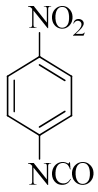
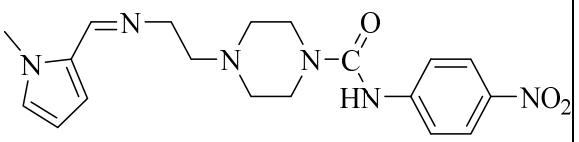
Supplementary table S4: Binding interaction of the compounds

Protein id	Compound	Binding score	Binding interaction
6FTB	5a	-8.25	GLU A:90, ASN A:256 – conventional hydrogen bonding, LYS A:203 – unfavourable bump, ASN A:253 – carbon hydrogen bond, MET A:88, LYS A:93, PRO A:89, TYR A:91, GLN A:259, TYR A:254, ILE A:255 – van der waals.
	5b	-8.51	M A: 0E301 – Pi- alkyl, M A: 0E303 – Pi-sigma and Pi-Pi stacked, PHE A:150 – van der waals, PO A:4313 – Pi-anion and carbon hydrogen bond.
	5c	-8.50	MET A:88, LYS A:93, PRO A:89, TYR A:91,GLN A:259, TYR A:254, ILE A:255 – van der waals, ASN A:253 – carbon hydrogen bond, LYS A:203 – unfavourable bump, GLU A:90, ASN A:256 – conventional hydrogen bond.
	5d	-8.00	ASN A:185 – carbon hydrogen bond, LEU A:61, TYR A:62, PHE A:63, AS A:60, LYS A:79, TYR A:187, THR A:188, SER A: 91, GLY A:191, GLN A:186, GLU A:59 – van der waals.
	5e	-8.62	VAL A: 154 – van der waals, M A: 0E301 – alkyl, PHE A: 150 – Pi-alkyl.
	5f	-8.09	SER A:81, GLN A:186 – conventional hydrogen bond, GLY A:198, ASN A:185, TYR A;187,LYS A:79, THR A:188 – van der waals, GLY A:198,AS A:194 – carbon hydrogen bond, HIS A:195 – Pi-alkyl.

	5g	-8.48	M A: 0E301 – conventional hydrogen bond, VAL A: 228 – Pi-alkyl, SER A: 227, EDO A: 310, ASP A: 145, A: 10W314 – van der waals, VAL A: 228 – Pi-alkyl.
	5h	-8.95	GLN A:64, TYR A:62 – carbon hydrogen bond, LEU A:61 – Pi-sigma, LYS A:75 – Pi-carbon, GLU A:59, TYR A:144, GLU A:72, GLY A:65 – van der waals.
	5i	-9.11	THR A:239 – Pi-sigma, LEU A:214 – Pi-alkyl, PHE A:197, MET A:234 – alkyl, GLU AA:236,GLN A:266,THR A:212,LEU A:267,GLN A:215,ILE A:218 – van der waals.
	5j	-8.48	M A:0E301 – conventional hydrogen bond, EDO A:310 van der waals, ARG A:148 – alkyl and Pi-alkyl.
	5k	-8.75	LYS A:79 – alkyl, GLU A:59 – carbon hydrogen bond, GLN A:186,THR A:188,PHE A:63,HIS A:195,ASN A:194,GLY A:191,SER A:81, TYR A:187,LEU A:61,ASN A:60,TYR A:62 – van der waals.
	5l	-8.15	PHE A:63 – Pi-Pi T shaped, LYS A:79 – Pi-alkyl, SER A:81 – conventional hydrogen bond, GLN A:186 – carbon hydrogen bond, ASN A:78,SER A:80,ASN A:194,GLY A:191,THR A:188,ASN A:185,TYR A:187,ASN A:60.

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		

Supplementary Table S6 : Fatty acid profile of standard 37 FAME mixture

Standard FAME components	Ret. Time (min)	Area (mV*s)	Area (%)	Height (mV)
Methyl butyrate (C4:0)	12.431	124.662	2.907	53.461
Methyl caproate (C6:0)	14.692	147.934	3.450	52.662
Methyl caprylate (C8:0)	18.471	168.311	3.925	50.194
Methyl decanoate (C10:0)	23.479	185.376	4.323	50.853
Methyl undecanoate (C11:0)	26.173	95.802	2.234	25.724
Methyl dodecanoate (C12:0)	28.863	199.420	4.650	52.569
Methyl tridecanoate (C13:0)	31.490	101.493	2.367	26.764
Methyl myristate (C14:0)	34.039	207.393	4.836	54.823
Methyl myristoleate (C14:1 cis-9)	36.112	102.095	2.381	26.331
Methyl pentadecenoate (C15:0)	36.479	104.185	2.430	27.192
Methyl pentadecenoate (C15:1 [cis-10])	38.504	102.641	2.394	26.224
Methyl palmitate (C16:0)	38.823	314.102	7.325	80.745
Methyl palmitoleate (C16:1[cis-9])	40.485	102.588	2.392	26.148
Methyl heptadecanoate (C17:0)	41.059	103.209	2.407	26.951
Methyl heptadecenoate (C17:1[cis-10])	42.674	101.549	2.368	26.040
Methyl stearate (C18:0)	43.205	202.394	4.720	51.787
Methyl octadecenoate (C18:1 [trans-9])	44.175	99.654	2.324	25.507
Methyl oleate (C18:1[cis-9])	44.594	199.976	4.663	50.653
Methyl linoleaidate (C18:2 [trans-9,12])	45.691	94.054	2.193	24.024
Methyl linoleate (C18:2[cis-9,12])	46.617	97.928	2.284	25.387
Methyl arachidate (C20:0)	47.226	182.551	4.257	47.257
Methyl linolenate (C18:3[cis-6,9,12])	48.094	97.295	2.269	24.433
Methyl eicosenoate (C20:1 [cis -11])	48.533	86.013	2.006	21.692
Methyl linolenate (C18:3[cis -9,12,15])	48.881	91.888	2.143	23.833
Methyl heneicosanoate (C21:0)	49.116	83.389	1.945	21.206
Methyl eicosadienoate (C20:2[cis-11,14])	50.447	78.499	1.831	19.889
Methyl behenate (C22:0)	50.944	150.208	3.503	37.541
Methyl eicosatrienoate (C20:3 [cis-8. 11,14])	51.865	82.358	1.921	19.150
Methyl erucate (C22:1[cis-13])	52.227	64.697	1.509	14.910
Methyl eicosatrienoate (C20:3 [cis-11,14,17])	52.639	71.484	1.667	17.088
Methyl arachidonate (C20:4 [cis -5,8,11,14])	52.769	64.179	1.497	14.742
Methyl tricosanoate (C23:0)	53.005	77.725	1.813	17.998
Methyl docosadienoate (C22:2[cis 13,16])	54.221	53.869	1.256	12.088
Methyl lignocerate (C24:0)	54.681	100.576	2.345	21.902
Methyl eicosapentaenoate (C20:5 [cis5,8,11,14,17])	55.485	67.104	1.565	14.460
Methyl nervonate (C24:1 [cis-15])	56.128	39.054	0.911	7.921
Methyl docosahexaenoate (C22:6 [cis -4,7,10,13,16,19])	61.700	42.486	0.991	6.648
Total			100.000	

Supplementary Table S7: MRSA control bacterial culture fatty acid profile.

Control *S. aureus* FAME components	**Ret. Time (min)**	**Area (mV*s)**	**Area (%)**	**Height (mV)**
Methyl butyrate (C4:0)	0.000	0.000	0.000	0.000
Unknown	13.917	7.852	5.758	3.058
Methyl caproate (C6:0)	14.395	12.039	8.829	3.949
Methyl caprylate (C8:0)	18.835	8.669	6.358	2.671
Methyl decanoate (C10:0)	23.765	8.539	6.262	2.542
Methyl undecanoate (C11:0)	0.000	0.000	0.000	0.000
Methyl dodecanoate (C12:0)	0.000	0.000	0.000	0.000
Methyl tridecanoate (C13:0)	31.297	9.786	7.177	2.471
Methyl myristate (C14:0)	0.000	0.000	0.000	0.000
Methyl myristoleate (C14:1 cis-9)	0.000	0.000	0.000	0.000
Methyl pentadecenoate (C15:0)	0.000	0.000	0.000	0.000
Methyl pentadecenoate (C15:1 [cis-10])	38.356	8.108	5.946	0.951
Methyl palmitate (C16:0)	0.000	0.000	0.000	0.000
Methyl palmitoleate (C16:1[cis-9])	0.000	0.000	0.000	0.000
Methyl heptadecanoate (C17:0)	0.000	0.000	0.000	0.000
Methyl heptadecenoate (C17:1[cis-10])	0.000	0.000	0.000	0.000
Methyl stearate (C18:0)	0.000	0.000	0.000	0.000
Methyl octadecenoate (C18:1 [trans-9])	0.000	0.000	0.000	0.000
Methyl oleate (C18:1[cis-9])	0.000	0.000	0.000	0.000
Methyl linoleaidate (C18:2 [trans-9,12])	0.000	0.000	0.000	0.000
Methyl linoleate (C18:2[cis-9,12])	46.529	6.303	4.622	1.538
Methyl arachidate (C20:0)	0.000	0.000	0.000	0.000
Methyl linolenate (C18:3[cis-6,9,12])	0.000	0.000	0.000	0.000
Methyl eicosenoate (C20:1 [cis -11])	0.000	0.000	0.000	0.000
Methyl linolenate (C18:3[cis -9,12,15])	0.000	0.000	0.000	0.000
Methyl heneicosanoate (C21:0)	0.000	0.000	0.000	0.000
Methyl eicosadienoate (C20:2[cis-11,14])	0.000	0.000	0.000	0.000
Methyl behenate (C22:0)	0.000	0.000	0.000	0.000
Methyl eicosatrienoate (C20:3 [cis-8. 11,14])	0.000	0.000	0.000	0.000
Methyl erucate (C22:1[cis-13])	52.271	68.158	49.982	15.762
Methyl eicosatrienoate (C20:3 [cis-11,14,17])	0.000	0.000	0.000	0.000
Methyl arachidonate (C20:4 [cis -5,8,11,14])	0.000	0.000	0.000	0.000
Methyl tricosanoate (C23:0)	0.000	0.000	0.000	0.000
Methyl docosadienoate (C22:2[cis 13,16])	0.000	0.000	0.000	0.000
Methyl lignocerate (C24:0)	0.000	0.000	0.000	0.000
Methyl eicosapentaenoate (C20:5 [cis5,8,11,14,17])	55.355	6.910	5.067	1.366
Methyl nervonate (C24:1 [cis-15])	0.000	0.000	0.000	0.000

Methyl docosahexaenoate (C22:6 [cis - 4,7,10,13,16,19])	0.000	0.000	0.000	0.000
Total			100.000	

Supplementary Table S8: MRSA control bacterial culture treated with 5i analogue fatty acid profile.

5i analogue treated *S. aureus* FAME components	**Ret. Time (min)**	**Area (mV*s)**	**Area (%)**	**Height (mV)**
Methyl butyrate (C4:0)	0.000	0.000	0.000	0.000
Unidentified	13.935	11.608	6.142	4.182
Unidentified	14.167	8.737	4.623	2.186
Methyl caproate (C6:0)	14.415	17.511	9.265	5.364
Methyl caprylate (C8:0)	18.862	9.368	4.957	2.847
Methyl decanoate (C10:0)	23.784	9.287	4.914	2.614
Methyl undecanoate (C11:0)	0.000	0.000	0.000	0.000
Methyl dodecanoate (C12:0)	28.905	6.619	3.502	1.792
Methyl tridecanoate (C13:0)	0.000	0.000	0.000	0.000
Methyl myristate (C14:0)	0.000	0.000	0.000	0.000
Methyl myristoleate (C14:1 cis-9)	0.000	0.000	0.000	0.000
Methyl pentadecenoate (C15:0)	0.000	0.000	0.000	0.000
Methyl pentadecenoate (C15:1 [cis-10])	0.000	0.000	0.000	0.000
Methyl palmitate (C16:0)	38.724	14.999	7.936	4.005
Methyl palmitoleate (C16:1[cis-9])	0.000	0.000	0.000	0.000
Methyl heptadecanoate (C17:0)	0.000	0.000	0.000	0.000
Methyl heptadecenoate (C17:1[cis-10])	0.000	0.000	0.000	0.000
Methyl stearate (C18:0)	0.000	0.000	0.000	0.000
Methyl octadecenoate (C18:1 [trans-9])	44.825	26.842	14.203	5.972
Methyl oleate (C18:1[cis-9])	44.483	30.463	16.119	8.195
Methyl linoleaidate (C18:2 [trans-9,12])	0.000	0.000	0.000	0.000
Methyl linoleate (C18:2[cis-9,12])	46.505	33.104	17.516	8.159
Methyl arachidate (C20:0)	0.000	0.000	0.000	0.000
Methyl linolenate (C18:3[cis-6,9,12])	0.000	0.000	0.000	0.000
Methyl eicosenoate (C20:1 [cis -11])	0.000	0.000	0.000	0.000
Methyl linolenate (C18:3[cis -9,12,15])	0.000	0.000	0.000	0.000
Methyl heneicosanoate (C21:0)	0.000	0.000	0.000	0.000
Methyl eicosadienoate (C20:2[cis-11,14])	0.000	0.000	0.000	0.000
Methyl behenate (C22:0)	0.000	0.000	0.000	0.000
Methyl eicosatrienoate (C20:3 [cis-8. 11,14])	0.000	0.000	0.000	0.000
Methyl erucate (C22:1[cis-13])	52.256	20.458	10.824	5.013
Methyl eicosatrienoate (C20:3 [cis-11,14,17])	0.000	0.000	0.000	0.000
Methyl arachidonate (C20:4 [cis -5,8,11,14])	0.000	0.000	0.000	0.000
Methyl tricosanoate (C23:0)	0.000	0.000	0.000	0.000

Methyl docosadienoate (C22:2[cis 13,16])	0.000	0.000	0.000	0.000
Methyl lignocerate (C24:0)	0.000	0.000	0.000	0.000
Methyl eicosapentaenoate (C20:5 [cis5,8,11,14,17])	0.000	0.000	0.000	0.000
Methyl nervonate (C24:1 [cis-15])	0.000	0.000	0.000	0.000
Methyl docosahexaenoate (C22:6 [cis -4,7,10,13,16,19])	0.000	0.000	0.000	0.000
Total			100.000	