Supplementary Materials: Synthesis and Antimicrobial Activity of 1,2-Benzothiazine Derivatives

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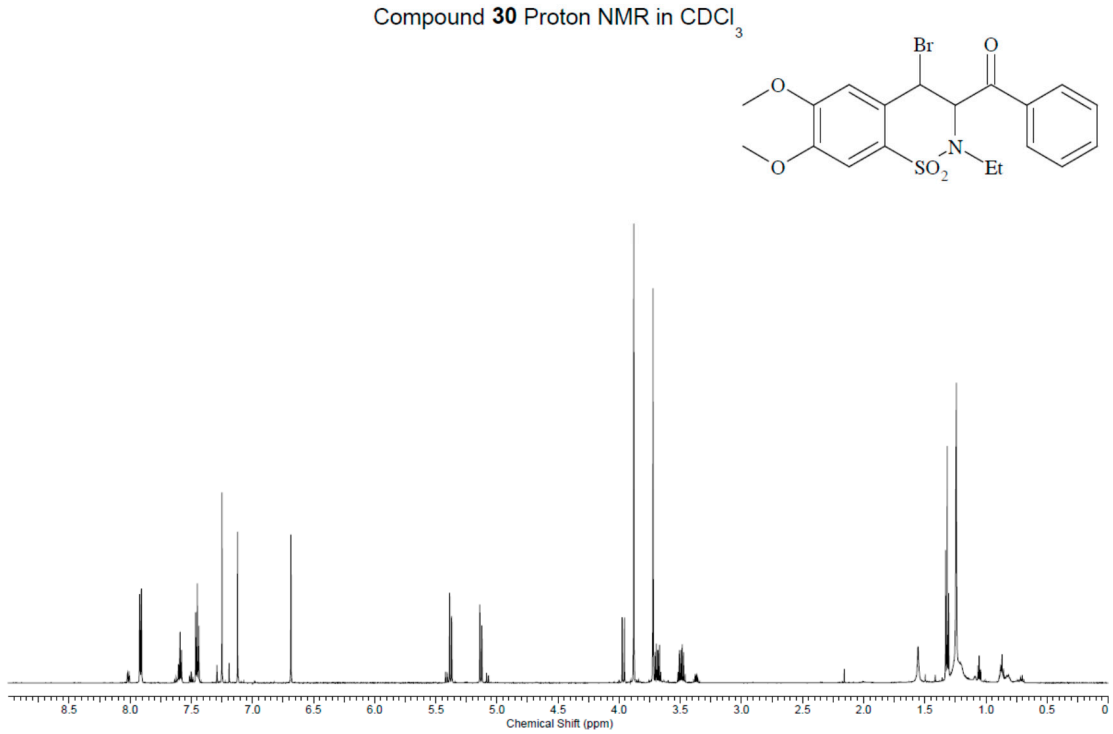
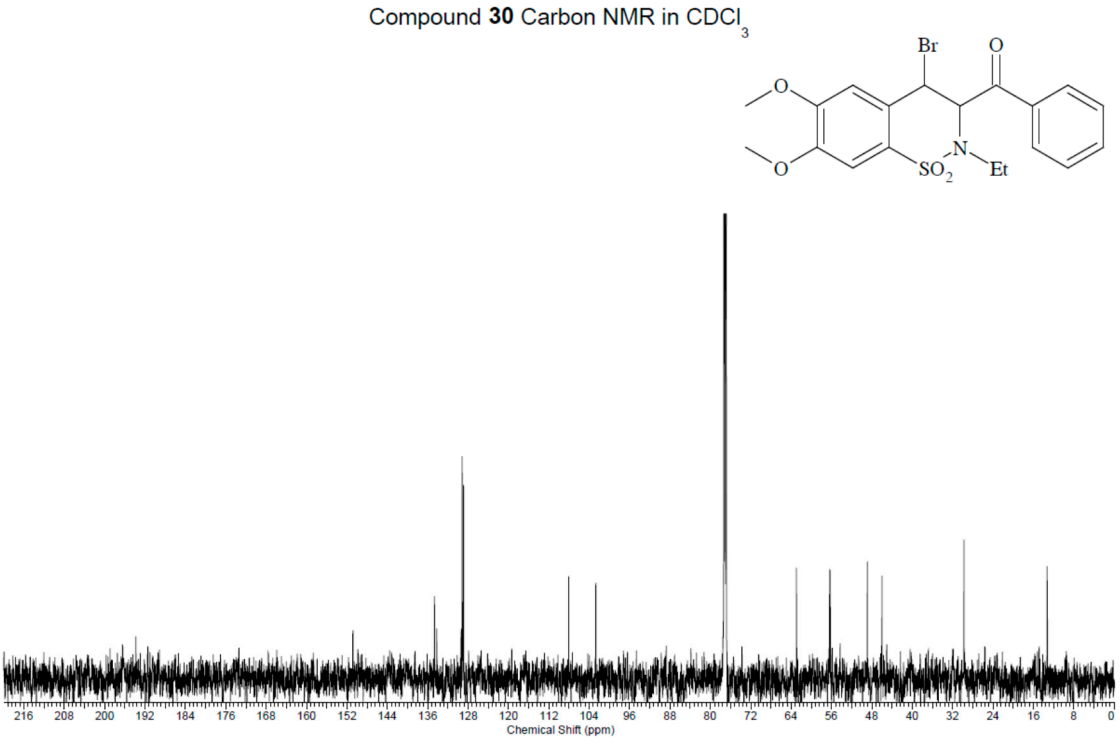
Content

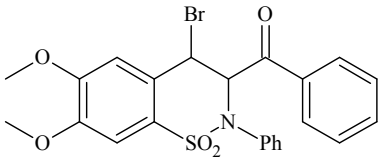
^{1}H-NMR and ^{13}C-NMR and HSMS data of representative compounds and micro data.

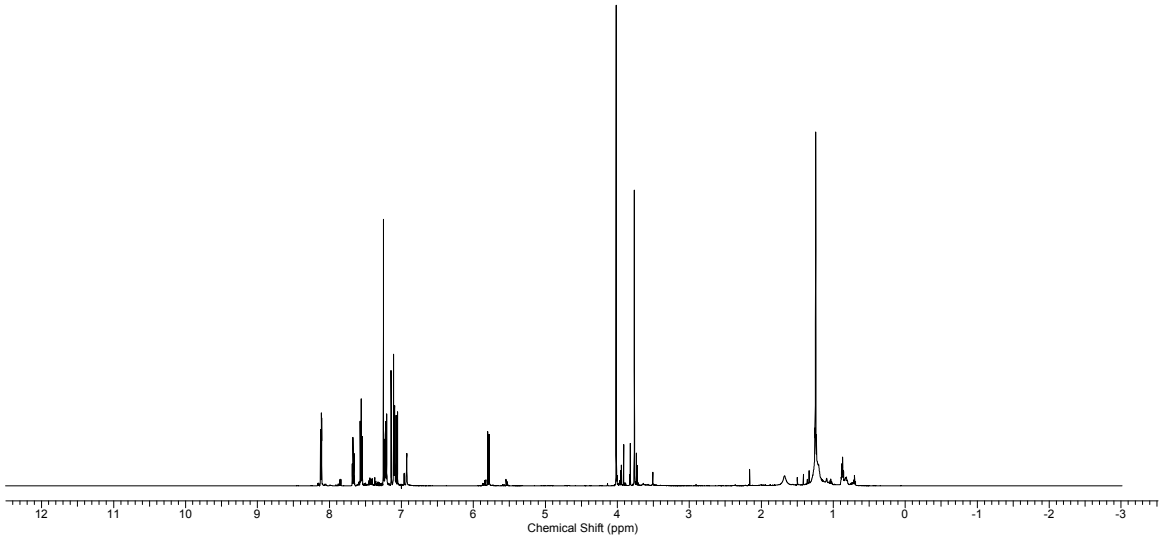
Table S1


Compound 30 Proton NMR in CDCl3
Br
O
O
O
N
SO2
Et
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

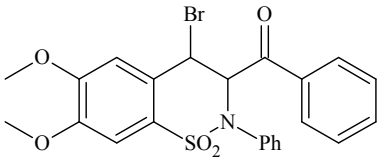

Compound 30 Carbon NMR in CDCl3
Br
O
O
O
N
SO2
Et
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

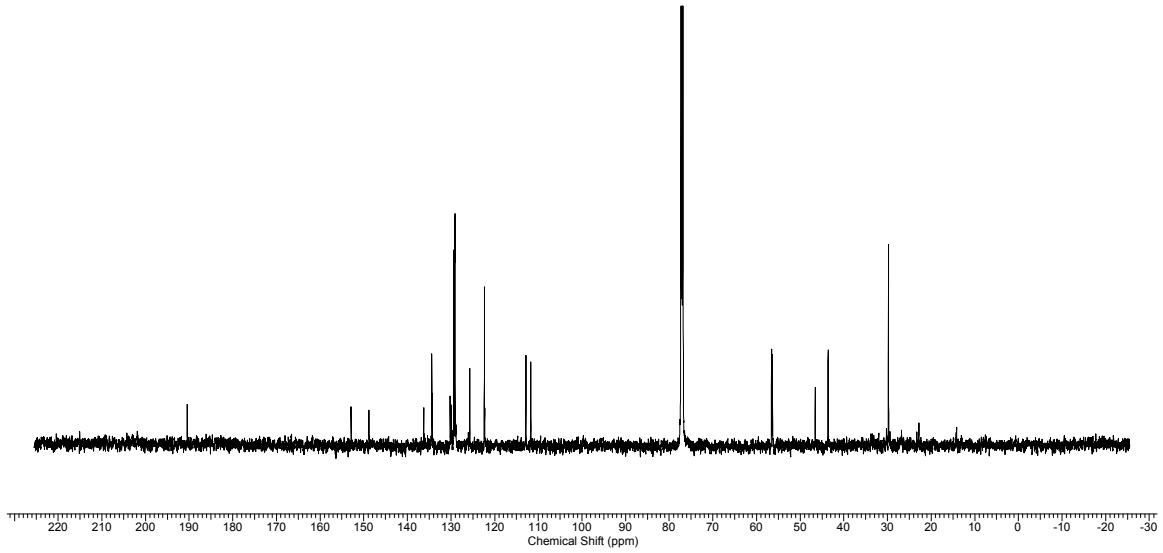
Compound **31** Proton NMR in CDCl3



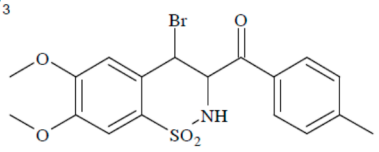


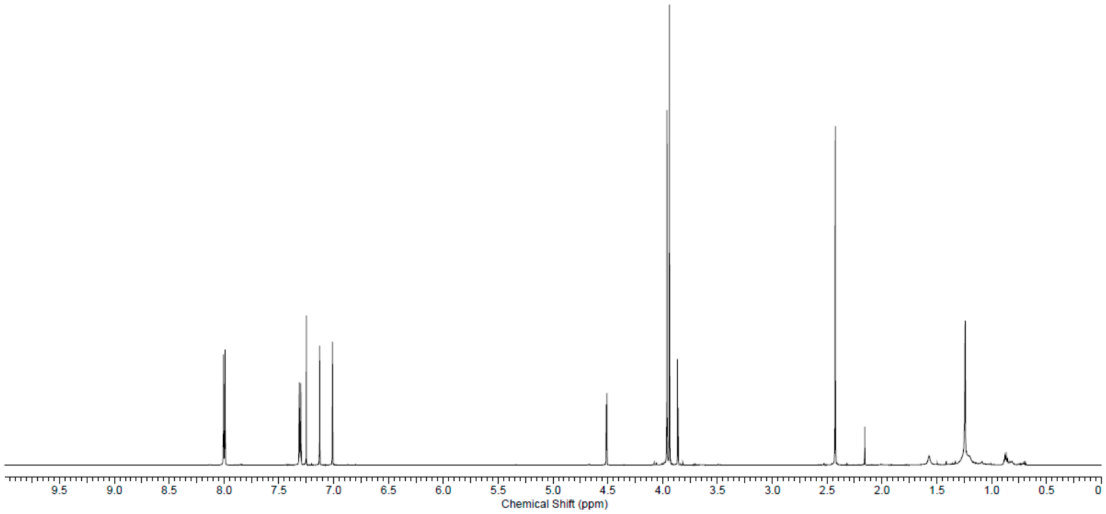
Compound 31 Carbon NMR in CDCl3



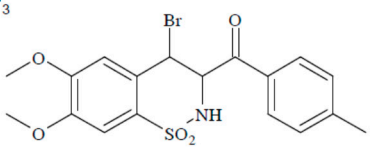


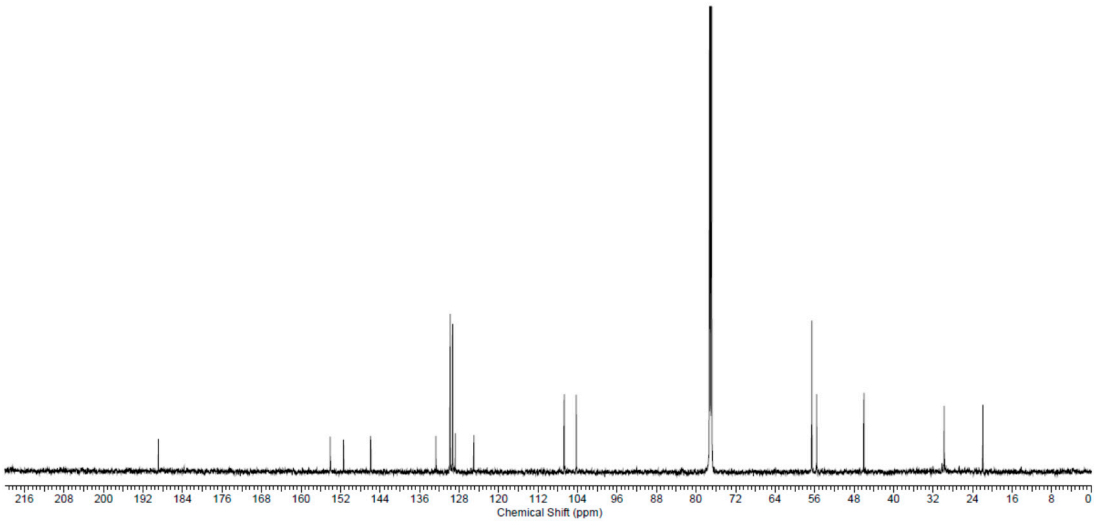
Compound **33** Proton NMR in $CDCl_3$



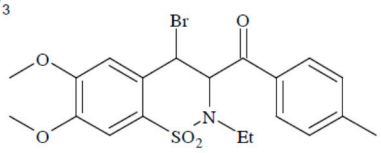


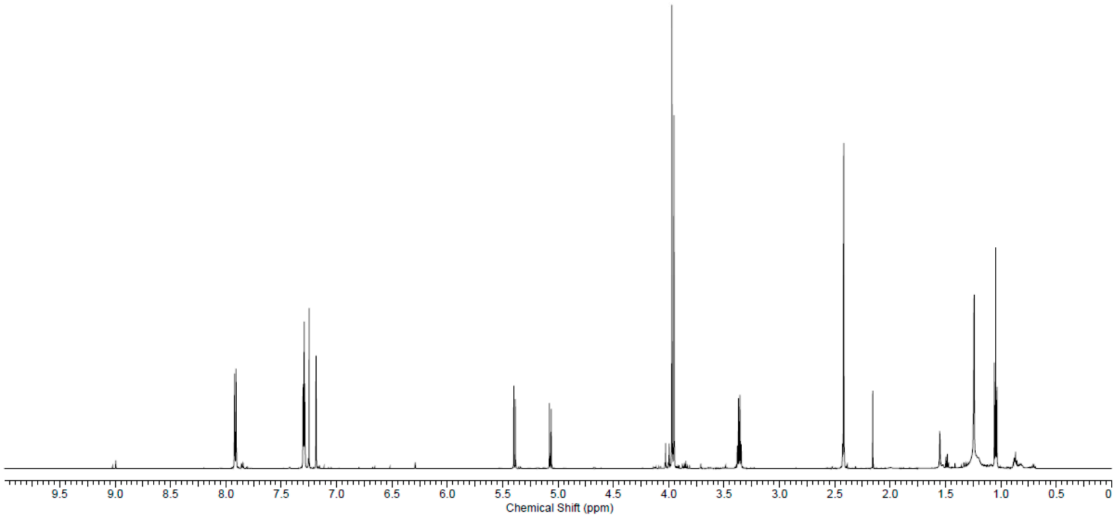
Compound **33** Carbon NMR in $CDCl_3$



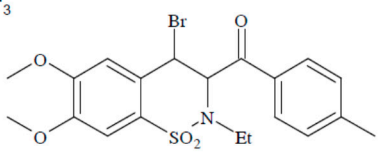


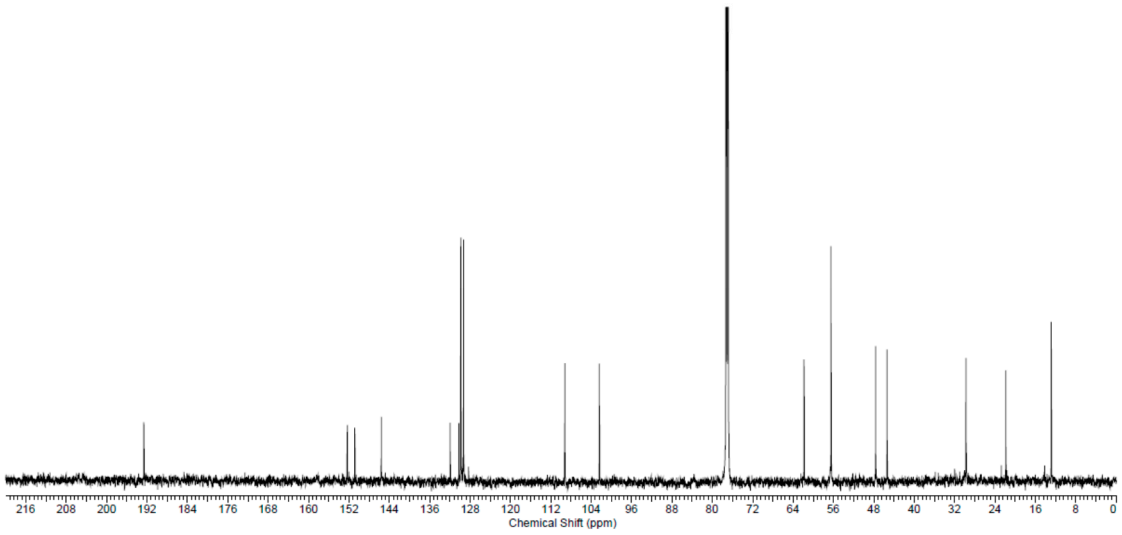
Compound **35** Proton NMR in $CDCl_3$



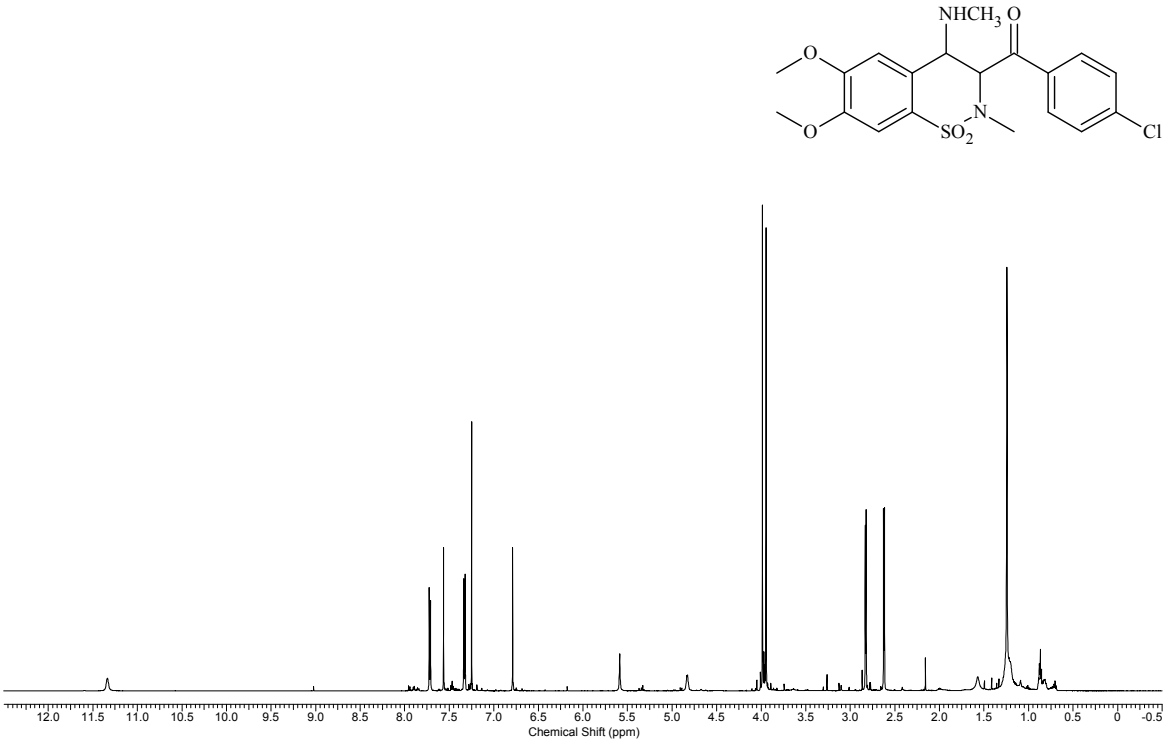


Compound **35** Carbon NMR in $CDCl_3$

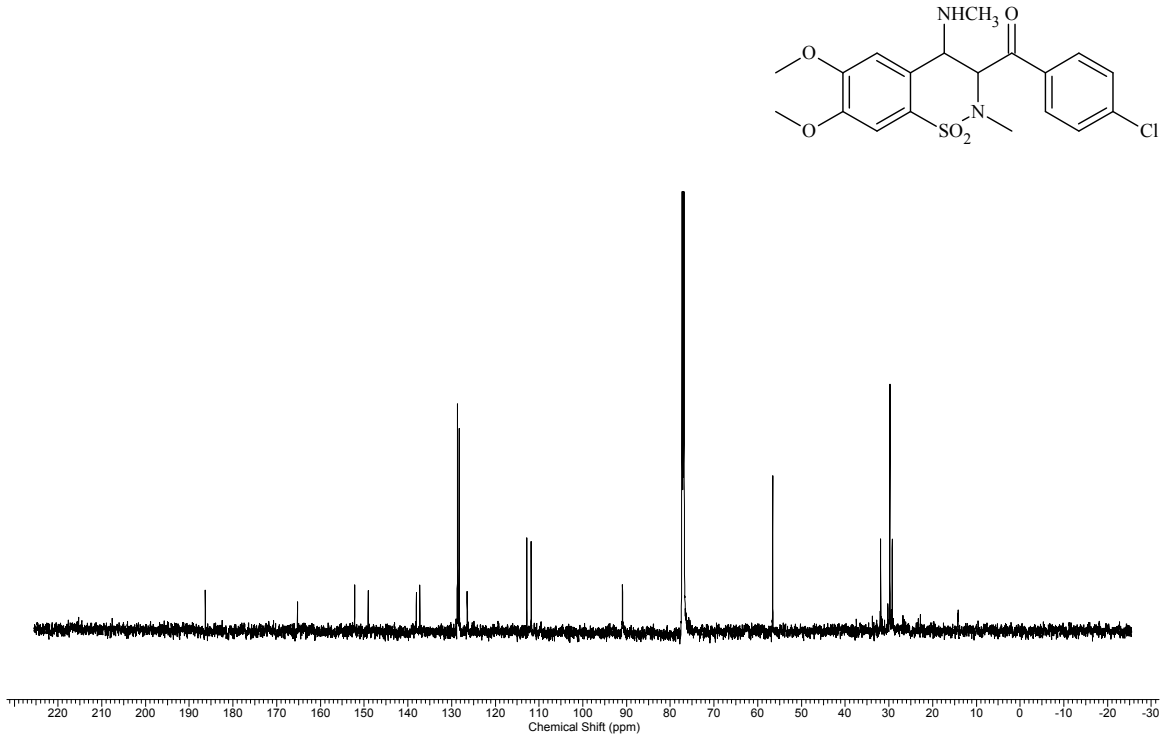




Compound 39 Proton NMR in CDCl3



Compound 39 Carbon NMR in CDCl3



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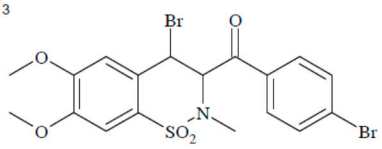
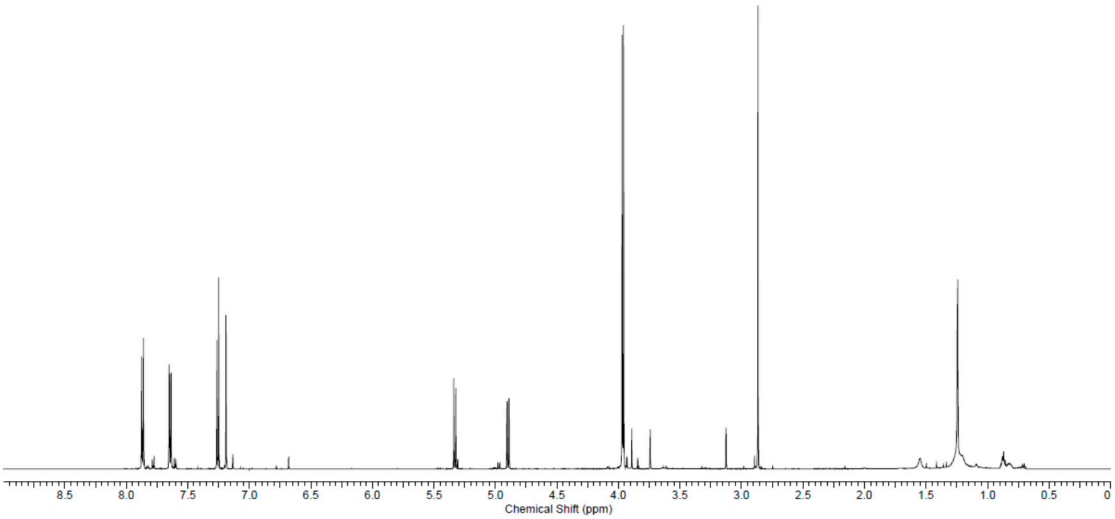
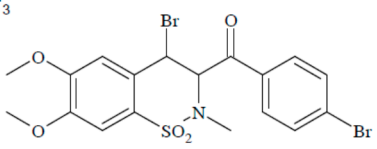
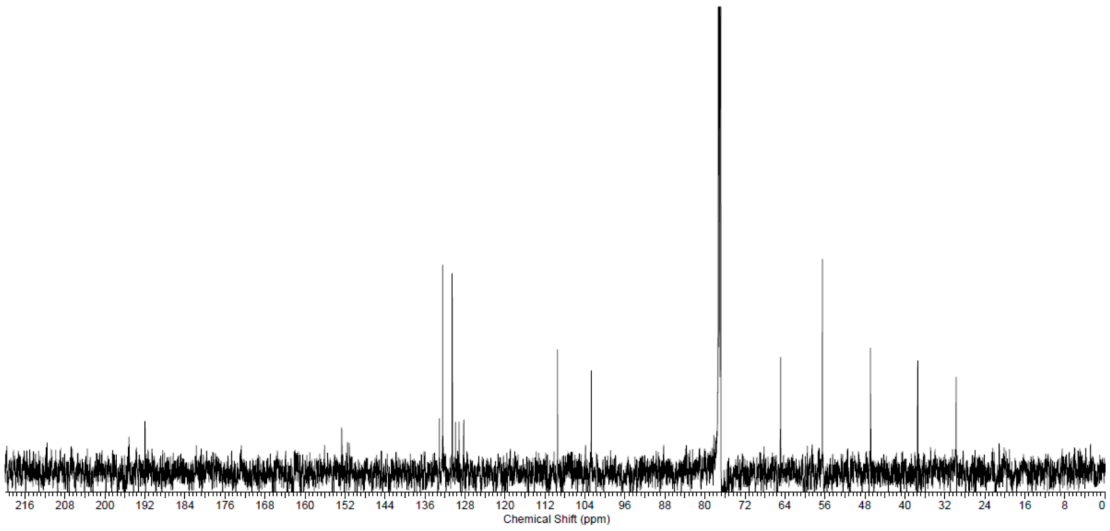




Compound **44** Carbon NMR in $CDCl_3$





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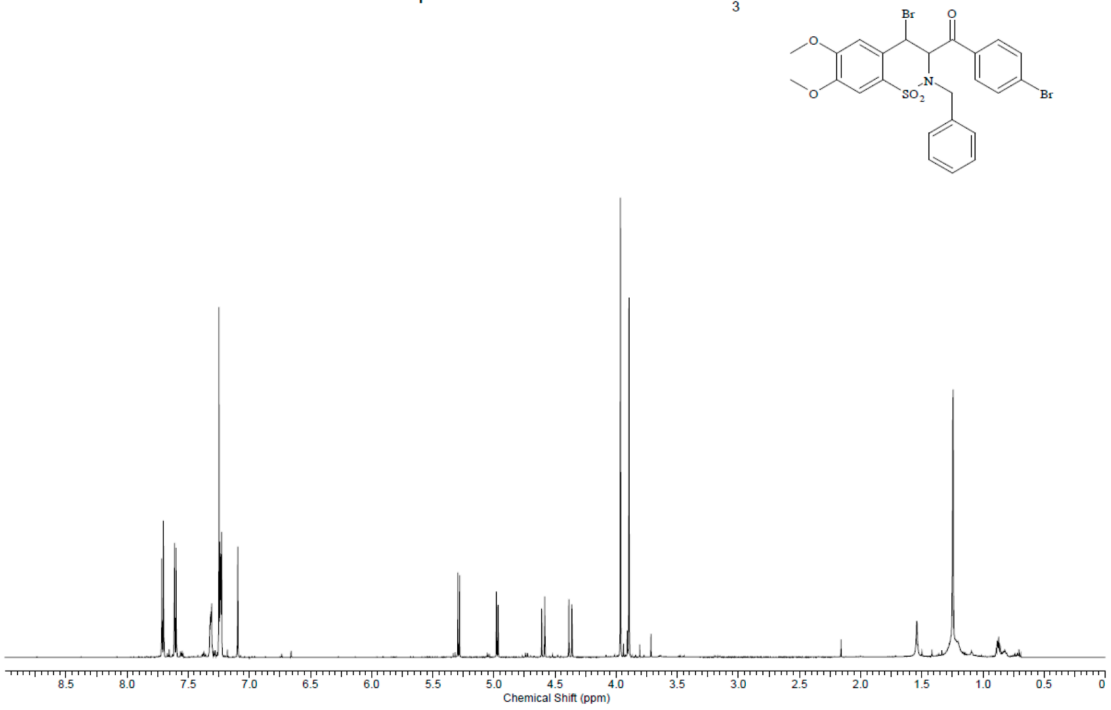
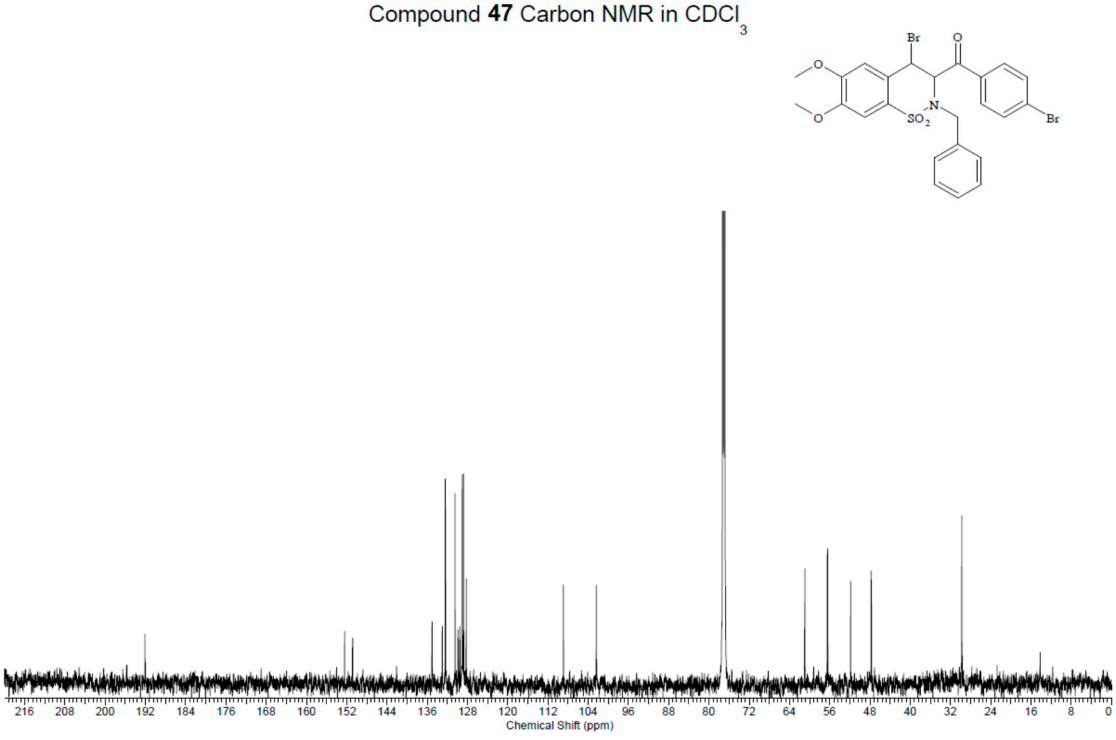


Compound **47** Carbon NMR in $CDCl_3$



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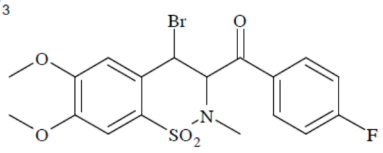
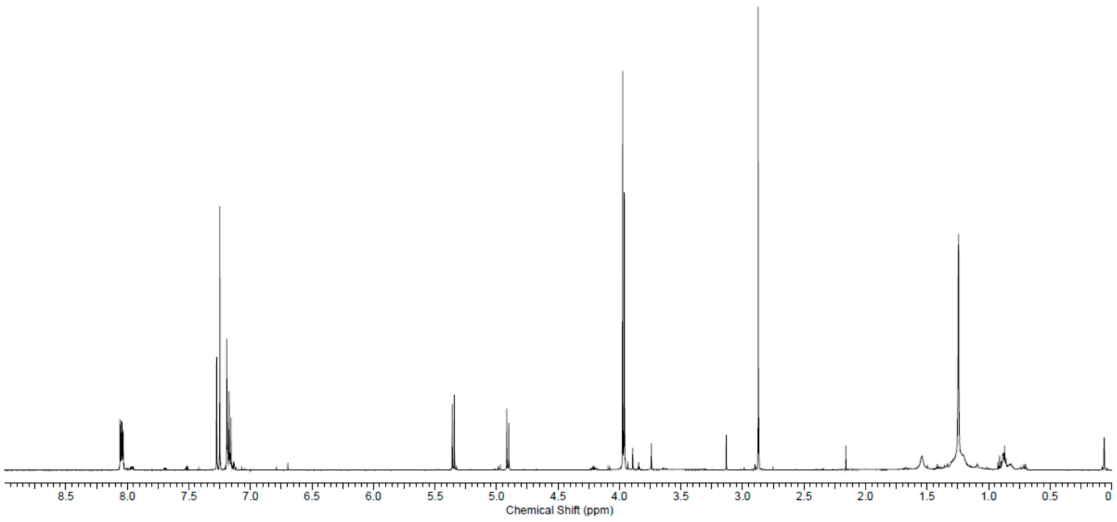
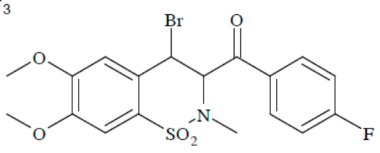
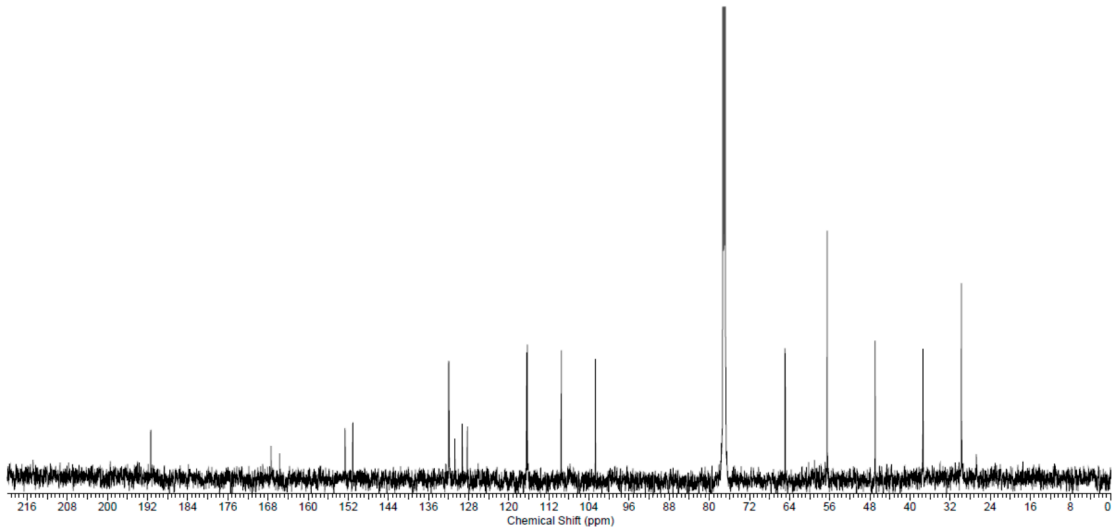


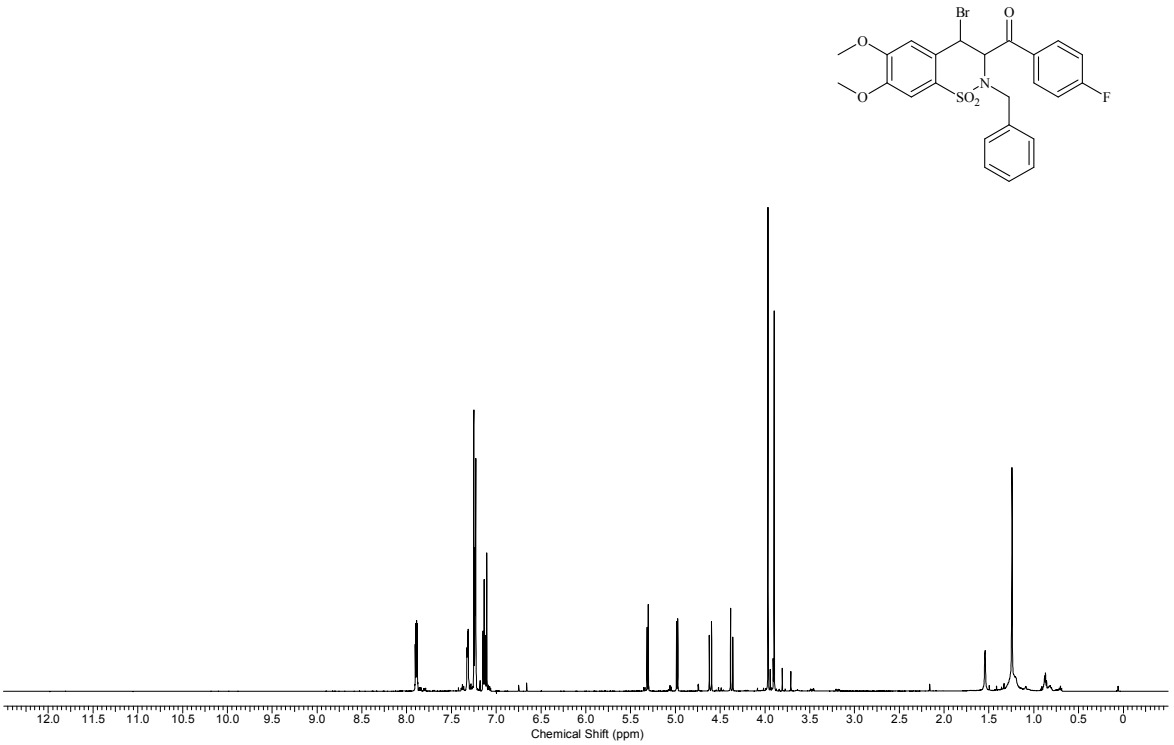


Compound **49** Carbon NMR in $CDCl_3$

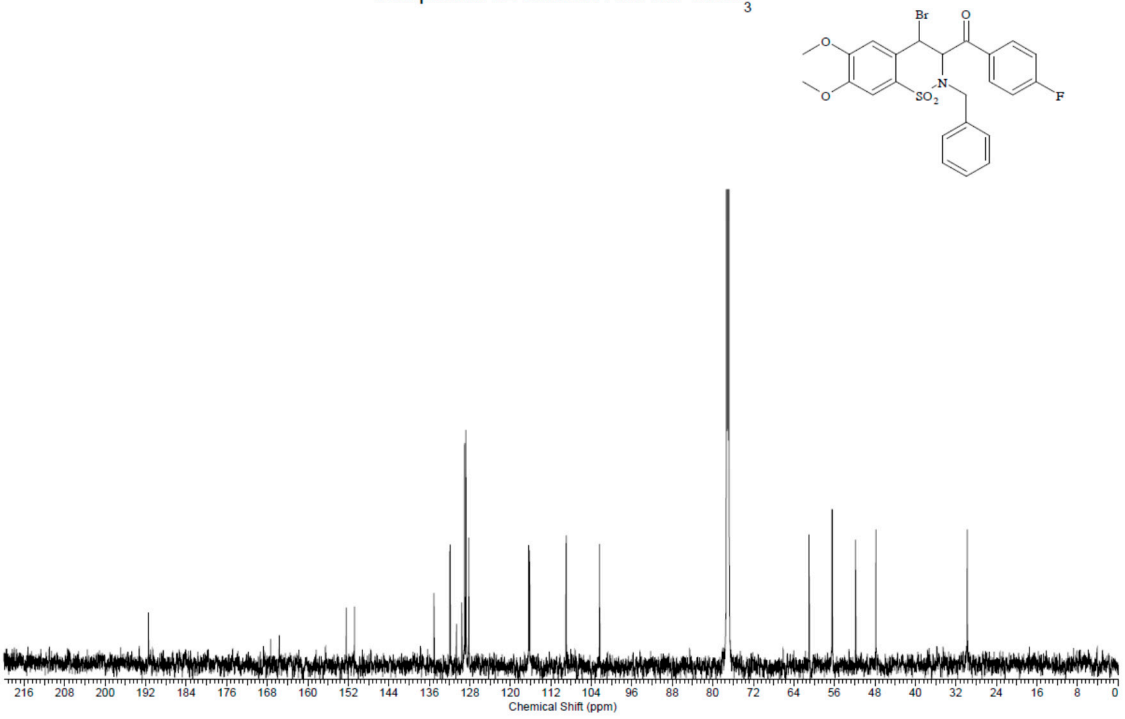




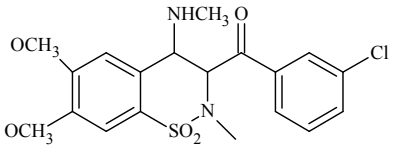
Compound **52** Proton NMR in CDCl3

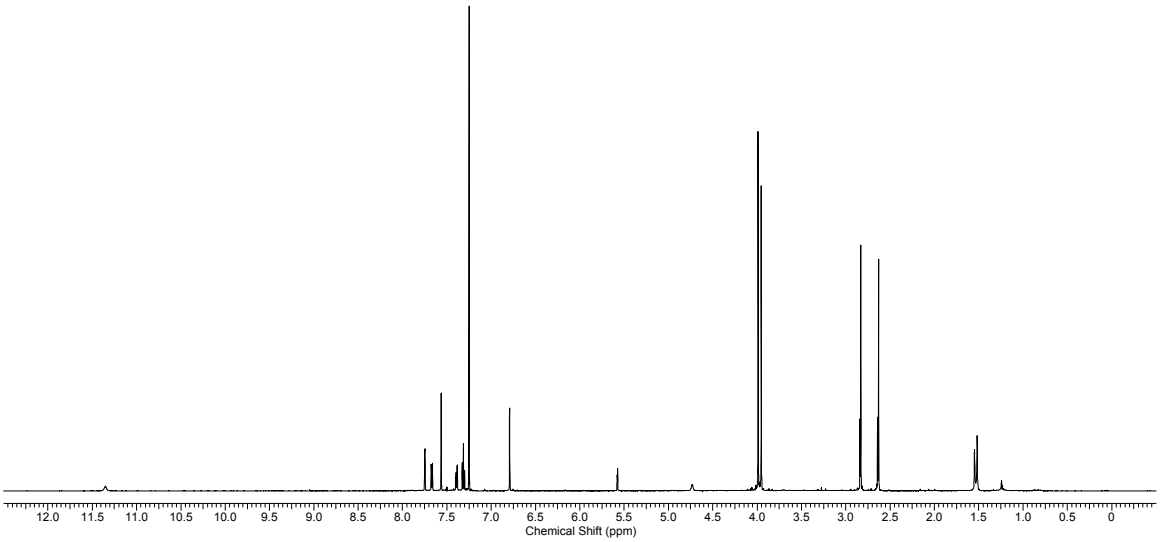


Compound **52** Carbon NMR in $CDCl_3$

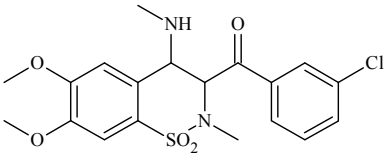


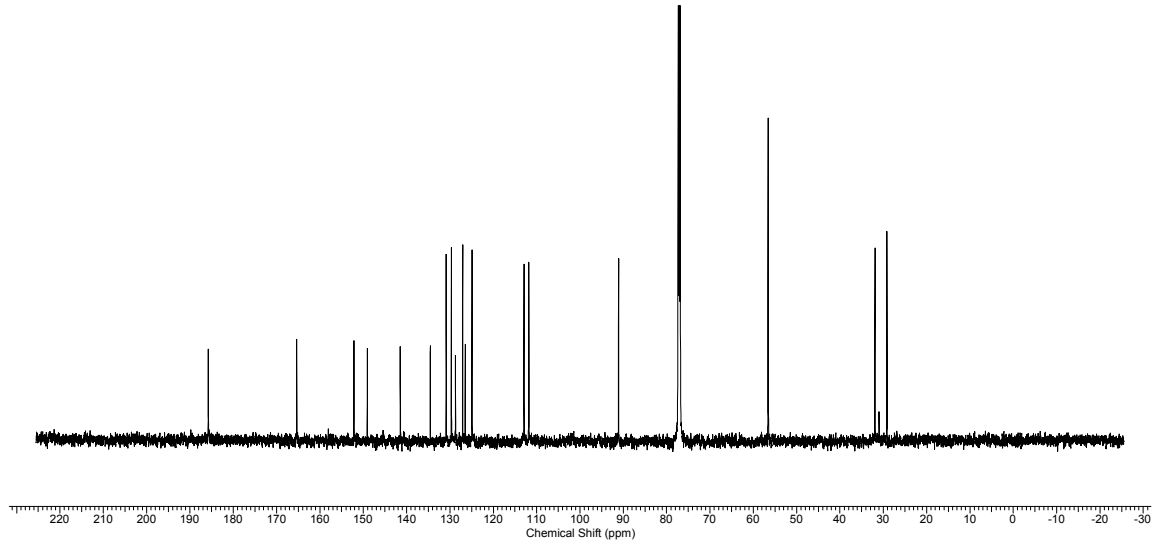
Compound **54** Proton NMR in CDCl3



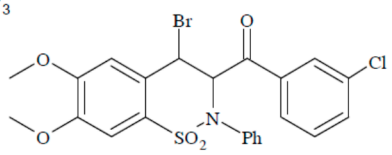


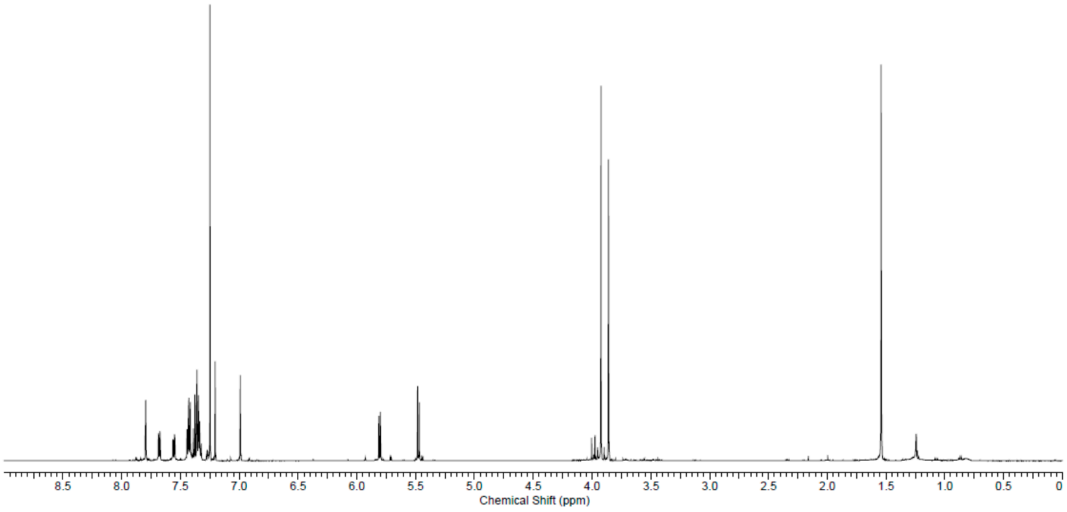
Compound 54 **Carbon NMR in CDCl3**



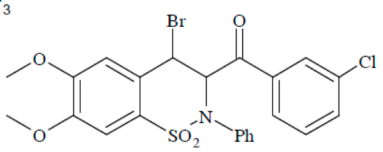


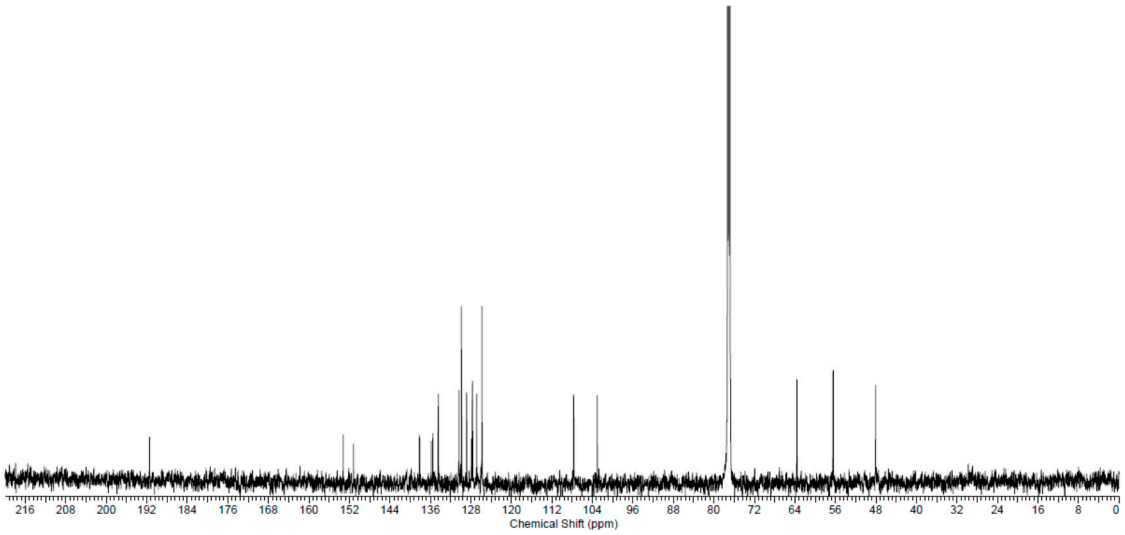
Compound **56** Proton NMR in $CDCl_3$





Compound **56** Carbon NMR in $CDCl_3$





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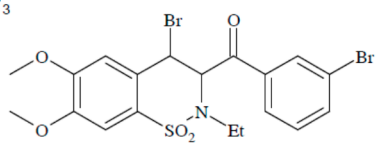
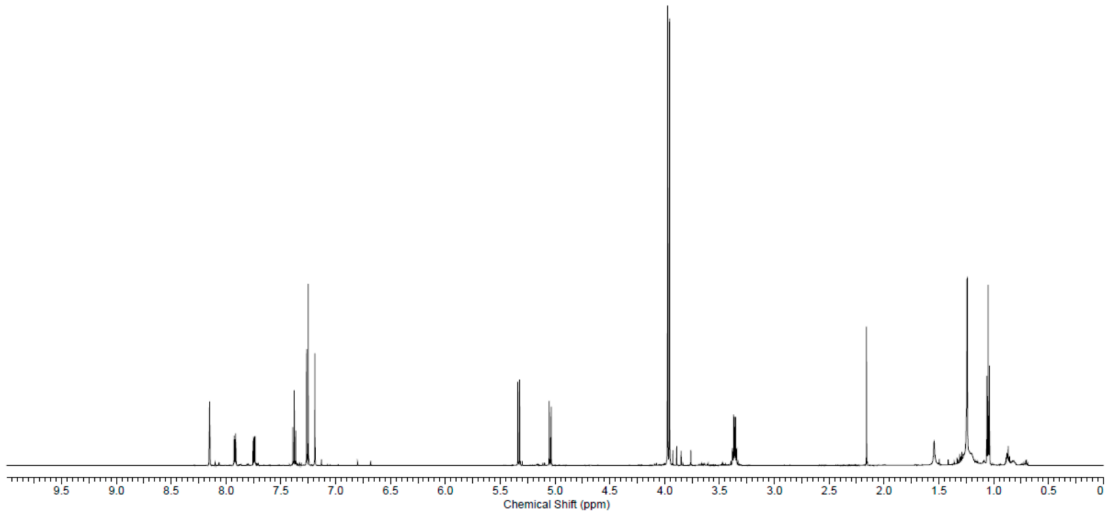
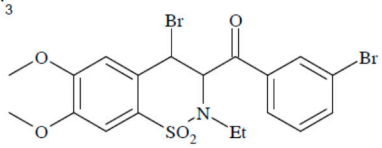
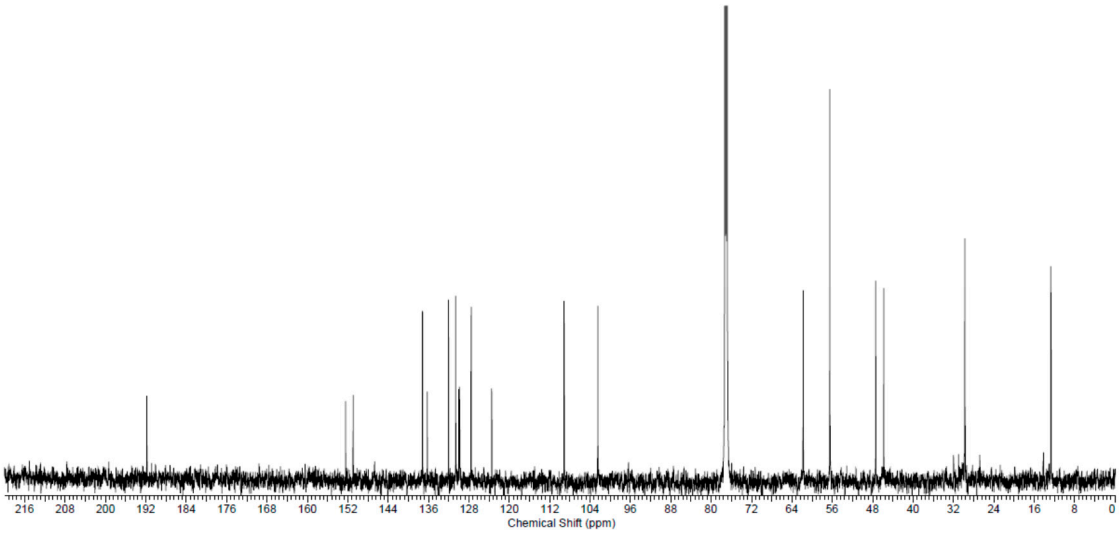




Compound **60** Carbon NMR in $CDCl_3$





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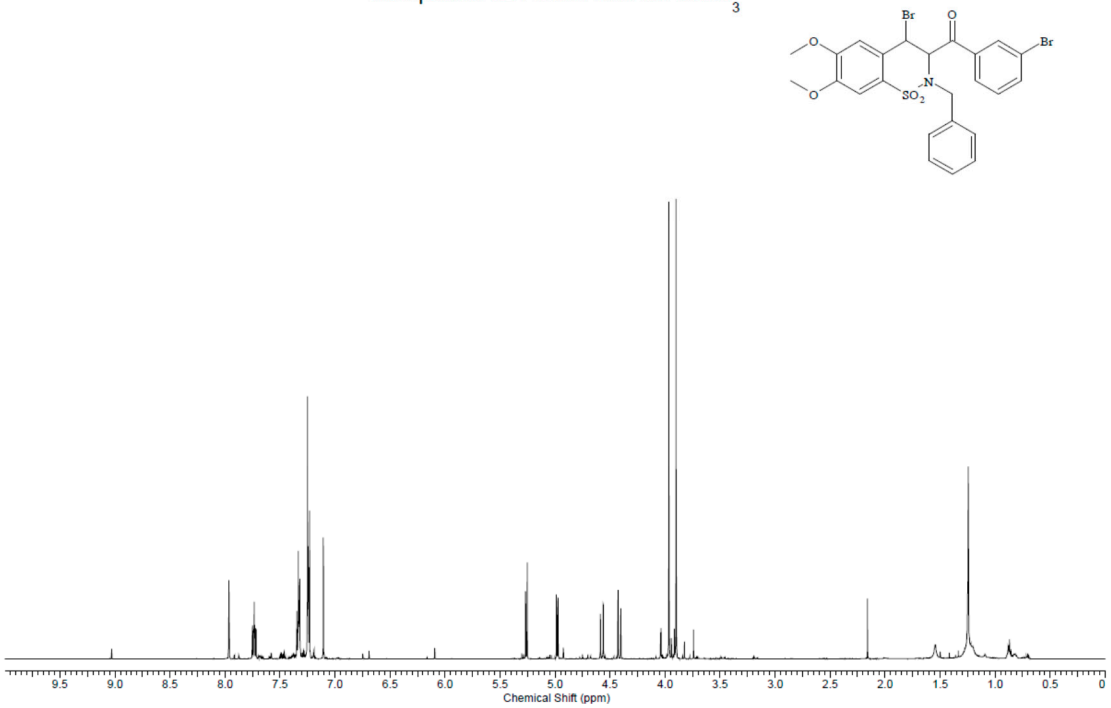
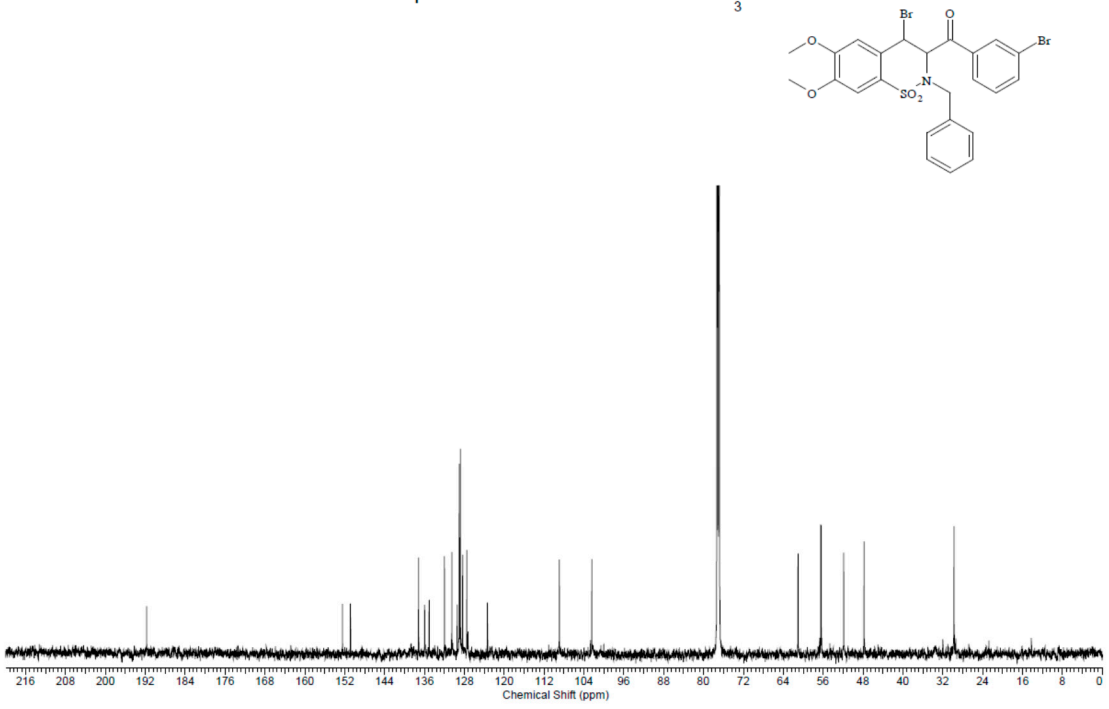


Compound **62** Carbon NMR in $CDCl_3$



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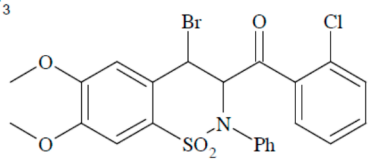
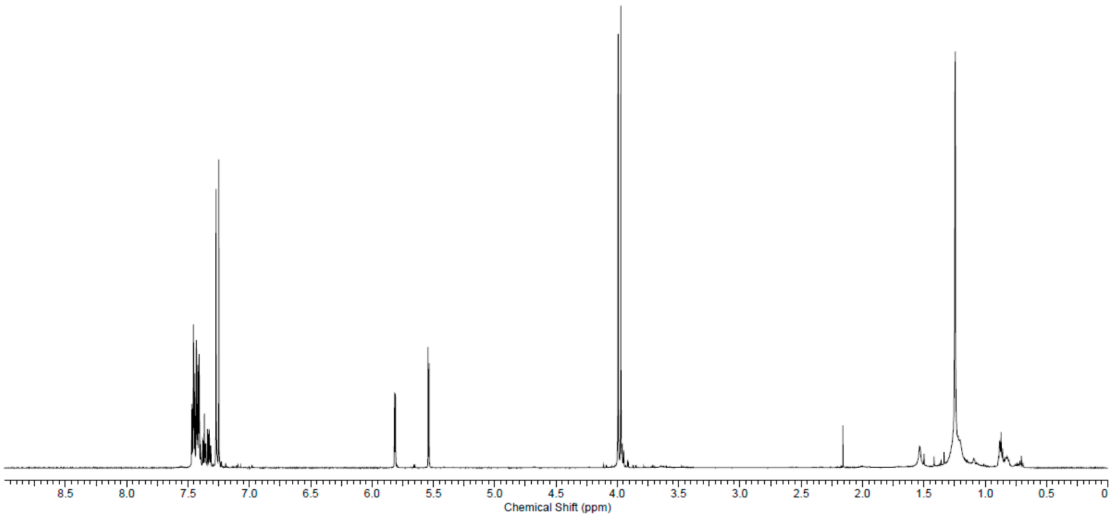
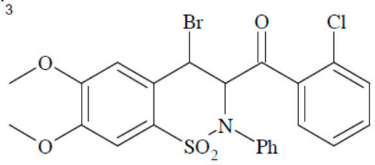
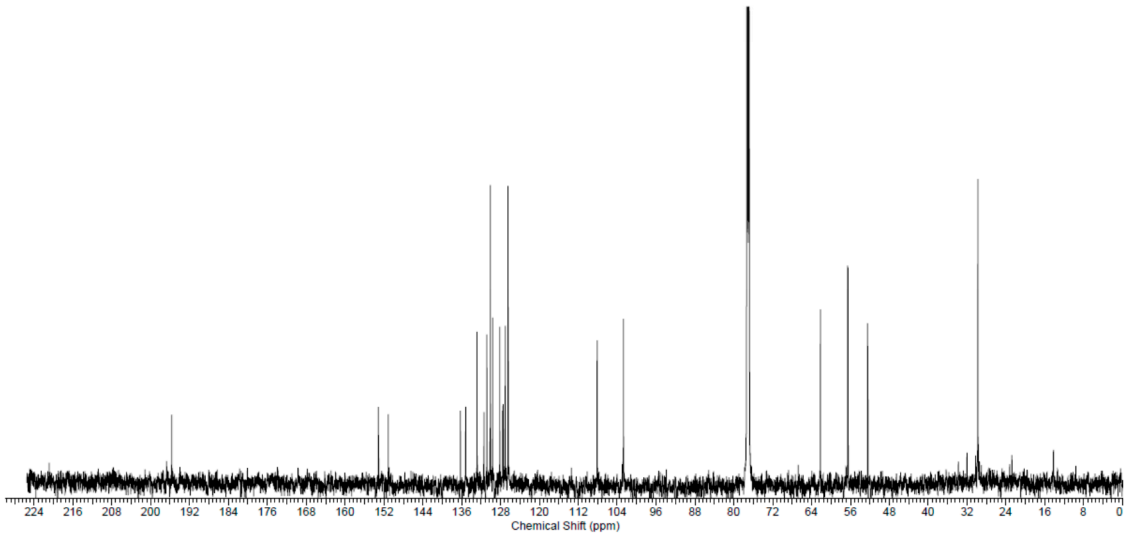


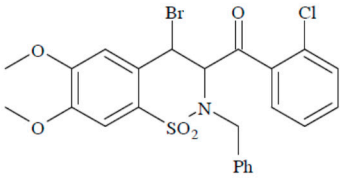


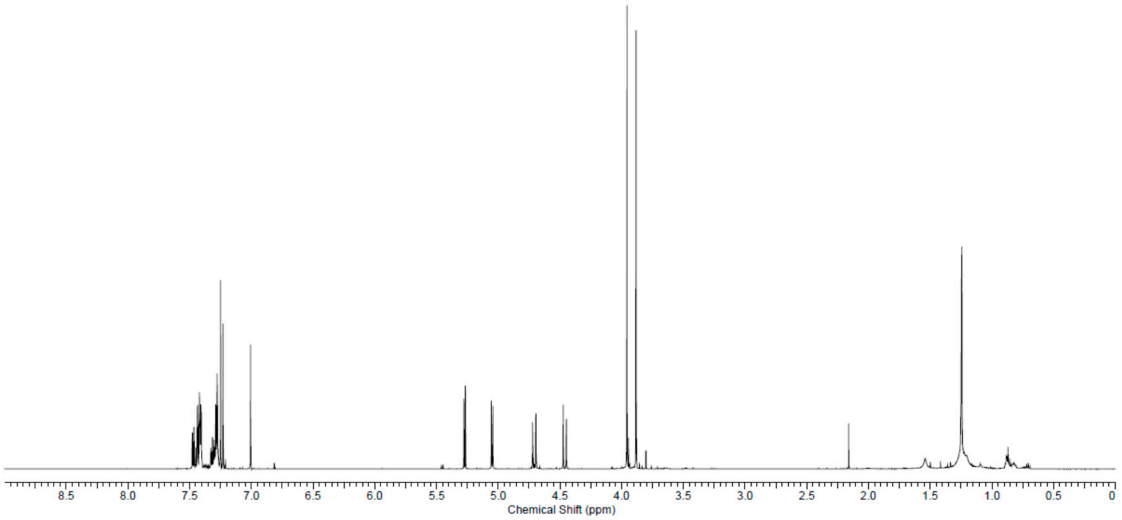
Compound **66** Carbon NMR in $CDCl_3$



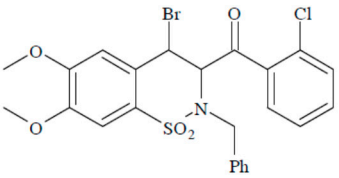


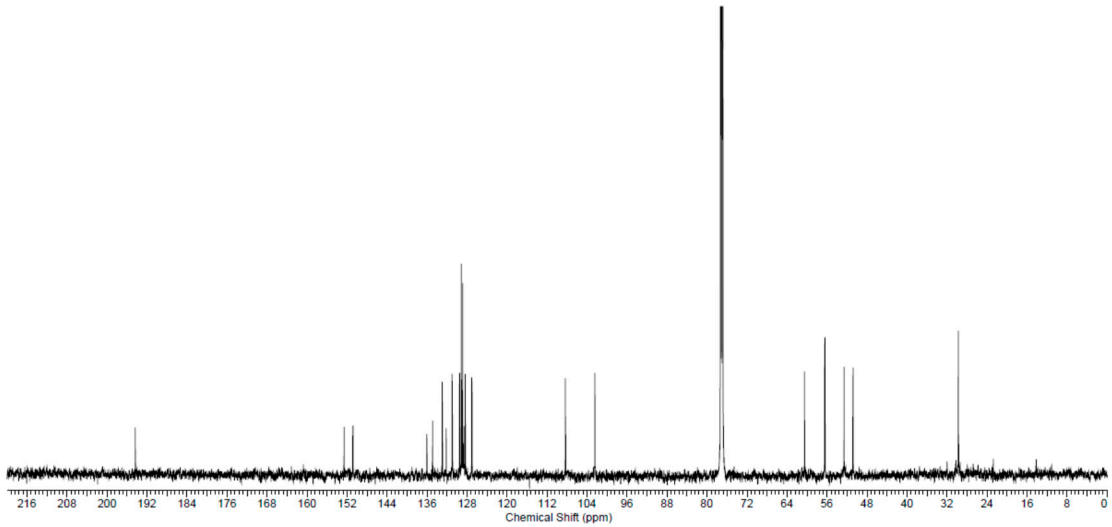
Compound **67** Proton NMR in $CDCl_3$



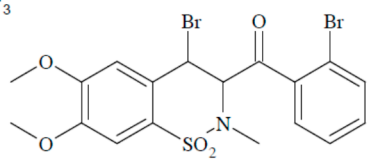


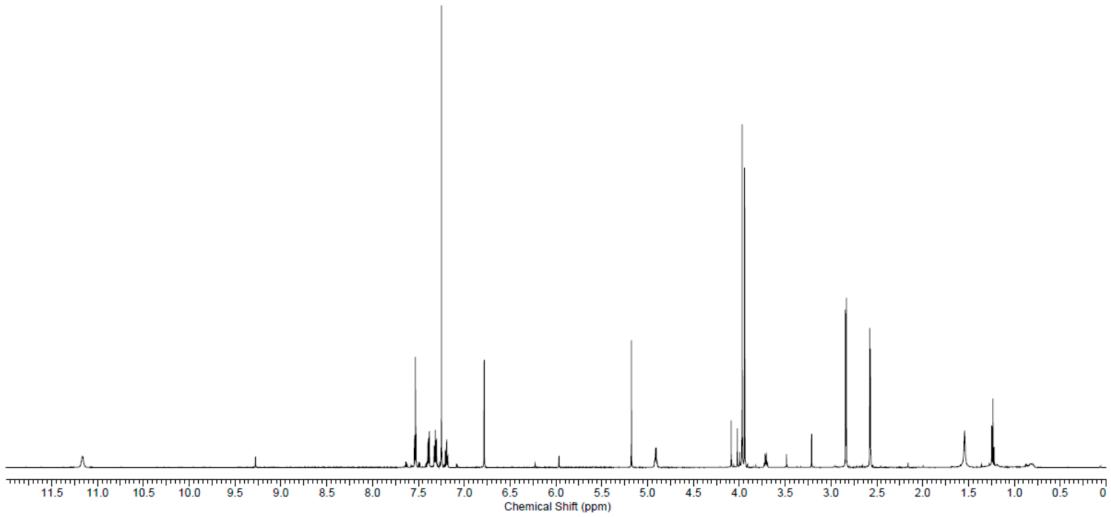
Compound **67** Carbon NMR in $CDCl_3$



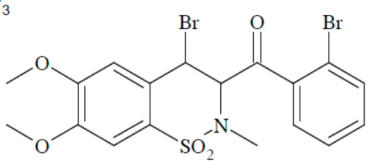


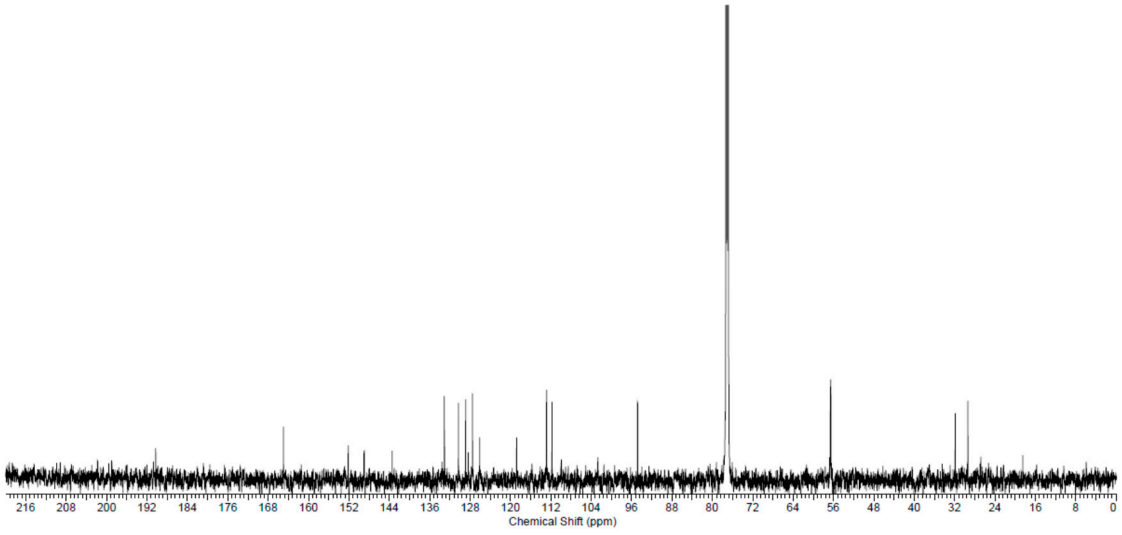
Compound **69** Proton NMR in $CDCl_3$



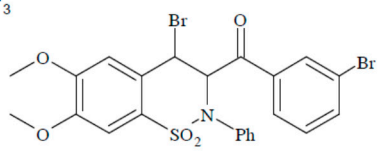


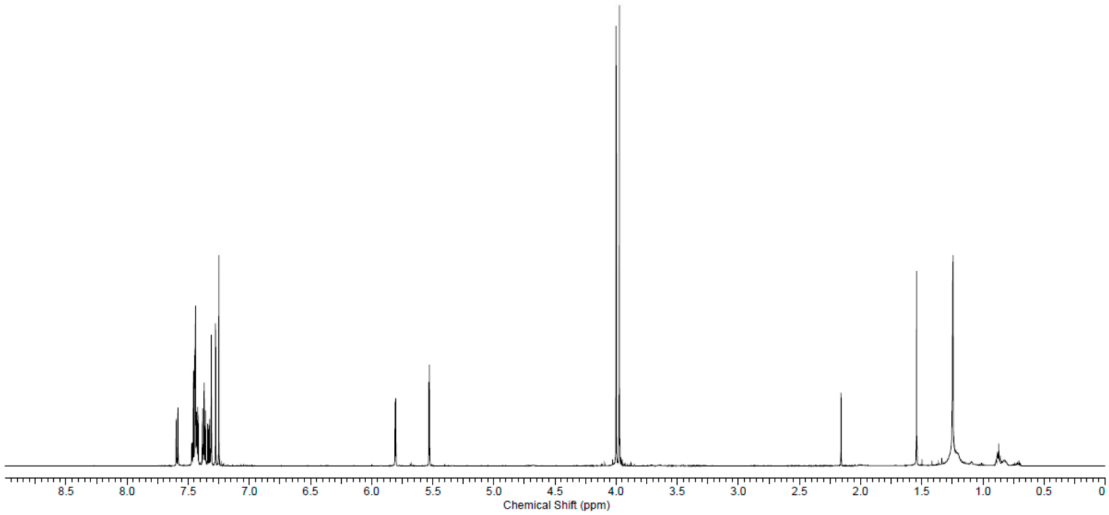
Compound **69** Carbon NMR in $CDCl_3$



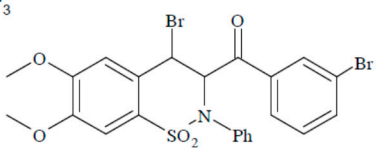


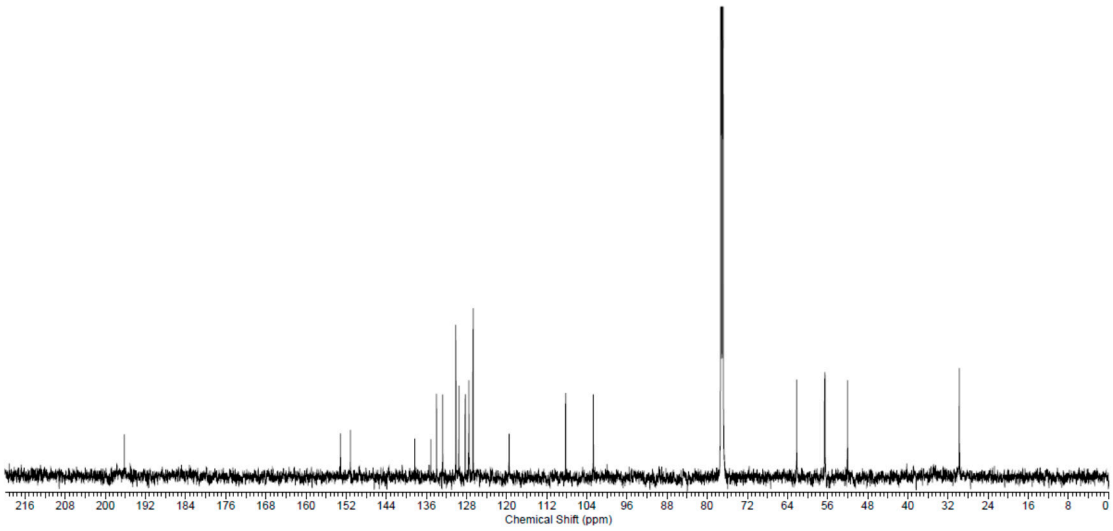
Compound **71** Proton NMR in $CDCl_3$



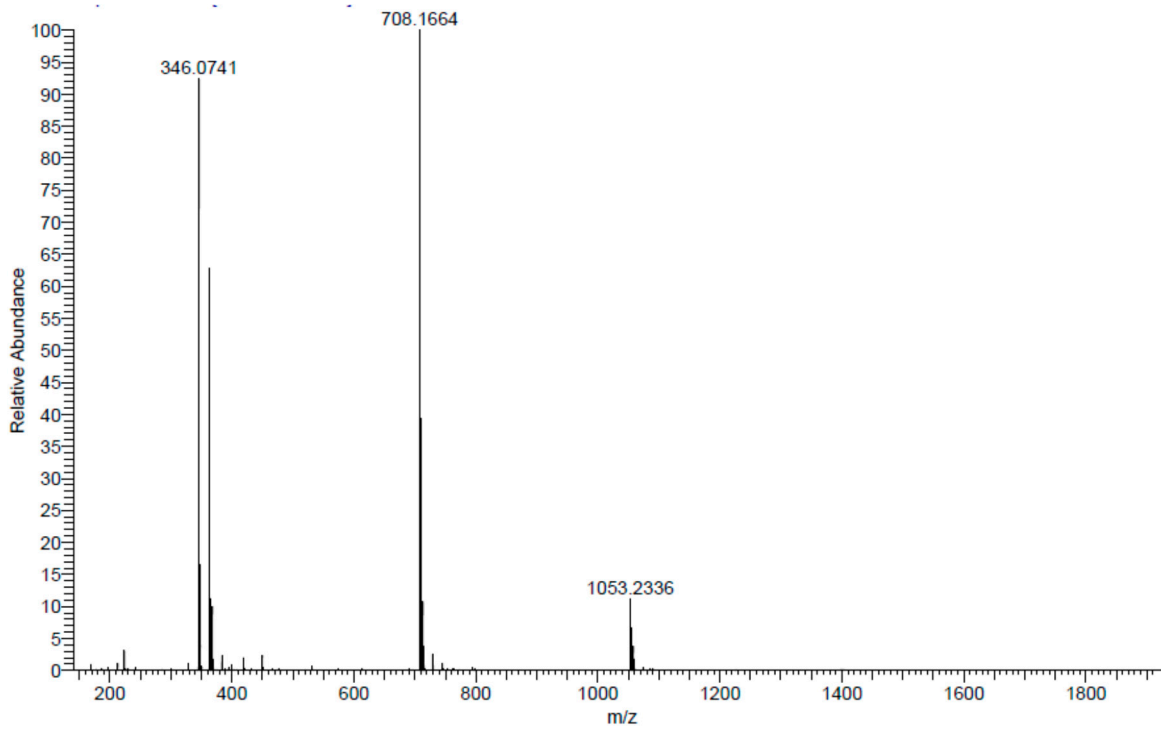


Compound **71** Carbon NMR in $CDCl_3$

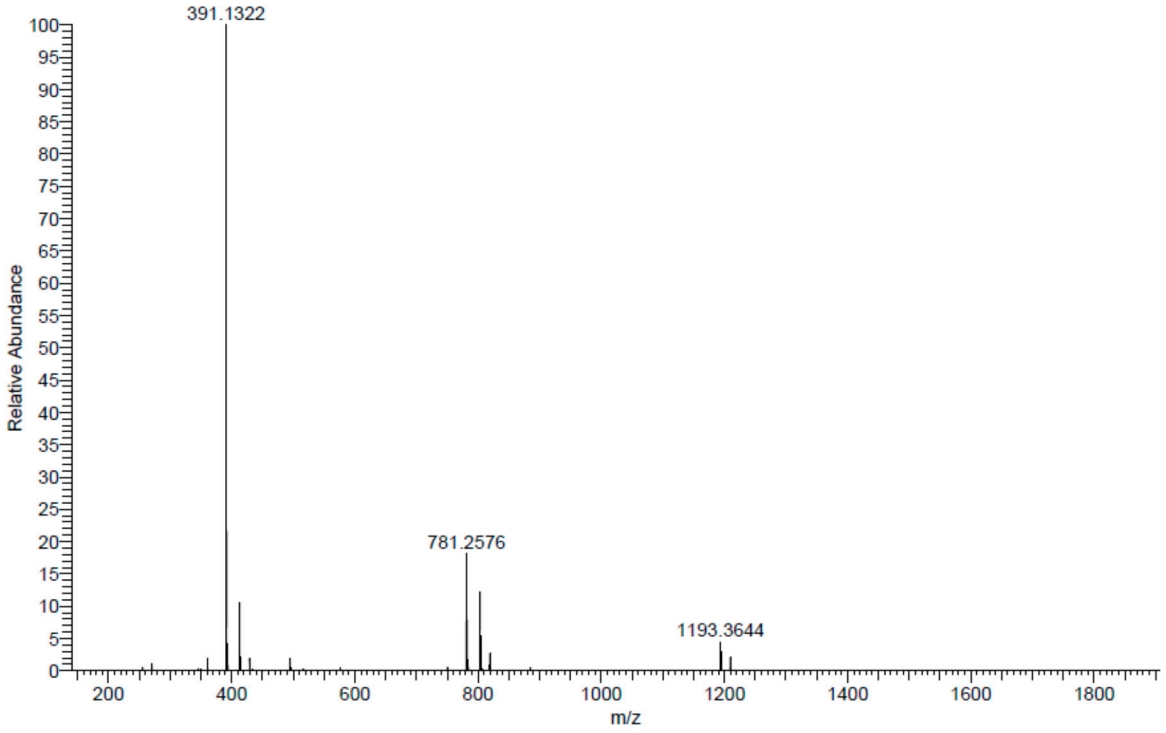




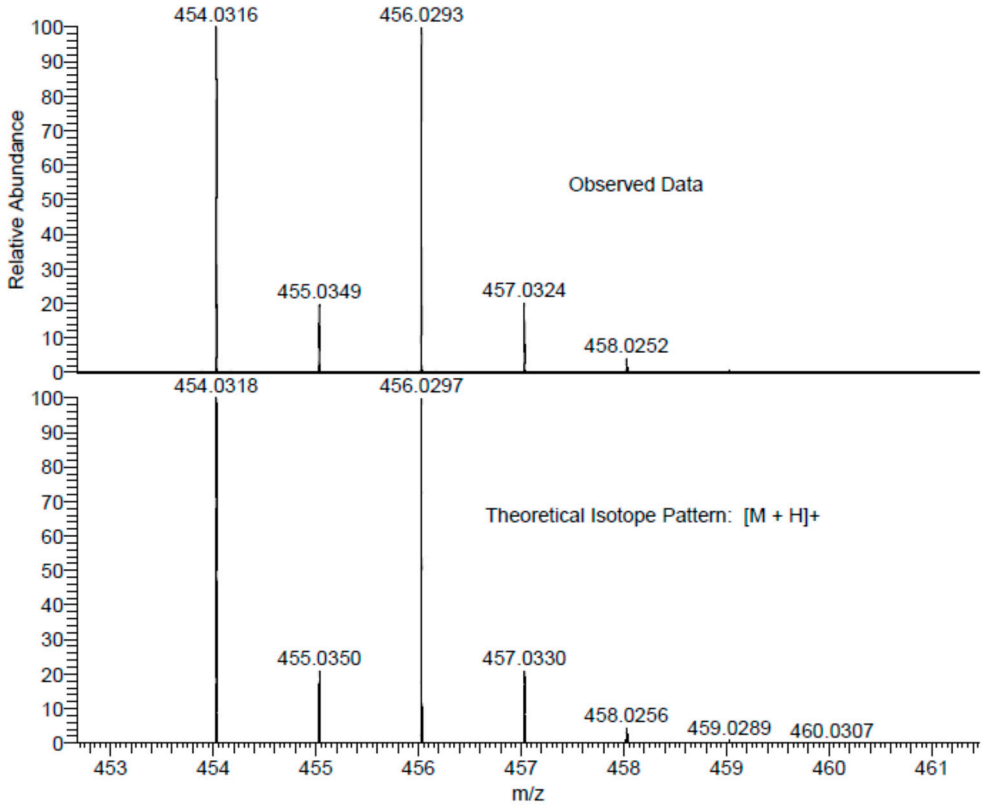
Compound **28** $[M + H]^+$



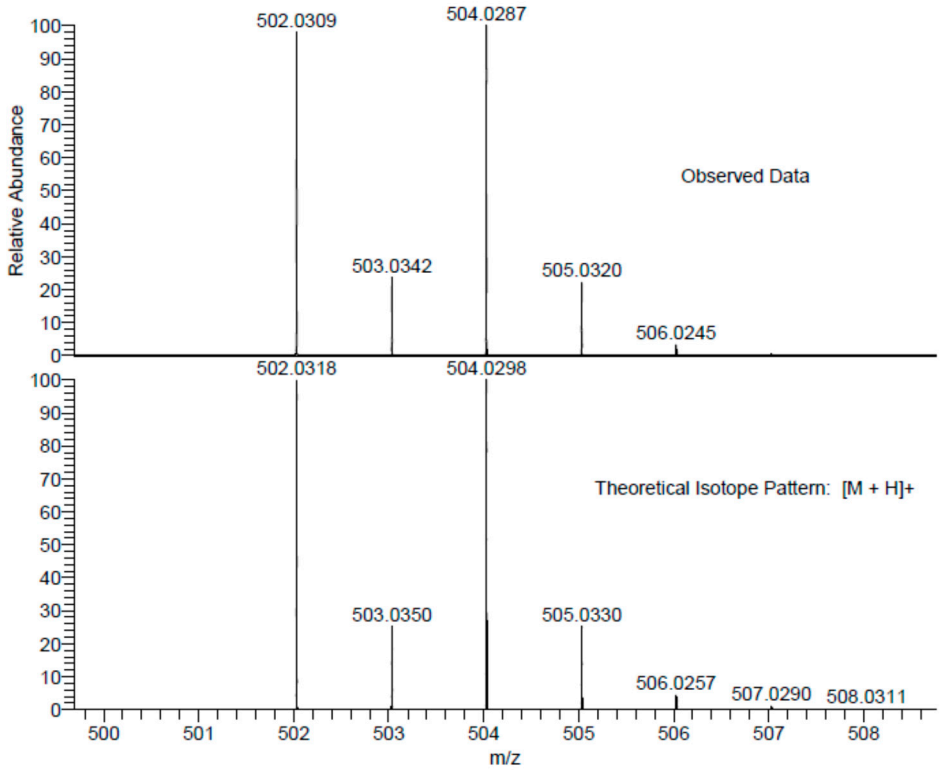
Compound **29** $[M + H]^+$



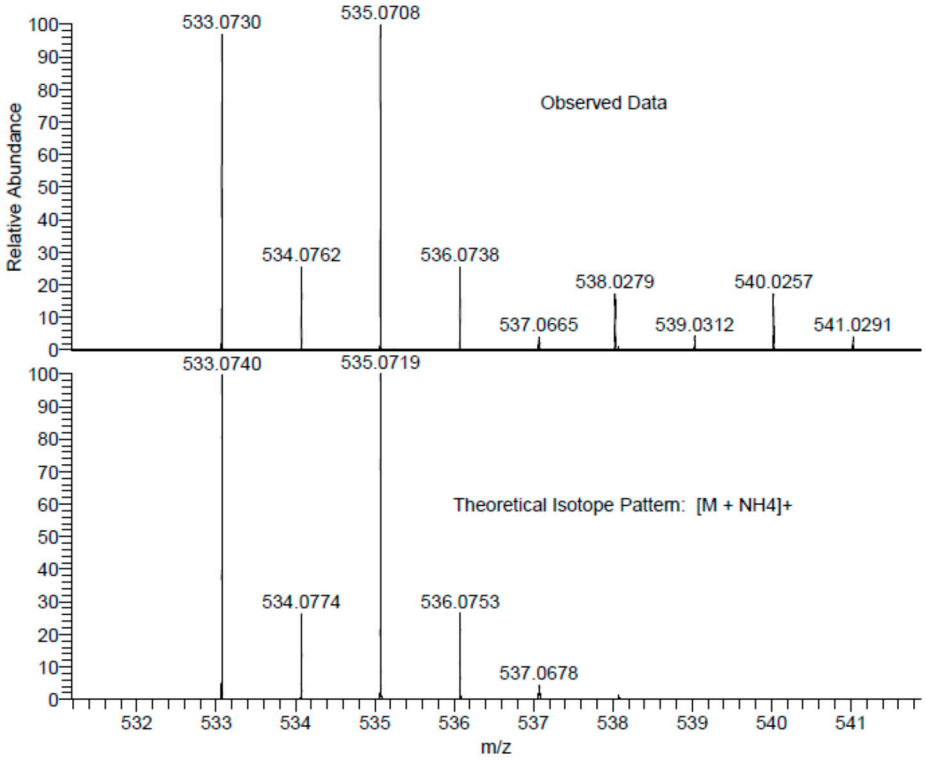
Compound **30** $[M + H]^+$



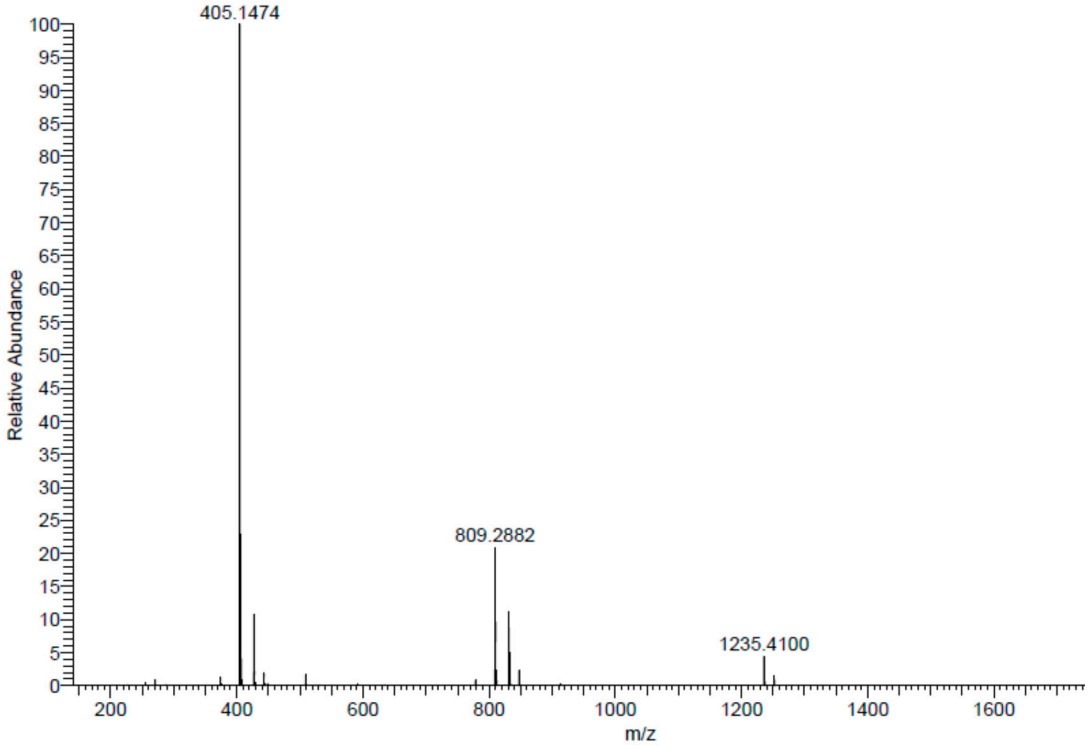
Compound **31** $[M + H]^+$



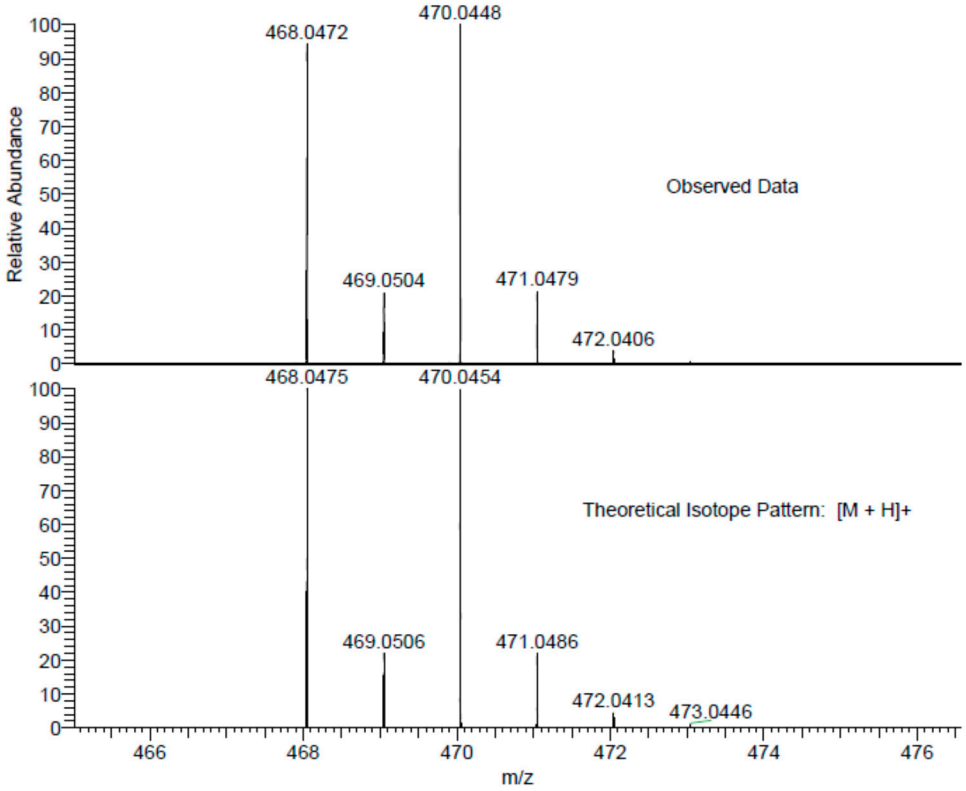
Compound **32** $[M + NH_4]^+$



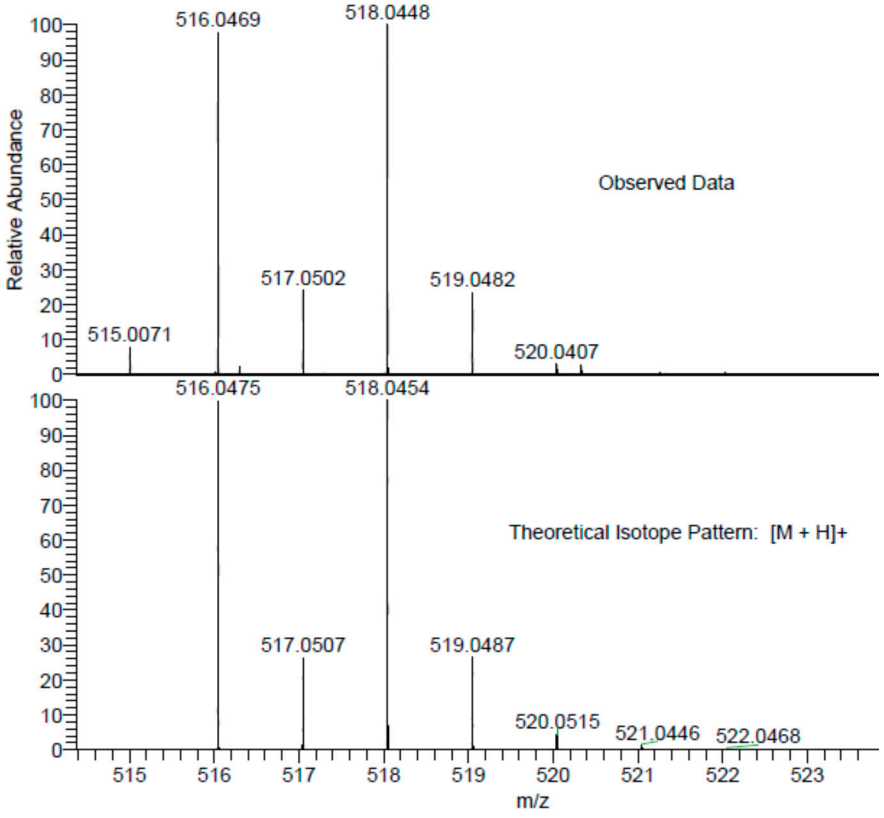
Compound **34** $[M + H]^+$



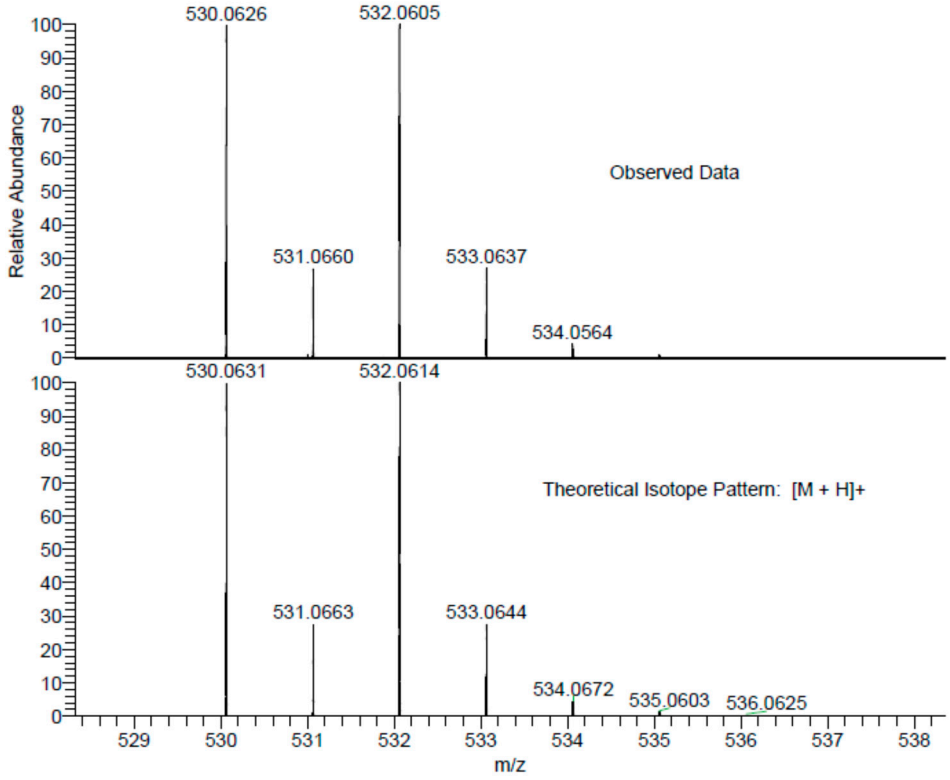
Compound **35** $[M + H]^+$



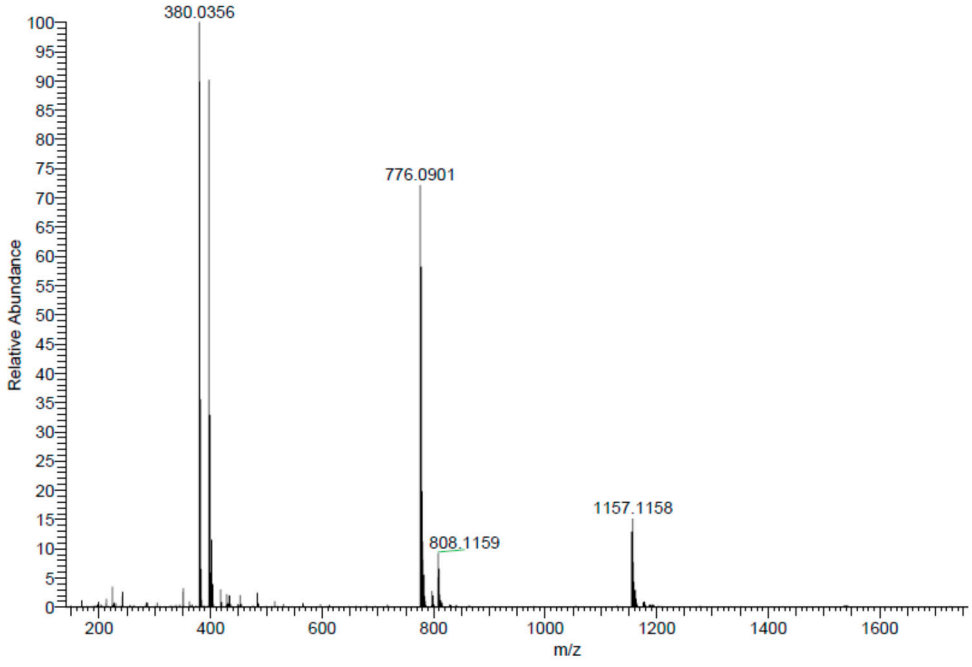
Compound **36** $[M + H]^+$



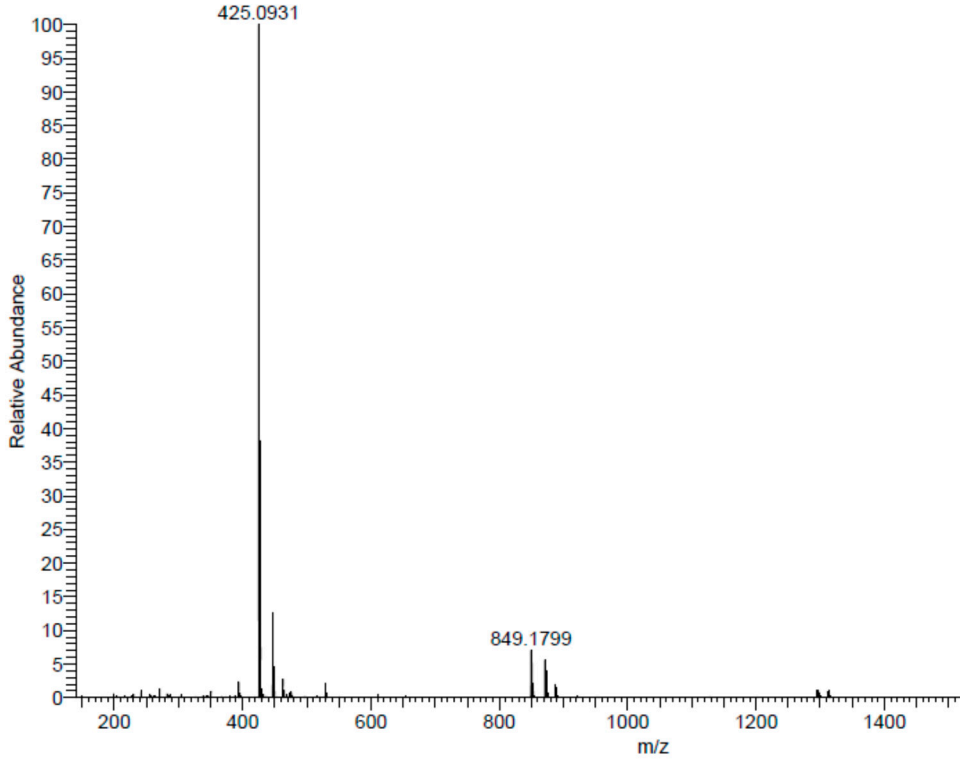
Compound **37** $[M + H]^+$



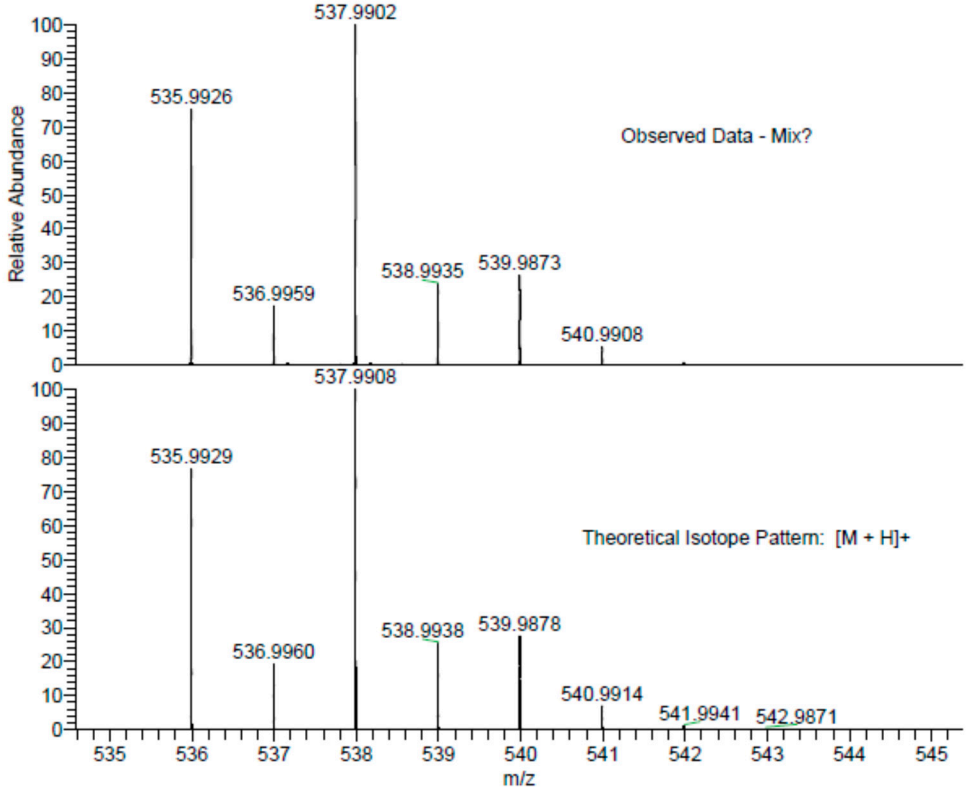
Compound **38** $[M - Br]^+$



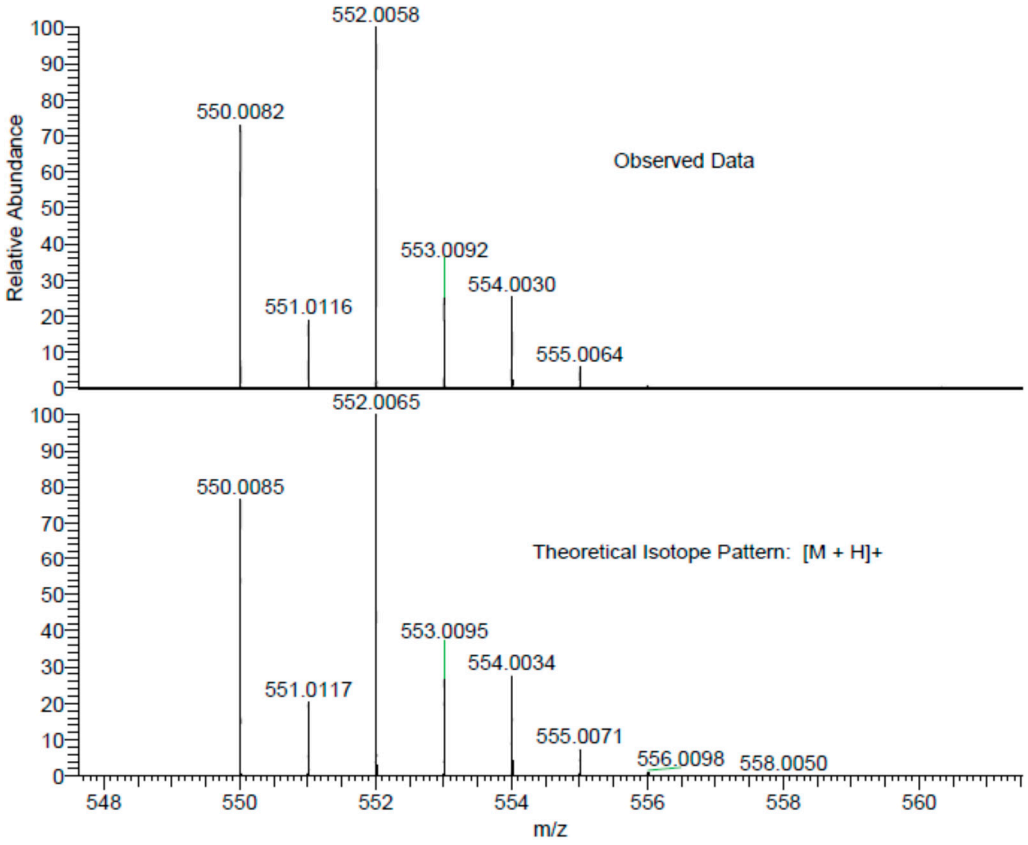
Compound **39** $[M + H]^+$



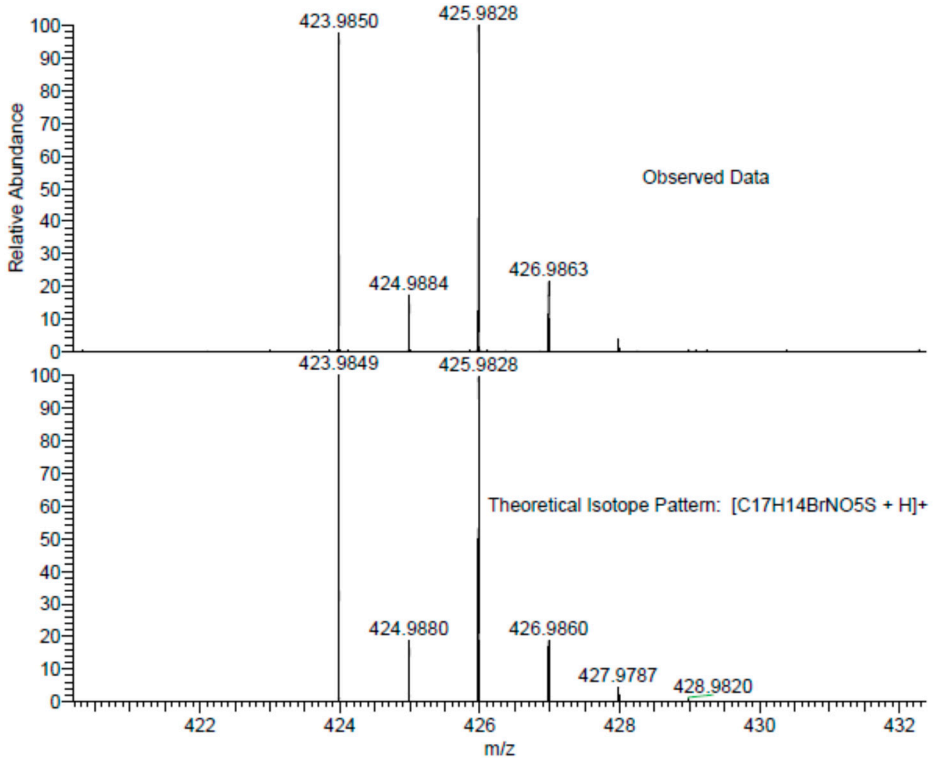
Compound **41** $[M + H]^+$



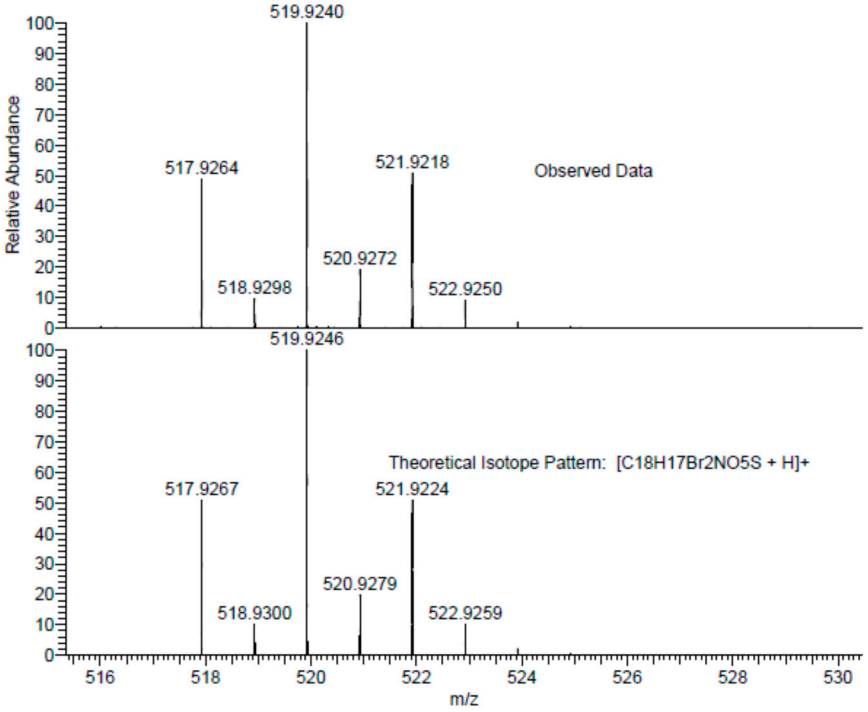
Compound **42** $[M + H]^+$



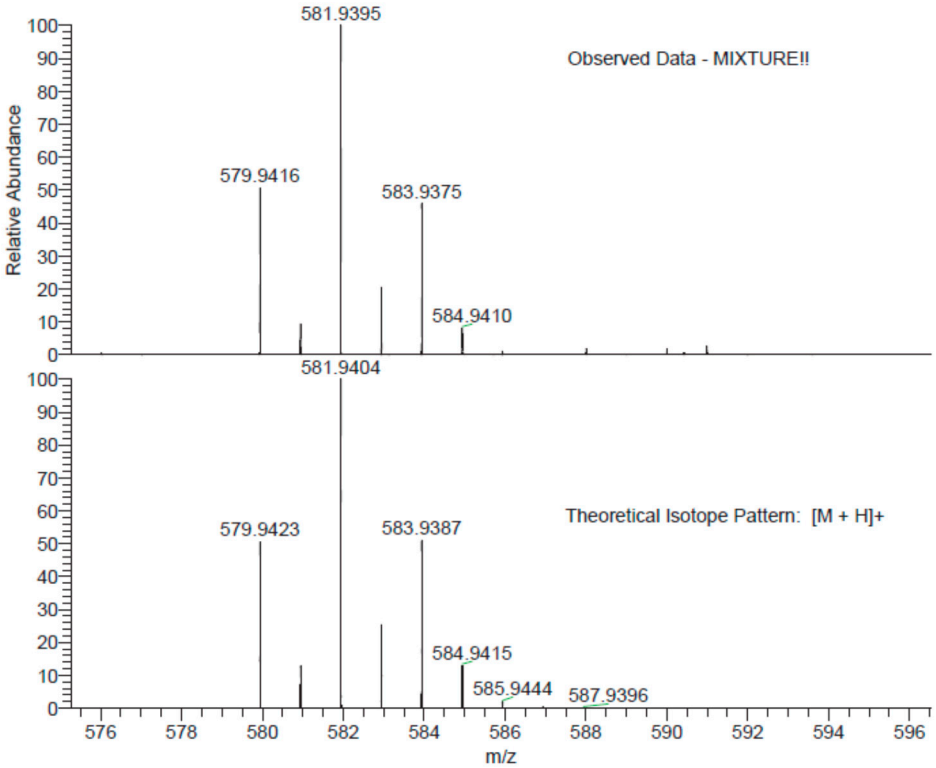
Compound **43** $[M - Br]^+$



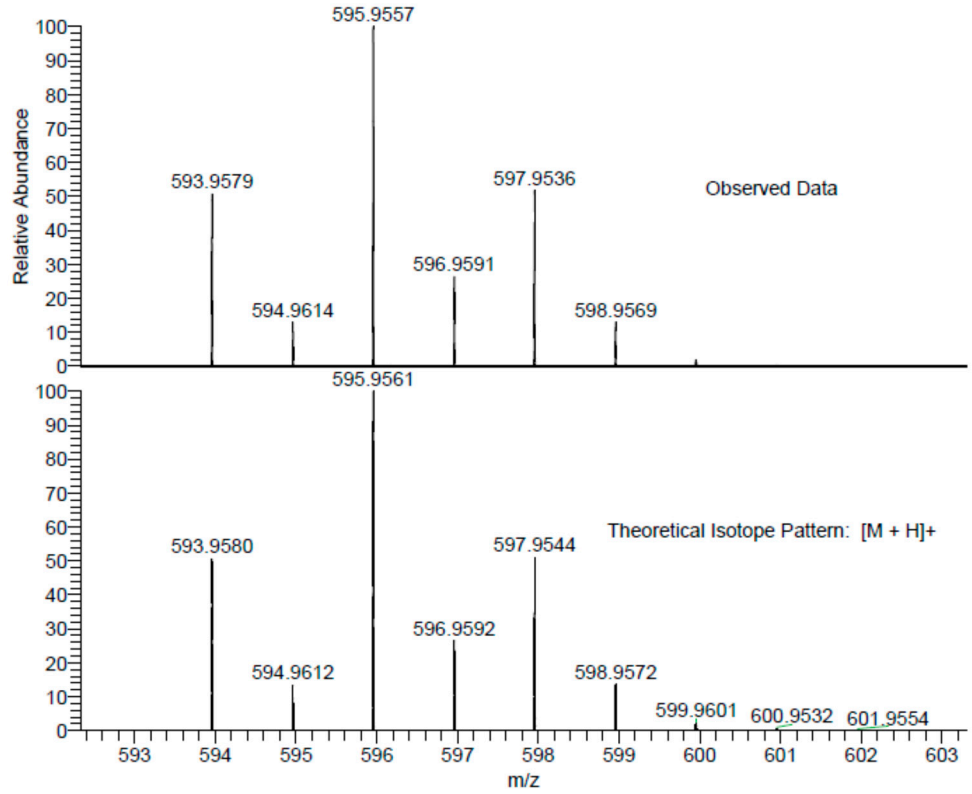
Compound **45** $[M + H]^+$



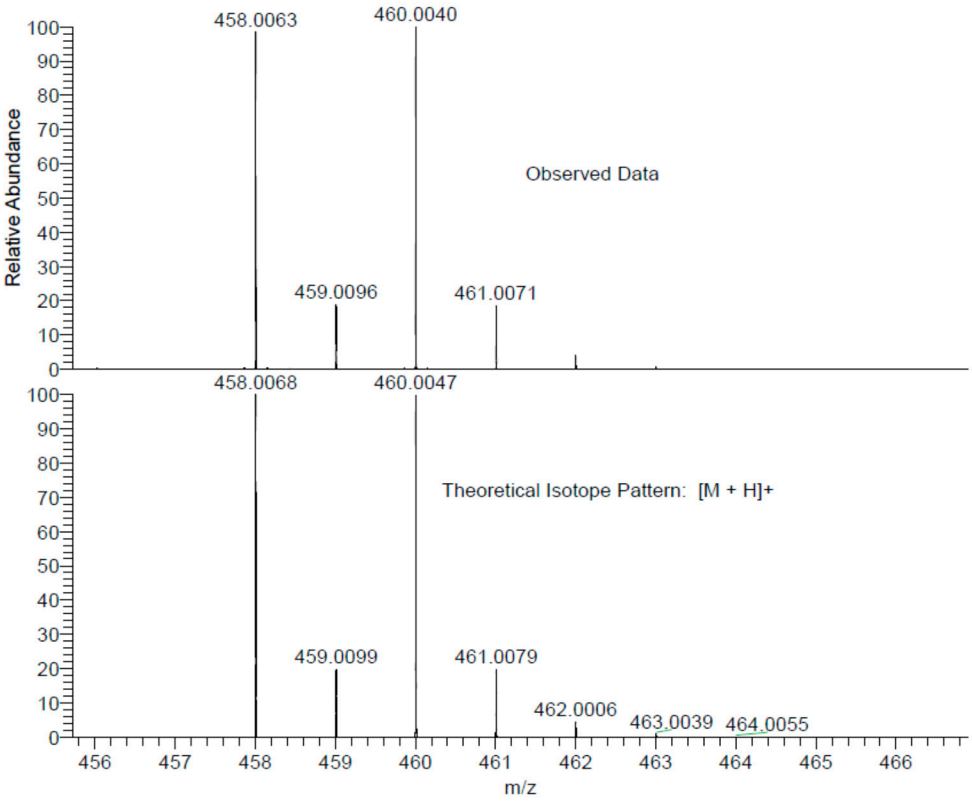
Compound **46** $[M + H]^+$



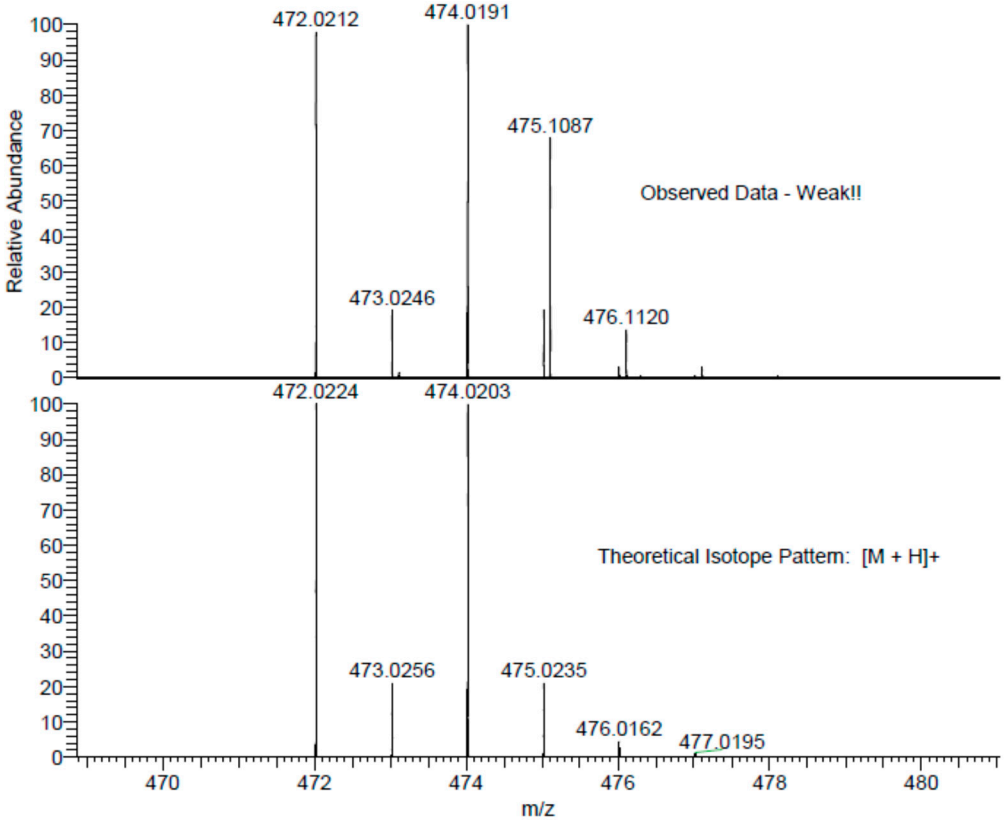
Compound **47** $[M + H]^+$



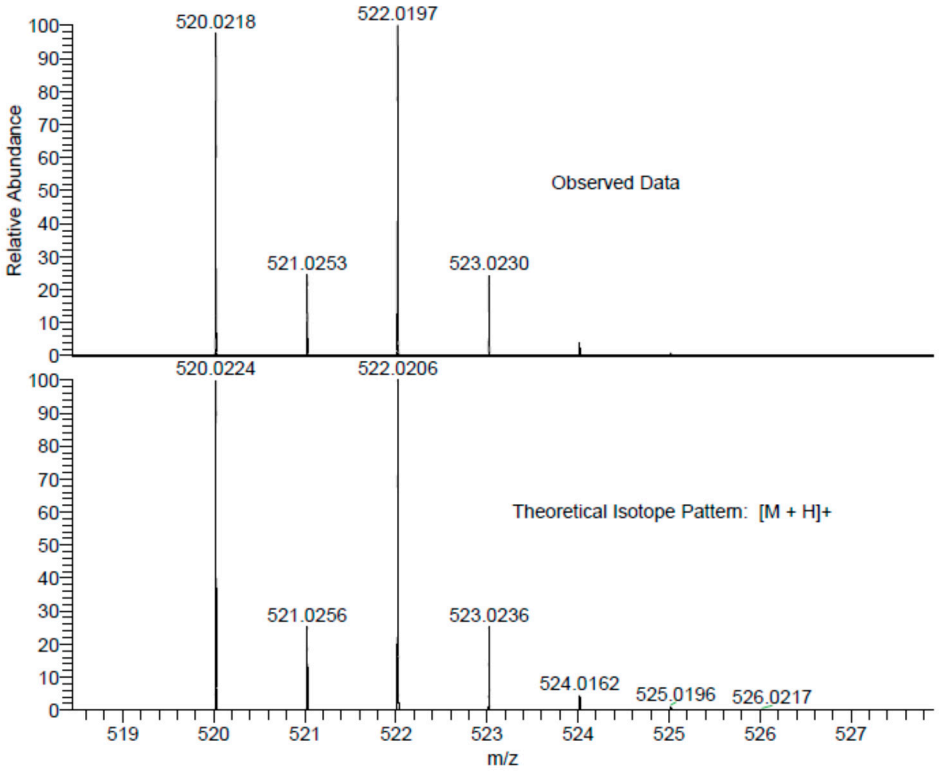
Compound **49** $[M + H]^+$



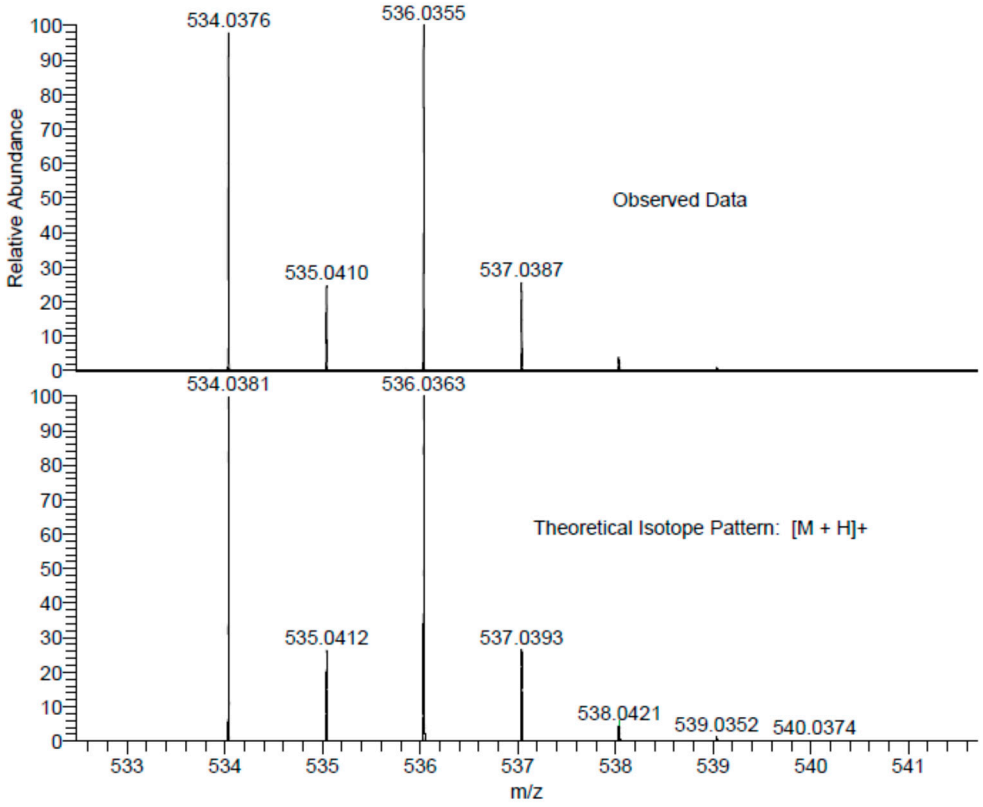
Compound **50** $[M + H]^+$



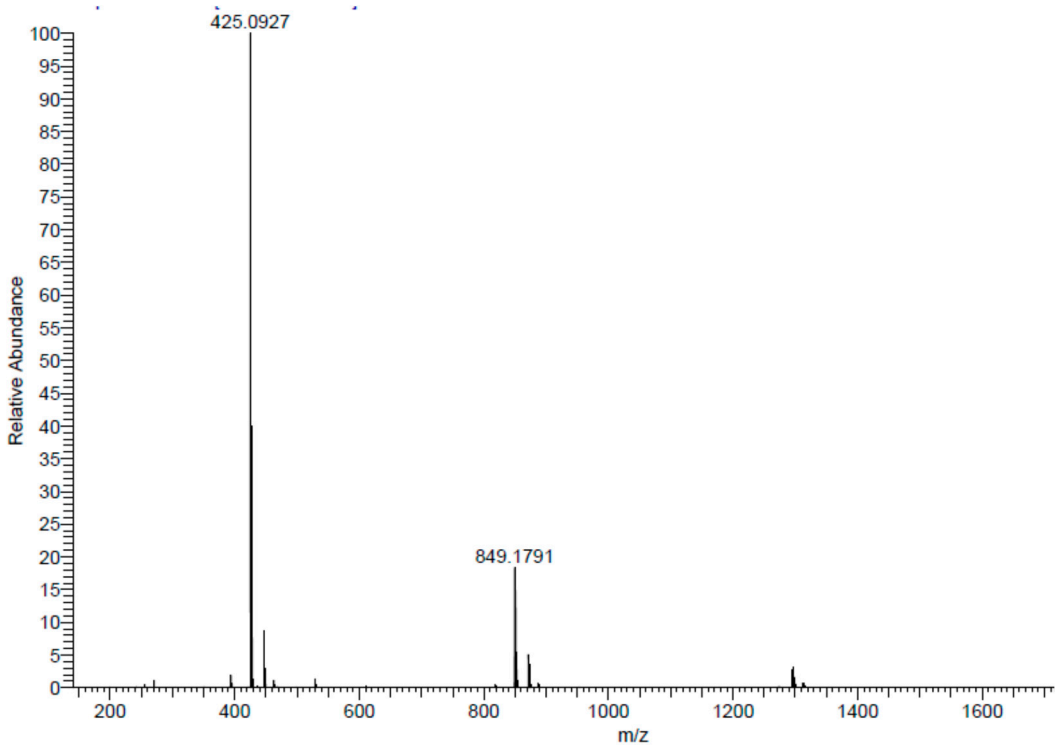
Compound **51** $[M + H]^+$



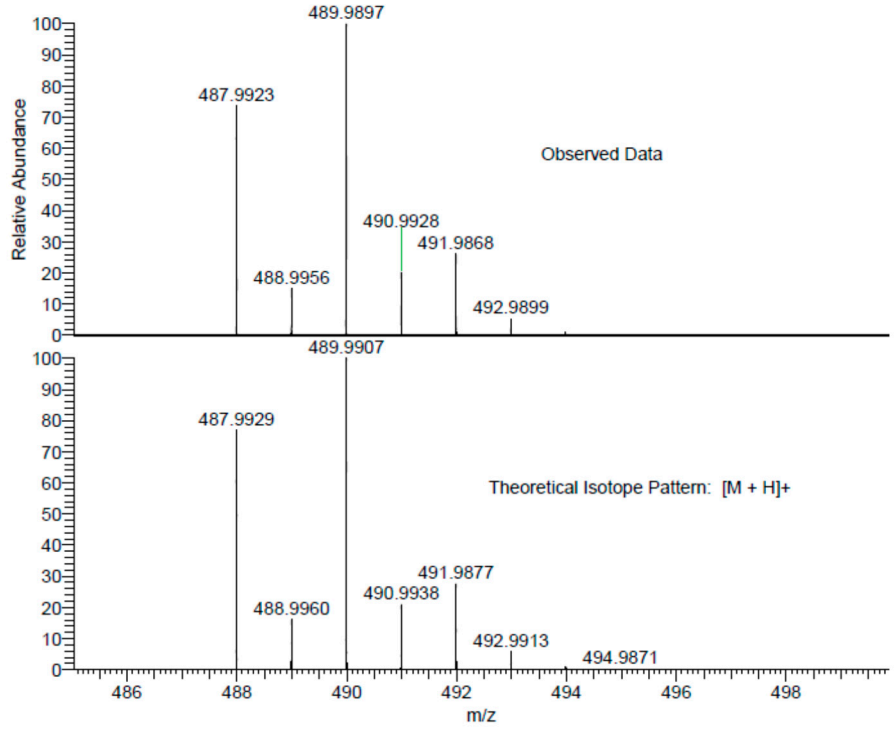
Compound **52** $[M + H]^+$



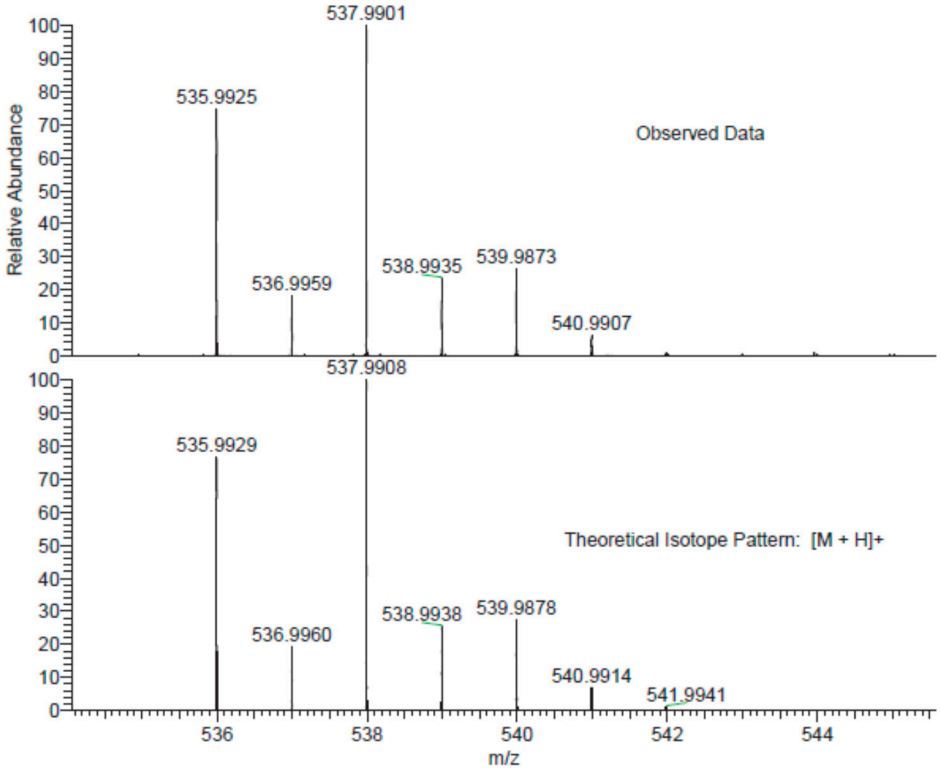
Compound **54** $[M + H]^+$



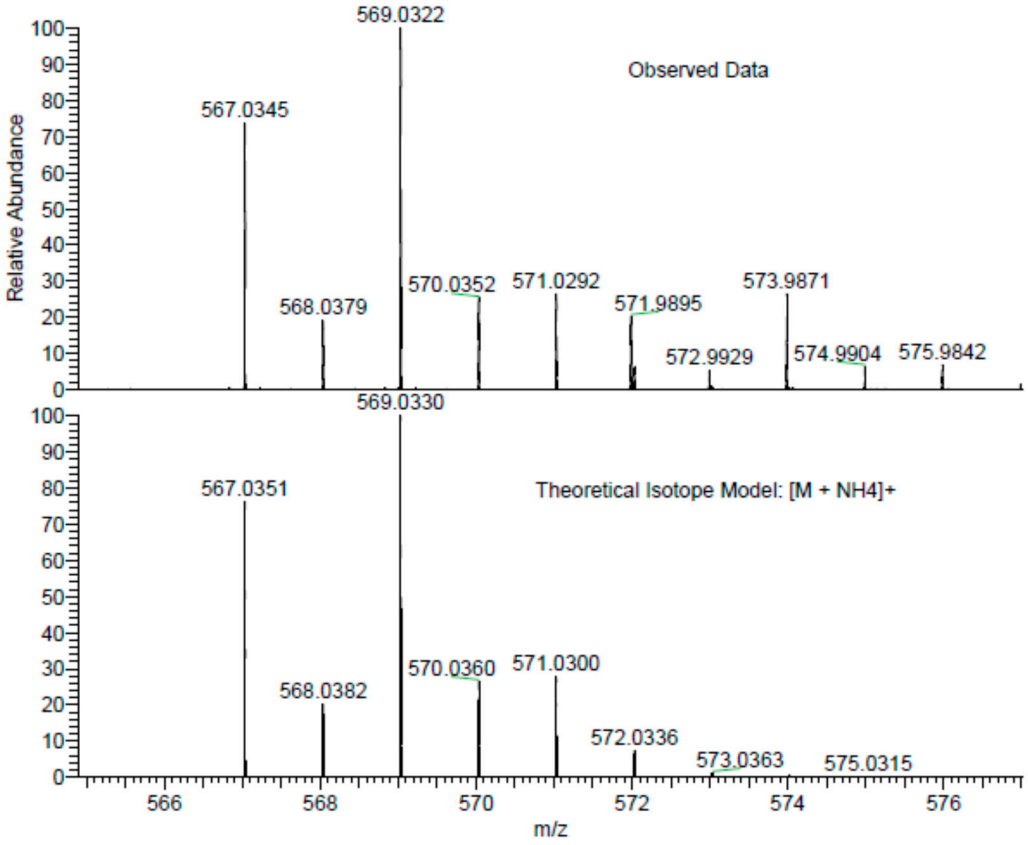
Compound **55** $[M + H]^+$



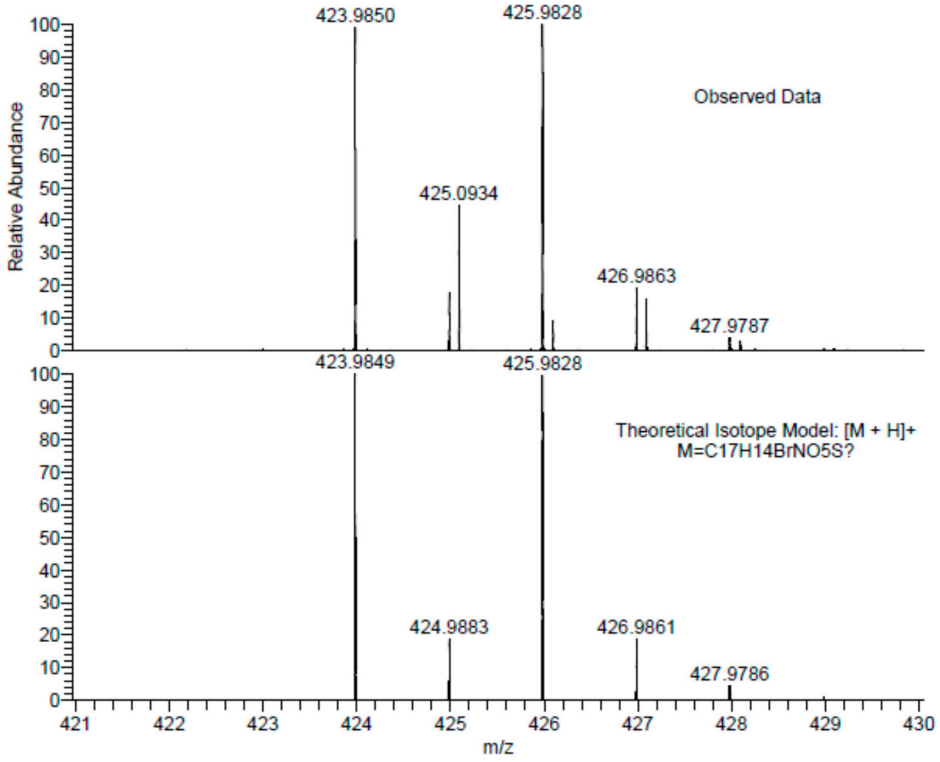
Compound **56** $[M + H]^+$



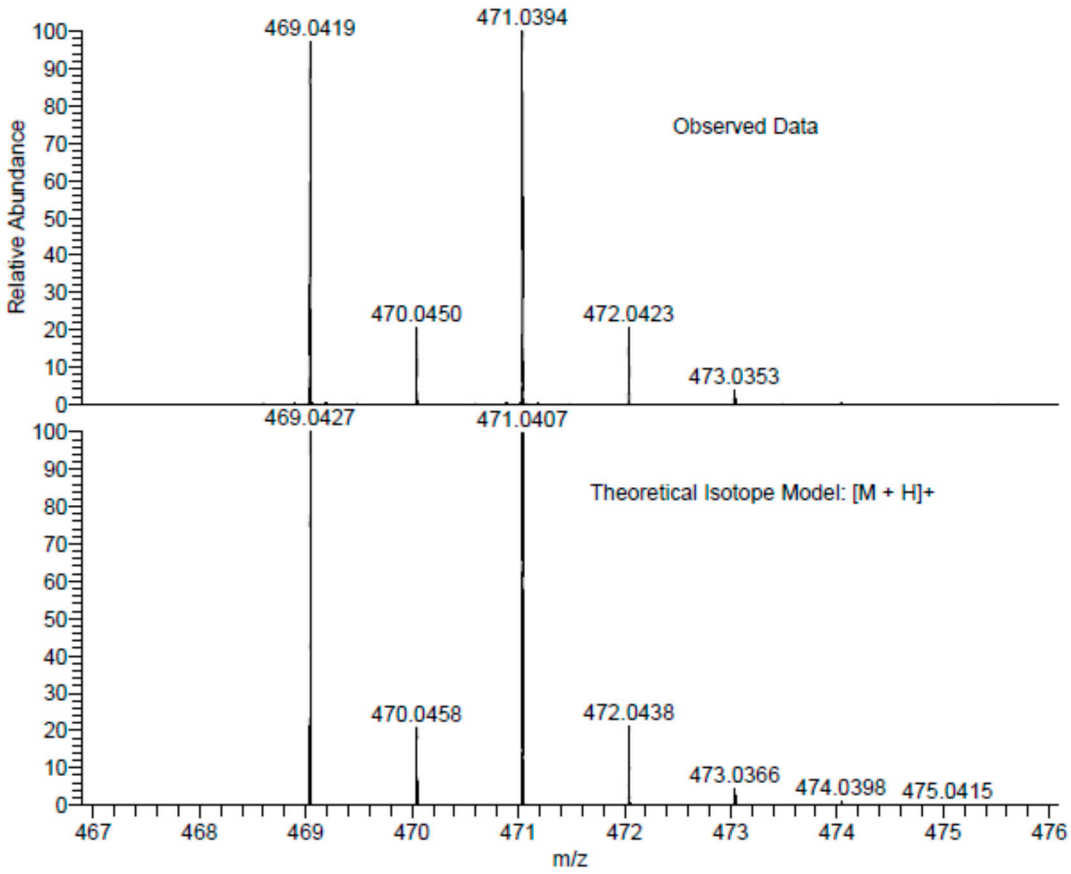
Compound **57** $[M + NH_4]^+$



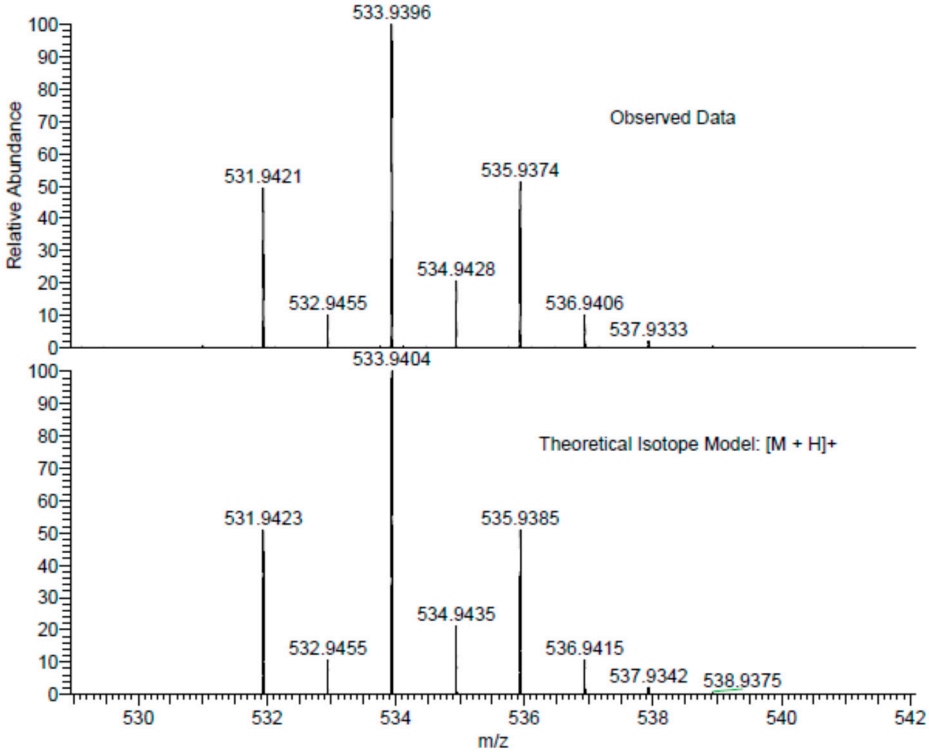
Compound **58** $[M - HBr]^+$



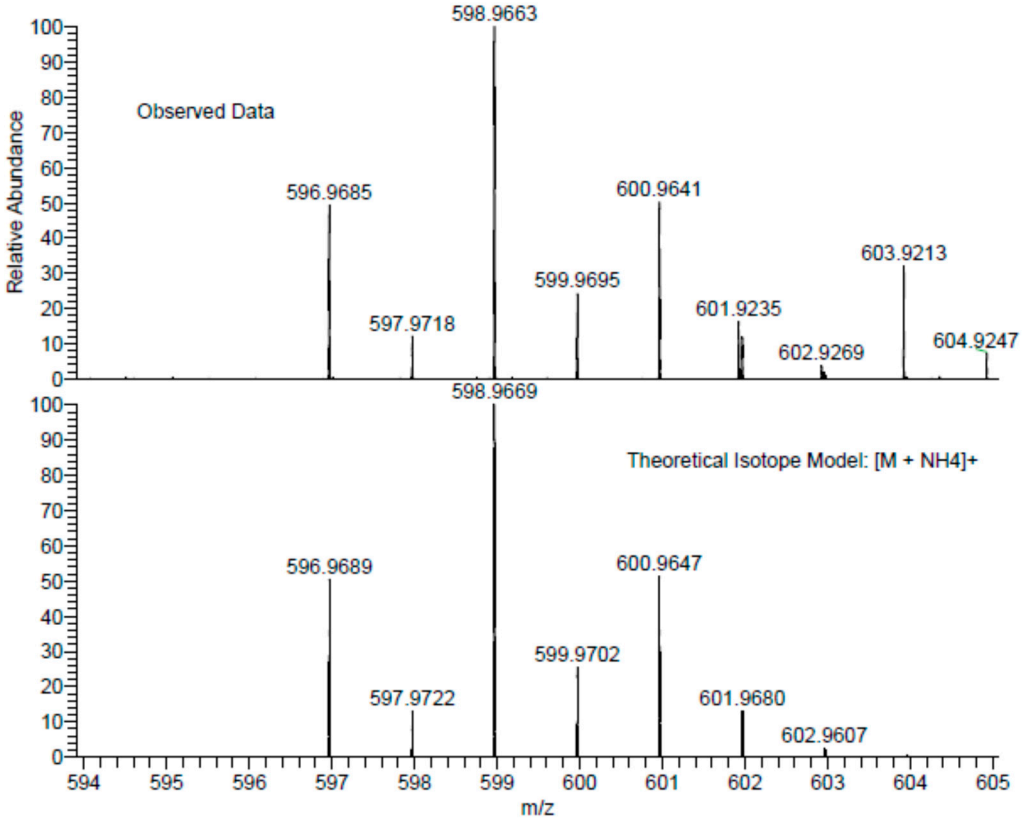
Compound **59** $[M + H]^+$



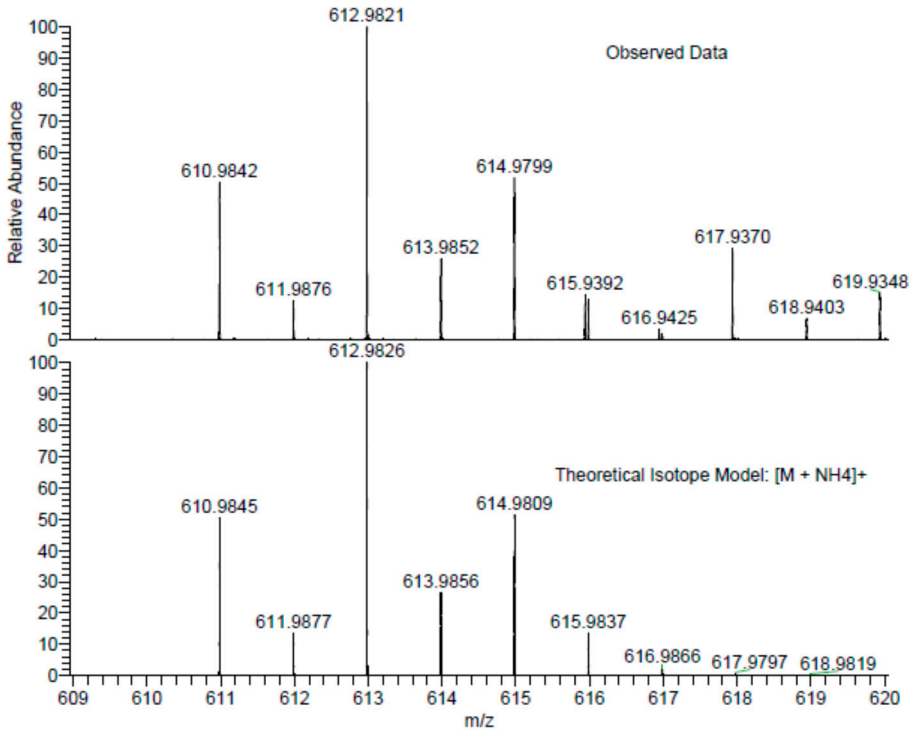
Compound **60** $[M + H]^+$



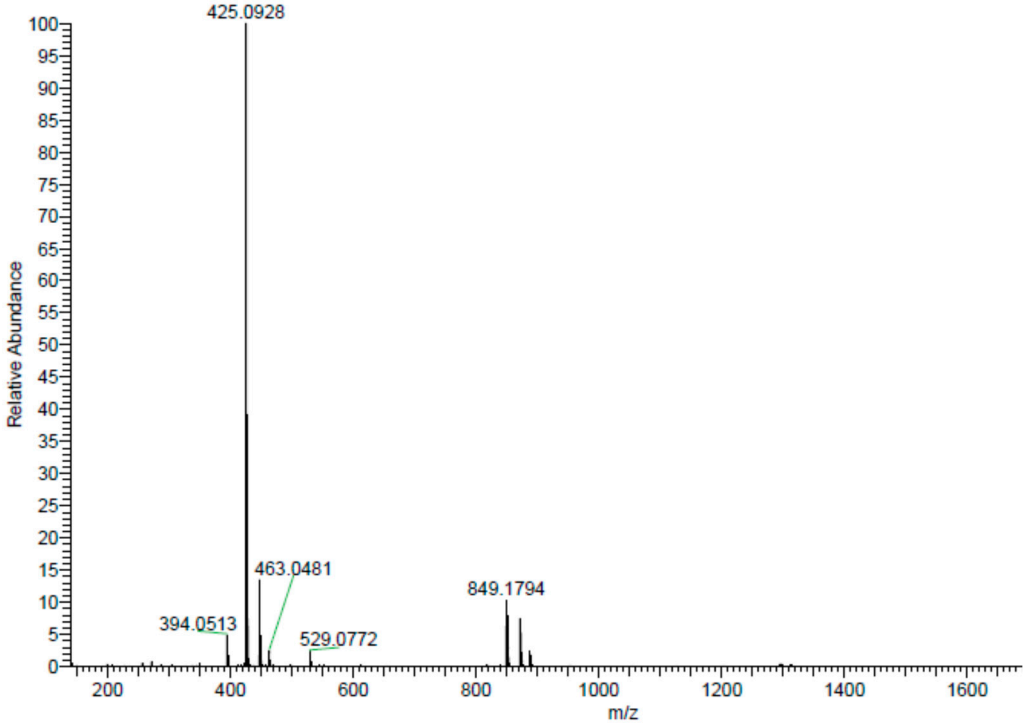
Compound **61** $[M + NH_4]^+$



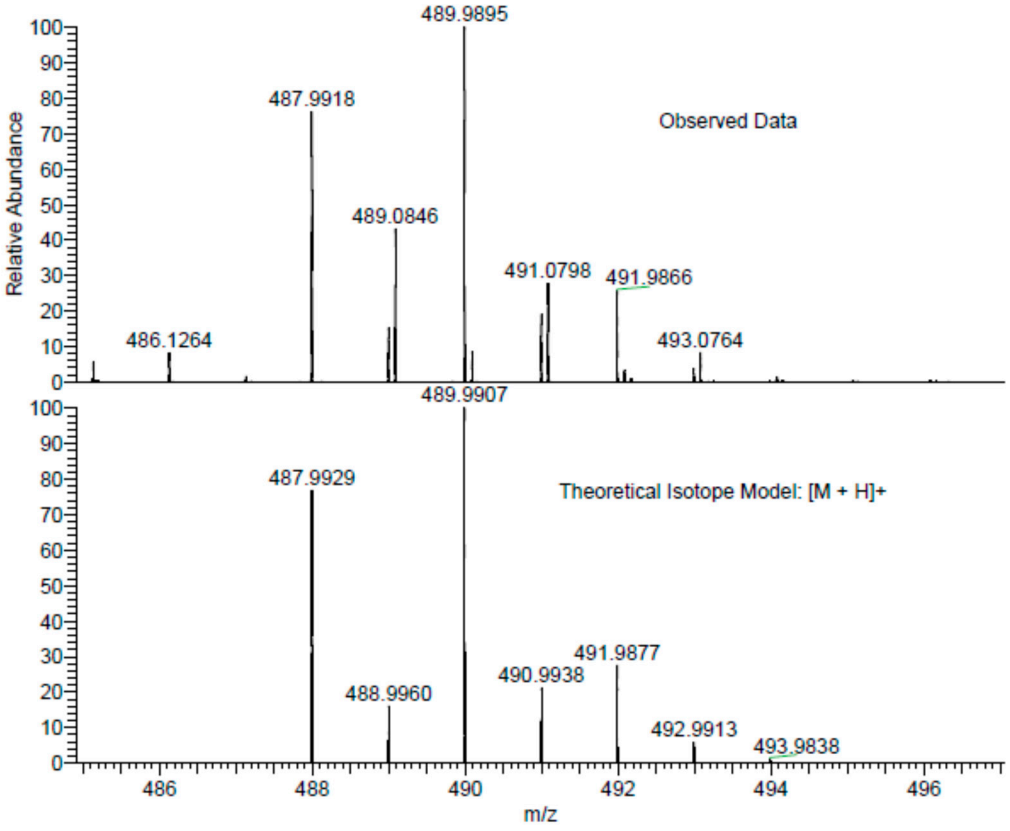
Compound **62** $[M + NH_4]^+$



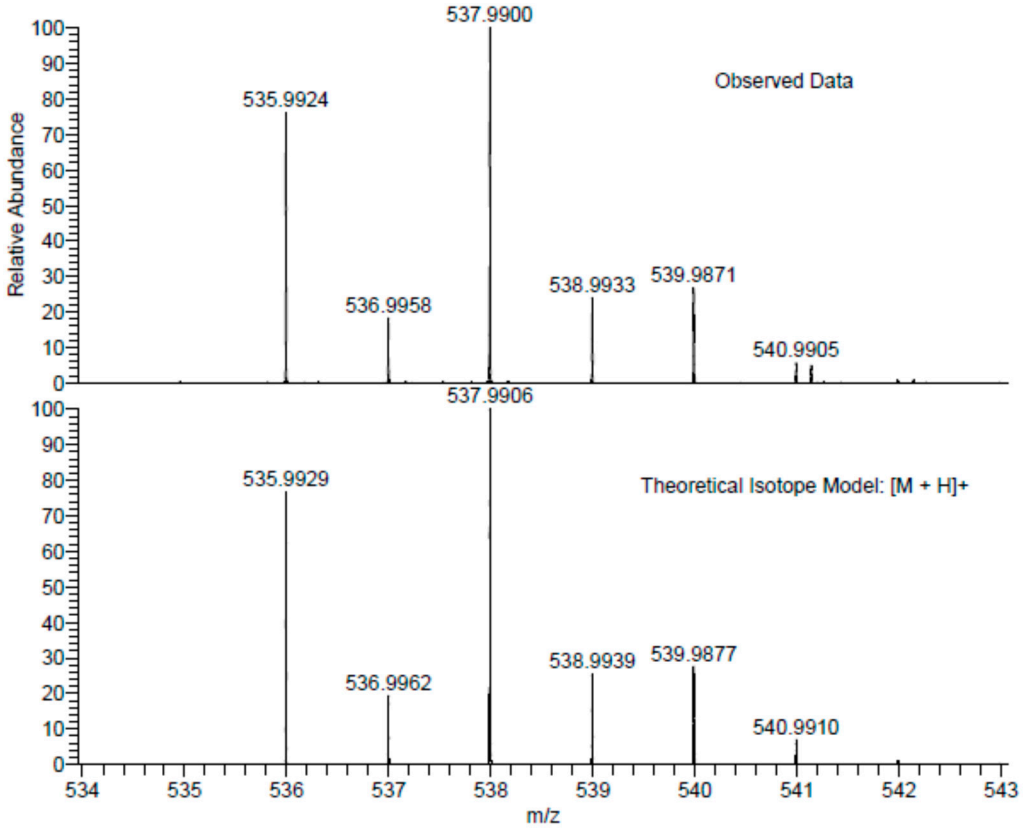
Compound **64** $[M + H]^+$



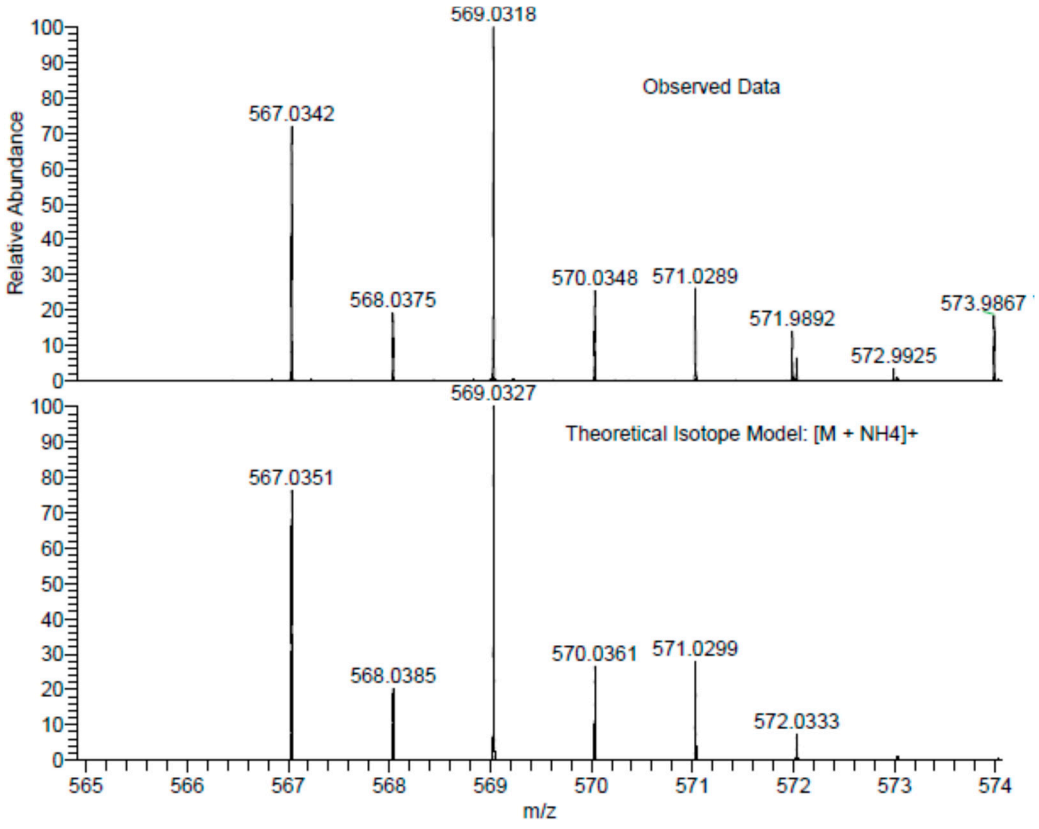
Compound **65** $[M + H]^+$



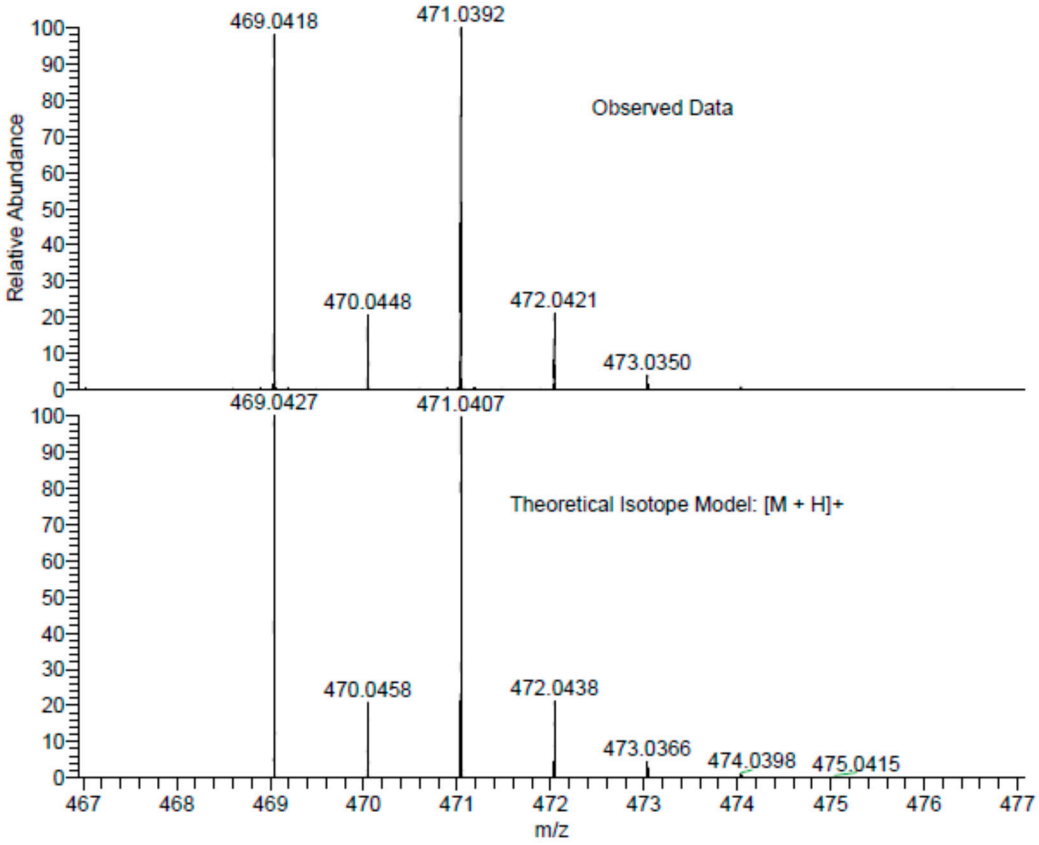
Compound **66** $[M + H]^+$



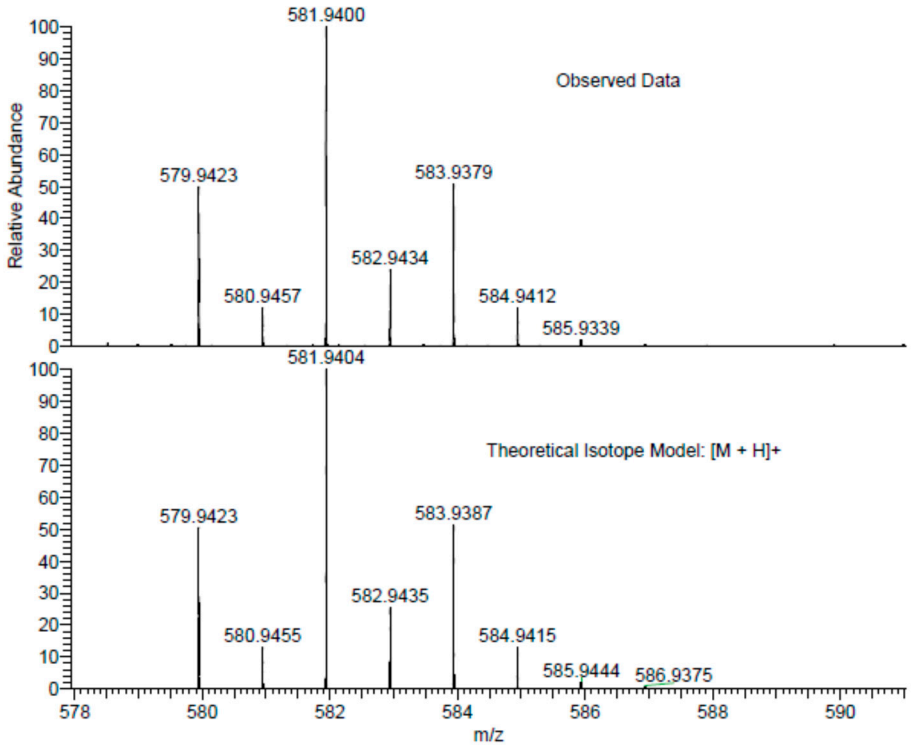
Compound **67** $[M + NH_4]^+$



Compound **69** $[M + H]^+$



Compound **71** $[M + H]^+$



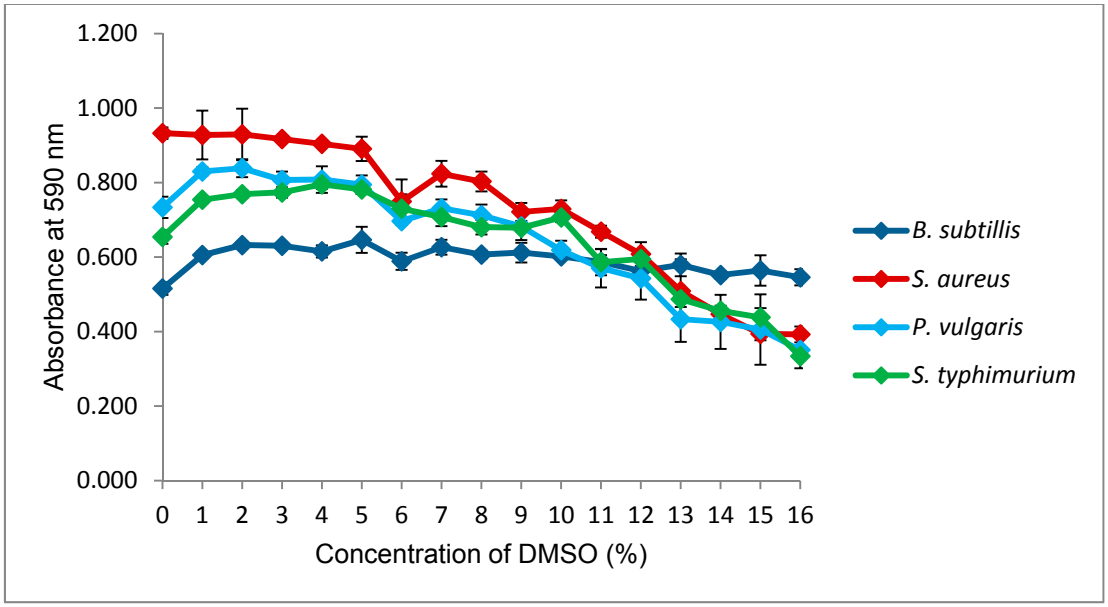


Figure S1. The absorbance measured at the 590 nm wave-length for *Bacillus subtilis*, *Staphylococcous aureus*, *Proteus vulgaris* and *Salmonella typhimurium* with different percentages of DMSO ranging from 0% to 16%. The experiment was conducted in triplicate. There is no decrease in absorbance up to 5% DMSO, meaning there is no inhibition of growth.

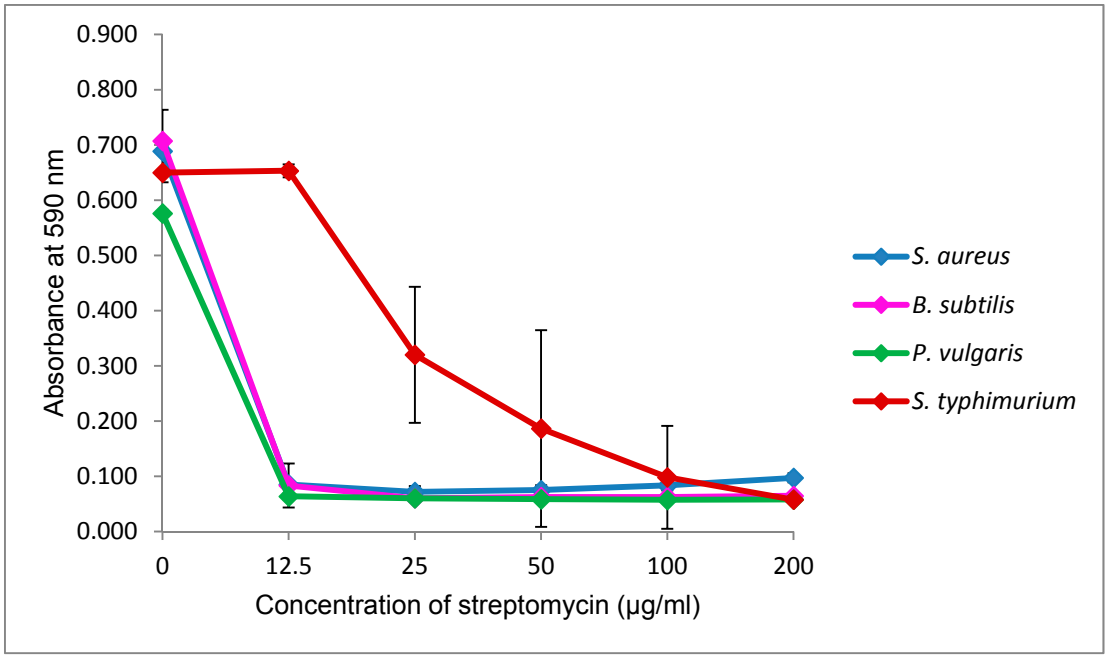


Figure S2. The graph shows the absorbance measured at the 590 nm wave-length after 16 h of incubation for *Bacillus subtilis*, *Staphylococcous aureus*, *Proteus vulgaris* and *Salmonella typhimurium* with different concentrations of streptomycin ranging from 12.5 µg/mL to 600 µg/mL. The experiment was conducted in triplicate.

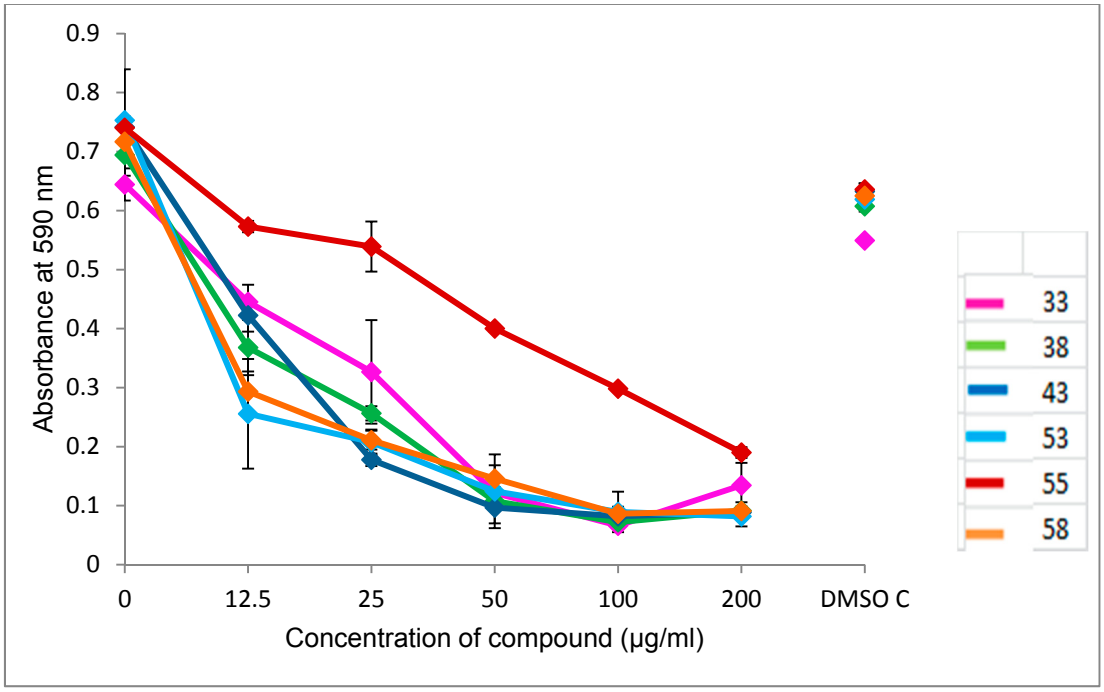


Figure S3. The graph shows the absorbance measured at the 590 nm wave-length after 16 h of incubation for *Staphylococcus aureus* with different concentrations of compounds **33**, **38**, **43**, **53**, **55** and **58** ranging from 12.5 µg/mL to 200 µg/mL. As there is decrease in absorbance meaning the growth of the bacteria is inhibited. At the end of the graph the results of DMSO plus compounds without bacteria are given as a control.

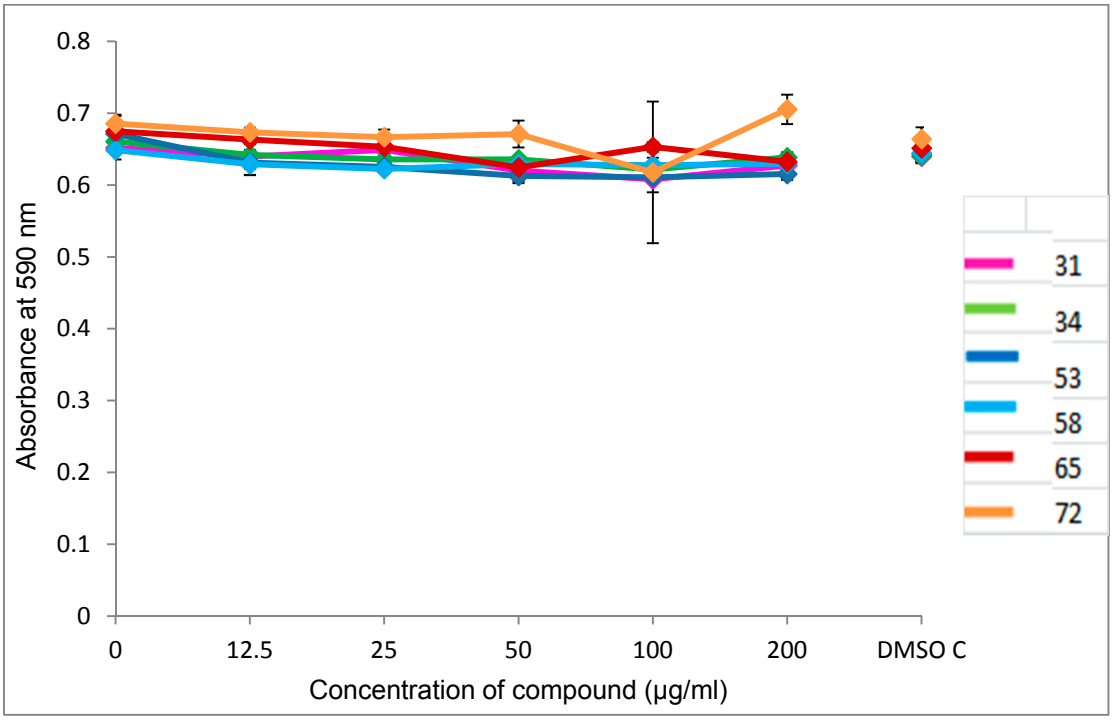


Figure S4. The graph shows the absorbance measured at the 590 nm wave-length after 16 h of incubation for *Salmonella typhimurium* with different concentrations of compounds **31**, **34**, **53**, **58**, **65** and **72** ranging from 12.5 µg/mL to 600 µg/mL. There is no decrease in absorbance for any of the compounds, meaning there is no inhibition of growth. At the end is the DMSO control.

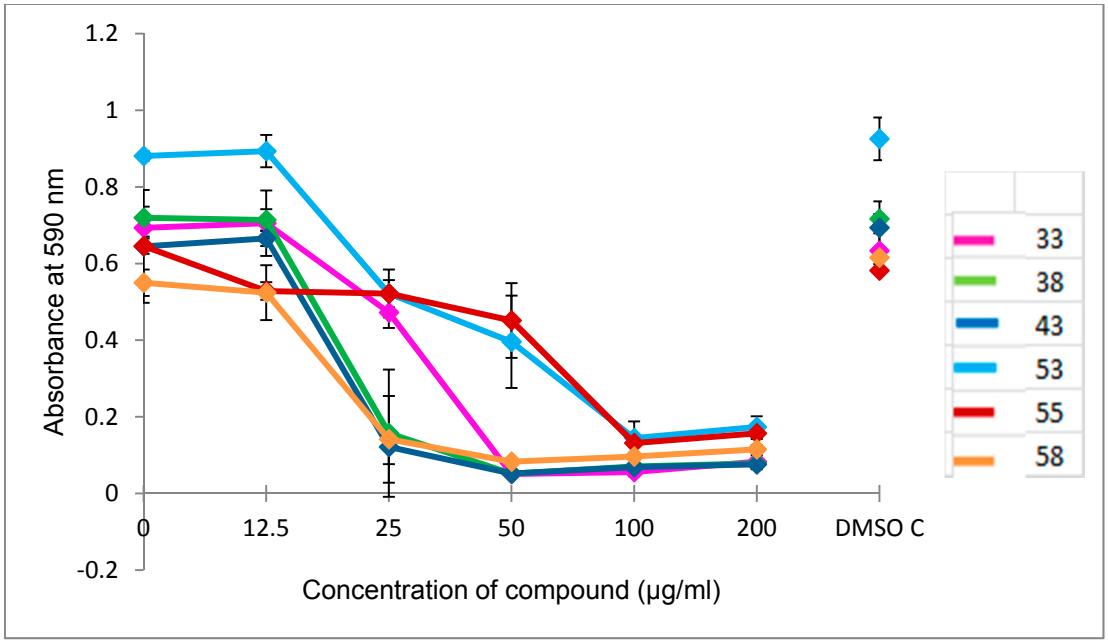


Figure S5. The graph shows the absorbance measured at the 590 nm wave-length after 16 h of incubation for *Bacillus subtilis* with different concentrations of compounds **33**, **38**, **43**, **53**, **55**, and **58** ranging from 12.5 µg/mL to 200 µg/mL. As there is decrease in absorbance meaning, the growth of bacteria is inhibited. At the end of the graph the results of DMSO plus compounds without bacteria are given as a control.

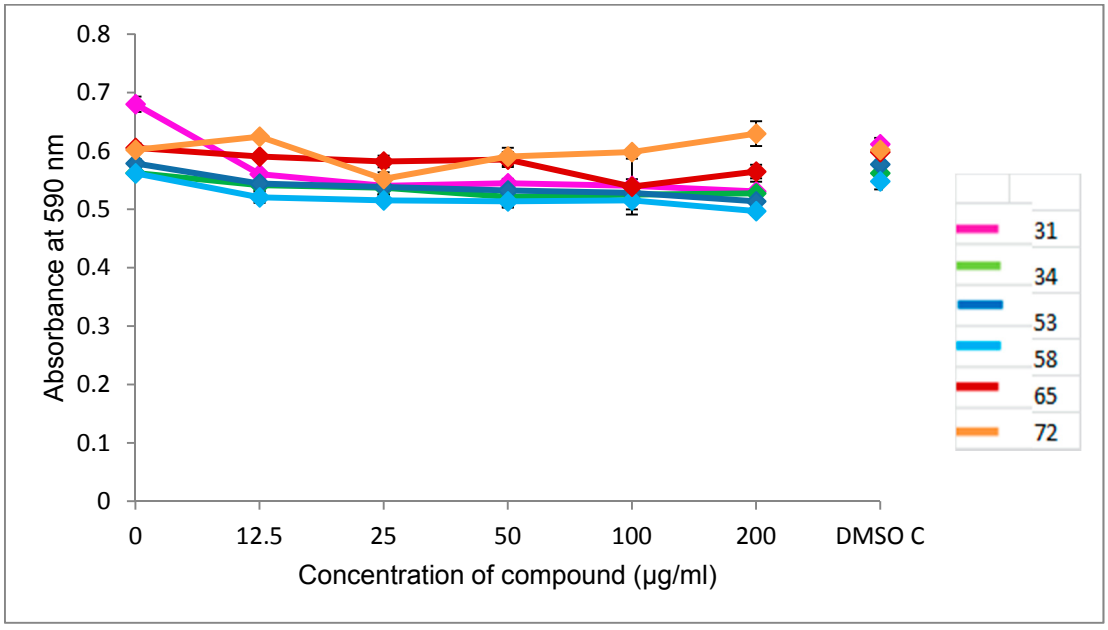


Figure S6. The graph shows the absorbance measured at the 590 nm wave-length after 16 h of incubation for *Proteus vulgaris* with different concentrations of compounds **31**, **34**, **53**, **58**, **65** and **72** ranging from 12.5 µg/mL to 200 µg/mL. There is no decrease in absorbance for any of the compounds, meaning there is no inhibition of growth. At the end is the DMSO control.

Table S1. MIC and MBC (μmol/mL) of selected compounds and Streptomycin against Gram-positive bacteria *B. subtilis*, *S. aureus* and Gram-negative bacteria *P. vulgaris*, *S. typhimurium*.

Compound	*B. subtilis*		*S. aureus*		*P. vulgaris*		*S. typhimurium*	
	MIC	**MBC**	**MIC**	**MBC**	**MIC**	**MBC**	**MIC**	**MBC**
31	996	996	996	>1195	>1195	>1195	>1195	>1195
33	113	113	227	>1363	>1363	>1363	>1363	>1363
38	108	108	216	>1301	>1301	>1301	>1301	>1301
43	49.5	99	198	-	>1188	>1188	>1188	>1188
45	938	938	938	-	>1125	>1125	>1125	>1125
50	1059	1271	847	>1271	>1271	>1271	>1271	>1271
53	216	216	216	433	>1301	>1301	>1301	>1301
55	204	204	408	>1226	>1226	>1226	>1226	>1226
58	49.5	99	198	396	>1188	>1188	>1188	>1188
60	1125	>1125	750	750	>1125	>1125	>1125	>1125
63	>1301	>1301	867	>1301	>1301	>1301	>1301	>1301
68	>1188	>1188	990	>1188	>1188	>1188	>1188	>1188
Streptomycin	21.4	21.4	21.4	42.9	10.7	10.7	171.9	171.9