

Design, synthesis, and evaluation of novel 3-carboranyl-1,8-naphthalimide derivatives as potential anticancer agents.

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Table of contents

Figure S1. ¹ H NMR spectrum of 6	7
Figure S2. ¹³ C NMR spectrum of 6	8
Figure S3. ¹¹ B NMR { ¹ H BB} spectrum of 6	9
Figure S4. UV spectrum of 6	10
Figure S5. IR spectrum of 6	11
Figure S6. HPLC analysis of 6	12
Figure S7. MS spectrum of 6	13
Figure S8. ¹ H NMR spectrum of 7	14
Figure S9. ¹³ C NMR spectrum of 7	15
Figure S10. ¹¹ B NMR { ¹ H BB} spectrum of 7	16
Figure S11. UV spectrum of 7	17
Figure S12. IR spectrum of 7	18
Figure S13. HPLC analysis of 7	19
Figure S14. MS spectrum of 7	20
Figure S15. ¹ H NMR spectrum of 8	21
Figure S16. ¹³ C NMR spectrum of 8	22
Figure S17. ¹¹ B NMR { ¹ H BB} spectrum of 8	23
Figure S18. UV spectrum of 8	24
Figure S19. IR spectrum of 8	25
Figure S20. HPLC analysis of 8	26
Figure S21. MS spectrum of 8	27
Figure S22. HRMS spectrum of 8	28
Figure S23. ¹ H NMR spectrum of 9	29
Figure S24. ¹³ C NMR spectrum of 9	30
Figure S25. ¹¹ B NMR { ¹ H BB} spectrum of 9	31
Figure S26. UV spectrum of 9	32
Figure S27. IR spectrum of 9	33
Figure S28. HPLC analysis of 9	34
Figure S29. MS spectrum of 9	35
Figure S30. ¹ H NMR spectrum of 10	36
Figure S31. ¹³ C NMR spectrum of 10	37
Figure S32. ¹¹ B NMR { ¹ H BB} spectrum of 10	38
Figure S33. UV spectrum of 10	39
Figure S34. IR spectrum of 10	40
Figure S35. HPLC analysis of 10	41
Figure S36. MS spectrum of 10	42
Figure S37. ¹ H NMR spectrum of 11	43
Figure S38. ¹³ C NMR spectrum of 11	44
Figure S39. ¹¹ B NMR { ¹ H BB} spectrum of 11	45
Figure S40. UV spectrum of 11	46
Figure S41. IR spectrum of 11	47
Figure S42. HPLC analysis of 11	48
Figure S43. MS spectrum of 11	49
Figure S44. ¹ H NMR spectrum of 15	50
Figure S45. ¹³ C NMR spectrum of 15	51
Figure S46. ¹¹ B NMR { ¹ H BB} spectrum of 15	52
Figure S47. UV spectrum of 15	53
Figure S48. IR spectrum of 15	54
Figure S49. HPLC analysis of 15	55
Figure S50. MS spectrum of 15	56

Figure S51. ¹ H NMR spectrum of 16	57
Figure S52. ¹³ C NMR spectrum of 16	58
Figure S53. ¹¹ B NMR { ¹ H BB} spectrum of 16	59
Figure S54. UV spectrum of 16	60
Figure S55. IR spectrum of 16	61
Figure S56. HPLC analysis of 16	62
Figure S57. MS spectrum of 16	63
Figure S58. ¹ H NMR spectrum of 17	64
Figure S59. ¹³ C NMR spectrum of 17	65
Figure S60. ¹¹ B NMR { ¹ H BB} spectrum of 17	66
Figure S61. UV spectrum of 17	67
Figure S62. IR spectrum of 17	68
Figure S63. HPLC analysis of 17	69
Figure S64. MS spectrum of 17	70
Figure S65. ¹ H NMR spectrum of 18	71
Figure S66. ¹³ C NMR spectrum of 18	72
Figure S67. ¹¹ B NMR { ¹ H BB} spectrum of 18	73
Figure S68. UV spectrum of 18	74
Figure S69. IR spectrum of 18	75
Figure S70. HPLC analysis of 18	76
Figure S71. MS spectrum of 18	77
Figure S72. ¹ H NMR spectrum of 19	78
Figure S73. ¹³ C NMR spectrum of 19	79
Figure S74. ¹¹ B NMR { ¹ H BB} spectrum of 19	80
Figure S75. UV spectrum of 19	81
Figure S76. IR spectrum of 19	82
Figure S77. HPLC analysis of 19	83
Figure S78. MS spectrum of 19	84
Figure S79. ¹ H NMR spectrum of 20	85
Figure S80. ¹³ C NMR spectrum of 20	86
Figure S81. ¹¹ B NMR { ¹ H BB} spectrum of 20	87
Figure S82. UV spectrum of 20	88
Figure S83. IR spectrum of 20	89
Figure S84. HPLC analysis of 20	90
Figure S85. MS spectrum of 20	91
Figure S86. HRMS spectrum of 20	92
Figure S87. ¹ H NMR spectrum of 31	93
Figure S88. ¹³ C NMR spectrum of 31	94
Figure S89. ¹¹ B NMR { ¹ H BB} spectrum of 31	95
Figure S90. UV spectrum of 31	96
Figure S91. IR spectrum of 31	97
Figure S92. HPLC analysis of 31	98
Figure S93. MS spectrum of 31	99
Figure S94. ¹ H NMR spectrum of 32	100
Figure S95. ¹³ C NMR spectrum of 32	101
Figure S96. ¹¹ B NMR { ¹ H BB} spectrum of 32	102
Figure S97. UV spectrum of 32	103
Figure S98. IR spectrum of 32	104
Figure S99. HPLC analysis of 32	105
Figure S100. MS spectrum of 32	106
Figure S101. ¹ H NMR spectrum of 33	107

Figure S102. ^{13}C NMR spectrum of 33	108
Figure S103. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 33	109
Figure S104. UV spectrum of 33	110
Figure S105. IR spectrum of 33	111
Figure S106. HPLC analysis of 33	112
Figure S107. MS spectrum of 33	113
Figure S108. ^1H NMR spectrum of 34	114
Figure S109. ^{13}C NMR spectrum of 34	115
Figure S110. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 34	116
Figure S111. UV spectrum of 34	117
Figure S112. IR spectrum of 34	118
Figure S113. HPLC analysis of 34	119
Figure S114. MS spectrum of 34	120
Figure S115. ^1H NMR spectrum of 35	121
Figure S116. ^{13}C NMR spectrum of 35	122
Figure S117. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 35	123
Figure S118. UV spectrum of 35	124
Figure S119. IR spectrum of 35	125
Figure S120. HPLC analysis of 35	126
Figure S121. MS spectrum of 35	127
Figure S122. HRMS spectrum of 35	128
Figure S123. ^1H NMR spectrum of 36	1296
Figure S124. ^{13}C NMR spectrum of 36	130
Figure S125. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 36	131
Figure S126. UV spectrum of 36	132
Figure S127. IR spectrum of 36	133
Figure S128. HPLC analysis of 36	134
Figure S129. MS spectrum of 36	135
Figure S130. ^1H NMR spectrum of 39	136
Figure S131. ^{13}C NMR spectrum of 39	137
Figure S132. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 39	138
Figure S133. UV spectrum of 39	139
Figure S134. IR spectrum of 39	140
Figure S135. HPLC analysis of 39	141
Figure S136. MS spectrum of 39	142
Figure S137. ^1H NMR spectrum of 40	143
Figure S138. ^{13}C NMR spectrum of 40	144
Figure S139. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 40	145
Figure S140. UV spectrum of 40	146
Figure S141. IR spectrum of 40	147
Figure S142. HPLC analysis of 40	148
Figure S143. MS spectrum of 40	149
Figure S144. HRMS spectrum of 40	150
Figure S145. ^1H NMR spectrum of 41	151
Figure S146. ^{13}C NMR spectrum of 41	152
Figure S147. IR spectrum of 41	153
Figure S148. UV spectrum of 41	1540
Figure S149. IR spectrum of 41	155
Figure S150. HPLC analysis of 41	156
Figure S151. MS spectrum of 41	157
Figure S152. ^1H NMR spectrum of 42	158

Figure S153. ^{13}C NMR spectrum of 42	159
Figure S154. IR spectrum of 42	160
Figure S155. UV spectrum of 42	161
Figure S156. IR spectrum of 42	162
Figure S157. HPLC analysis of 42	163
Figure S158. MS spectrum of 42	166
Figure S159. Influence of compound 6 on cell cycle distribution in HepG2 cells	165
Figure S160. ROS production in HepG2 cells after 24 h incubation with compound 6-11, 16-20, 32, 39-42	166
Figure S161. Autofluorescence analysis of the tested compounds in HepG2 cells	167
Figure S162. Flow cytometry analysis of apoptosis/necrosis in HepG2 cells after cell toxicity induction with compound 6	168
Table 1S. Percentage distribution of early and late apoptotic and necrotic cells assessed by flow cytometry	169
Figure S163. Flow cytometry analysis of apoptosis/necrosis in HepG2 cells after cell toxicity induction with compound 31	170
Figure S164. Flow cytometry analysis of autophagy in HepG2 cells after cell toxicity induction with compound 8	171
Figure S1651. Flow cytometry analysis of lipid peroxidation in HepG2 cells after cell toxicity induction with compound 15	172
Figure S166. Human Topoisomerase II α relaxation assay	173
Figure S167. Melting curves of ct-DNA upon addition of 6-11	174
Figure S168. Melting curves of ct-DNA upon addition of 15-20	175
Figure S169. Melting curves of ct-DNA upon addition of 31-36	176
Figure S170. Melting curves of ct-DNA upon addition of 39-42	177
Figure S171. Melting curves of ct-DNA upon addition of mitonafide and pinafide	178
Figure S172. Changes in the CD spectrum of ct-DNA upon addition of mitonafide and pinafide	179
Figure S173. Changes in the CD spectrum of ct-DNA upon addition of 6 and 7	180
Figure S174. Changes in the CD spectrum of ct-DNA upon addition of 8 and 9	181
Figure S175. Changes in the CD spectrum of ct-DNA upon addition of 10 and 11	182
Figure S176. Changes in the CD spectrum of ct-DNA upon addition of 15 and 16	183
Figure S177. Changes in the CD spectrum of ct-DNA upon addition of 17 and 18	184
Figure S178. Changes in the CD spectrum of ct-DNA upon addition of 19 and 20	185
Figure S179. Changes in the CD spectrum of ct-DNA upon addition of 31 and 32	186
Figure S180. Changes in the CD spectrum of ct-DNA upon addition of 33 and 34	187
Figure S181. Changes in the CD spectrum of ct-DNA upon addition of 35 and 36	188
Figure S182. Changes in the CD spectrum of ct-DNA upon addition of 39 and 40	189
Figure S183. Changes in the CD spectrum of ct-DNA upon addition of 41 and 42	190
Figure S184. UV-vis absorption spectra of compound 6 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	191
Figure S185. UV-vis absorption spectra of compound 7 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	192
Figure S186. UV-vis absorption spectra of compound 8 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	193
Figure S187. UV-vis absorption spectra of compound 9 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	194

Figure S188. UV-vis absorption spectra of compound 10 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	195
Figure S189. UV-vis absorption spectra of compound 11 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	196
Figure S190. UV-vis absorption spectra of compound 15 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	197
Figure S191. UV-vis absorption spectra of compound 16 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	198
Figure S192. UV-vis absorption spectra of compound 17 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	199
Figure S193. UV-vis absorption spectra of compound 18 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	200
Figure S194. UV-vis absorption spectra of compound 19 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	201
Figure S195. UV-vis absorption spectra of compound 20 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	202
Figure S196. UV-vis absorption spectra of compound 33 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	203
Figure S197. UV-vis absorption spectra of compound 34 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	204
Figure S198. UV-vis absorption spectra of compound 35 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	205
Figure S199. UV-vis absorption spectra of compound 36 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	206
Figure S200. UV-vis absorption spectra of compound 39 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	207
Figure S201. UV-vis absorption spectra of compound 40 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	208
Figure S202. UV-vis absorption spectra of mitonafide (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	209
Figure S203. UV-vis absorption spectra of pinafide (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right)	210
Table 2S. Crystallographic data	211

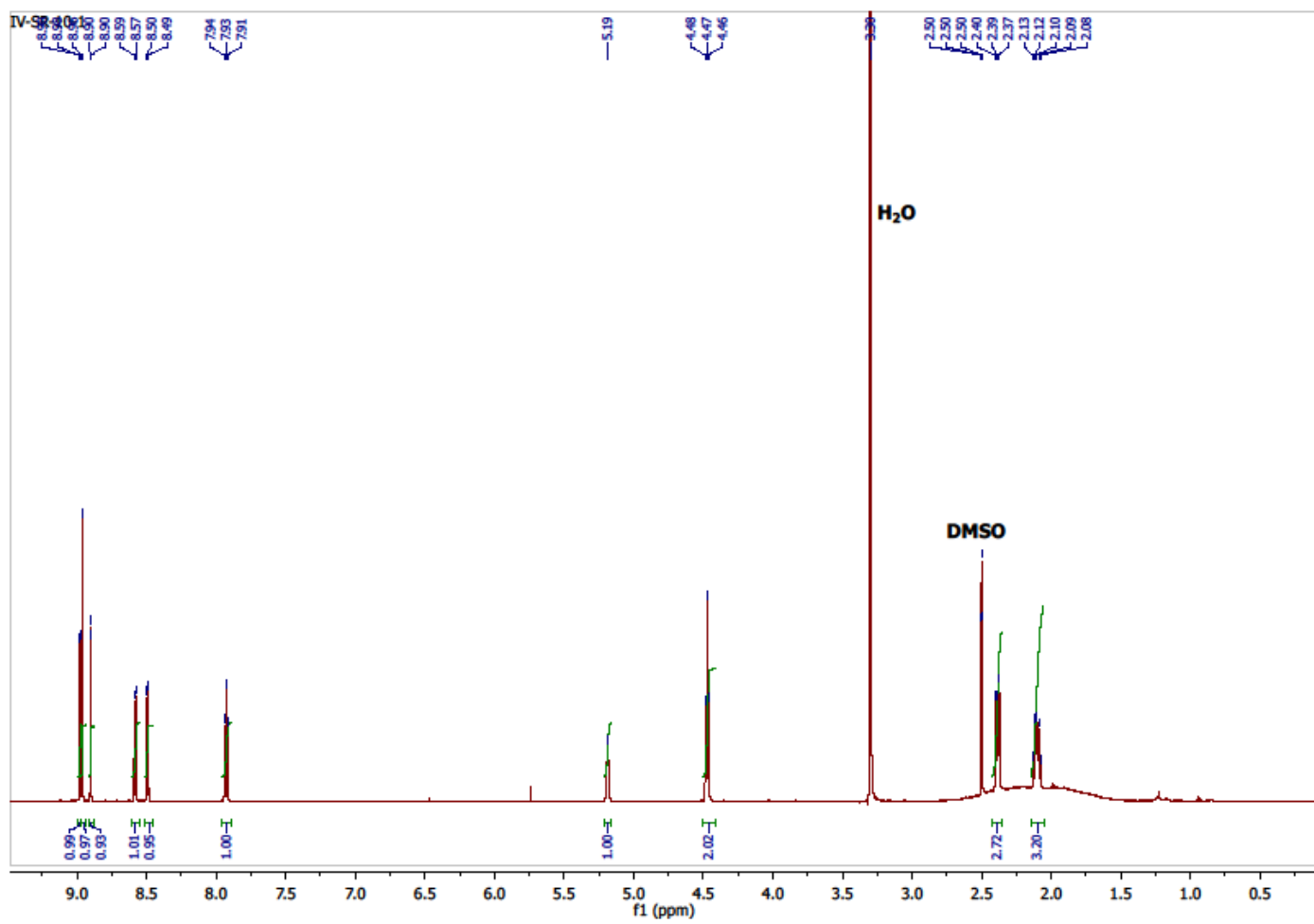


Figure S1. ¹H NMR spectrum of 6.

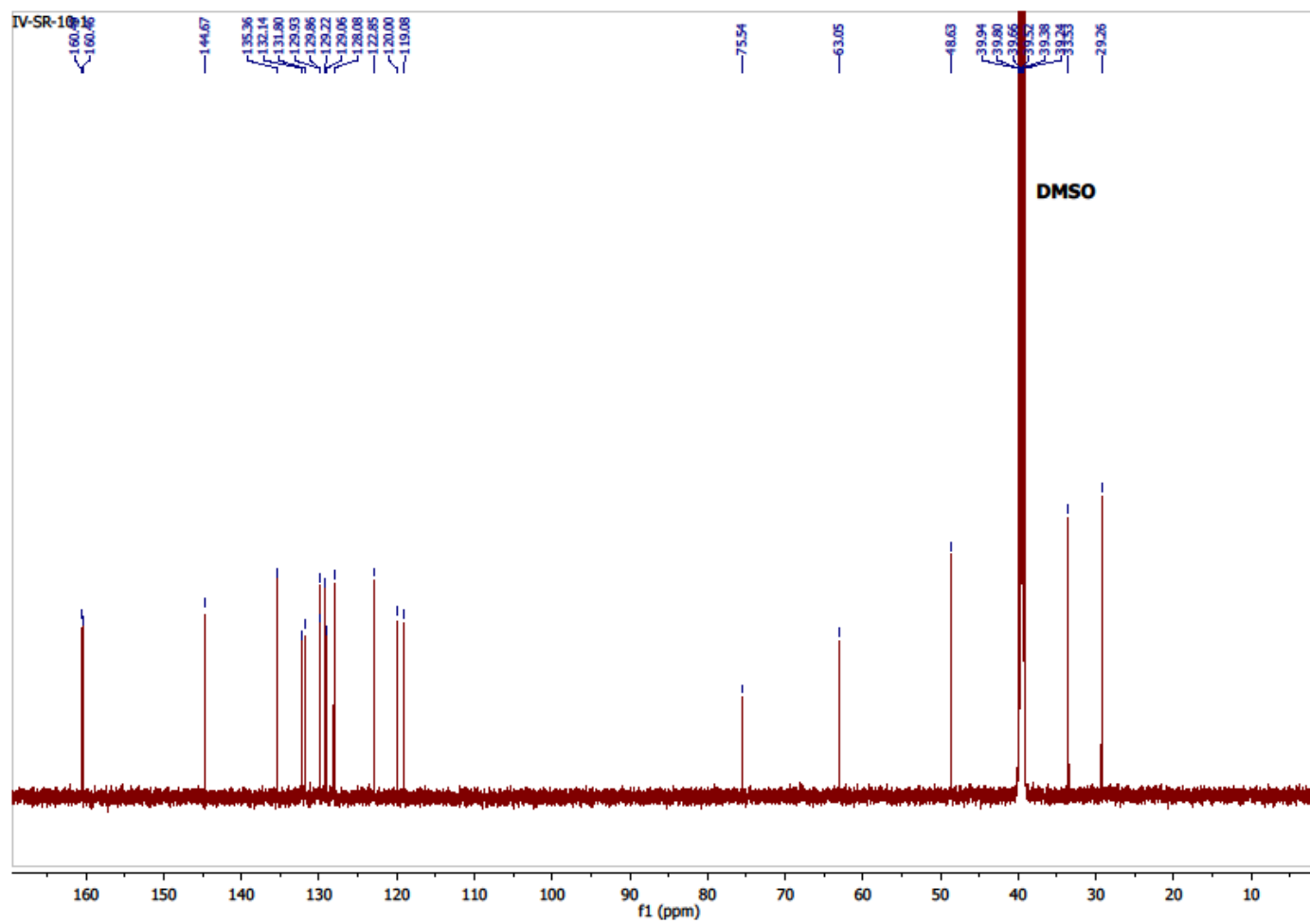


Figure S2. ^{13}C NMR spectrum of 6.

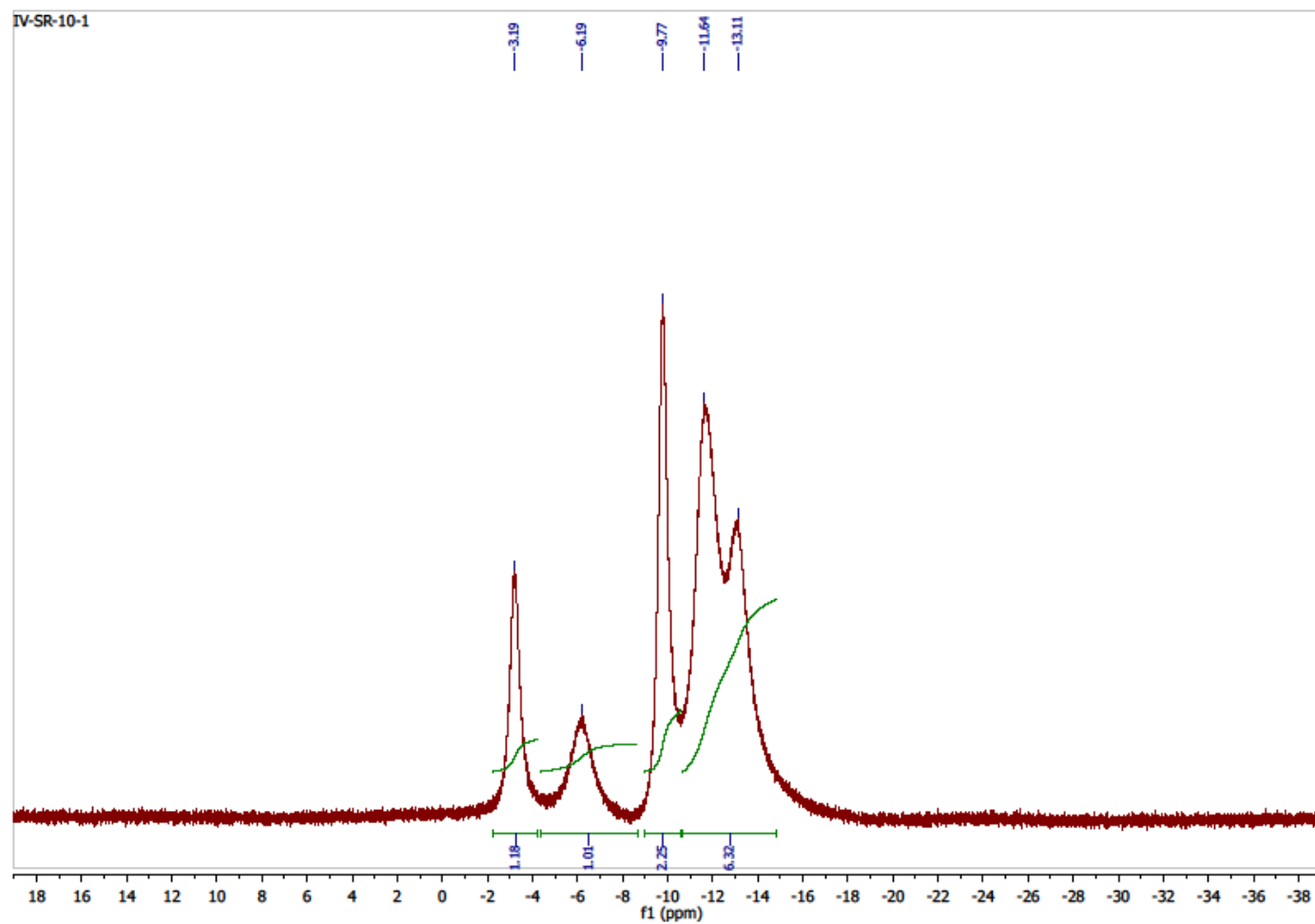


Figure S3. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of **6**.

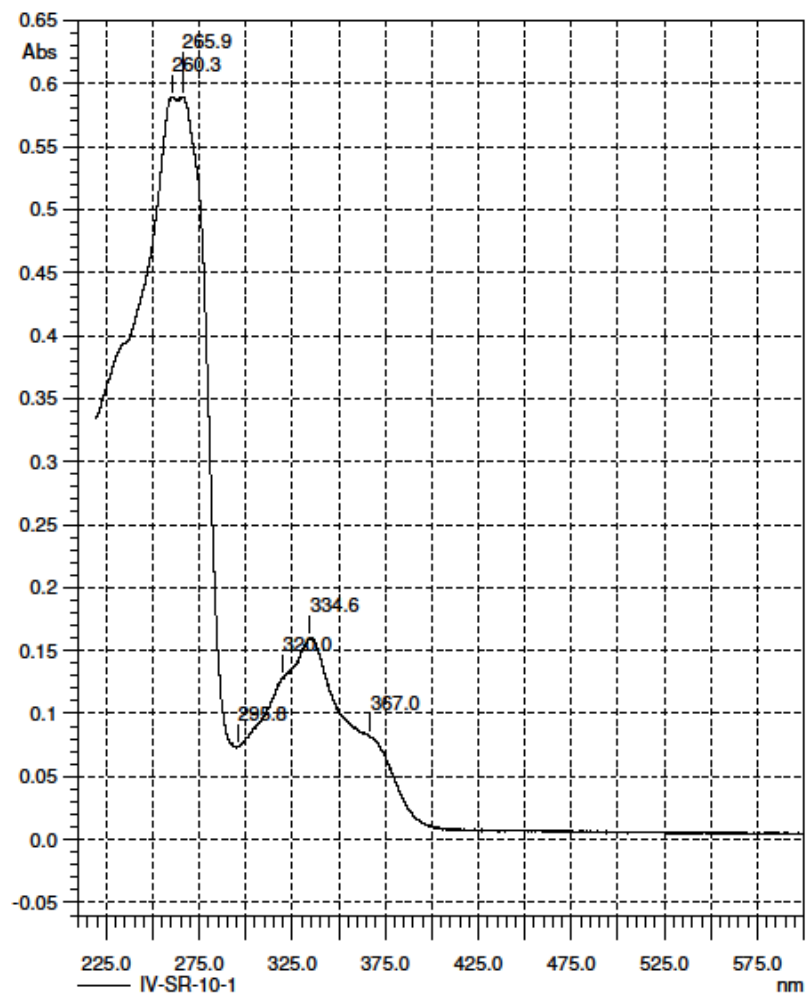


Figure S4. UV spectrum of 6.

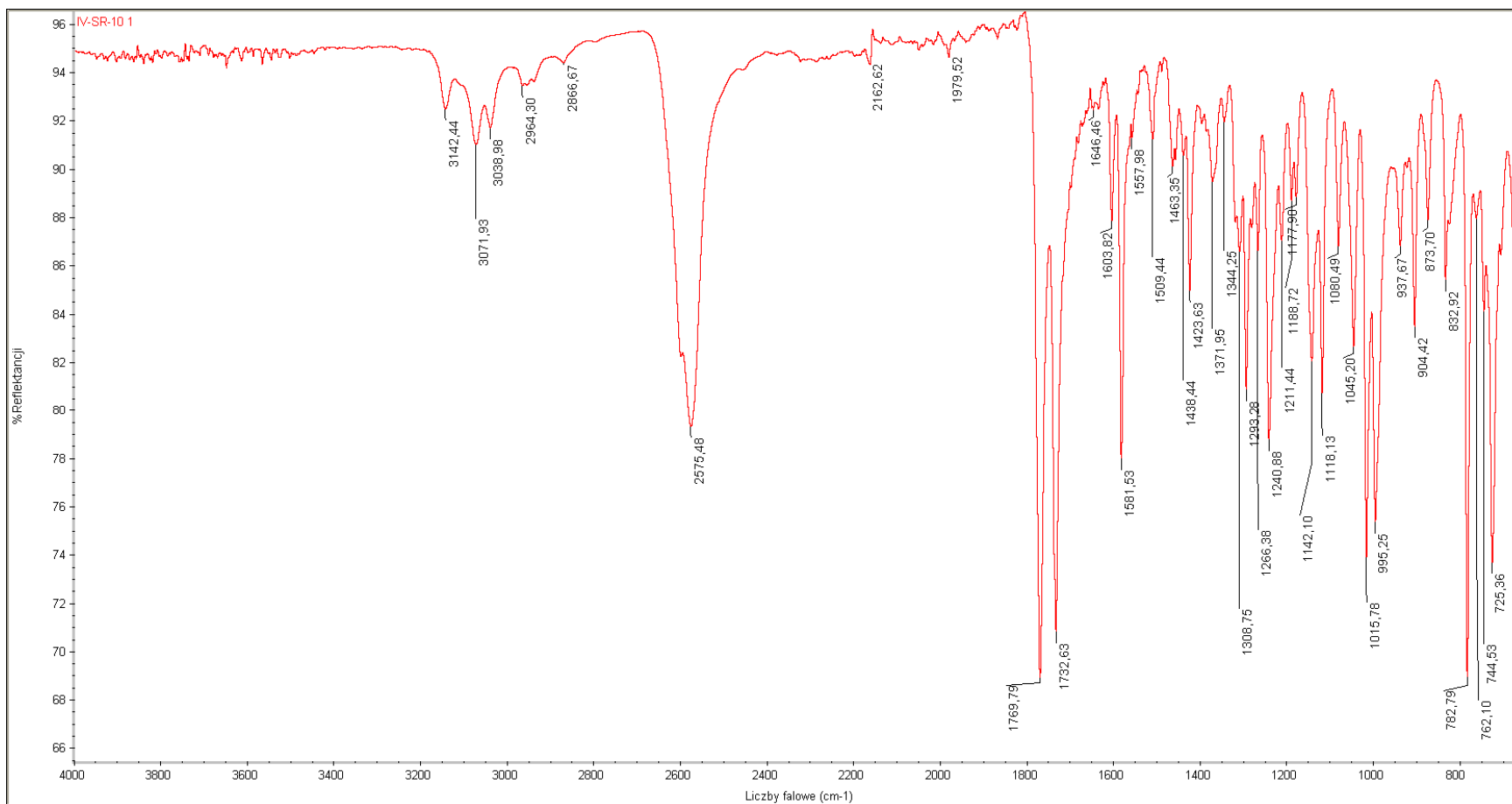
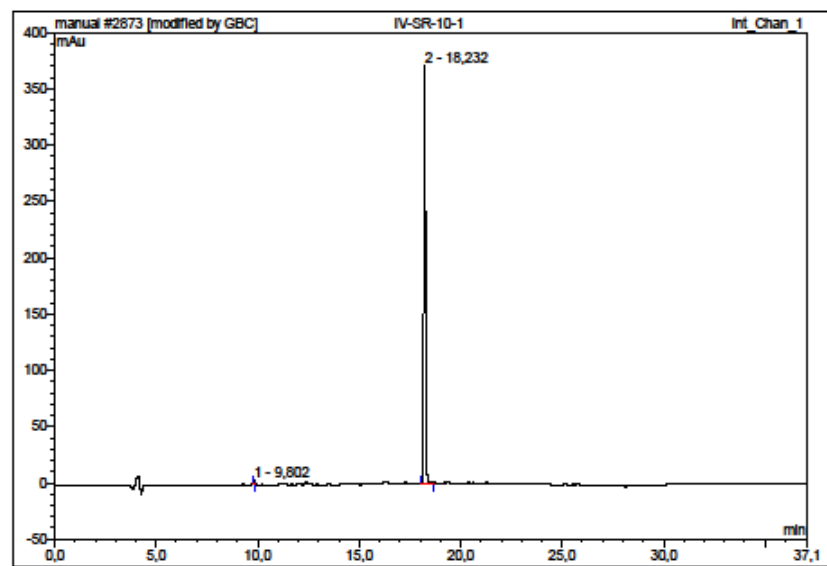


Figure S5. IR spectrum of 6.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	9,80	n.a.	2,985	0,240	0,63	n.a.	BMB*
2	18,23	n.a.	371,895	37,820	99,37	n.a.	BMB
Total:			374,880	38,060	100,00	0,000	

Figure S6. HPLC analysis of 6.

Spectrum Name: IV-SR-10_1_PT
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 180V 300C Offset: 30V Span: 20V

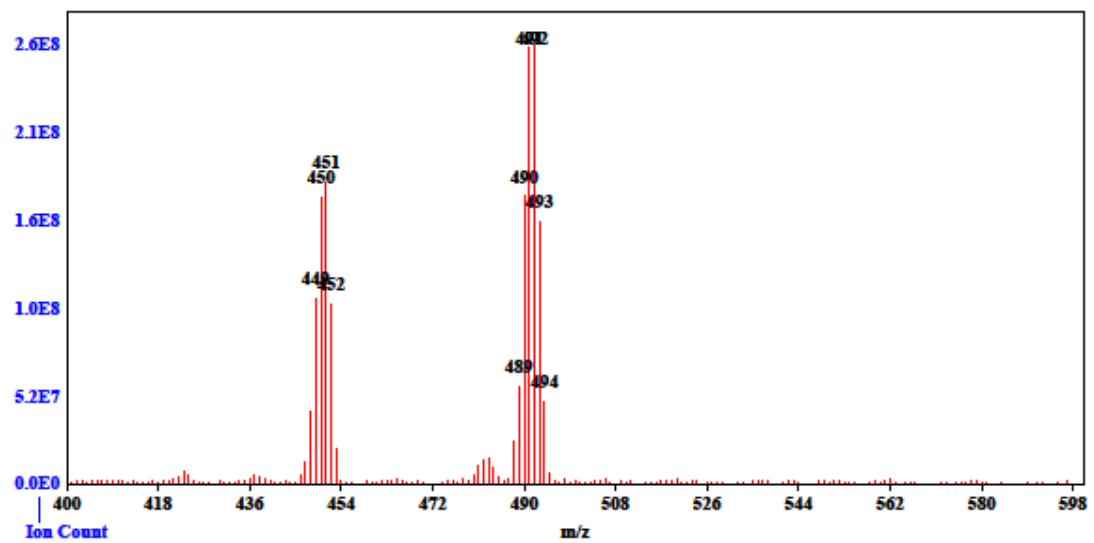


Figure S7. MS spectrum of 6.

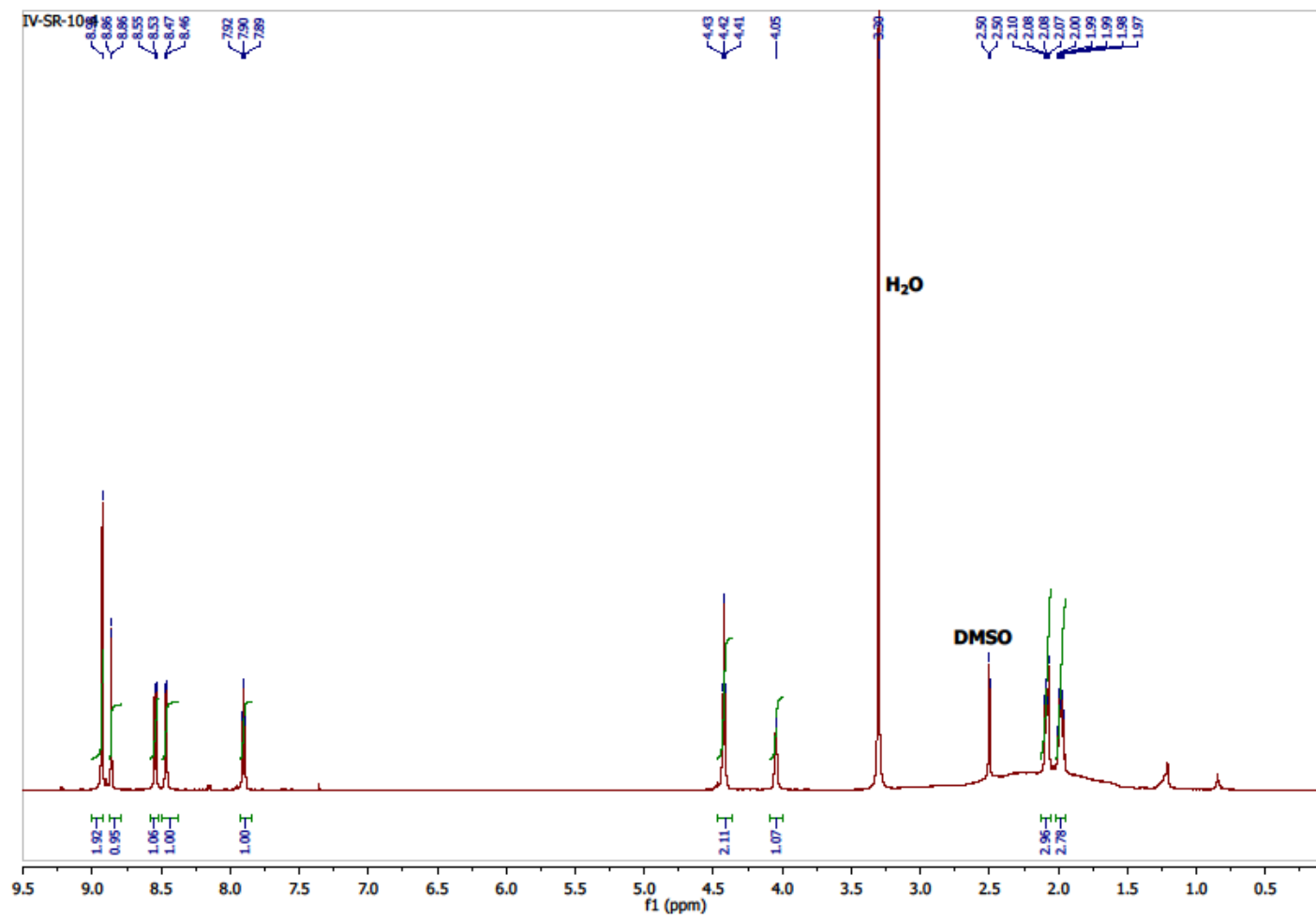


Figure S8. ¹H NMR spectrum of 7.

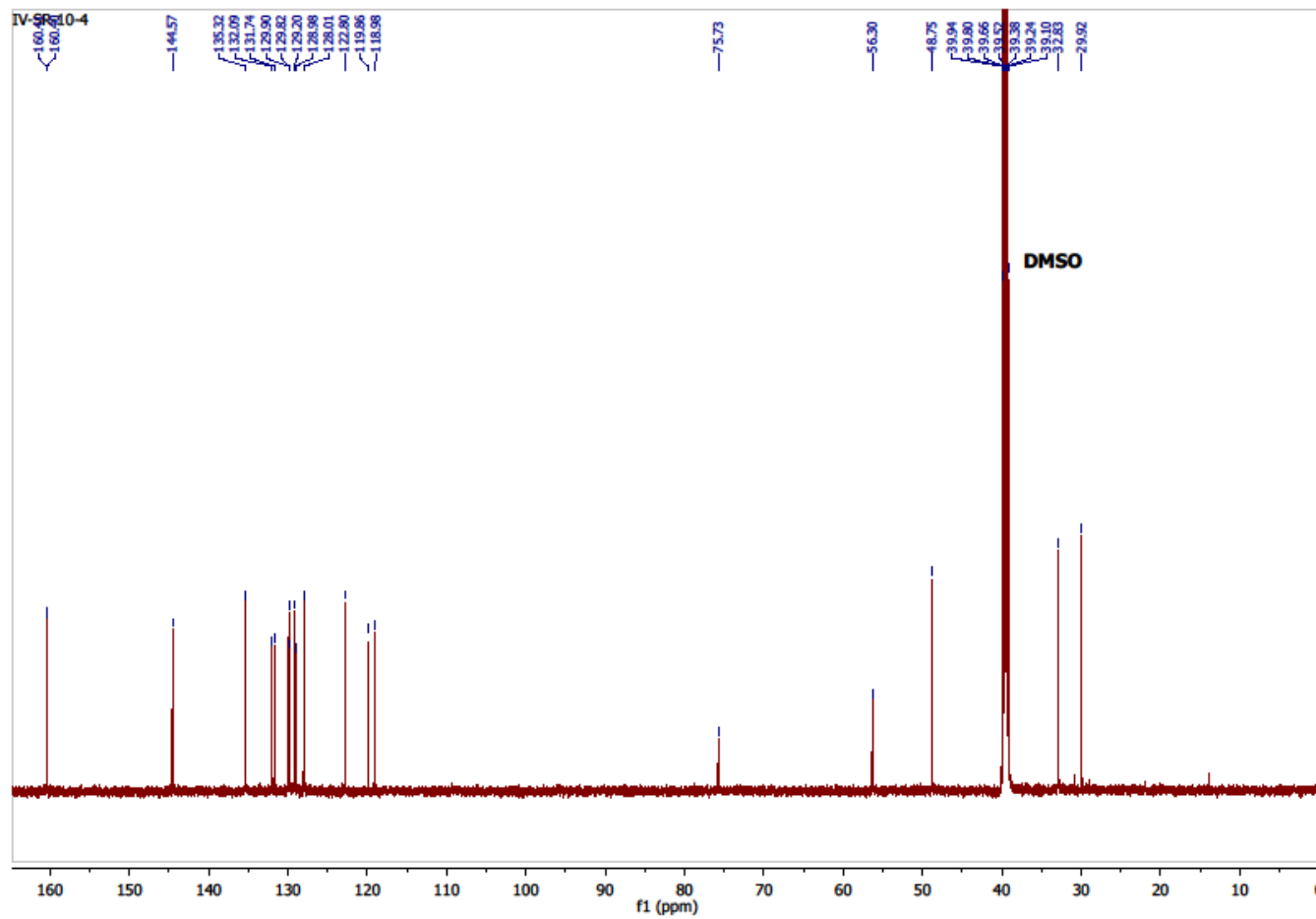


Figure S9. ^{13}C NMR spectrum of 7.

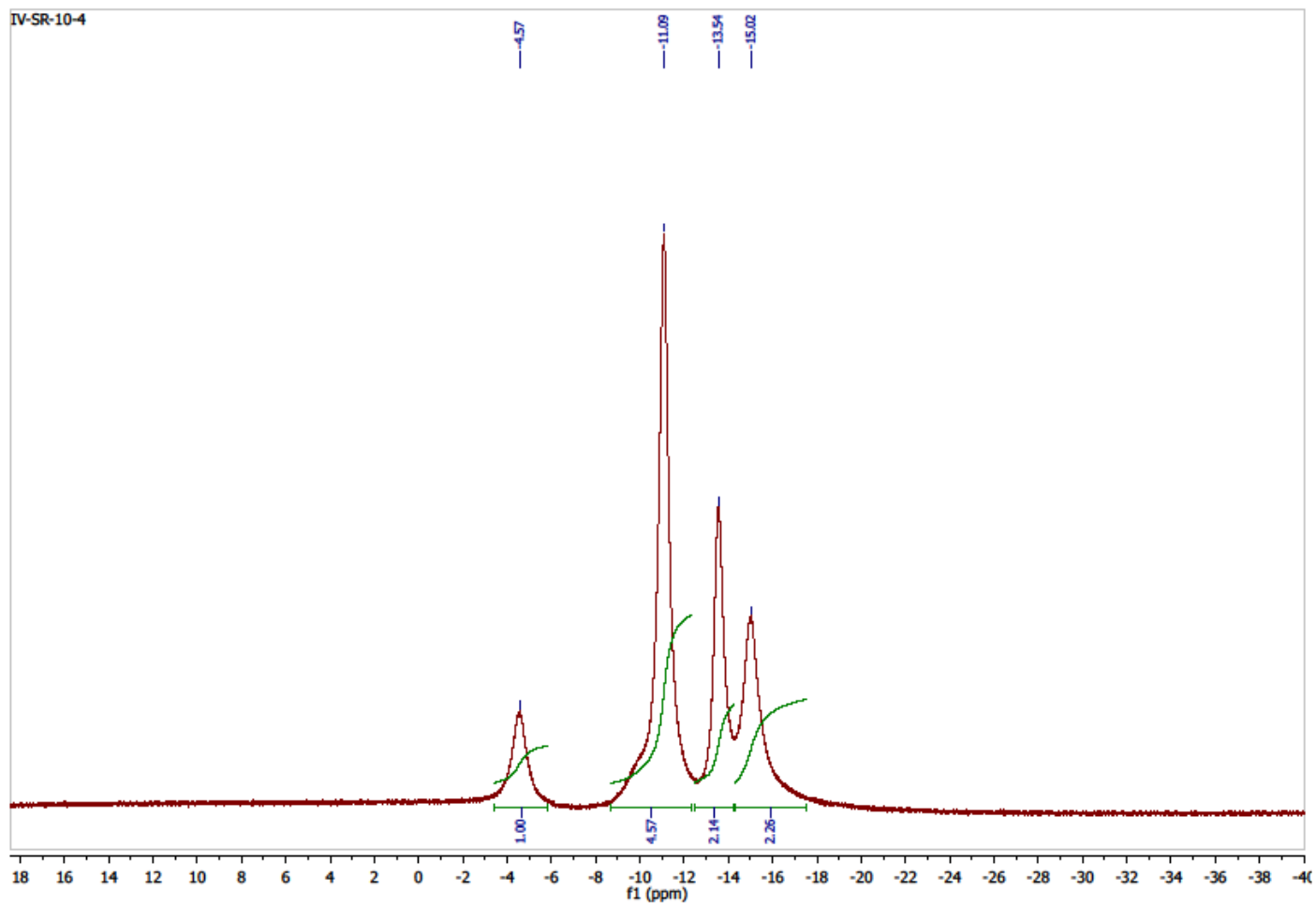


Figure S10. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 7.

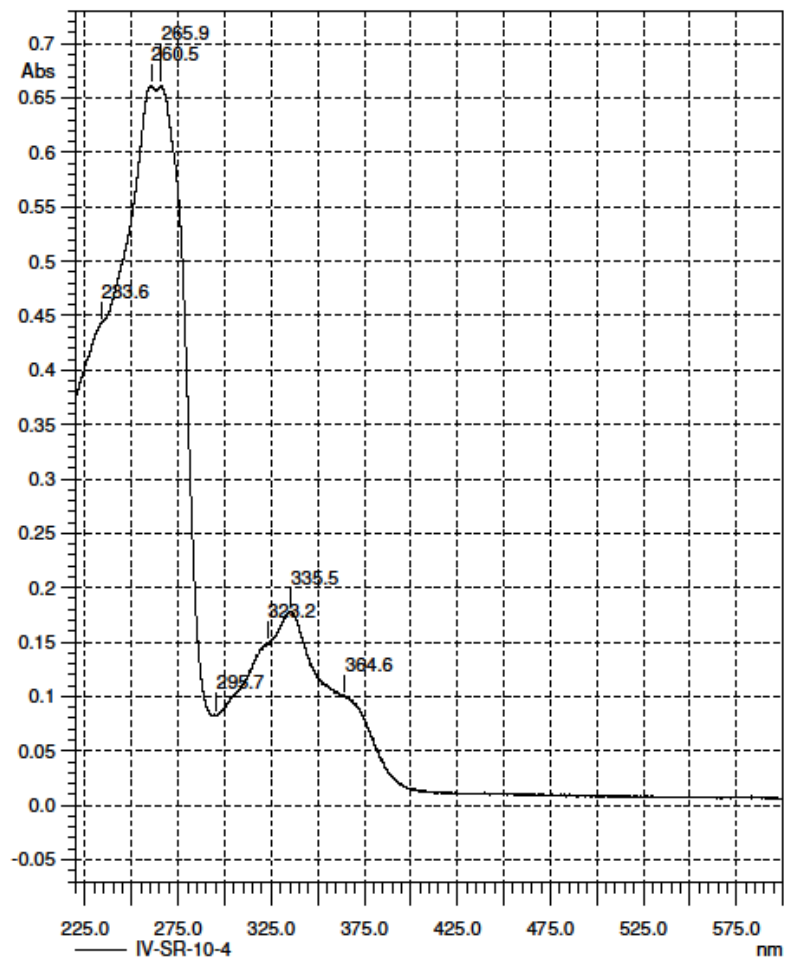


Figure S11. UV spectrum of 7.

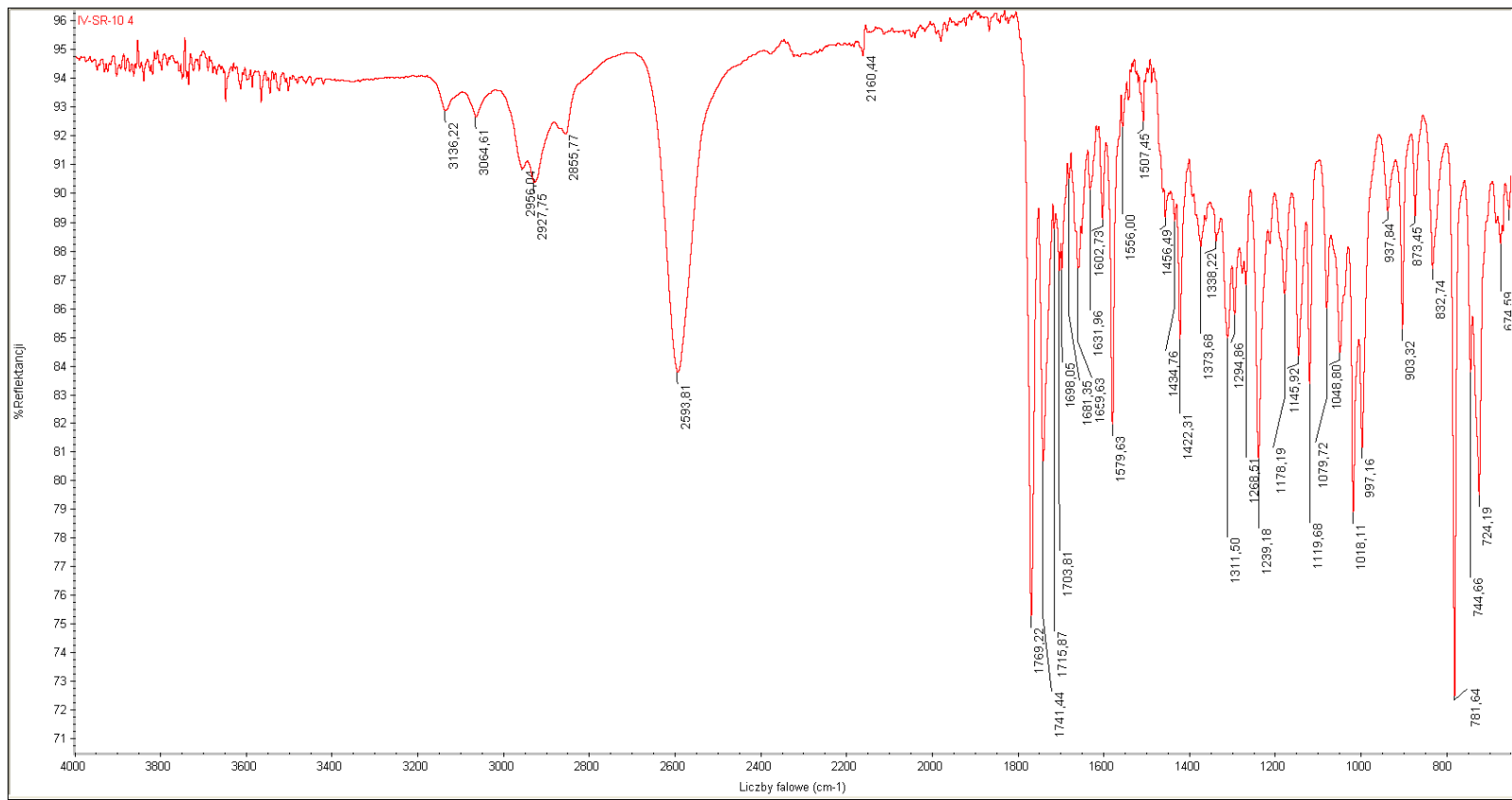
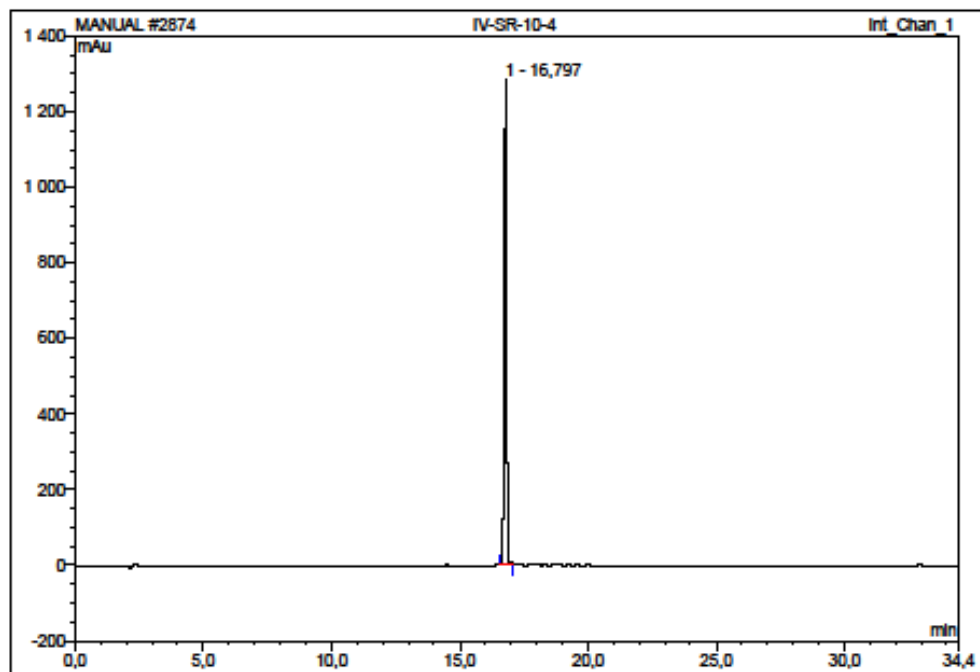


Figure S12. IR spectrum of 7.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu ² min	Rel.Area %	Amount	Type
1	16,80	n.a.	1281,764	135,115	100,00	n.a.	BMB
Total:			1281,764	135,115	100,00	0,000	

Figure S13. HPLC analysis of 7.

Spectrum Name: IV-SR-10_4
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 180V 300C Offset: 30V Span: 20V

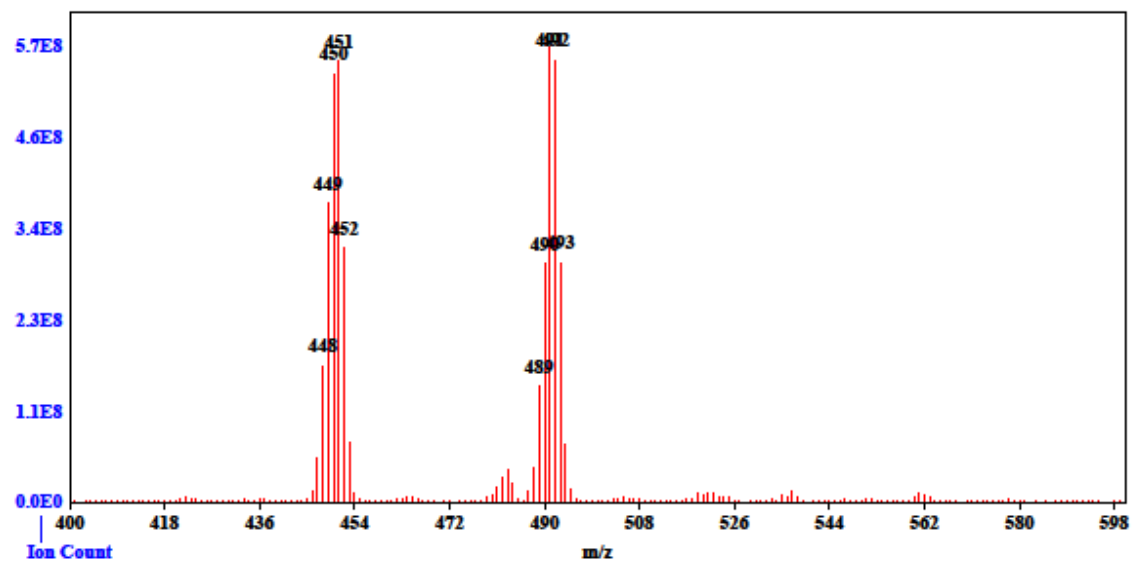


Figure S14. MS spectrum of 7.

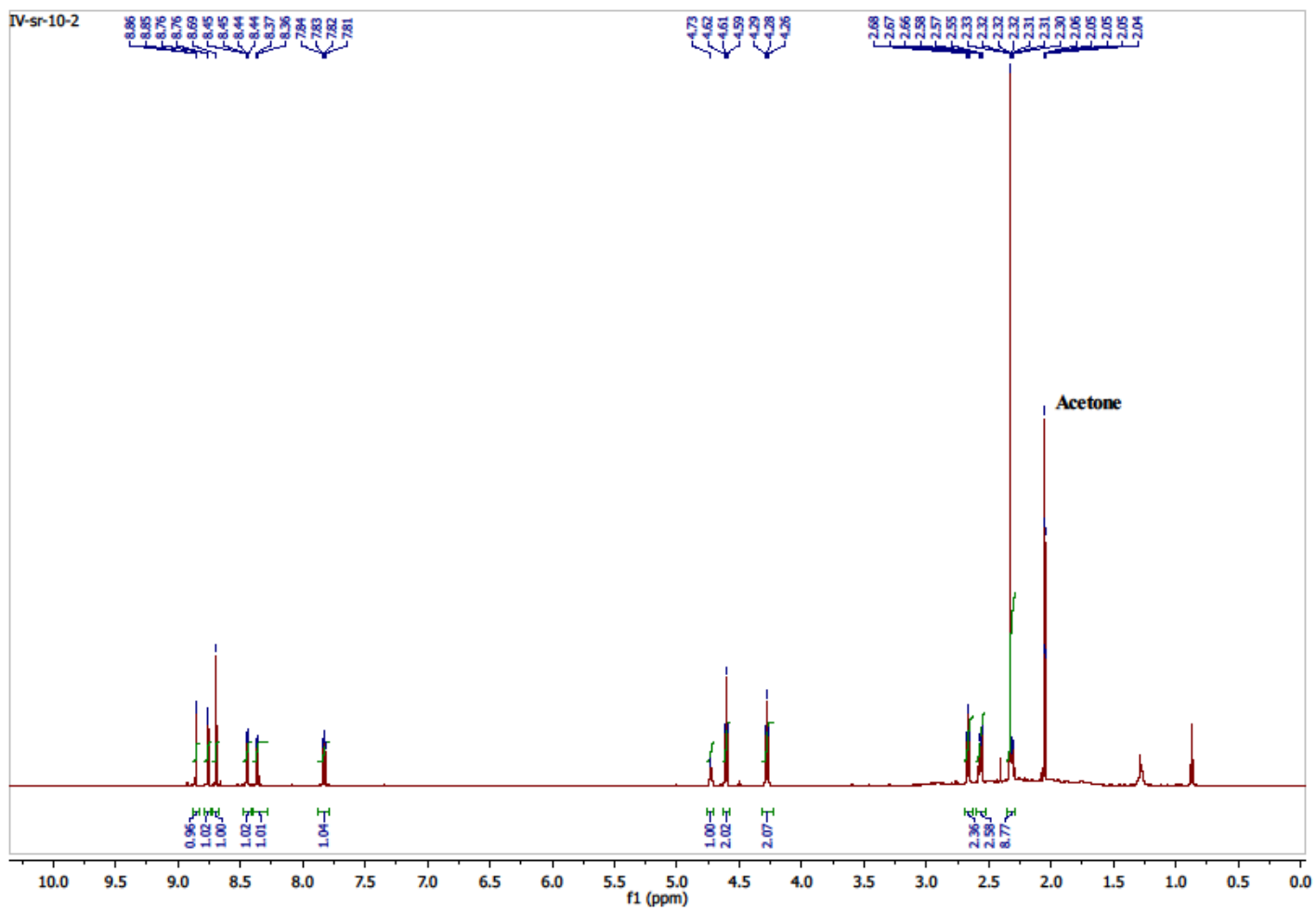


Figure S15. ¹H NMR spectrum of 8.

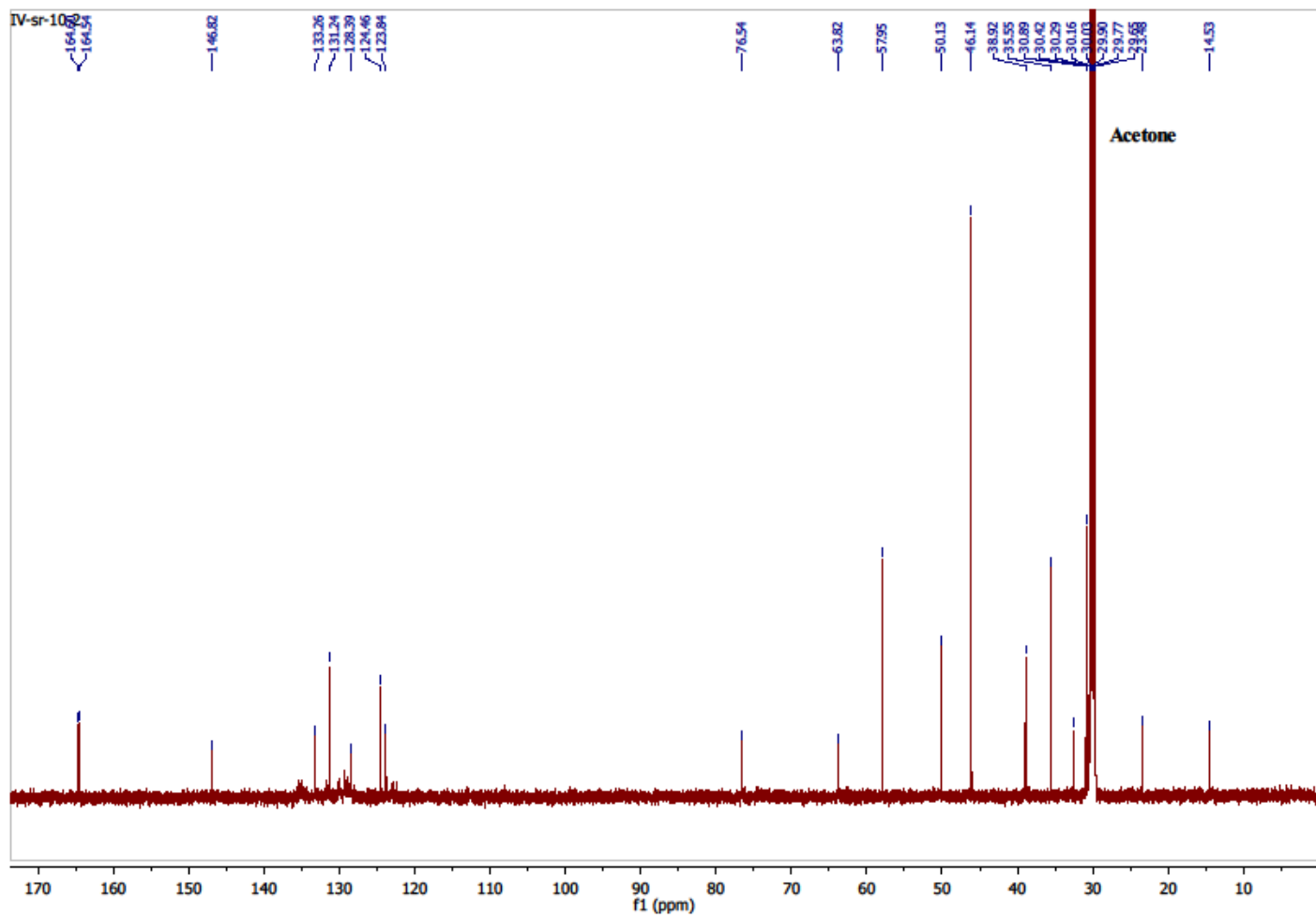


Figure S16. ^{13}C NMR spectrum of 8.

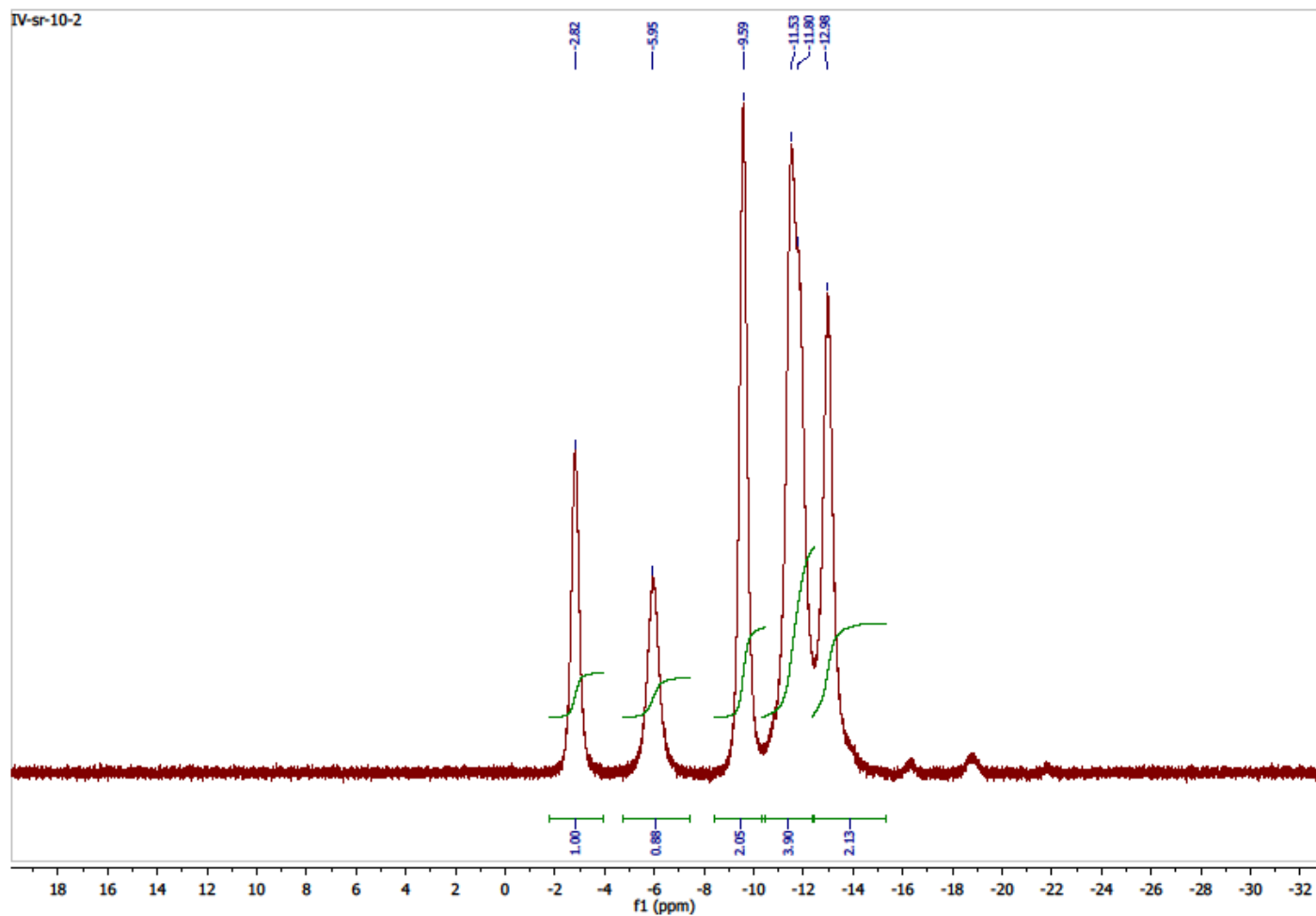


Figure S17. ^{11}B NMR (^1H BB) spectrum of 8.

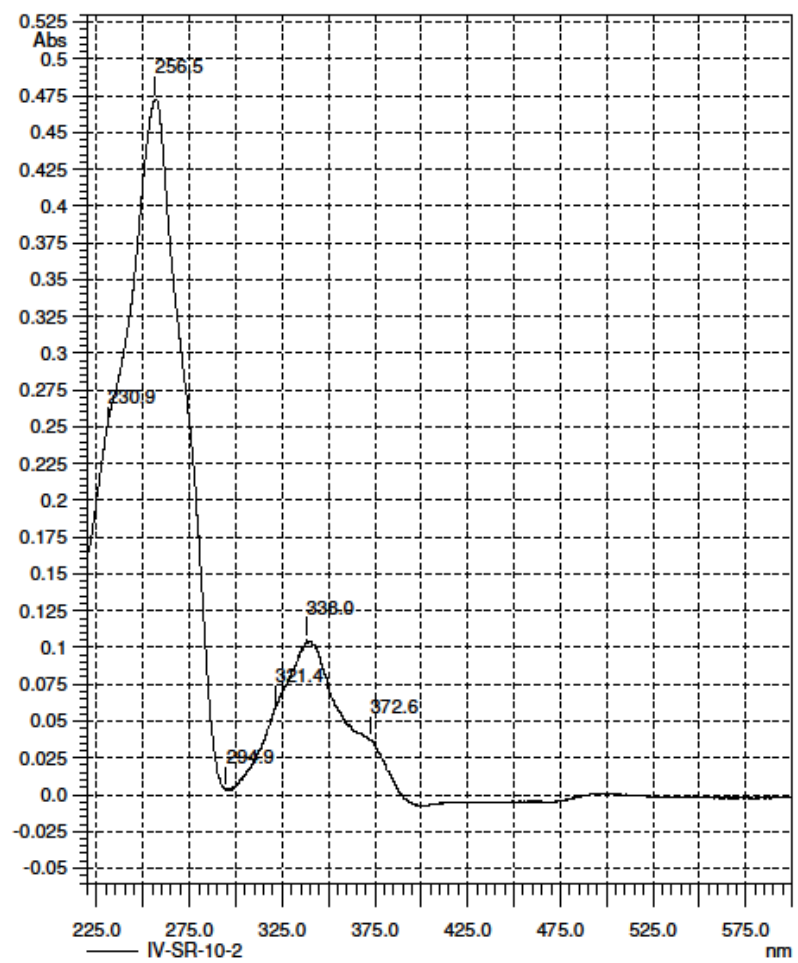


Figure S18. UV spectrum of 8.

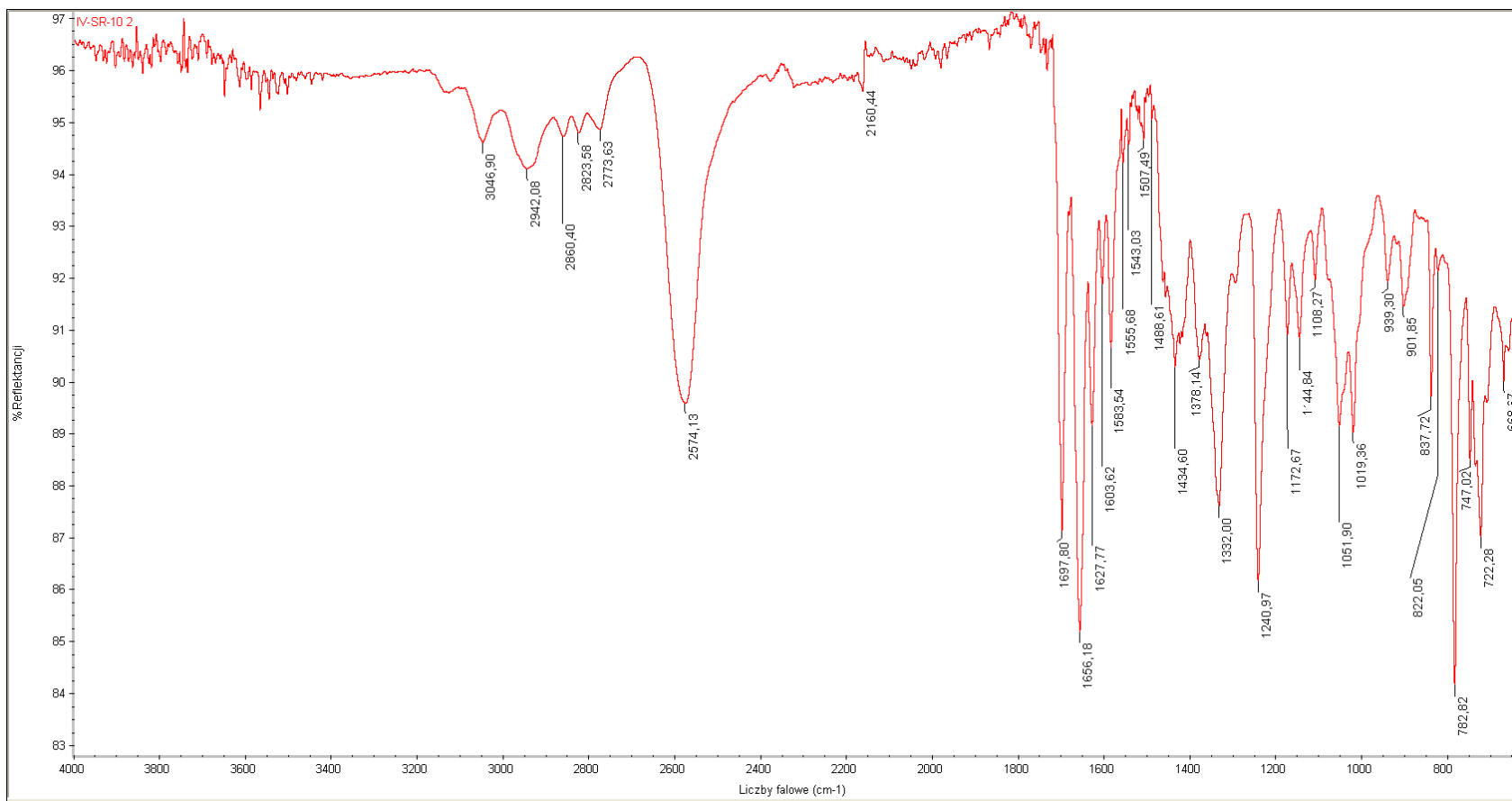
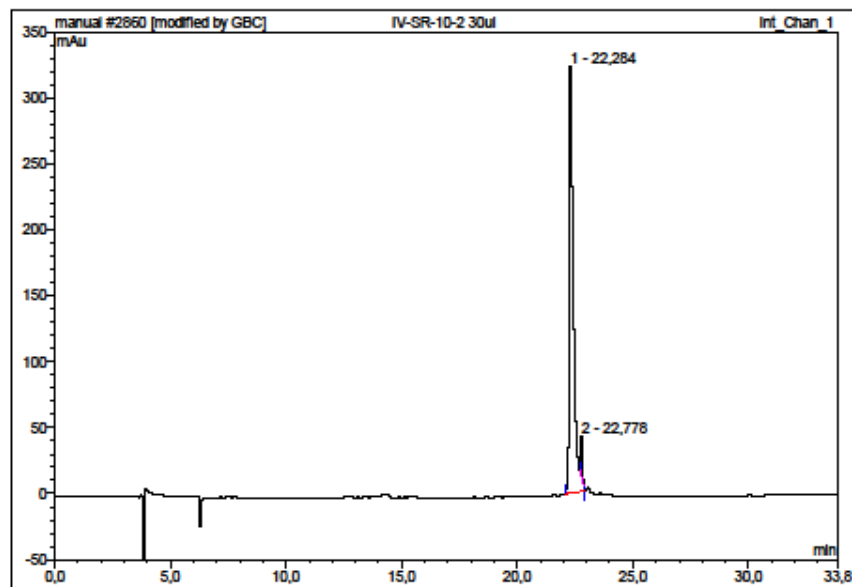


Figure S19. IR spectrum of 8.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	22,28	n.a.	324,260	69,327	96,50	n.a.	BMB*
2	22,78	n.a.	30,615	2,511	3,50	n.a.	Rd*
Total:			354,875	71,838	100,00	0,000	

Figure S20. HPLC analysis of 8.

Spectrum Name: IV-SR-10_2_PT
Start Ion: 300
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

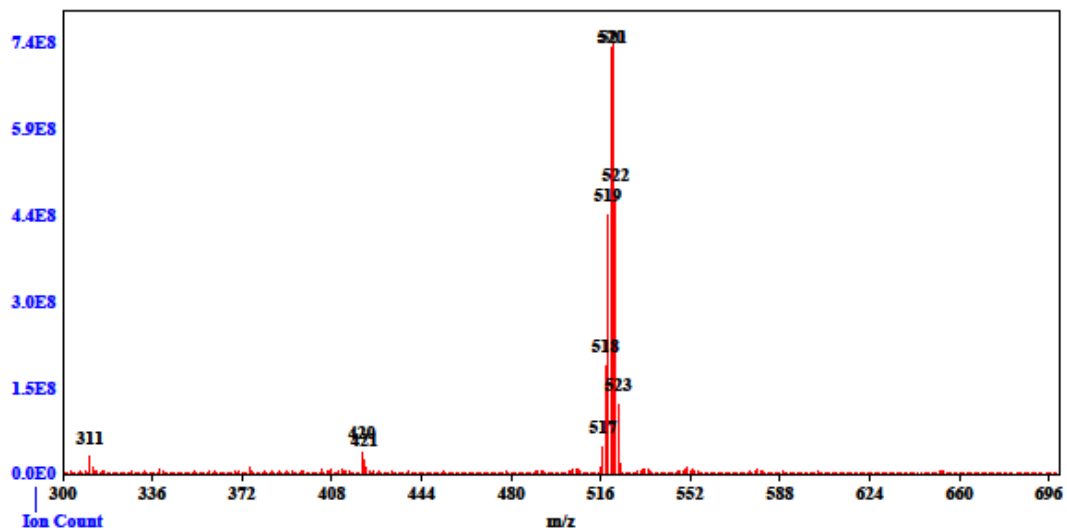


Figure S21. MS spectrum of 8.

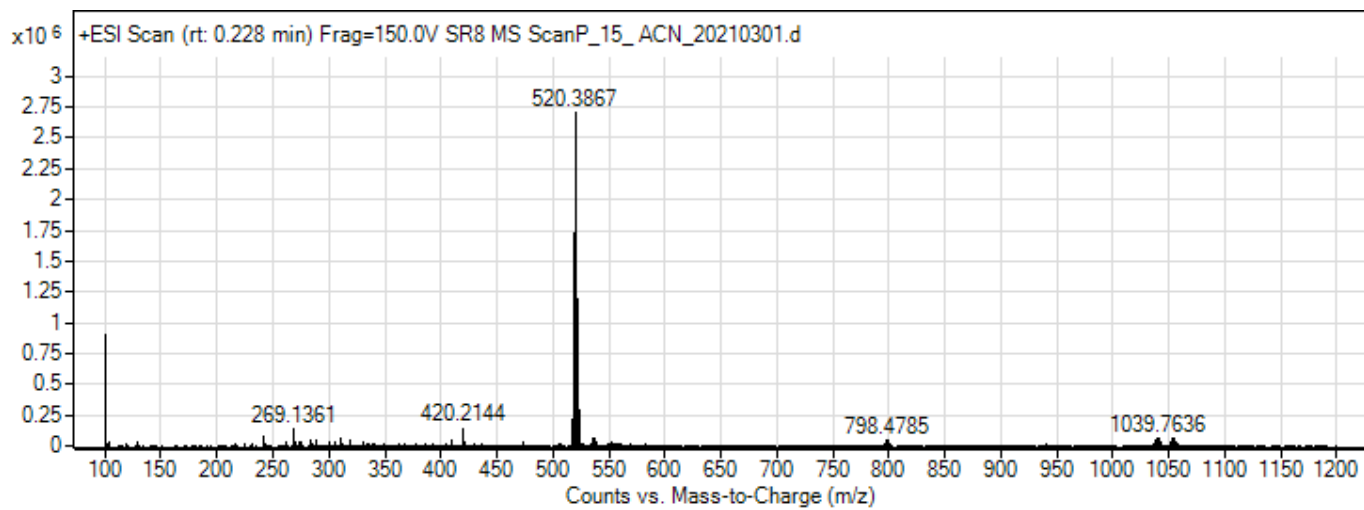


Figure S22. HRMS spectrum of 8.

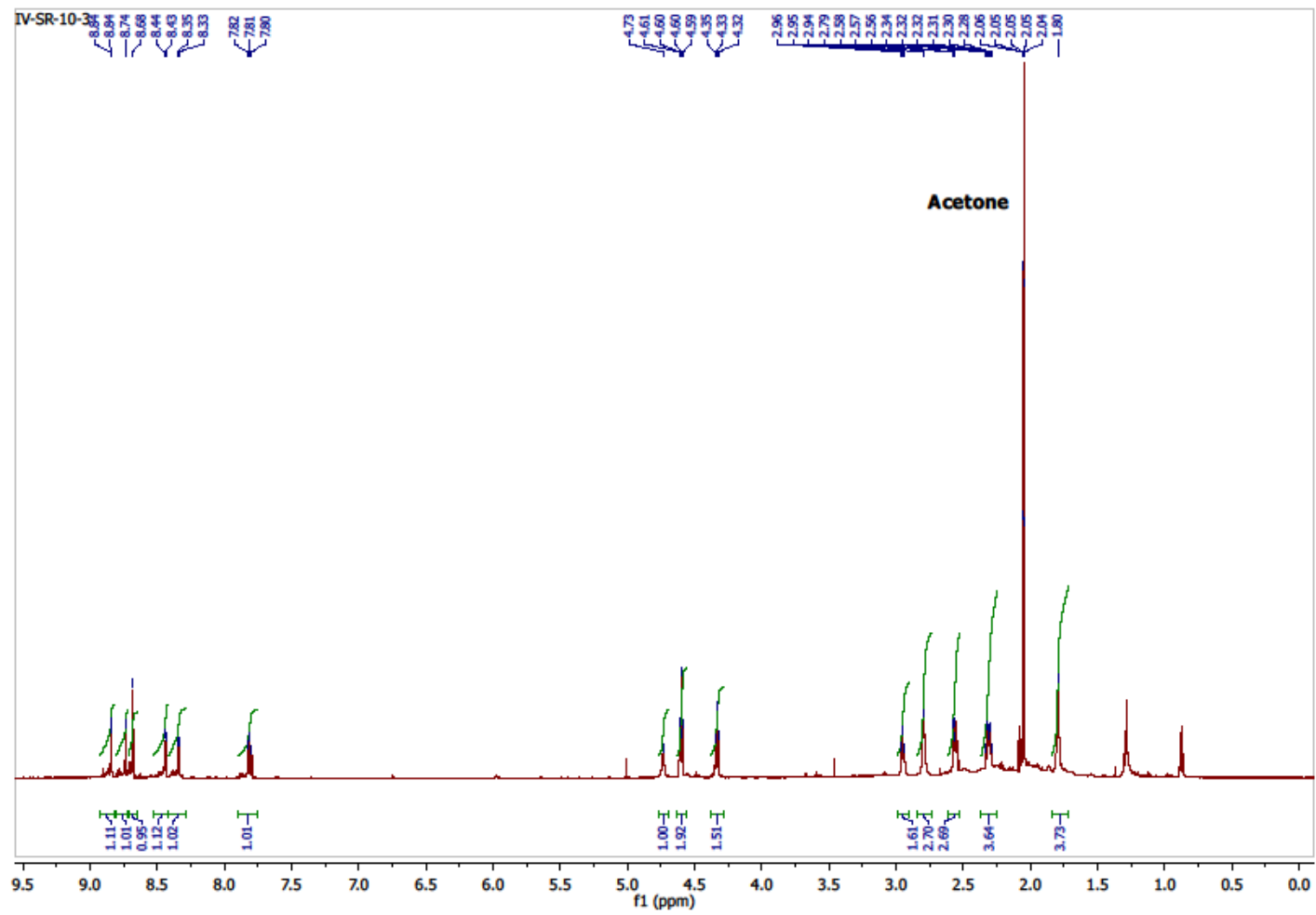


Figure S23. ¹H NMR spectrum of 9.

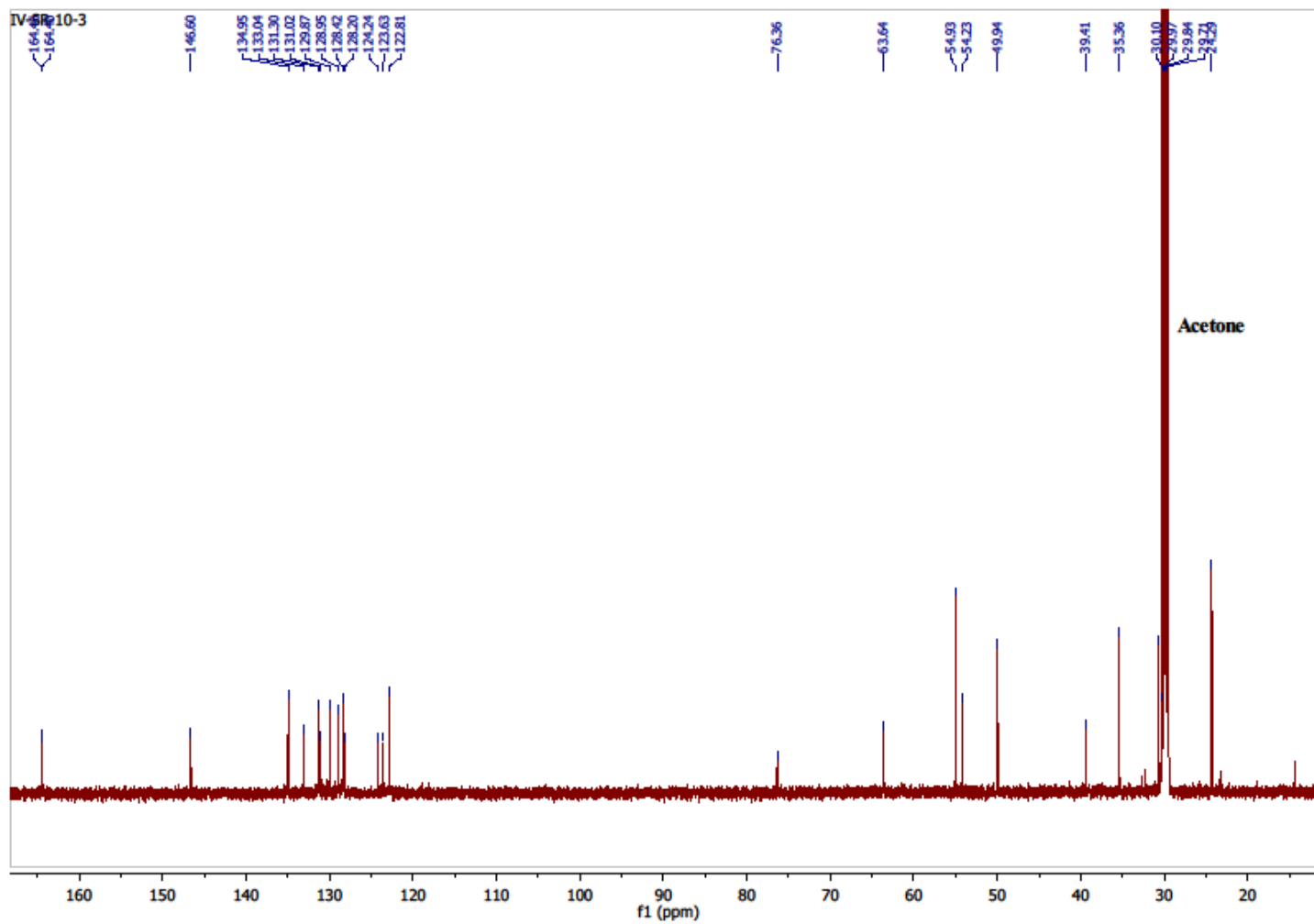


Figure S24. ^{13}C NMR spectrum of **9**.

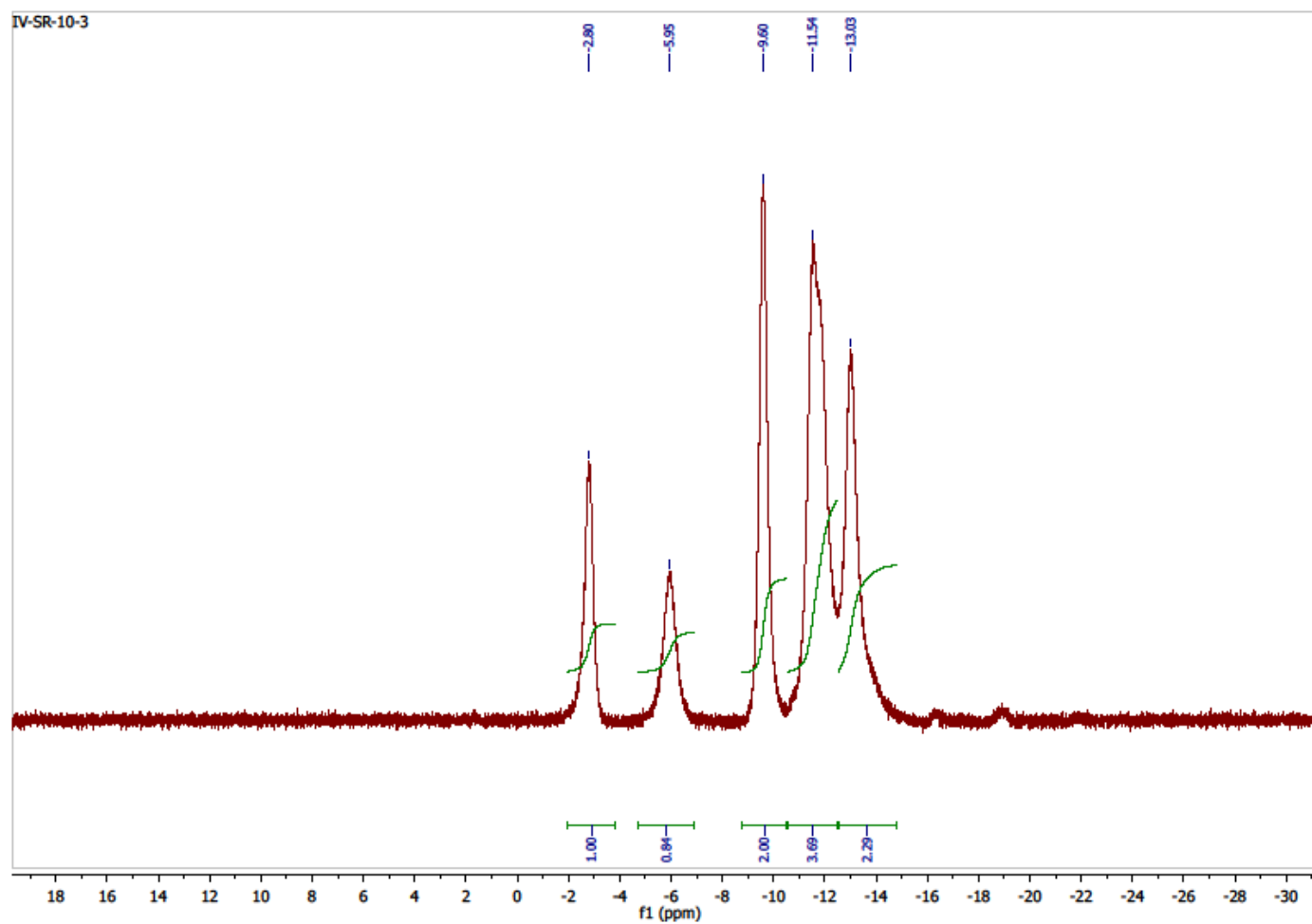


Figure S25. ^{11}B NMR (^1H BB) spectrum of 9.

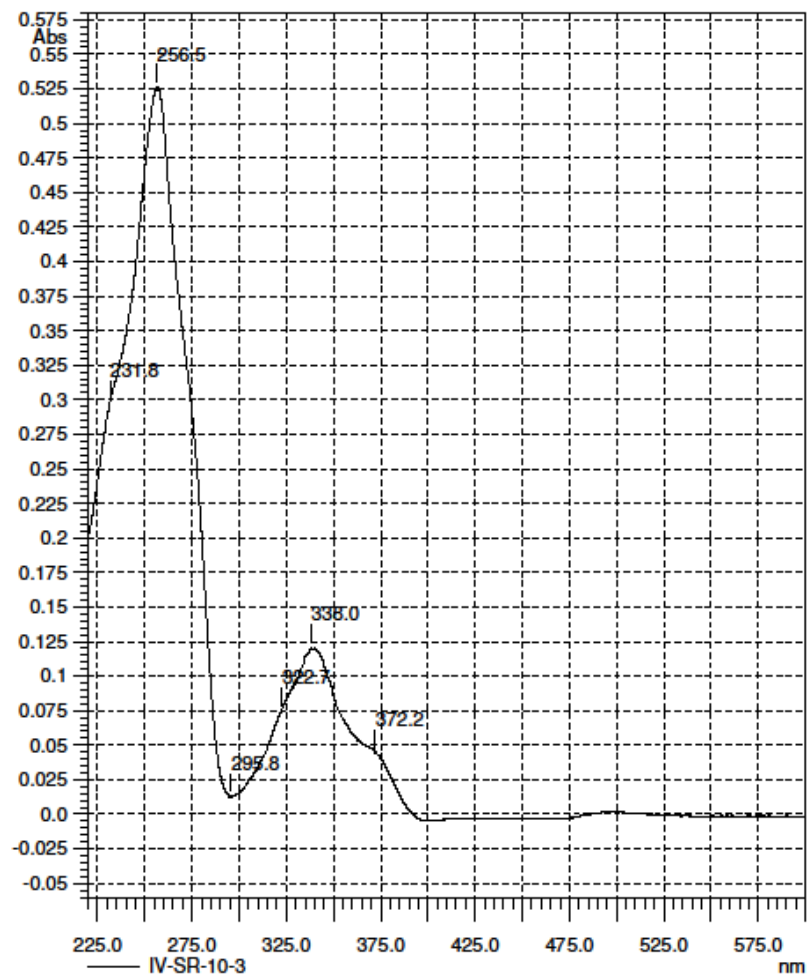


Figure S26. UV spectrum of 9.

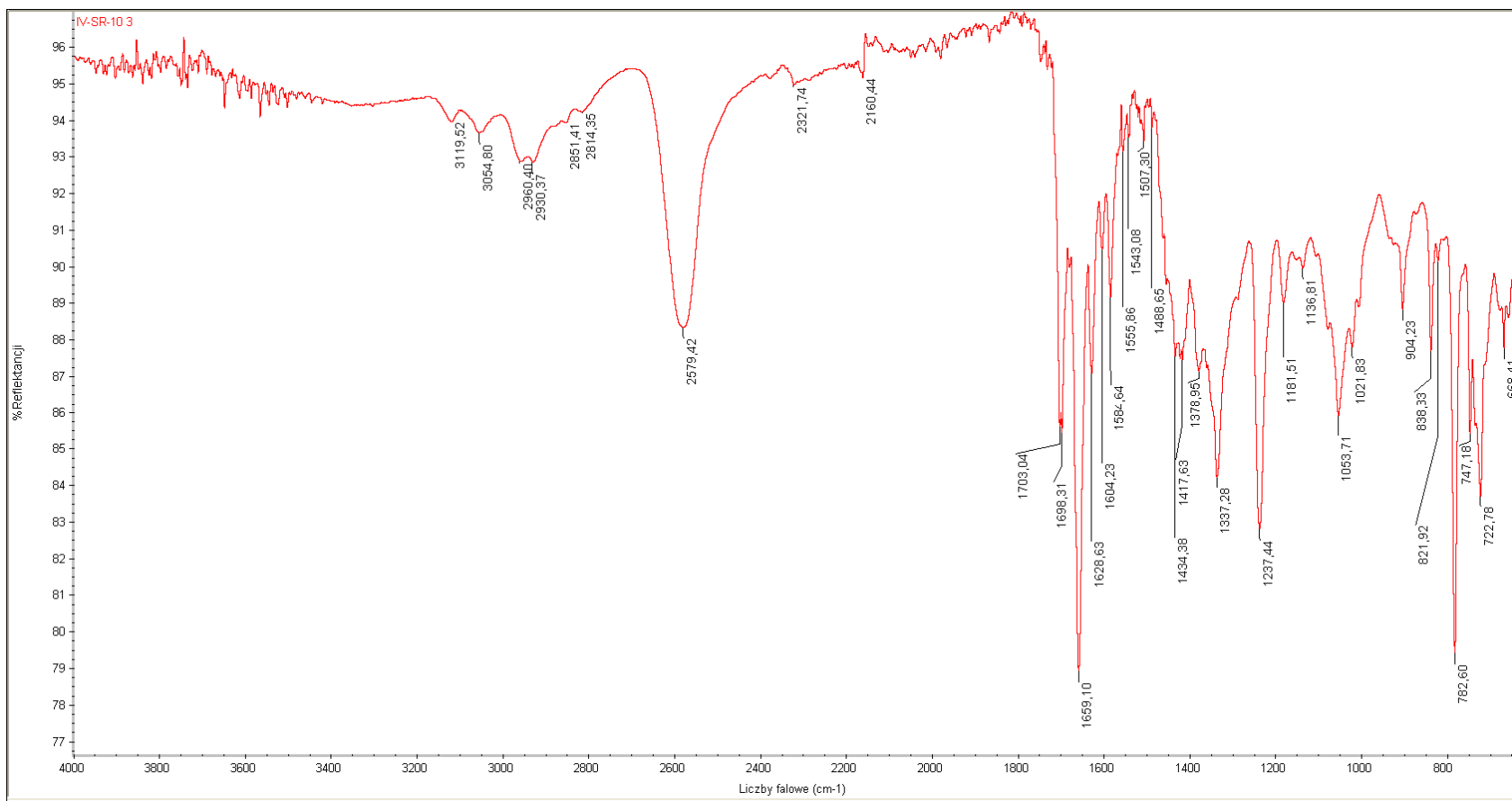
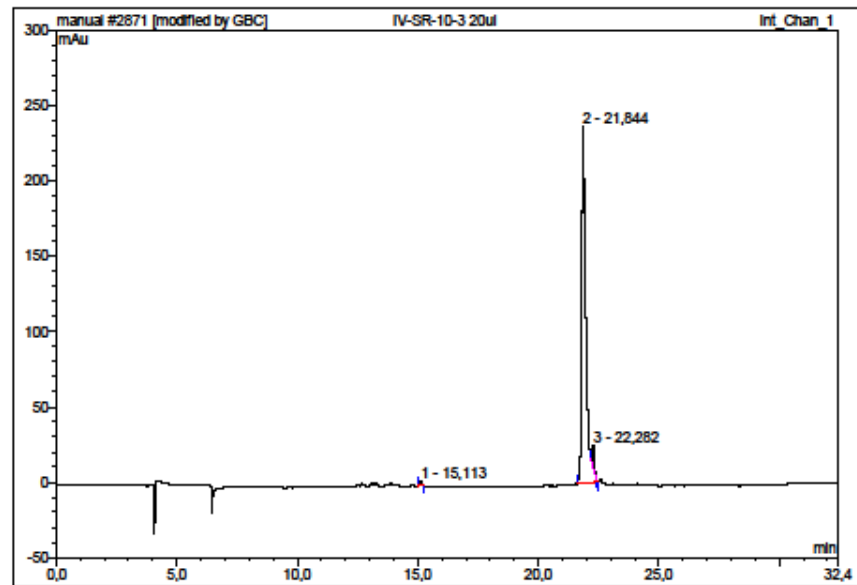


Figure S27. IR spectrum of 9.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	15,11	n.a.	3,035	0,348	0,72	n.a.	BMB*
2	21,84	n.a.	236,872	46,733	96,65	n.a.	BMB*
3	22,28	n.a.	15,135	1,272	2,63	n.a.	Rd*
Total:			255,042	48,353	100,00	0,000	

Figure S28. HPLC analysis of 9.

Spectrum Name: IV-SR-10_3_PT
Start Ion: 300
End Ion: 700
Source: APCI + 10.0μA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

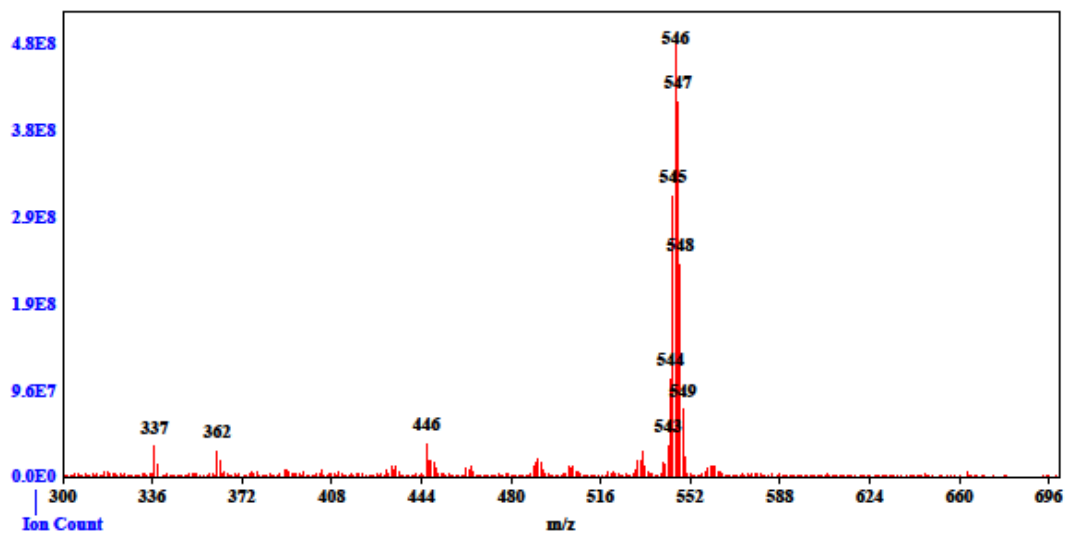


Figure S29. MS spectrum of 9.

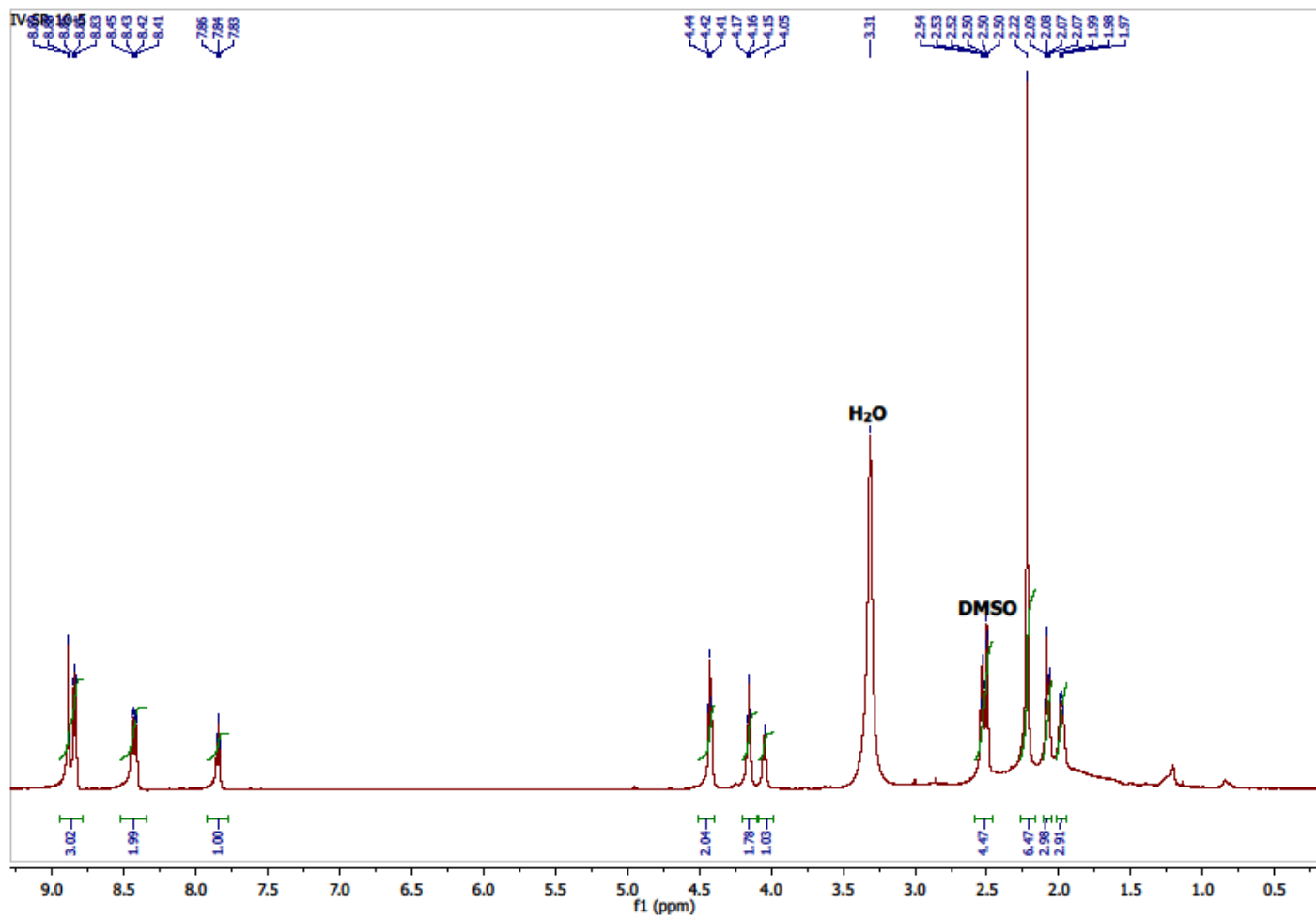


Figure S30. ¹H NMR spectrum of 10.

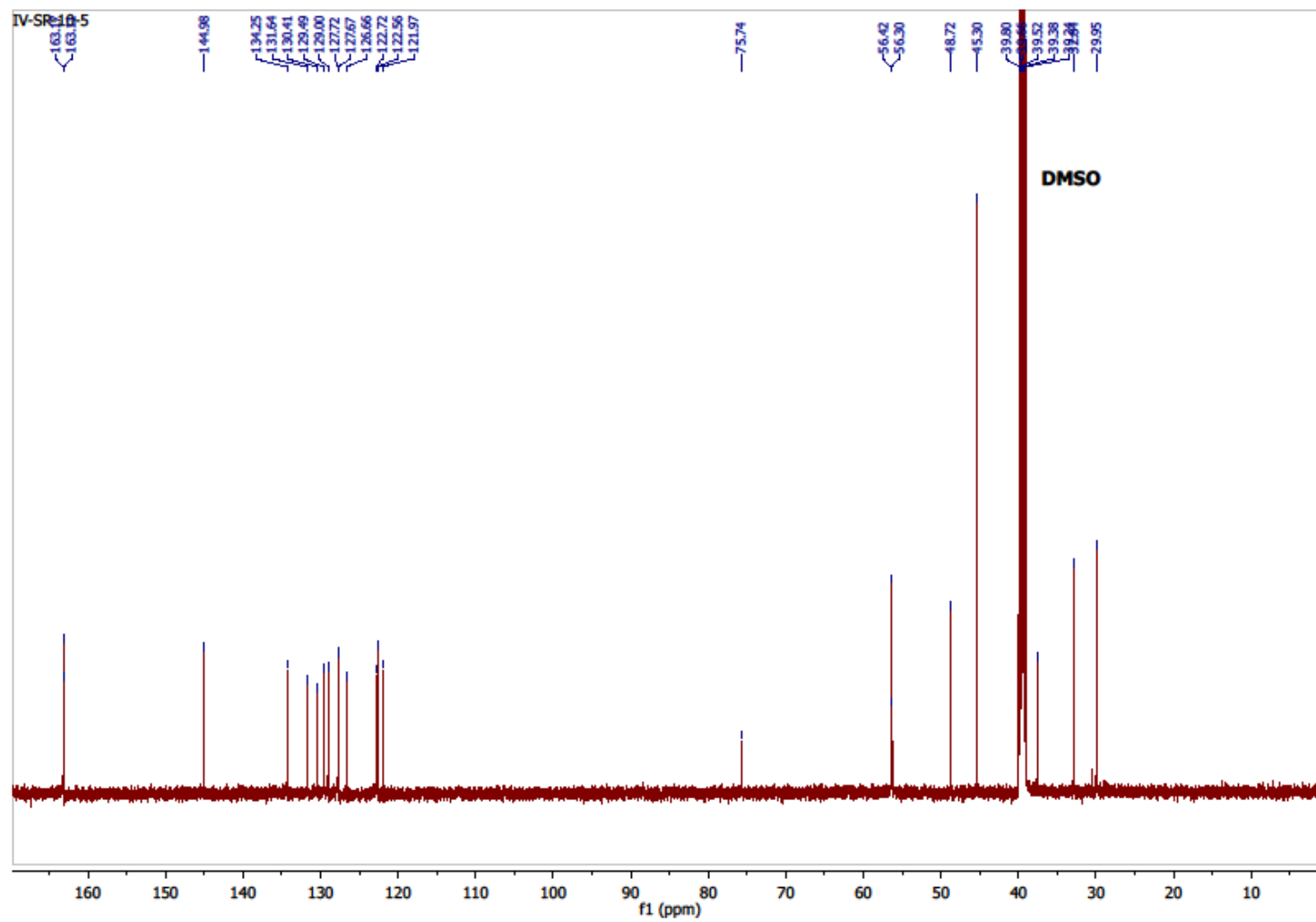


Figure S31. ^{13}C NMR spectrum of 10.

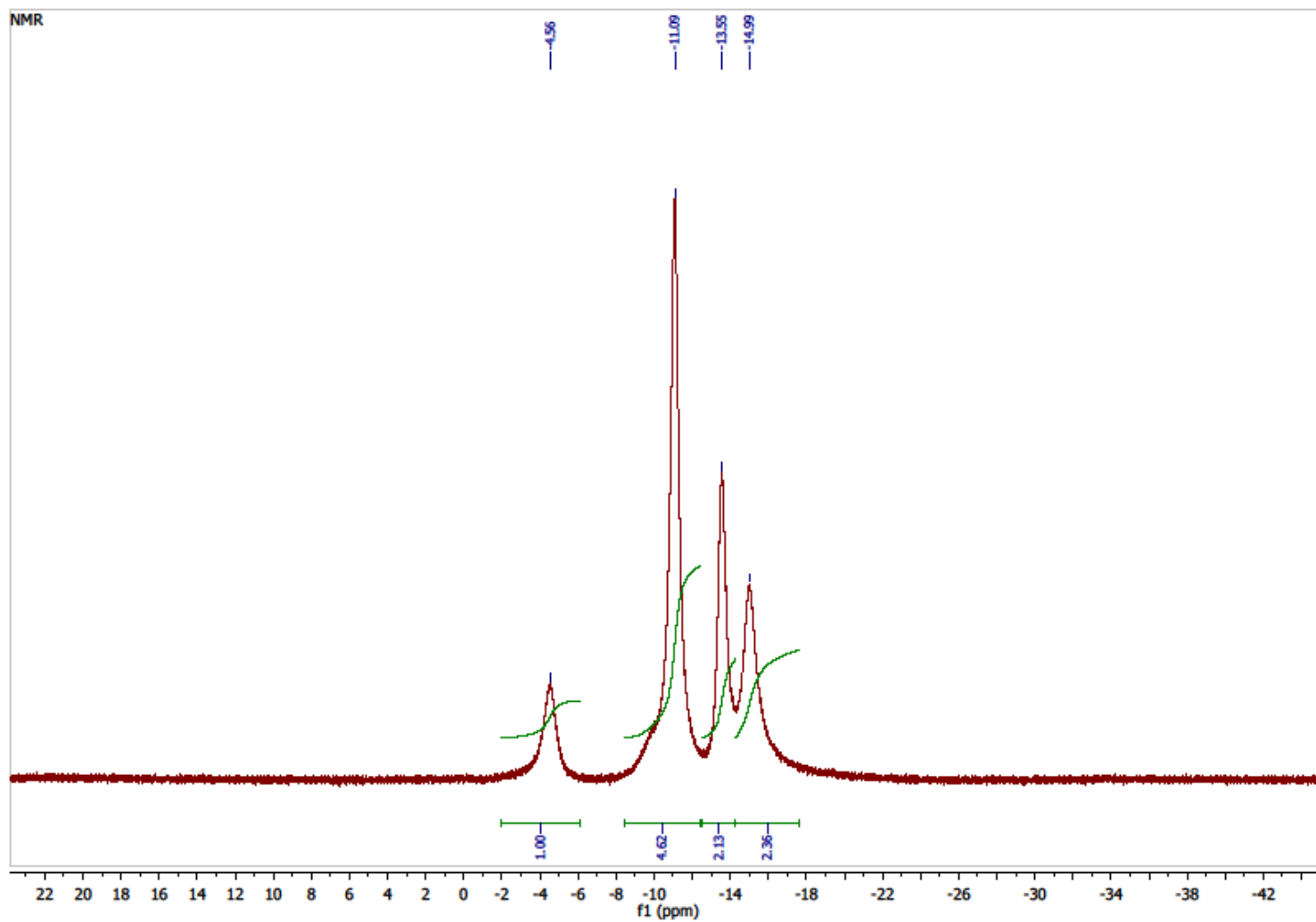


Figure S32. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 10.

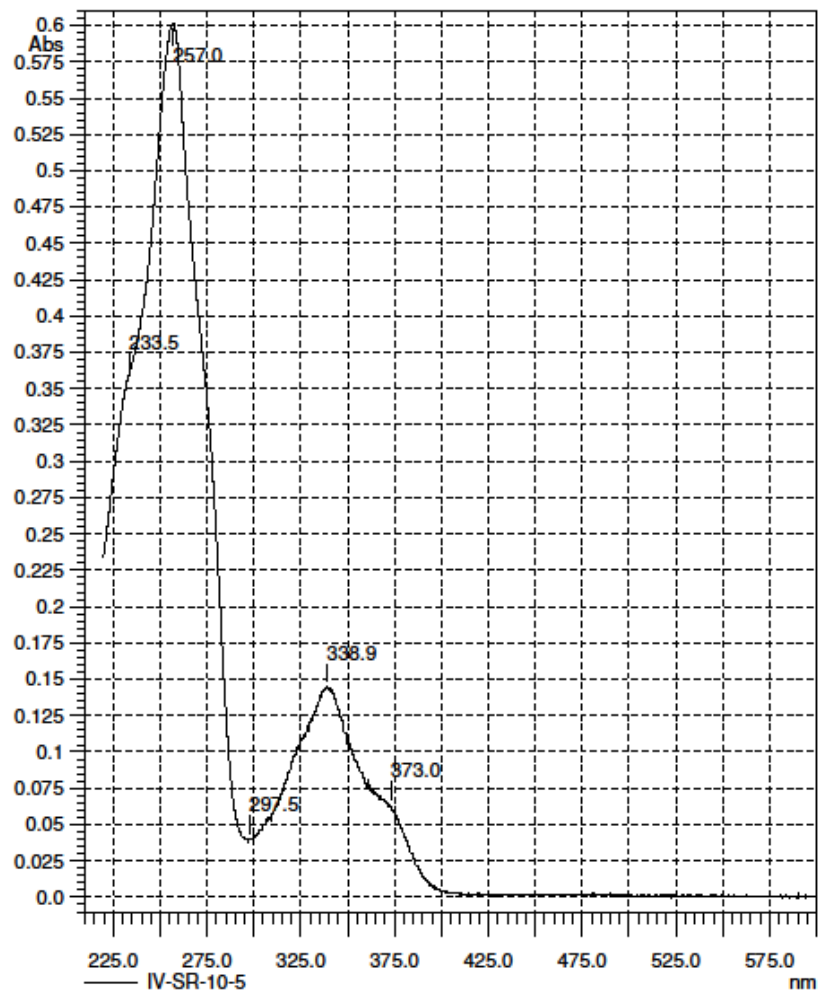


Figure S33. UV spectrum of 10.

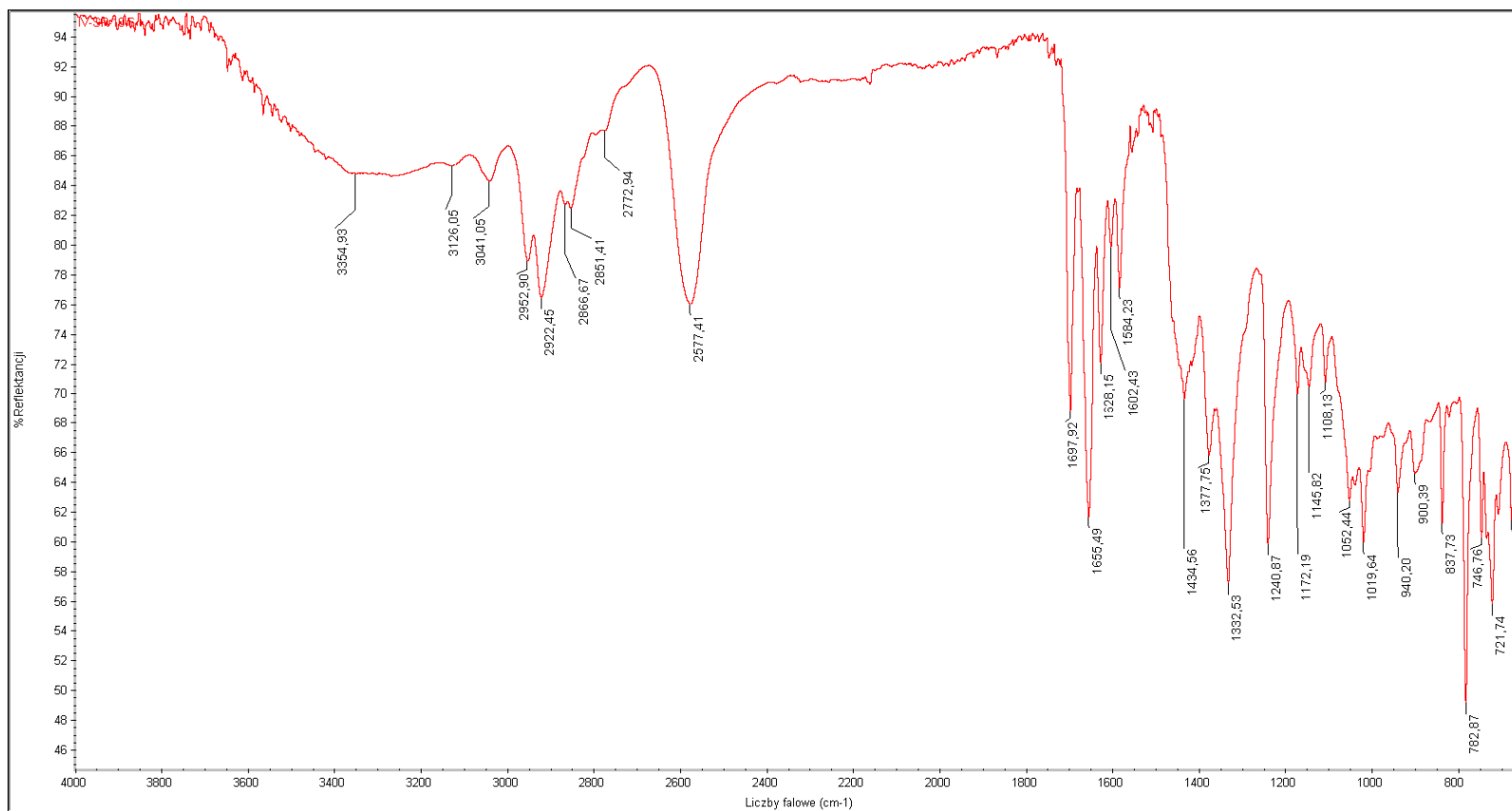
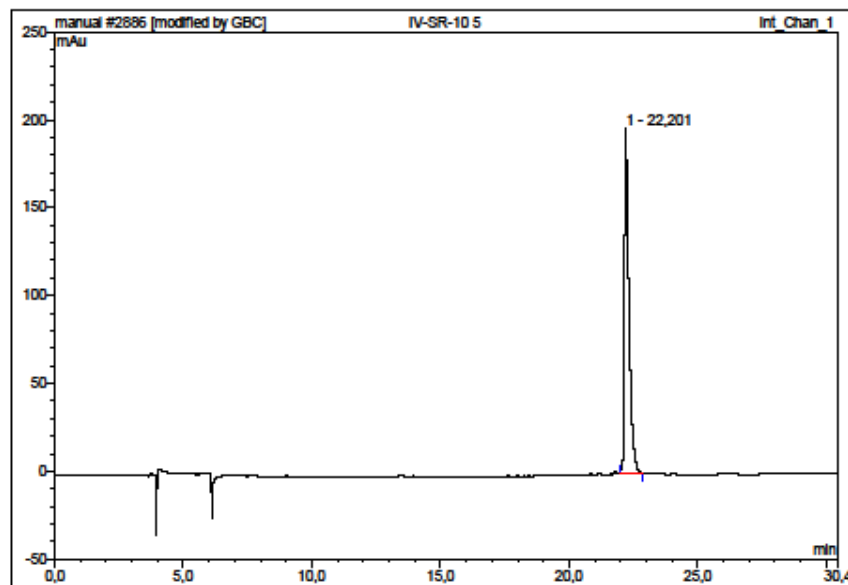


Figure S34. IR spectrum of 10.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	22,20	n.a.	196,209	39,594	100,00	n.a.	BMB
Total:			196,209	39,594	100,00	0,000	

Figure S35. HPLC analysis of 10.

Spectrum Name: IV-SR-10_5_PT
Start Ion: 300
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

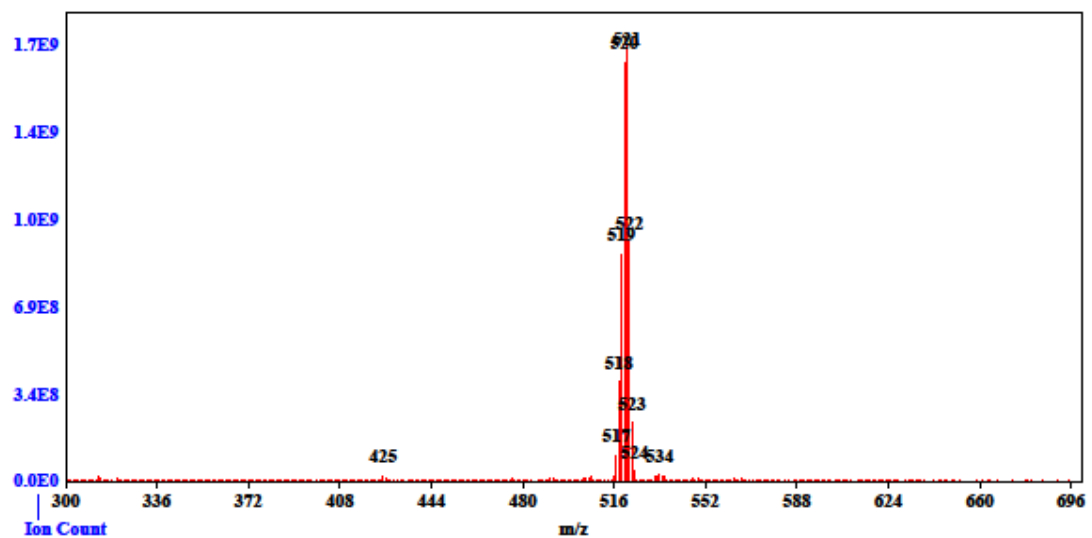


Figure S36. MS spectrum of 10.

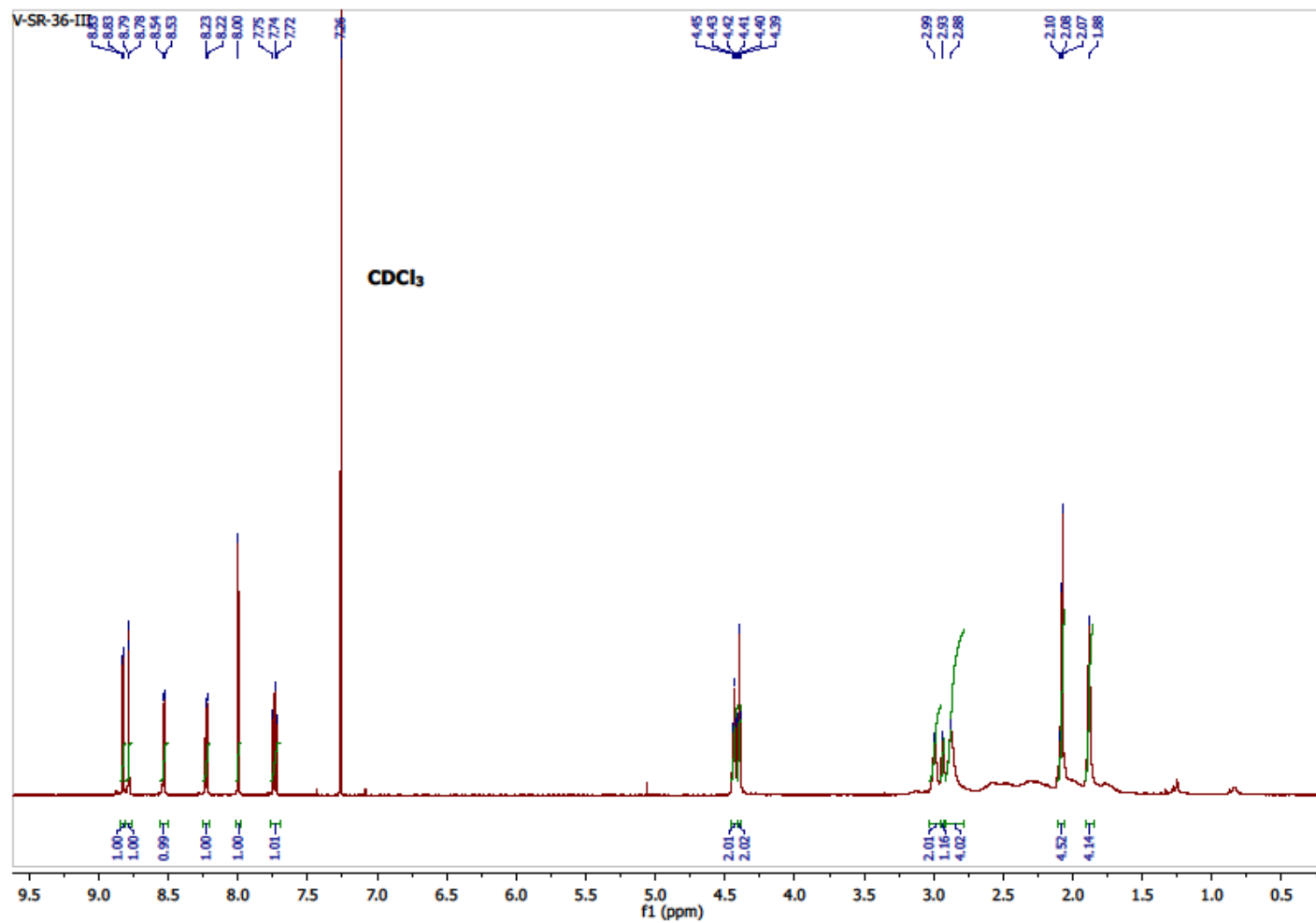


Figure S37. ¹H NMR spectrum of 11.

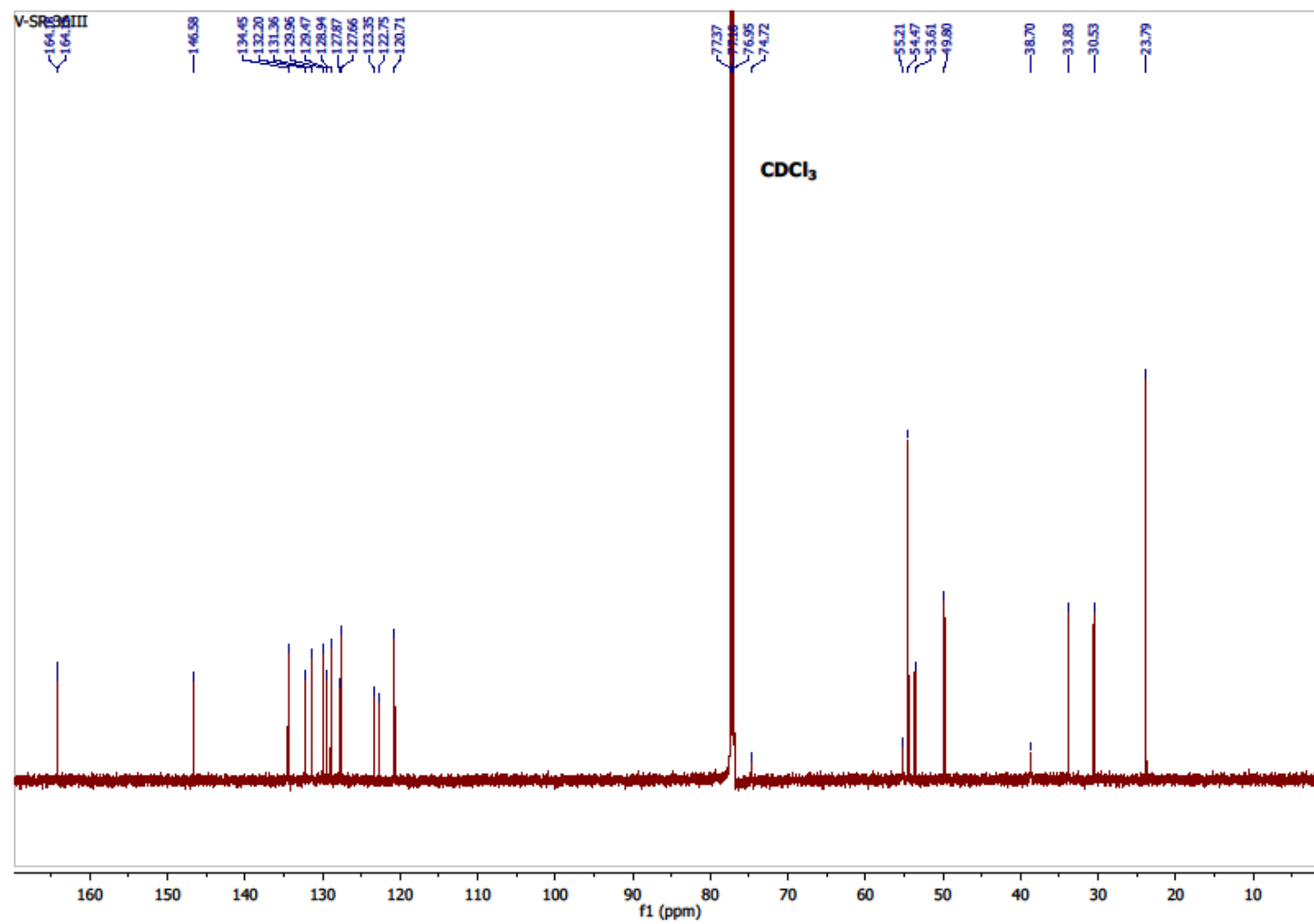


Figure S38. ¹³C NMR spectrum of 11.

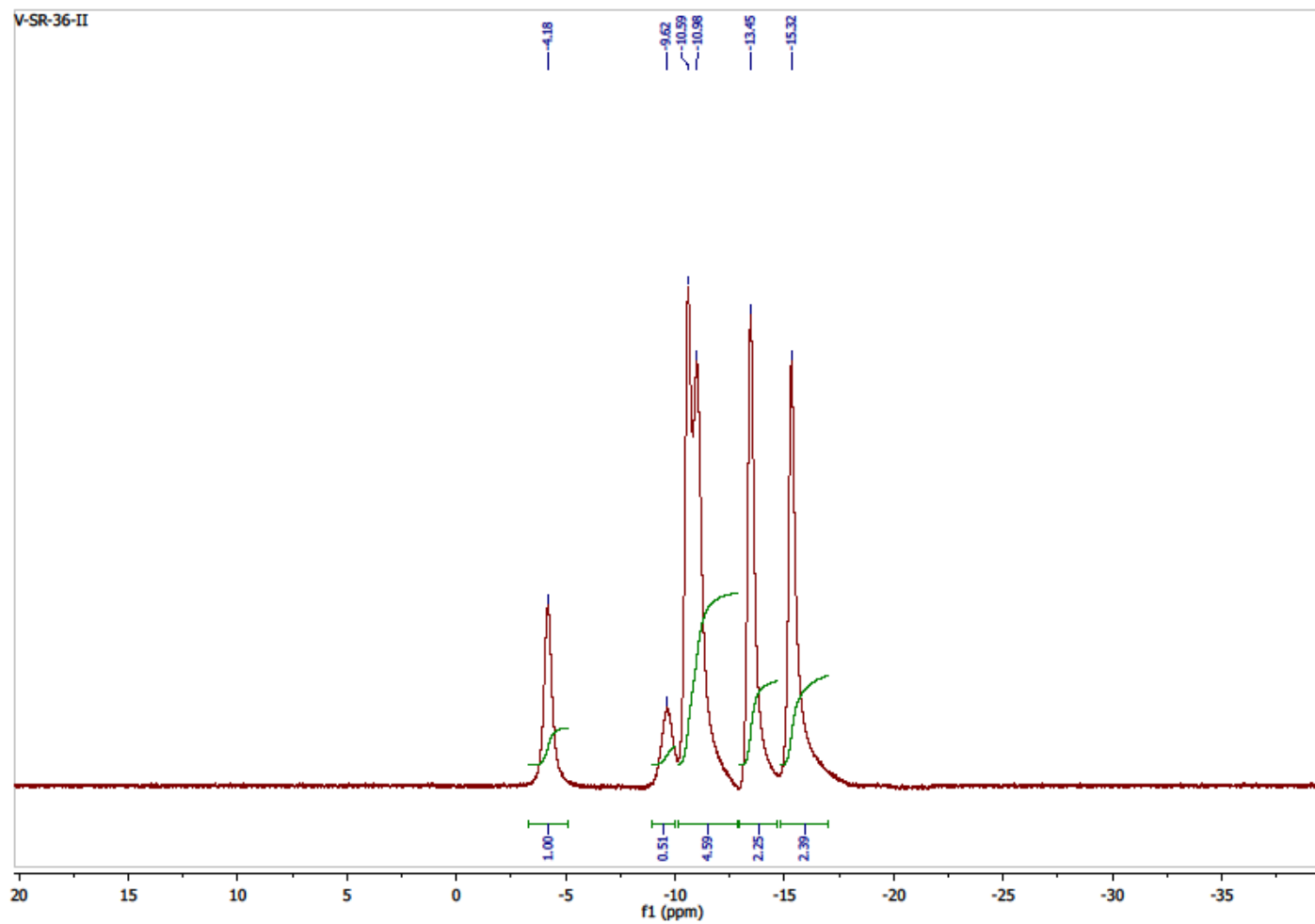


Figure S39. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 11.

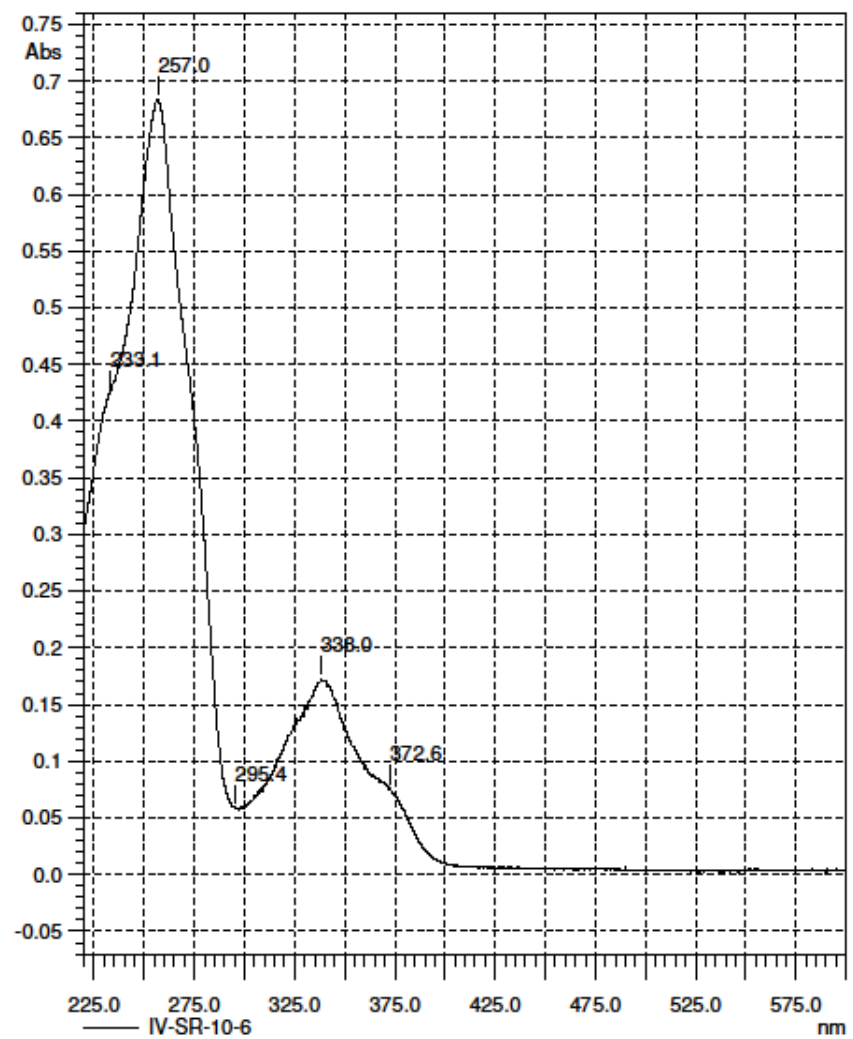


Figure S40. UV spectrum of 11.

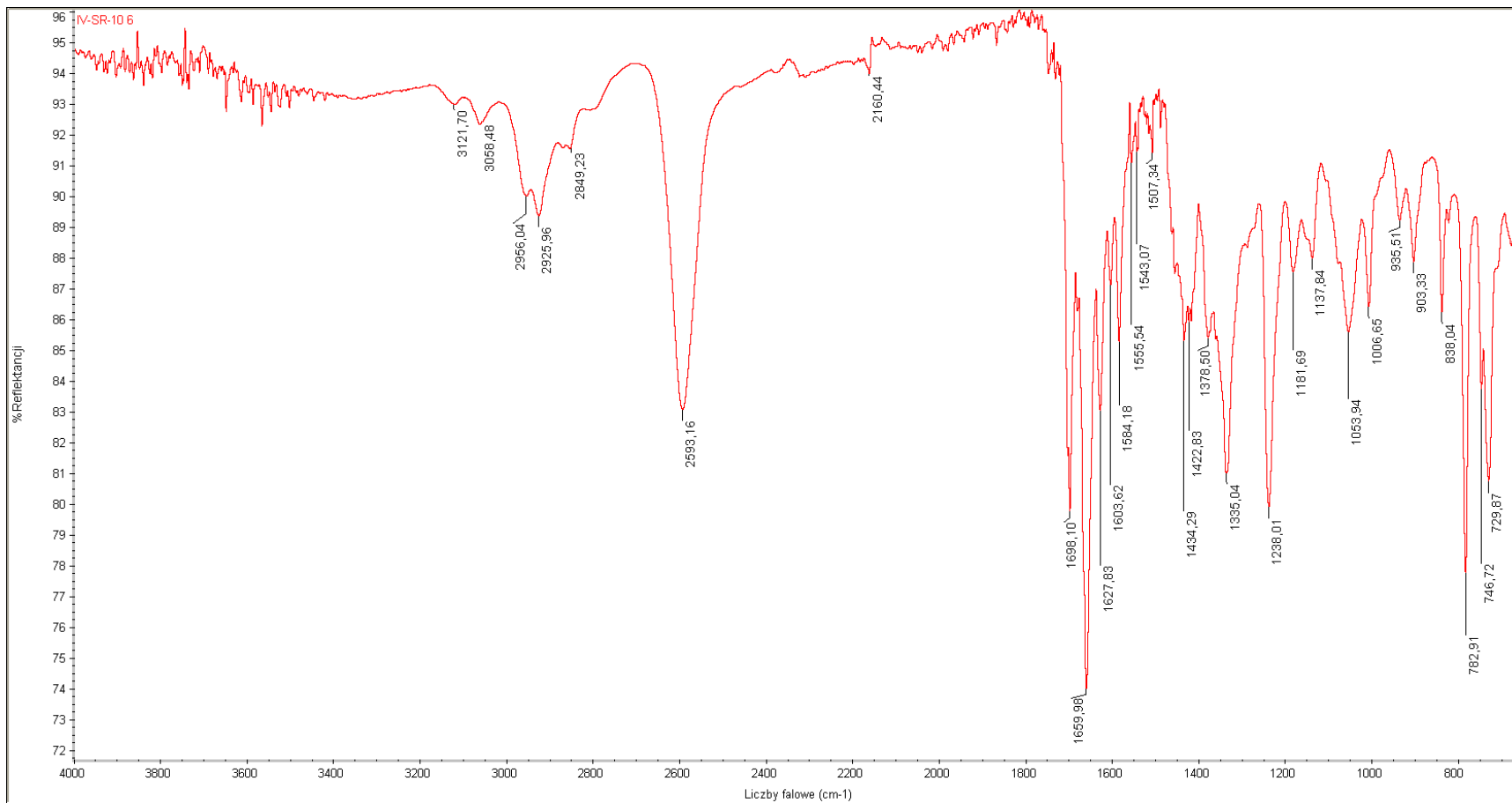
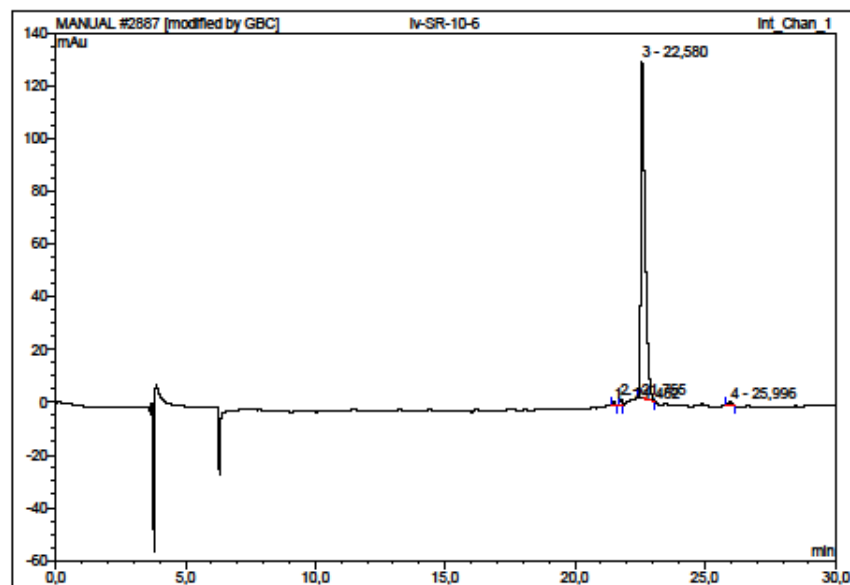


Figure S41. IR spectrum of 11.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	21,48	n.a.	0,983	0,114	0,46	n.a.	BMB*
2	21,76	n.a.	2,363	0,226	0,91	n.a.	BMB*
3	22,58	n.a.	127,847	24,210	97,63	n.a.	BMB*
4	26,00	n.a.	1,303	0,248	1,00	n.a.	BMB*
Total:			132,495	24,798	100,00	0,000	

Figure S42. HPLC analysis of 11.

Spectrum Name: IV-SR-10_6_PT
Start Ion: 450
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

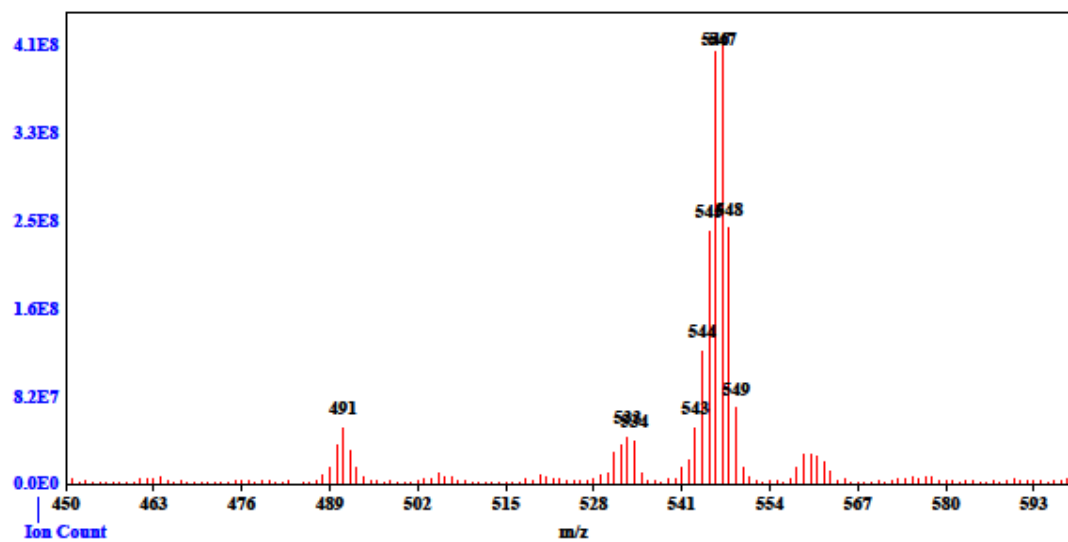


Figure S43. MS spectrum of 11.

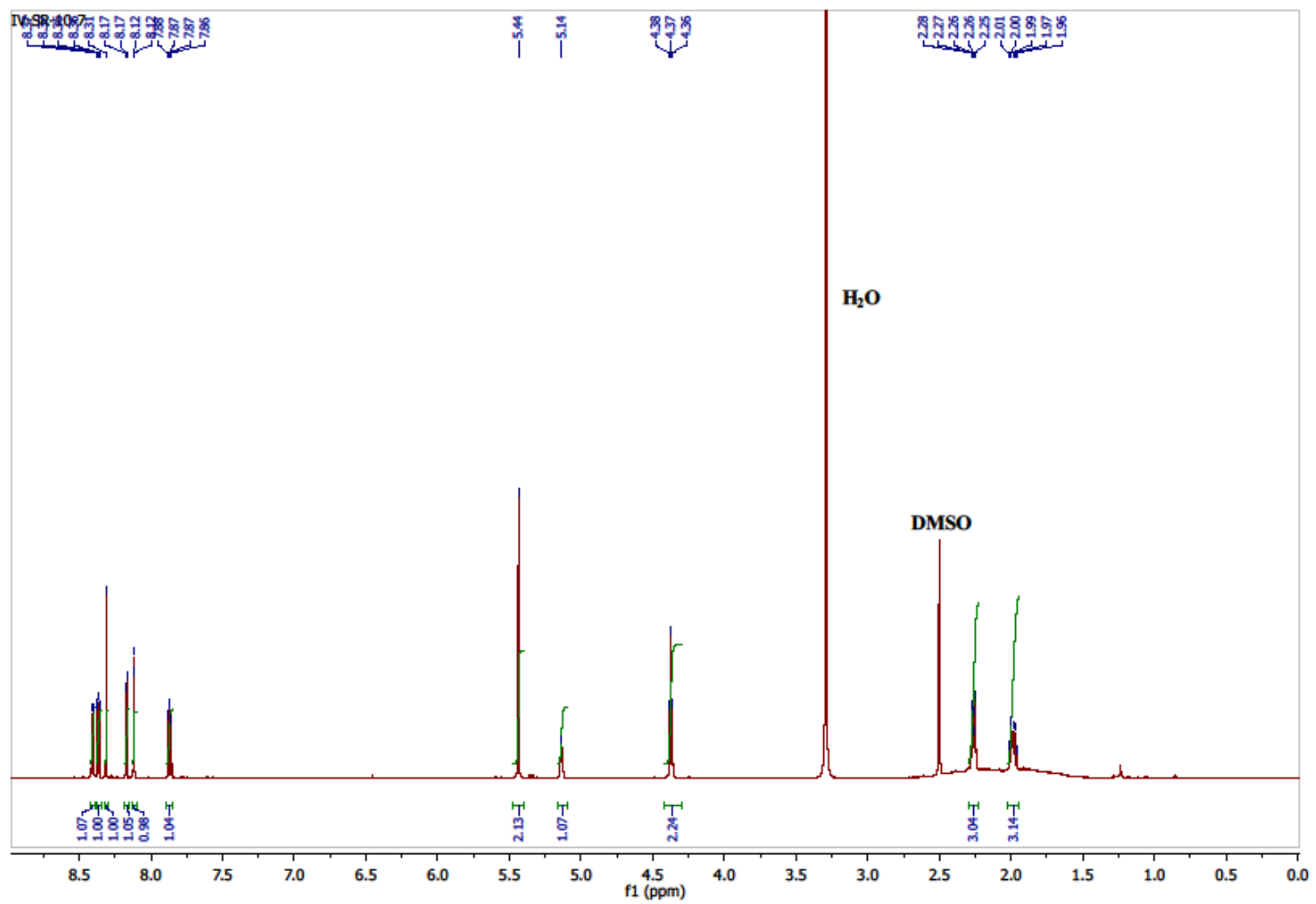


Figure S44. ¹H NMR spectrum of 15.

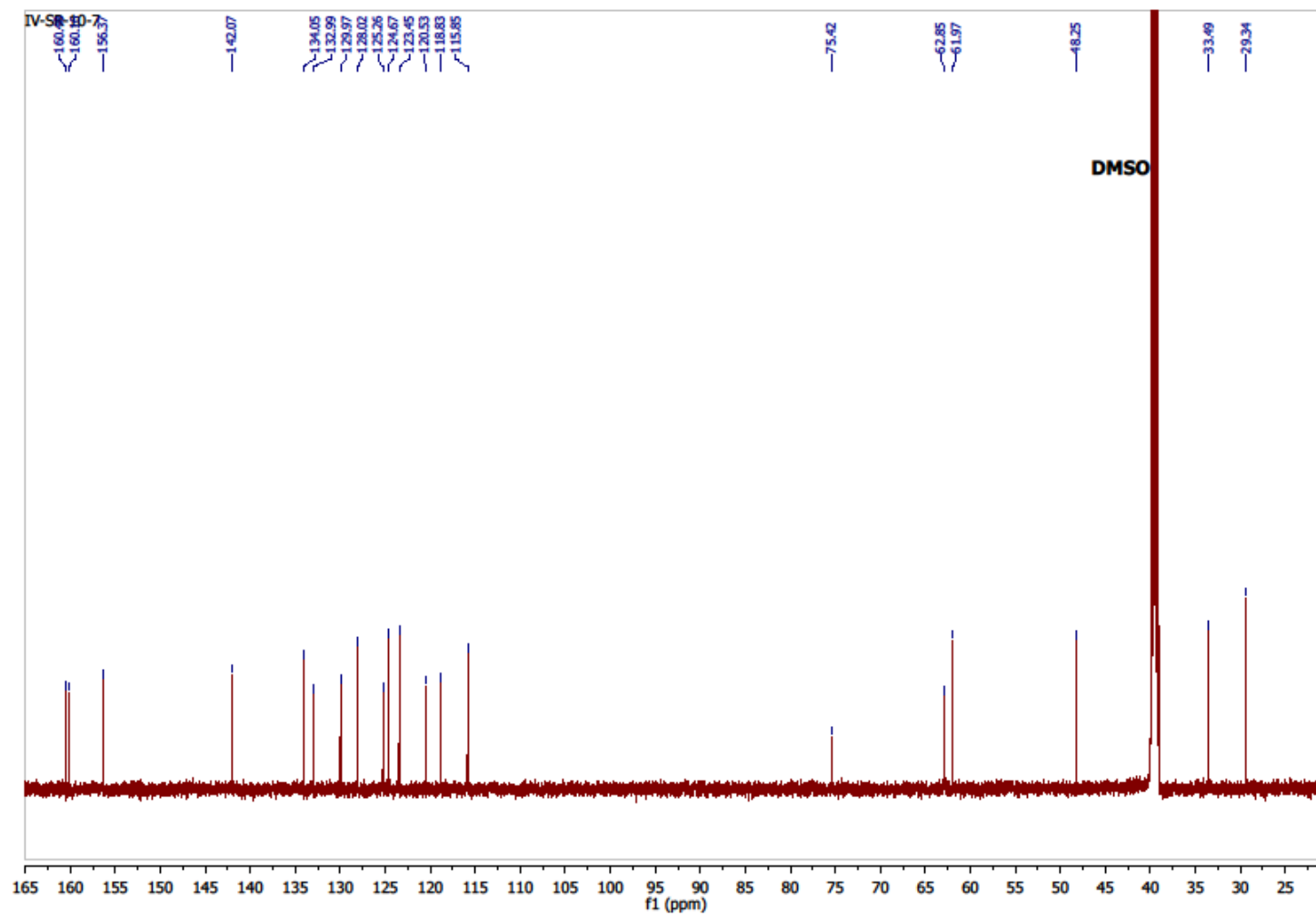


Figure S45. ^{13}C NMR spectrum of 15.

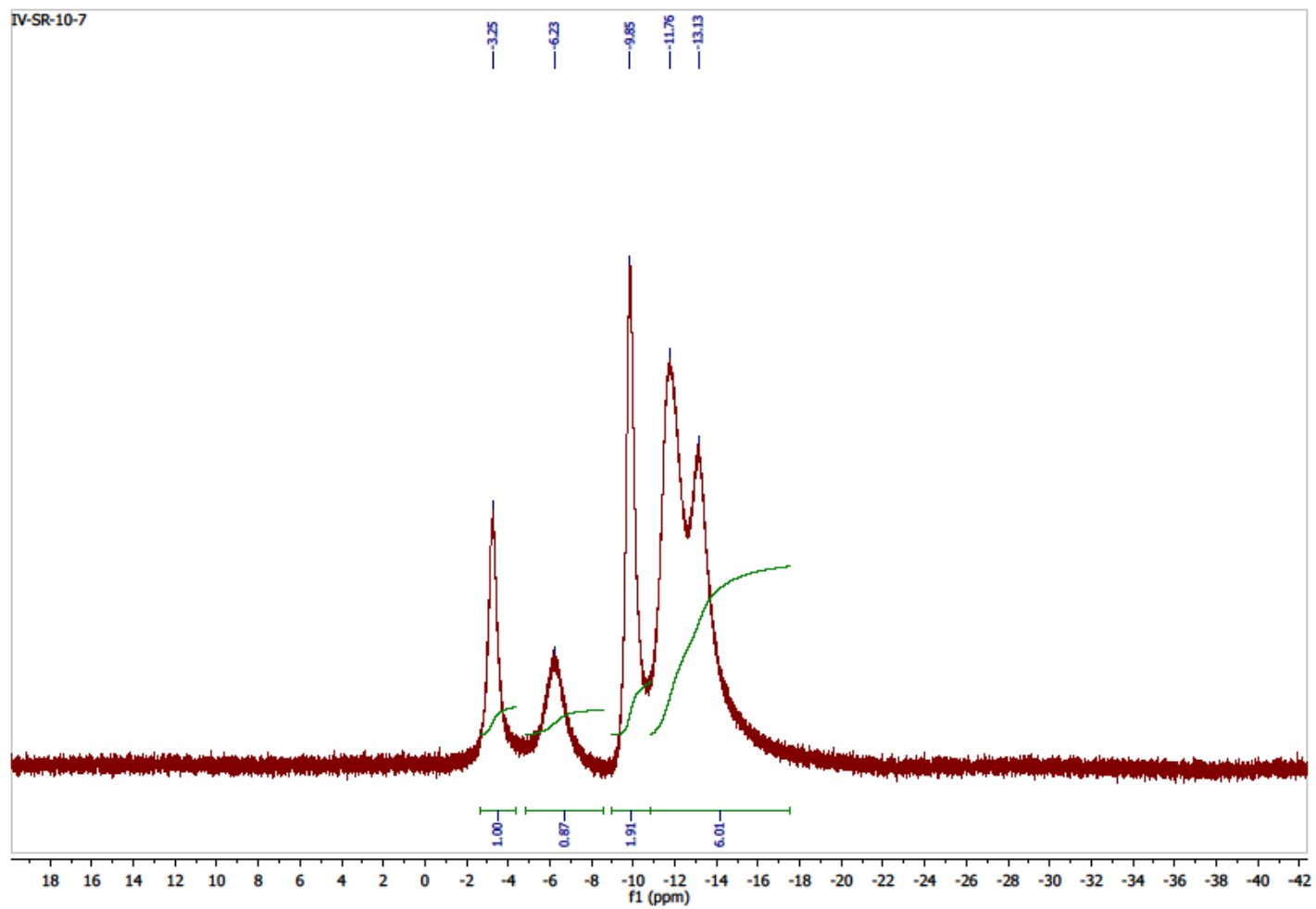


Figure S46. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 15.

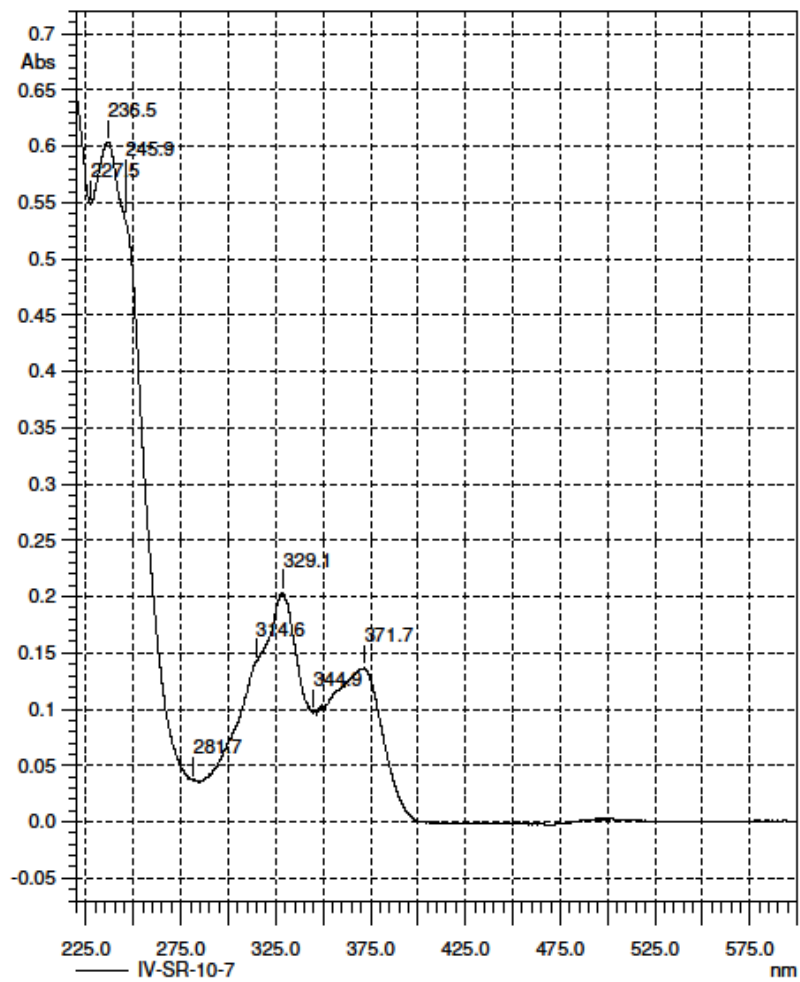


Figure S47. UV spectrum of 15.

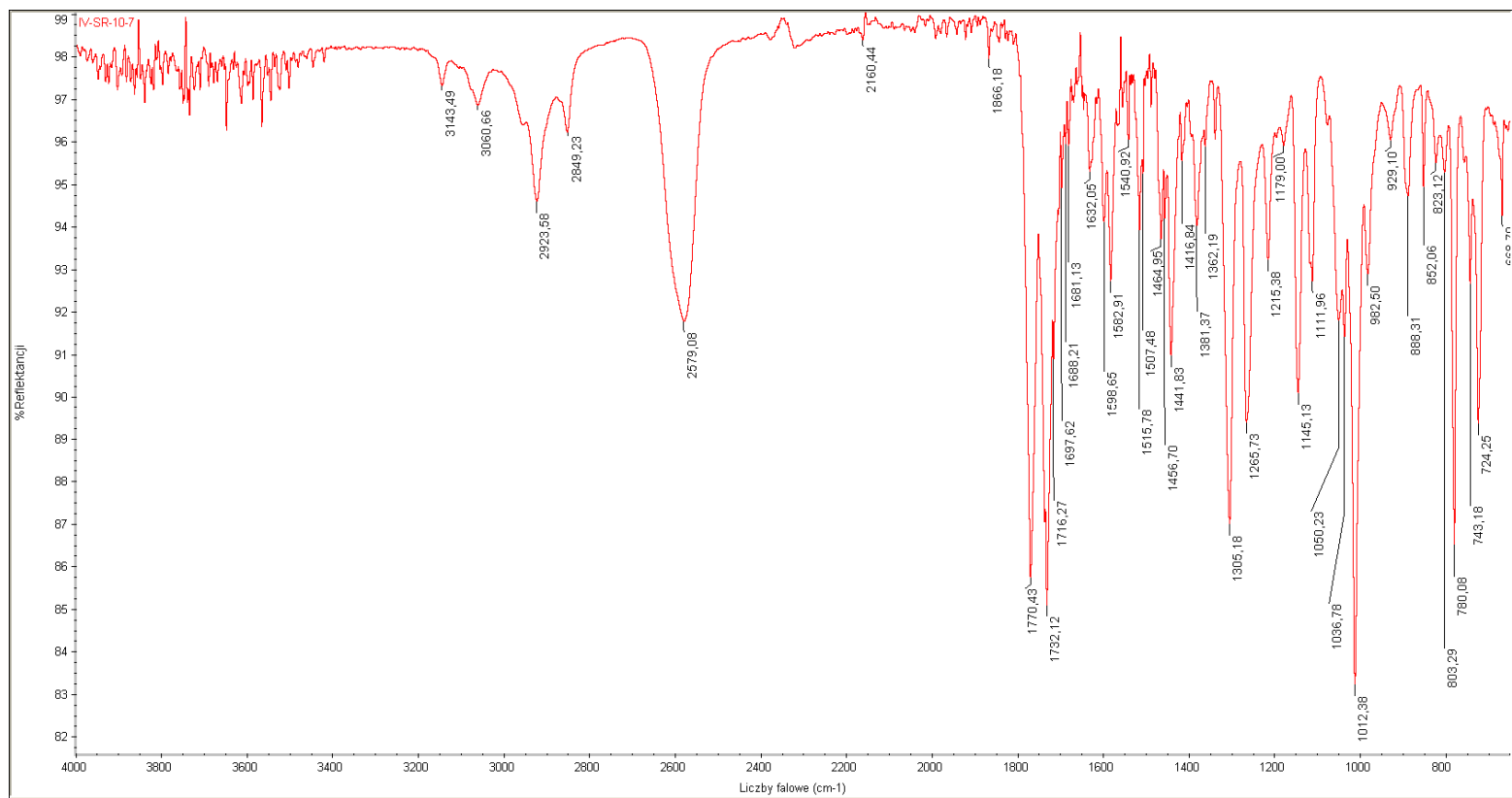


Figure S48. IR spectrum of 15.

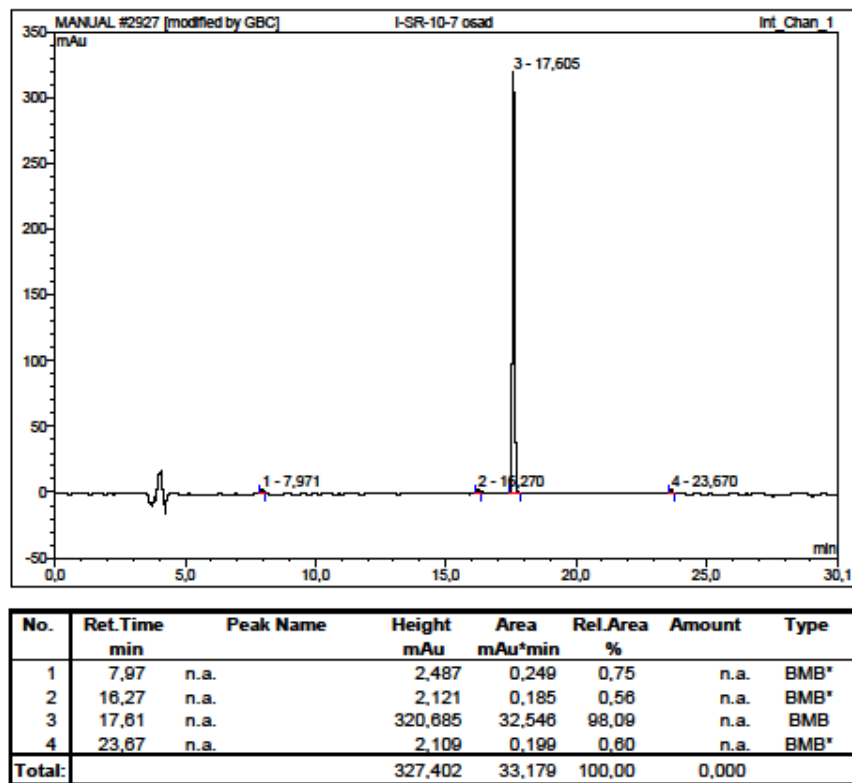


Figure S49. HPLC analysis of 15.

Spectrum Name: IV-SR-10_7
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

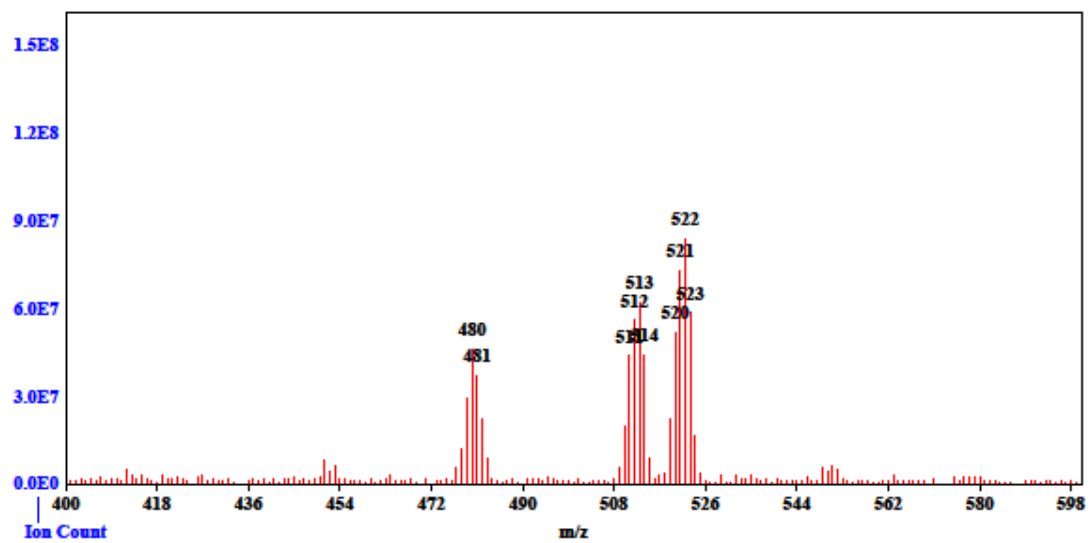


Figure S50. MS spectrum of 15.

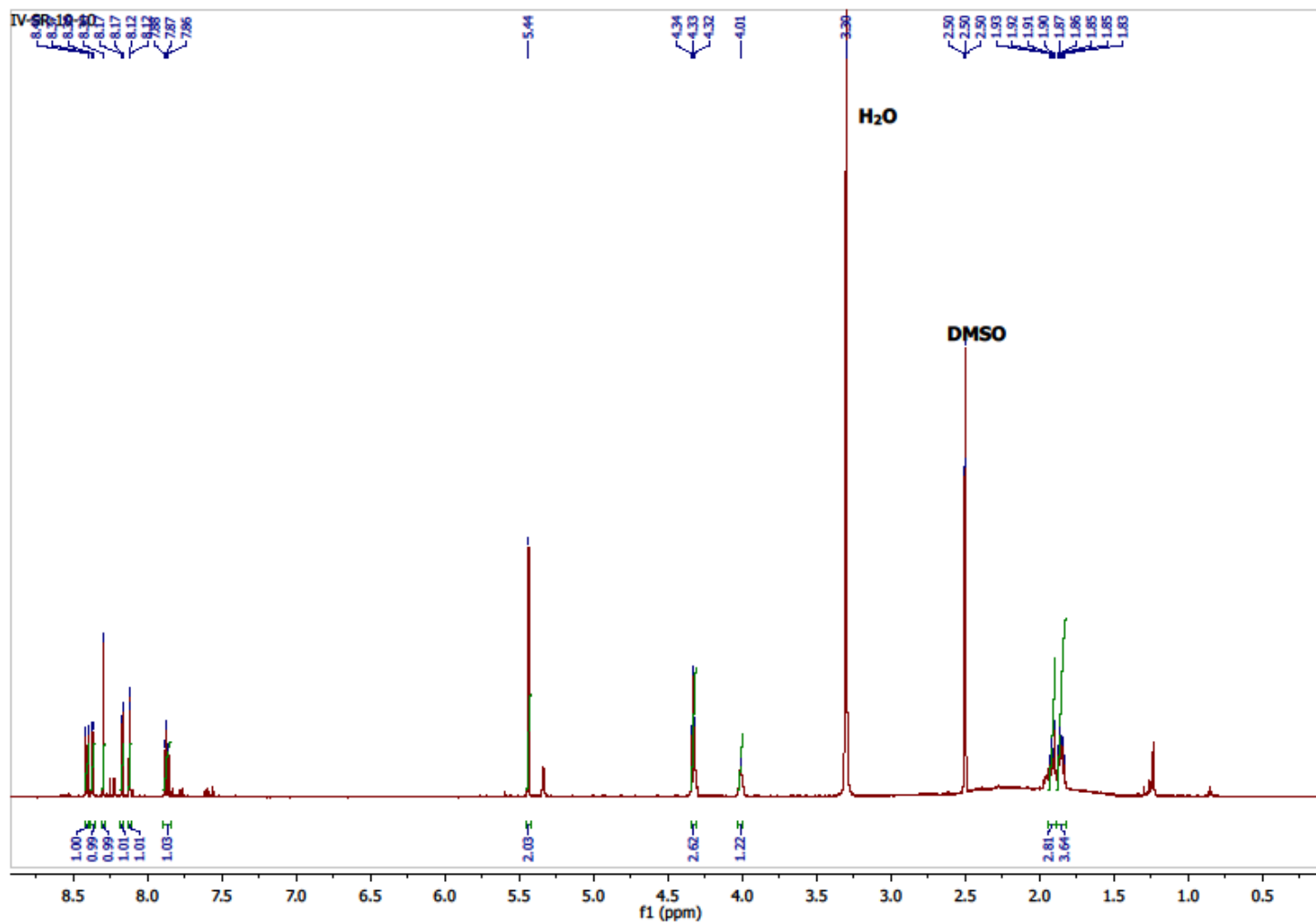


Figure S51. ¹H NMR spectrum of 16.

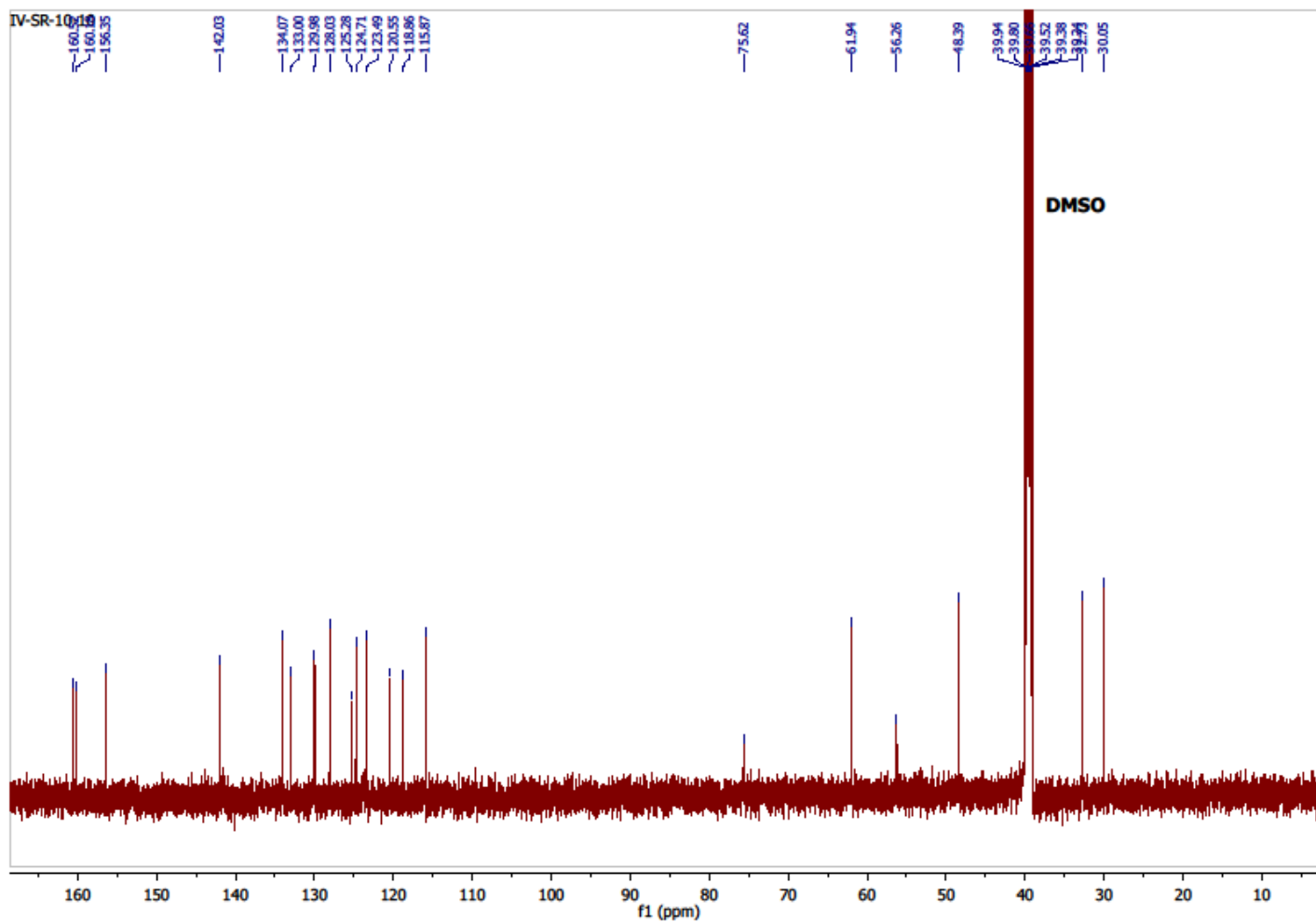


Figure S52. ^{13}C NMR spectrum of **16**.

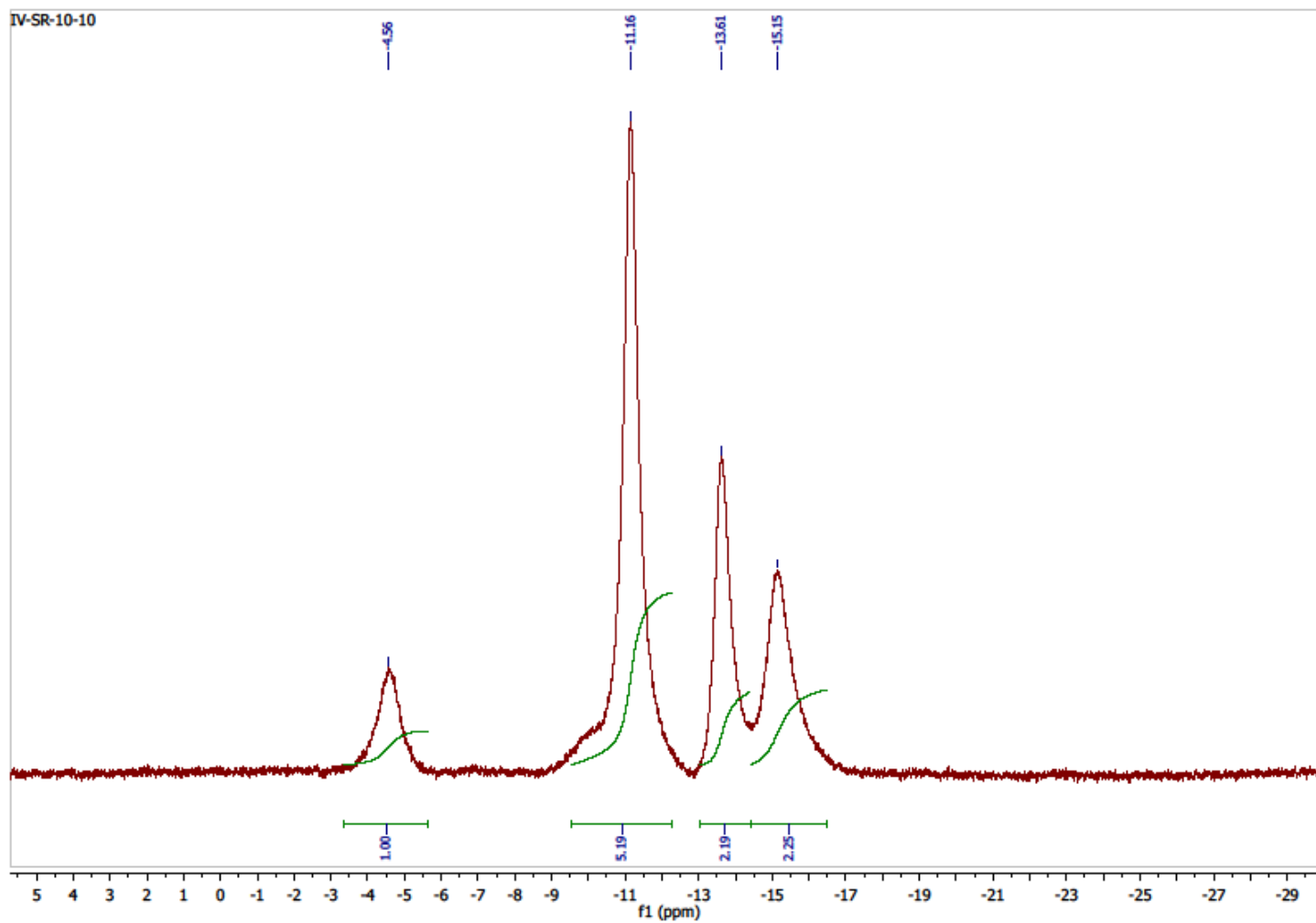


Figure S53. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 16.

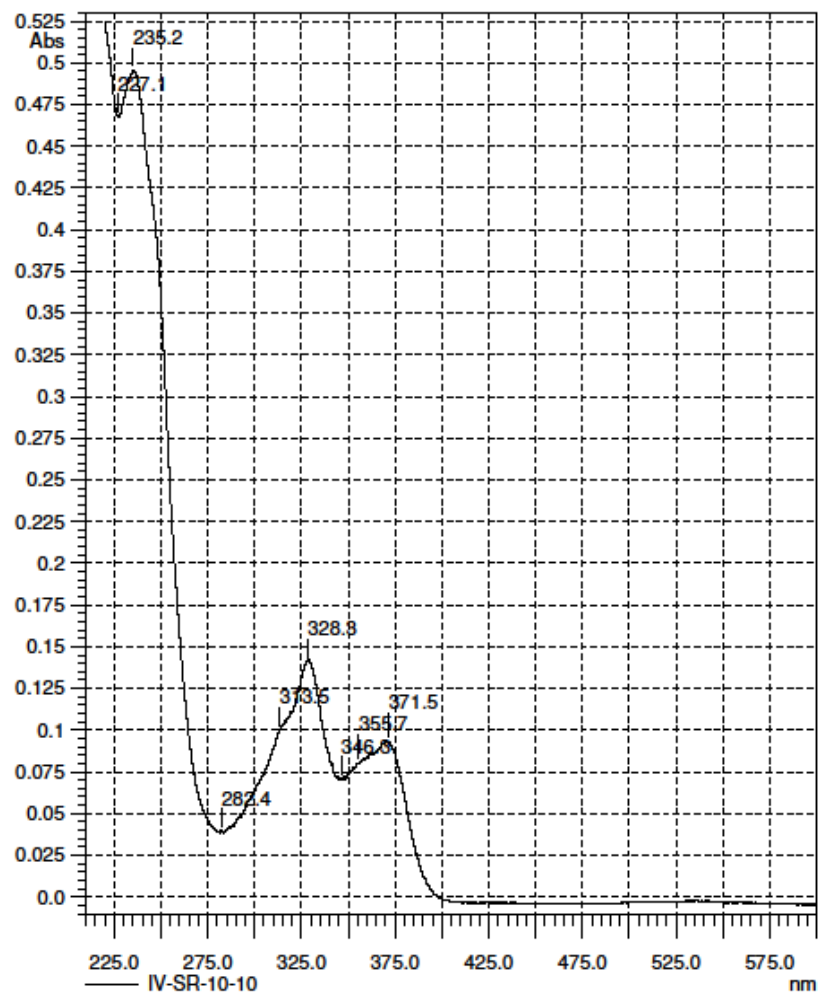


Figure S54. UV spectrum of 16.

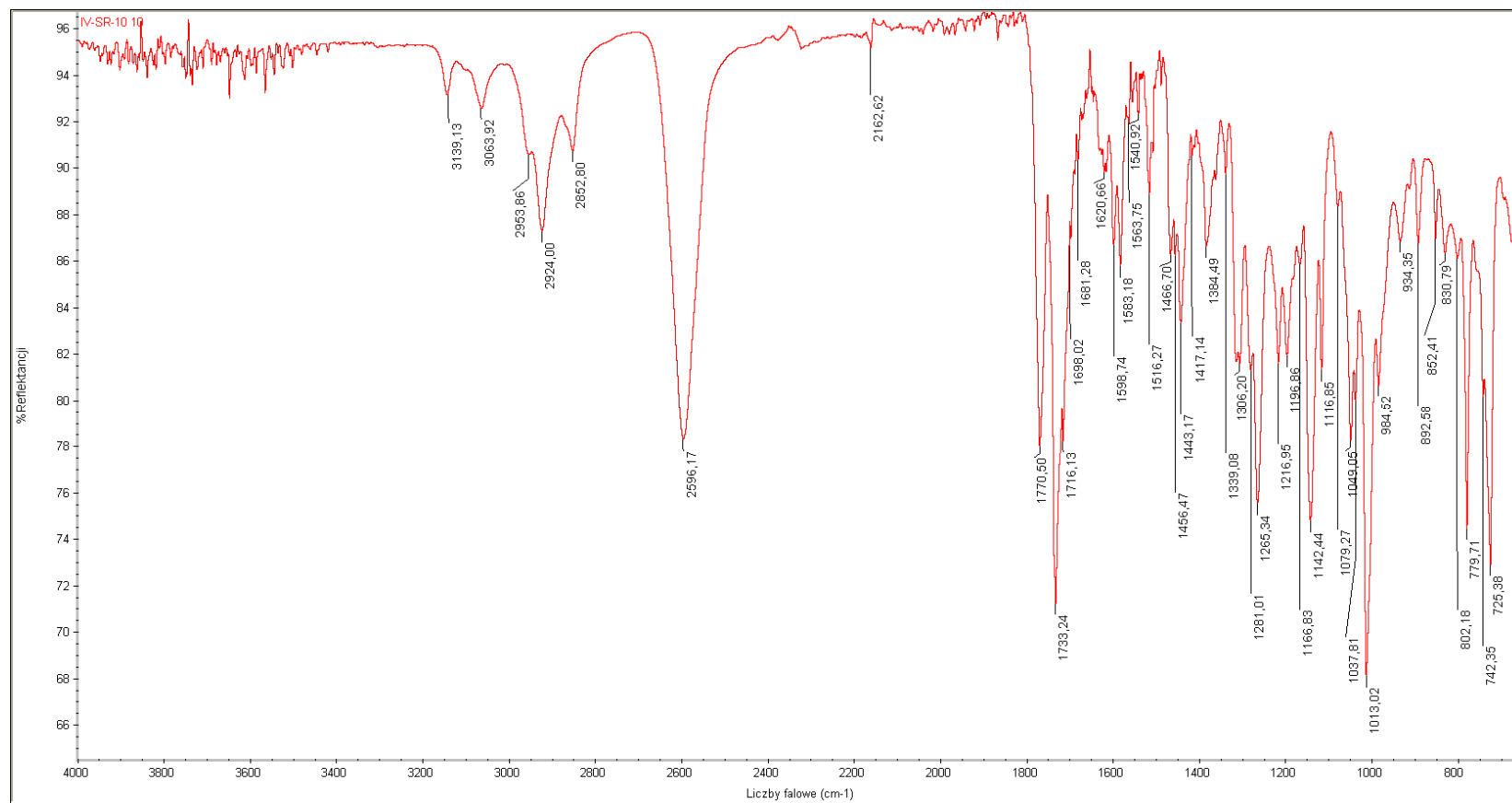
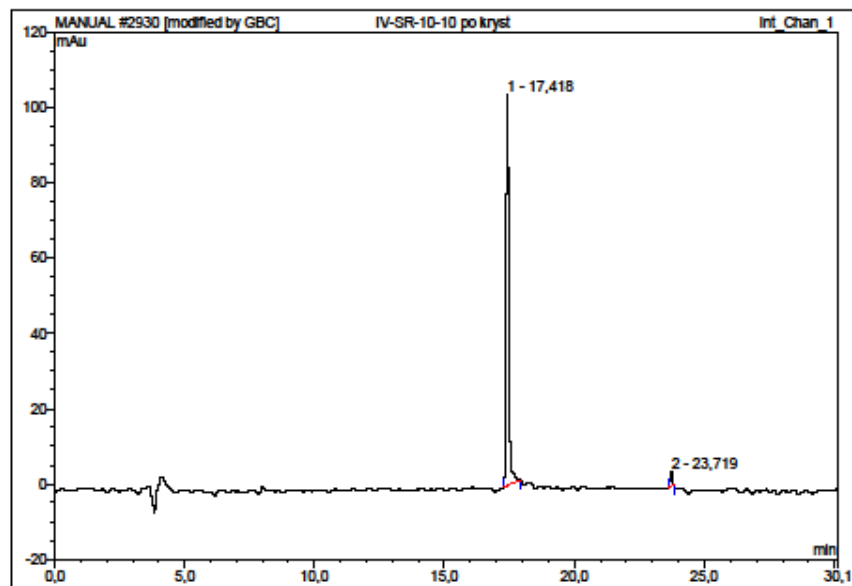


Figure S55. IR spectrum of 16.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	17,42	n.a.	103,998	11,152	96,15	n.a.	BMB
2	23,72	n.a.	4,200	0,446	3,85	n.a.	BMB*
Total:			108,198	11,598	100,00	0,000	

Figure S56. HPLC analysis of 16.

Spectrum Name: IV-SR-10_10
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

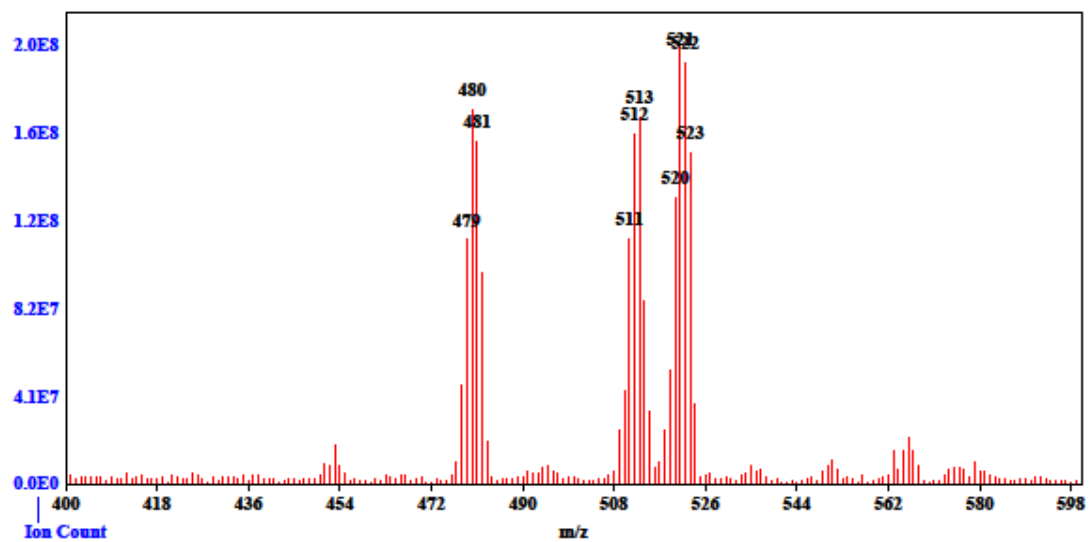


Figure S57. MS spectrum of 16.

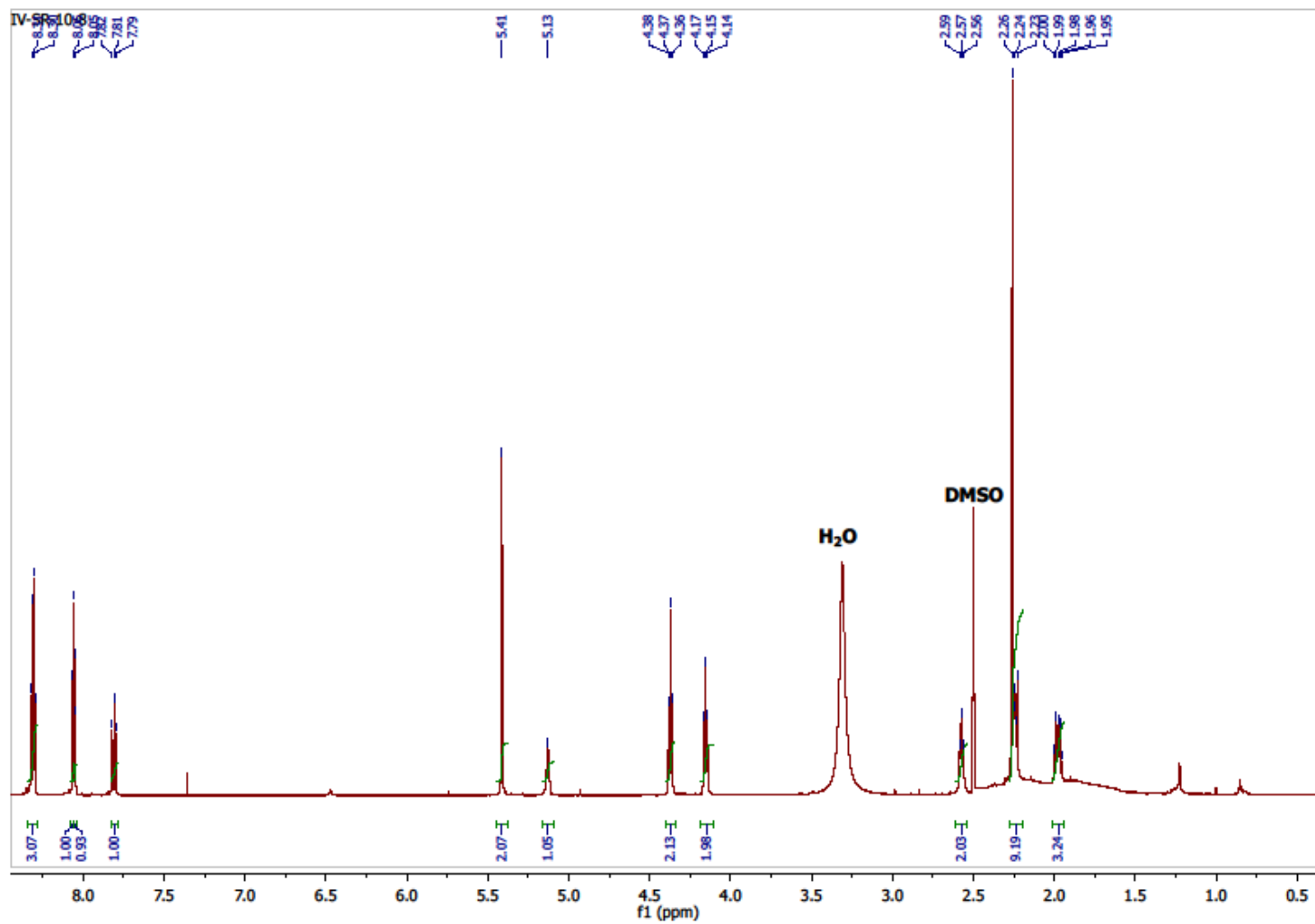


Figure S58. ^1H NMR spectrum of 17.

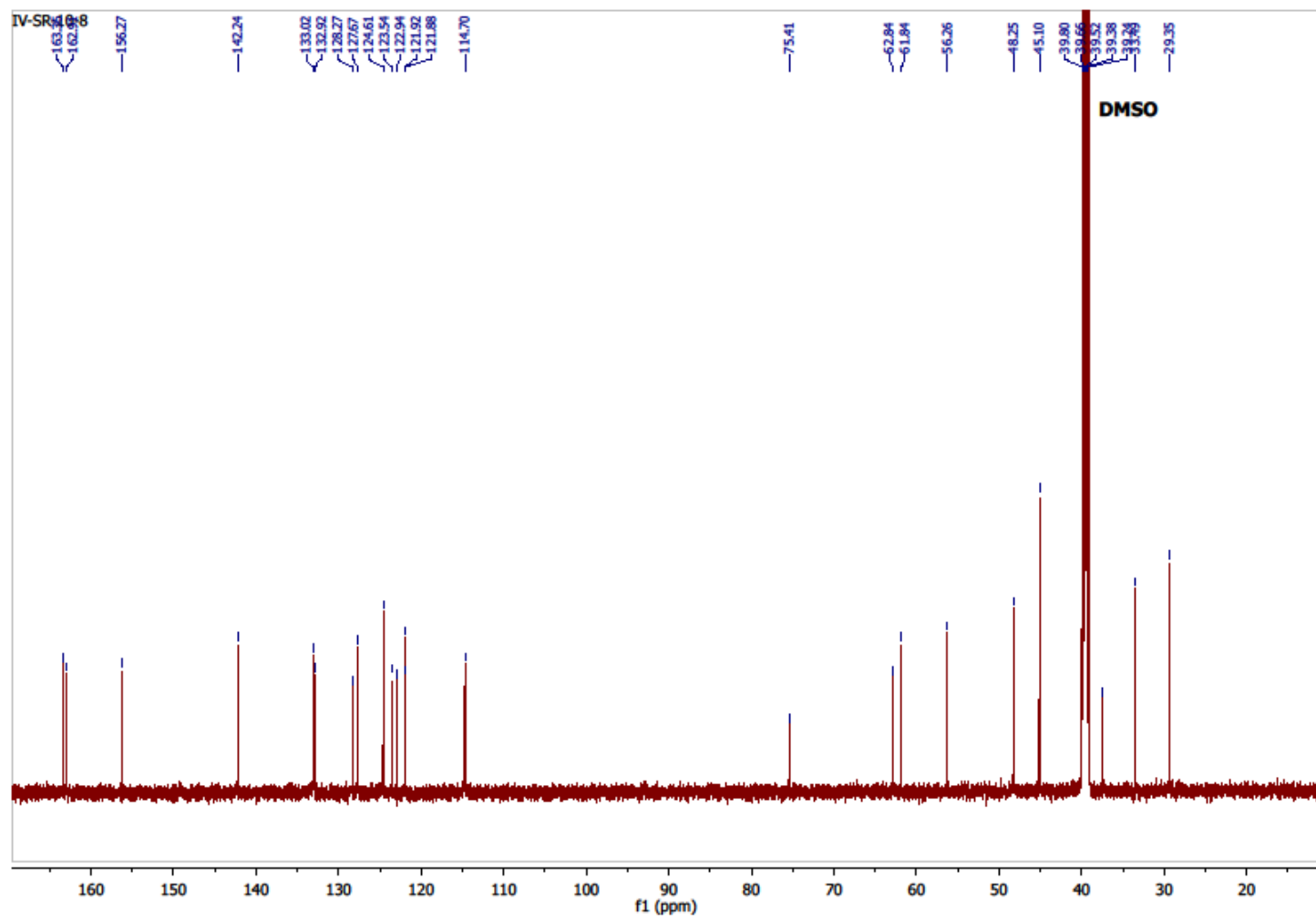


Figure S59. ^{13}C NMR spectrum of 17.

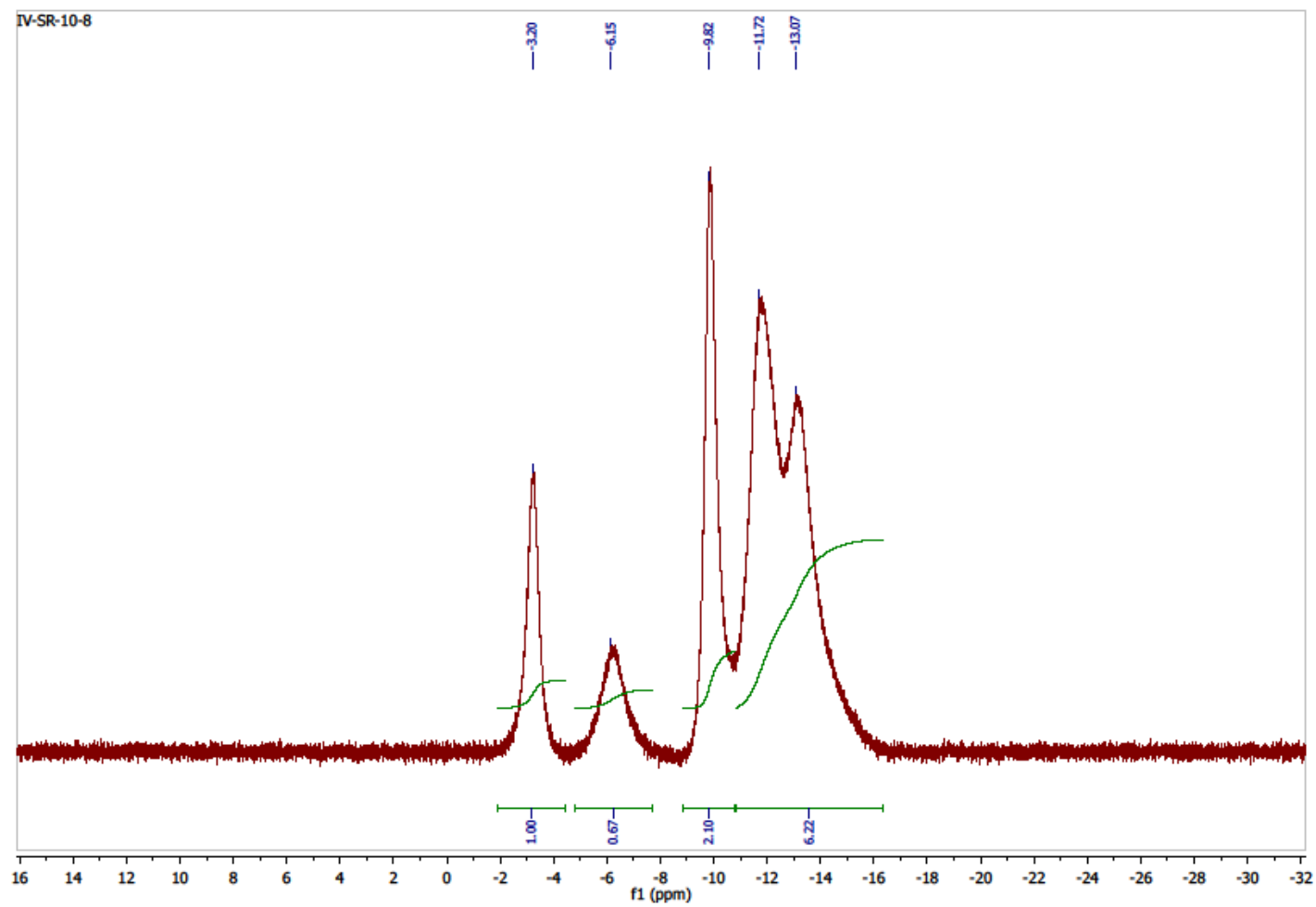


Figure S60. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 17.

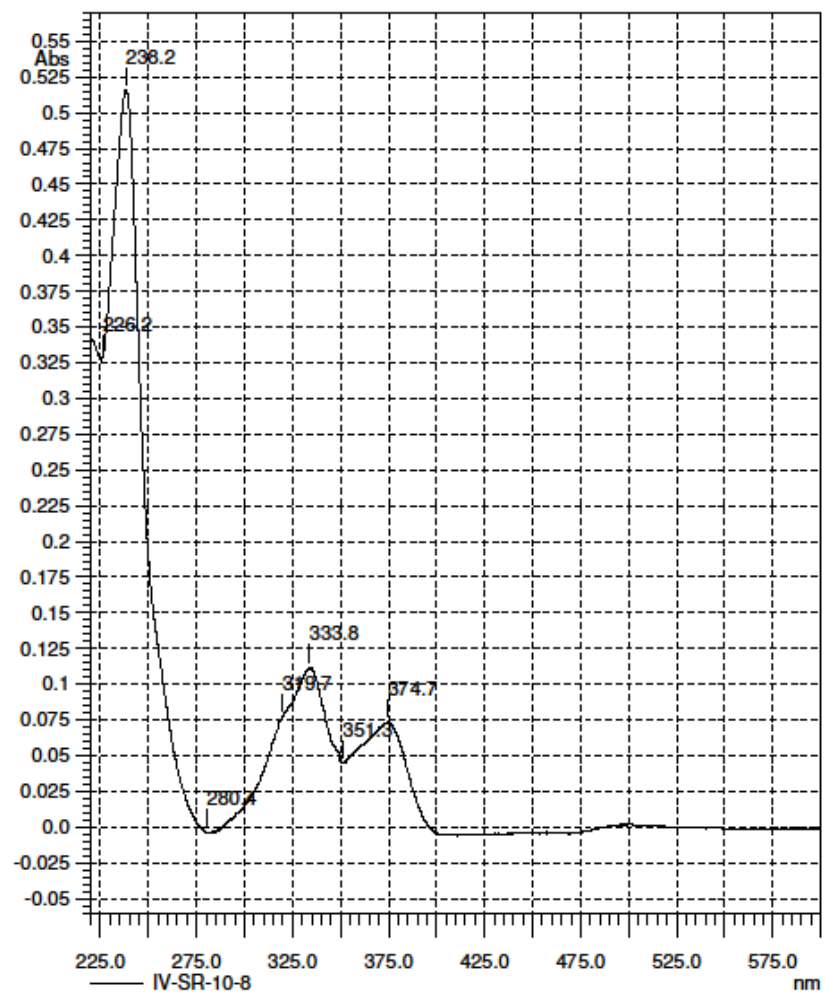


Figure S61. UV spectrum of 17.

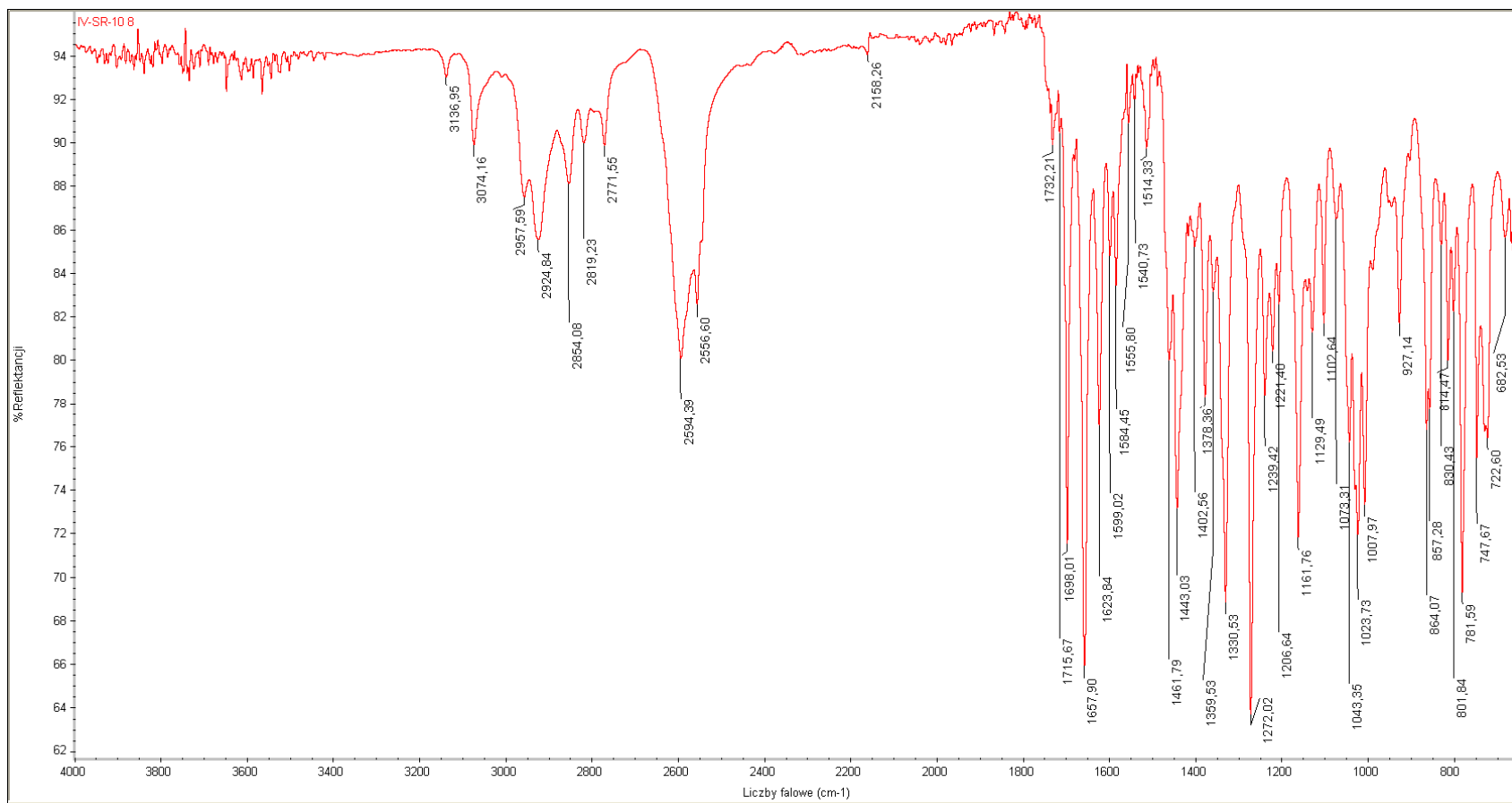


Figure S62. IR spectrum of 17.

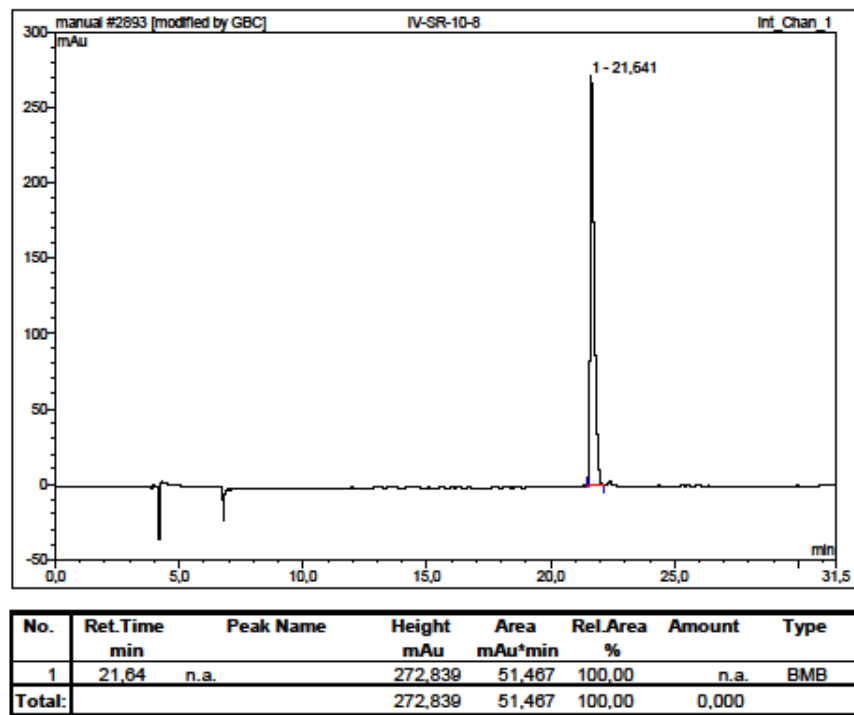


Figure S63. HPLC analysis of 17.

Spectrum Name: IV-SR-10_8_PT
Start Ion: 400
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

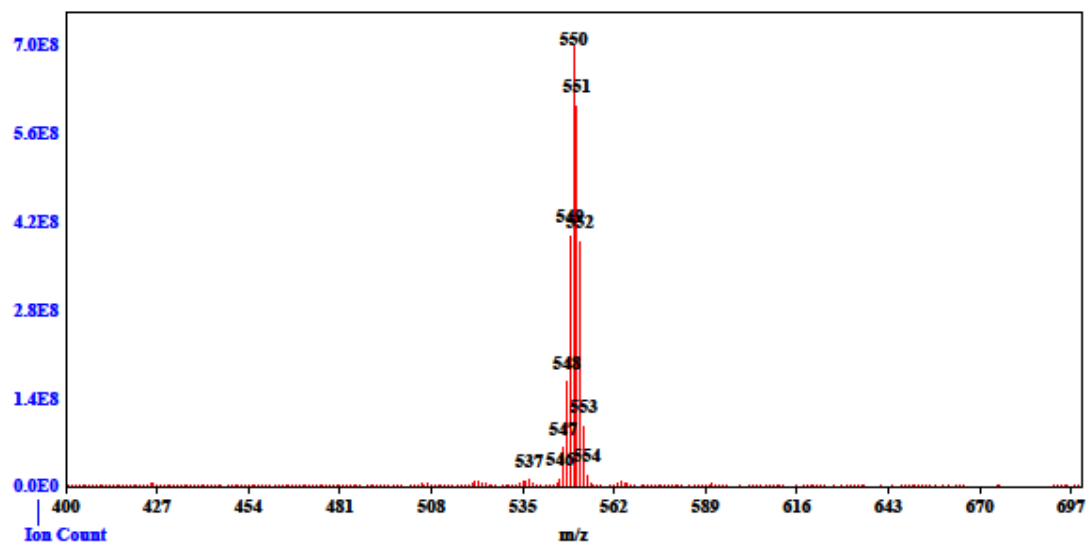


Figure S64. MS spectrum of 17.

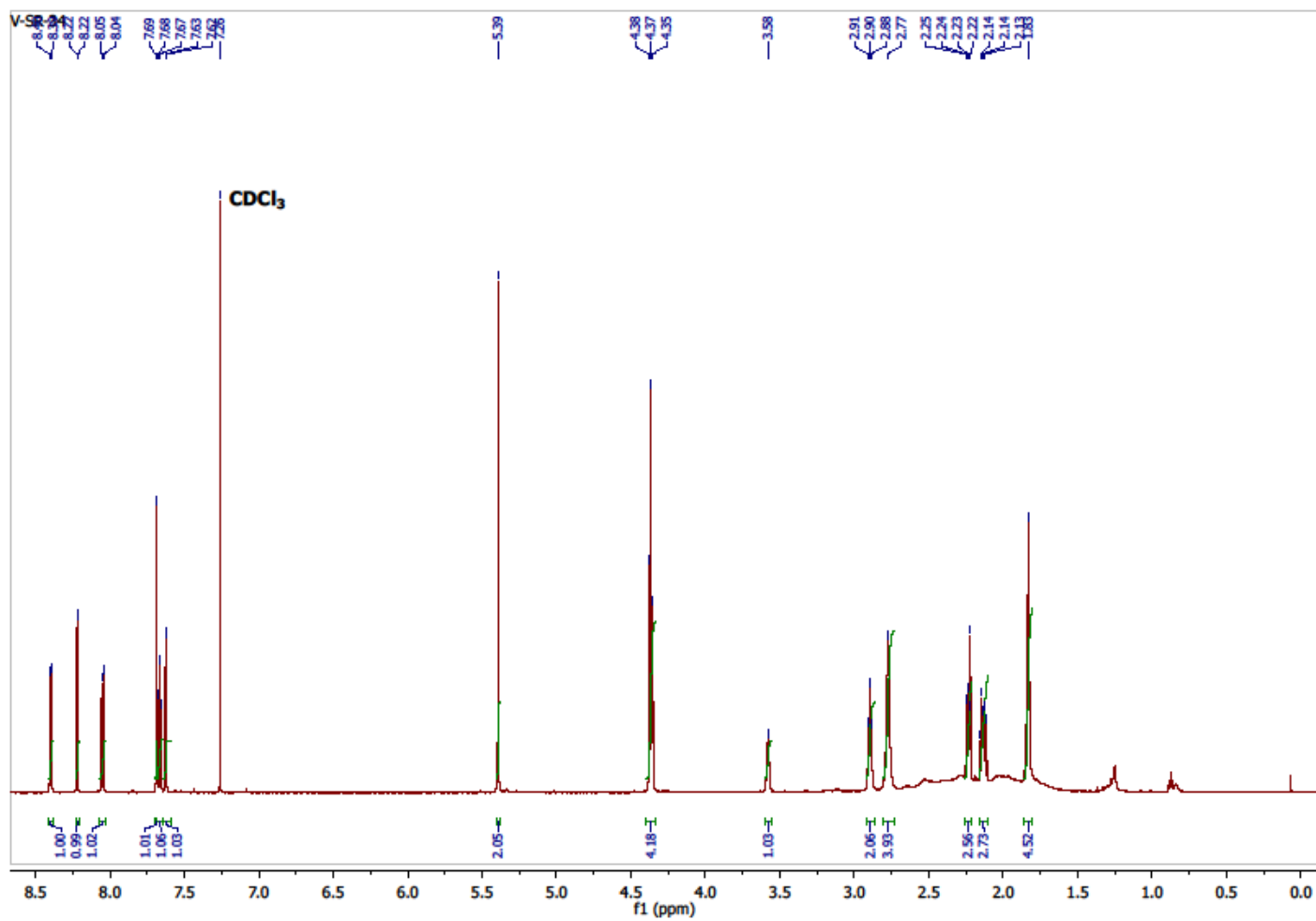


Figure S65. ^1H NMR spectrum of 18.

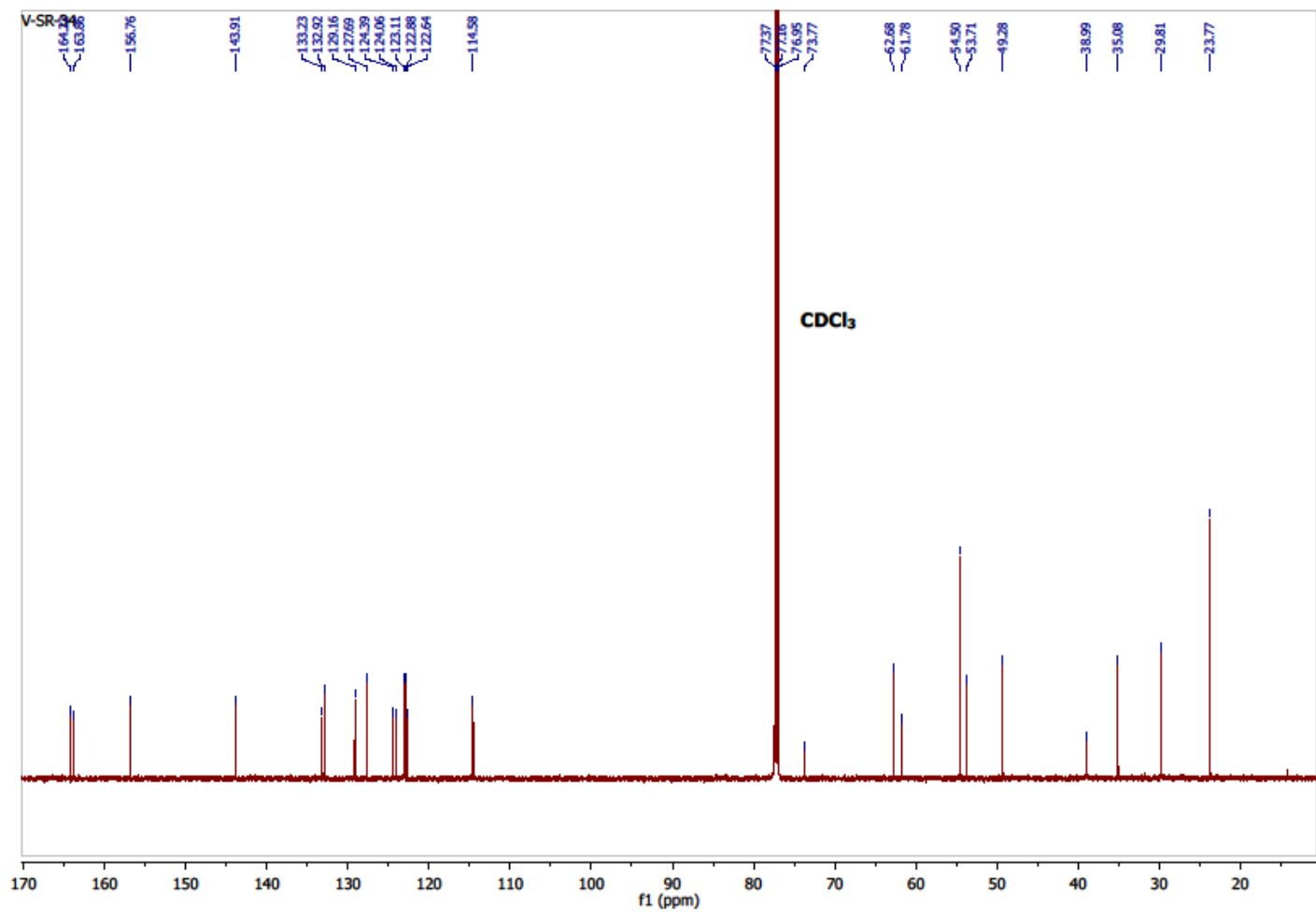


Figure S66. ¹³C NMR spectrum of 18.

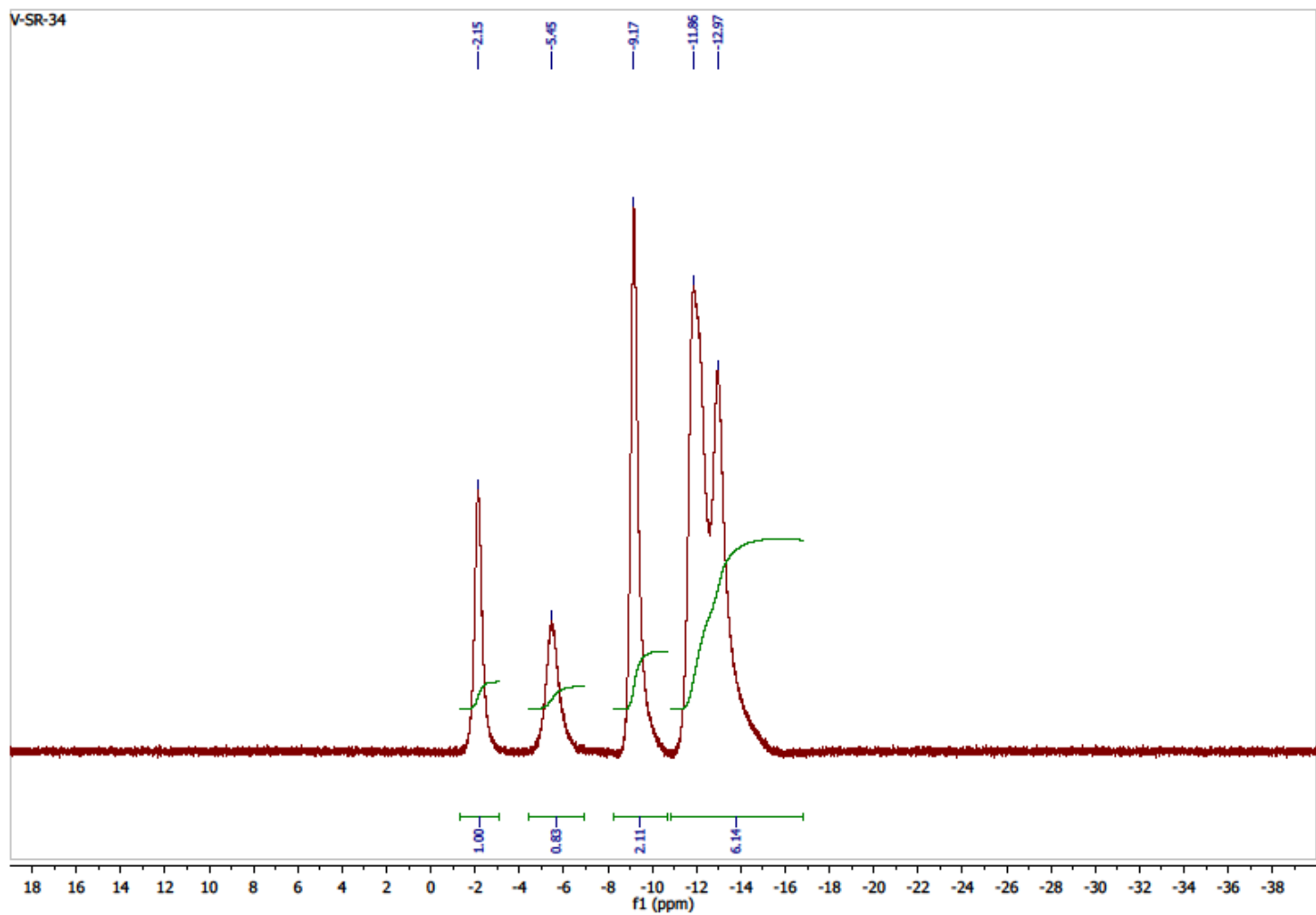


Figure S67. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 18.

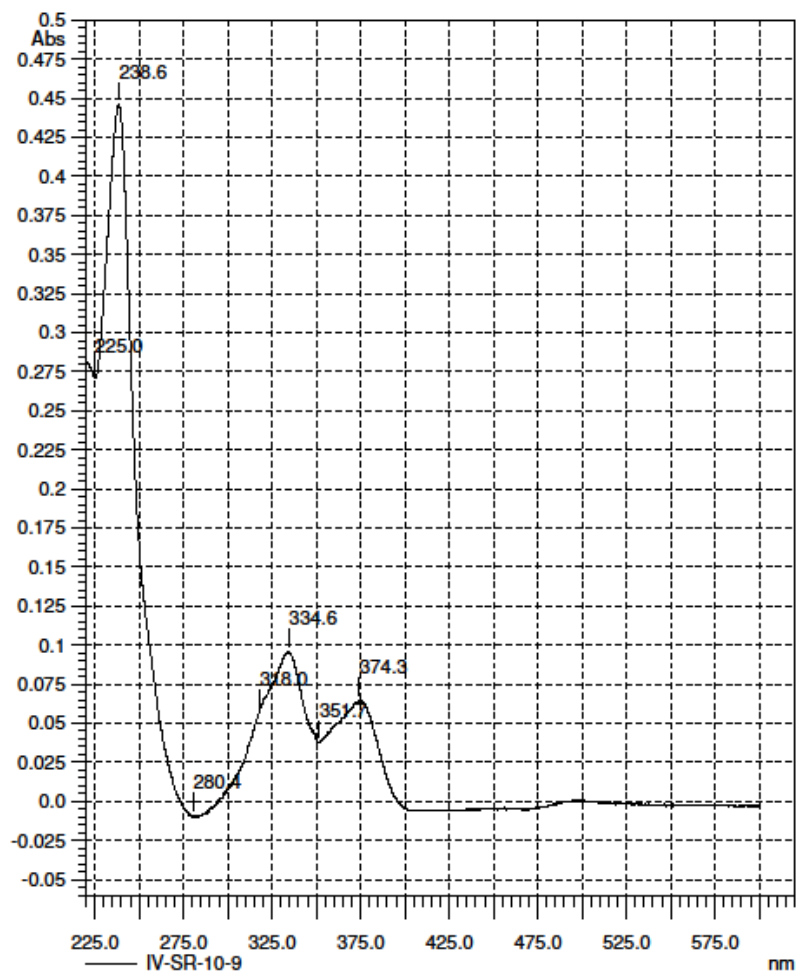


Figure S68. UV spectrum of 18.

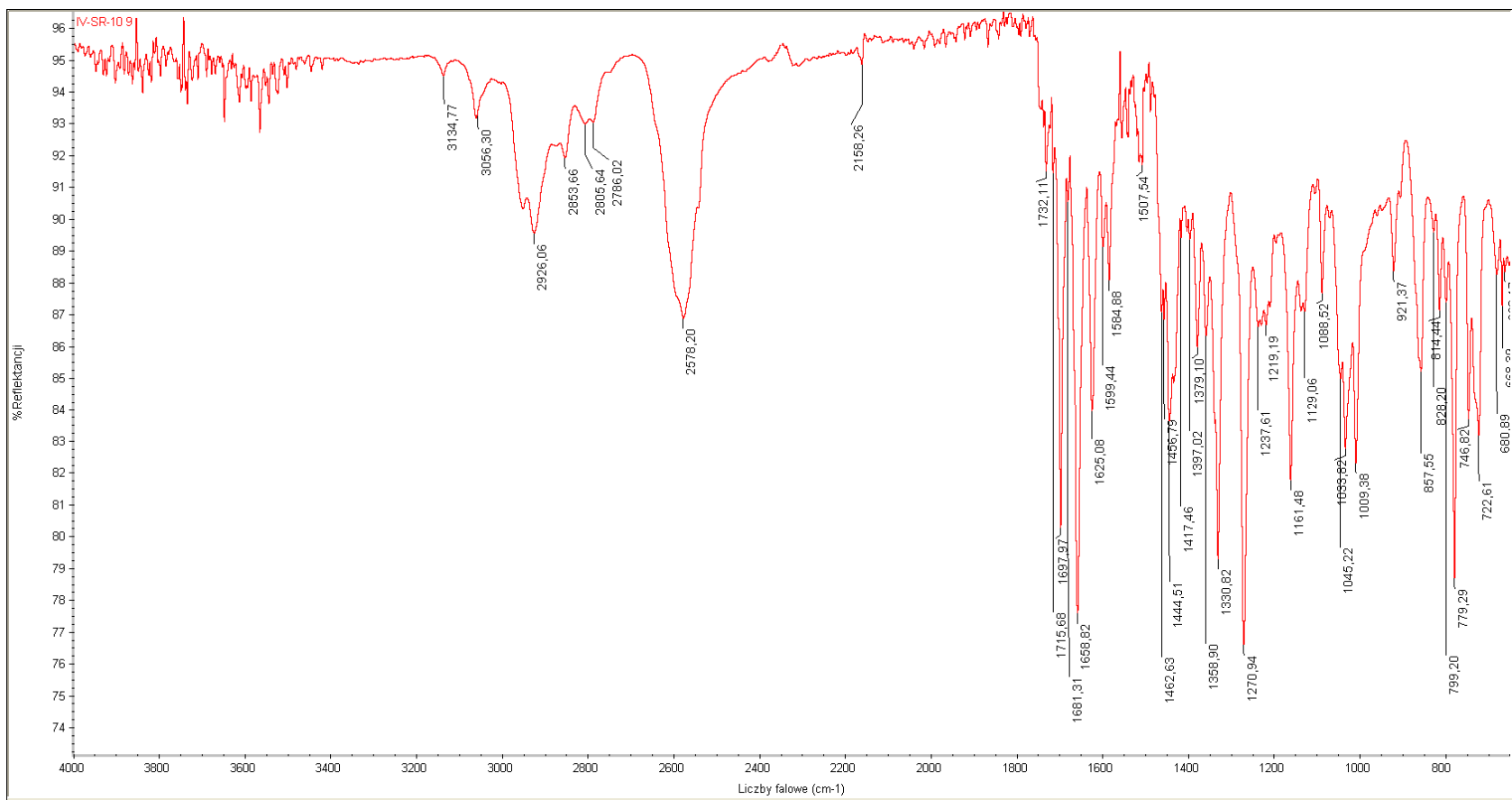
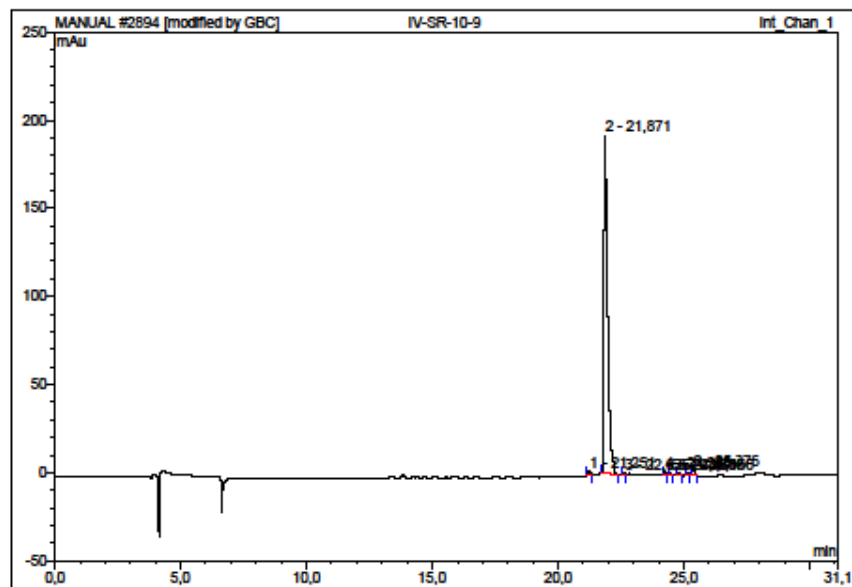


Figure S69. IR spectrum of 18.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	21,25	n.a.	1,985	0,193	0,56	n.a.	BMB*
2	21,87	n.a.	191,502	33,011	96,79	n.a.	BMB
3	22,64	n.a.	0,708	0,071	0,21	n.a.	BMB*
4	24,27	n.a.	1,989	0,186	0,54	n.a.	BMB*
5	24,48	n.a.	0,728	0,065	0,19	n.a.	BMB*
6	24,80	n.a.	1,215	0,127	0,37	n.a.	BMB*
7	25,17	n.a.	0,822	0,078	0,23	n.a.	BMB*
8	25,38	n.a.	2,904	0,375	1,10	n.a.	BMB*
Total:			201,851	34,108	100,00	0,000	

Figure S70. HPLC analysis of 18.

Spectrum Name: IV-SR-10_9_PT
Start Ion: 400
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

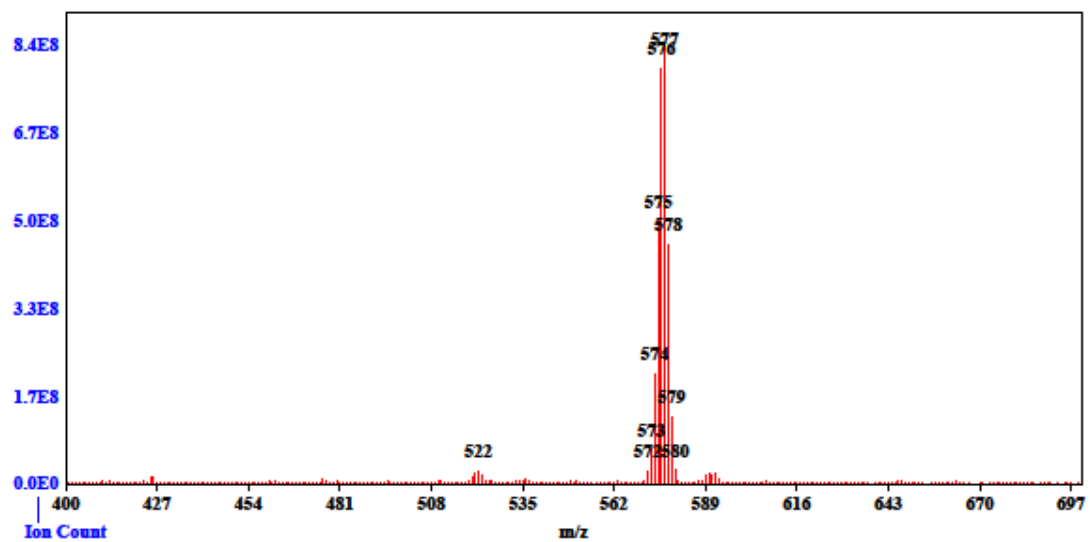


Figure S71. MS spectrum of 18.

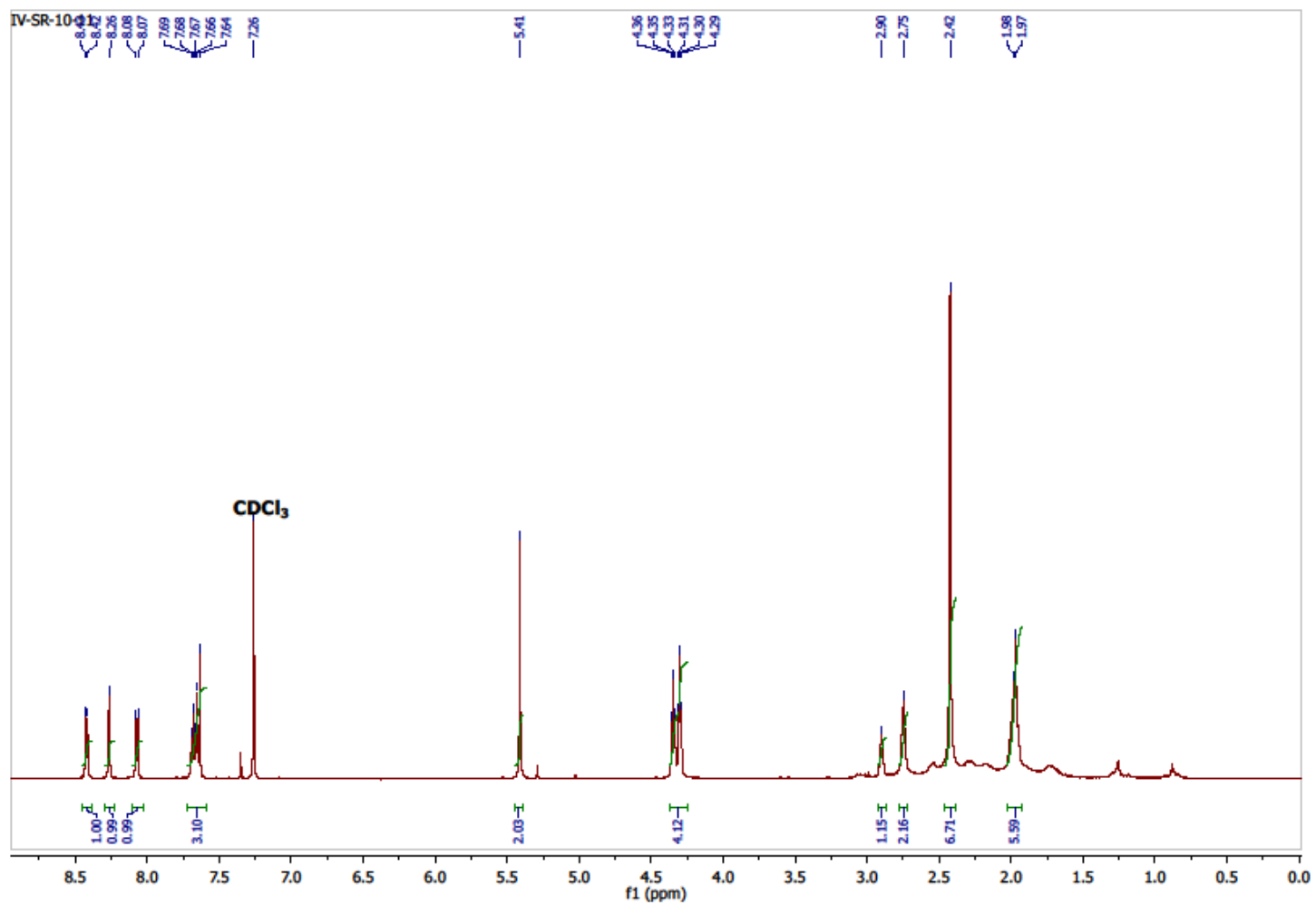


Figure S72. ¹H NMR spectrum of 19.

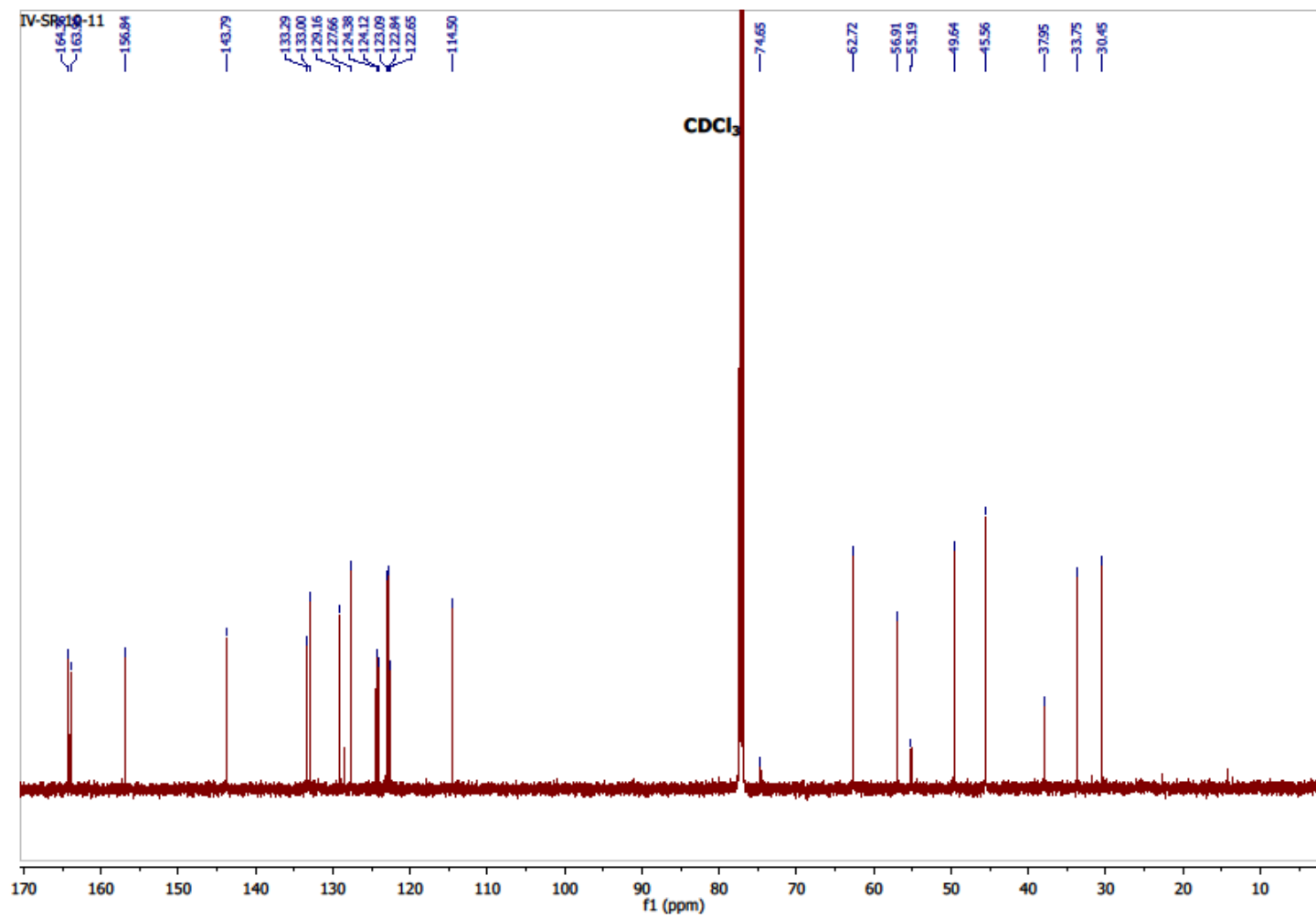


Figure S73. ¹³C NMR spectrum of 19.

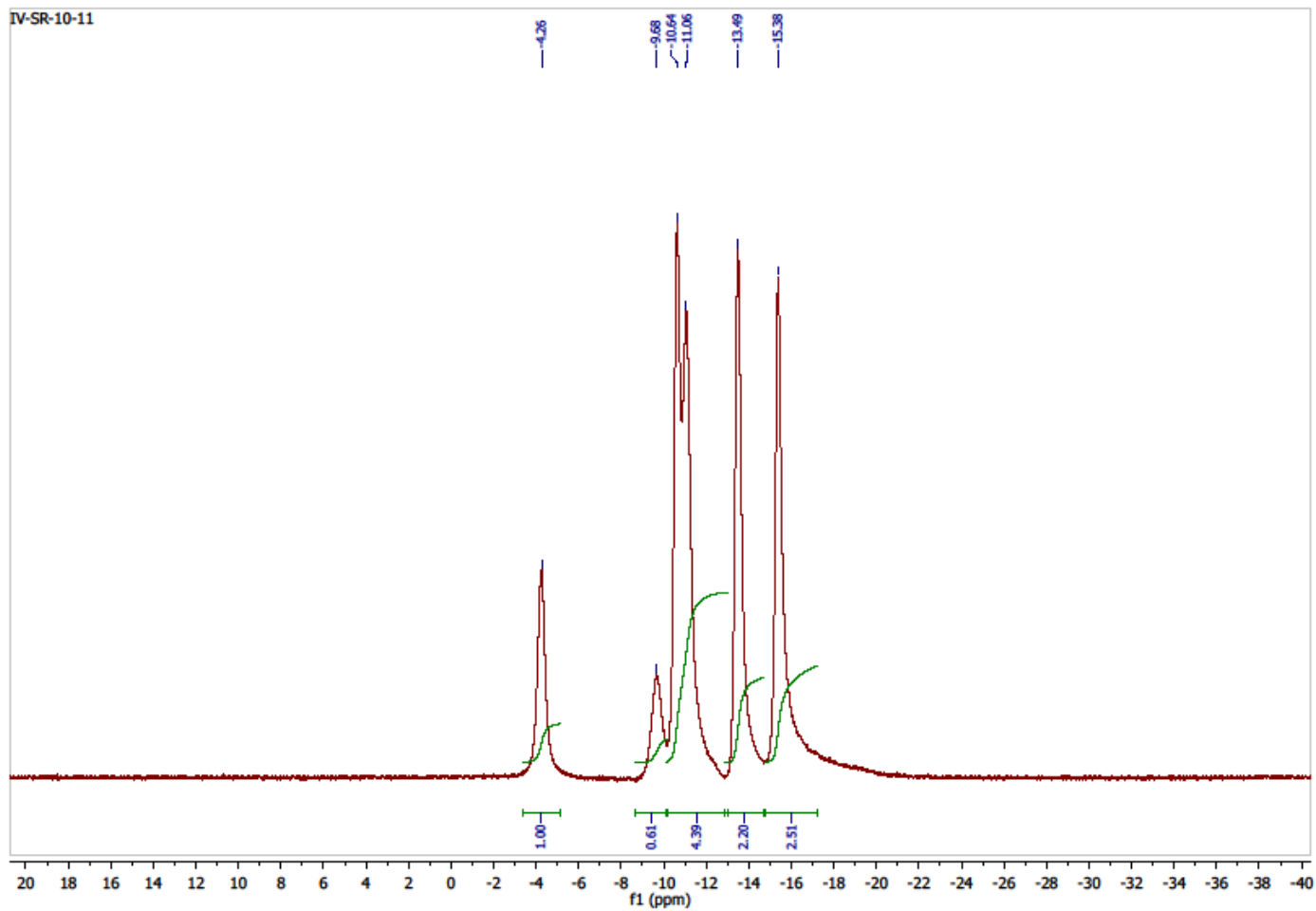


Figure S74. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 19.

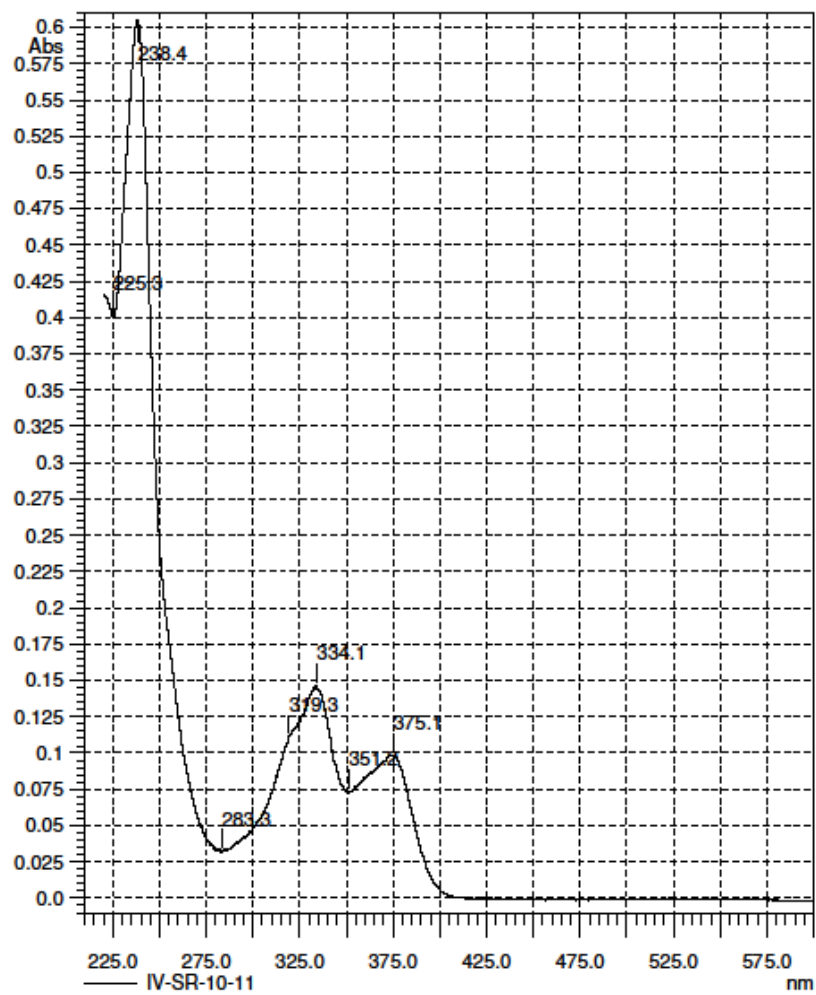


Figure S75. UV spectrum of 19.

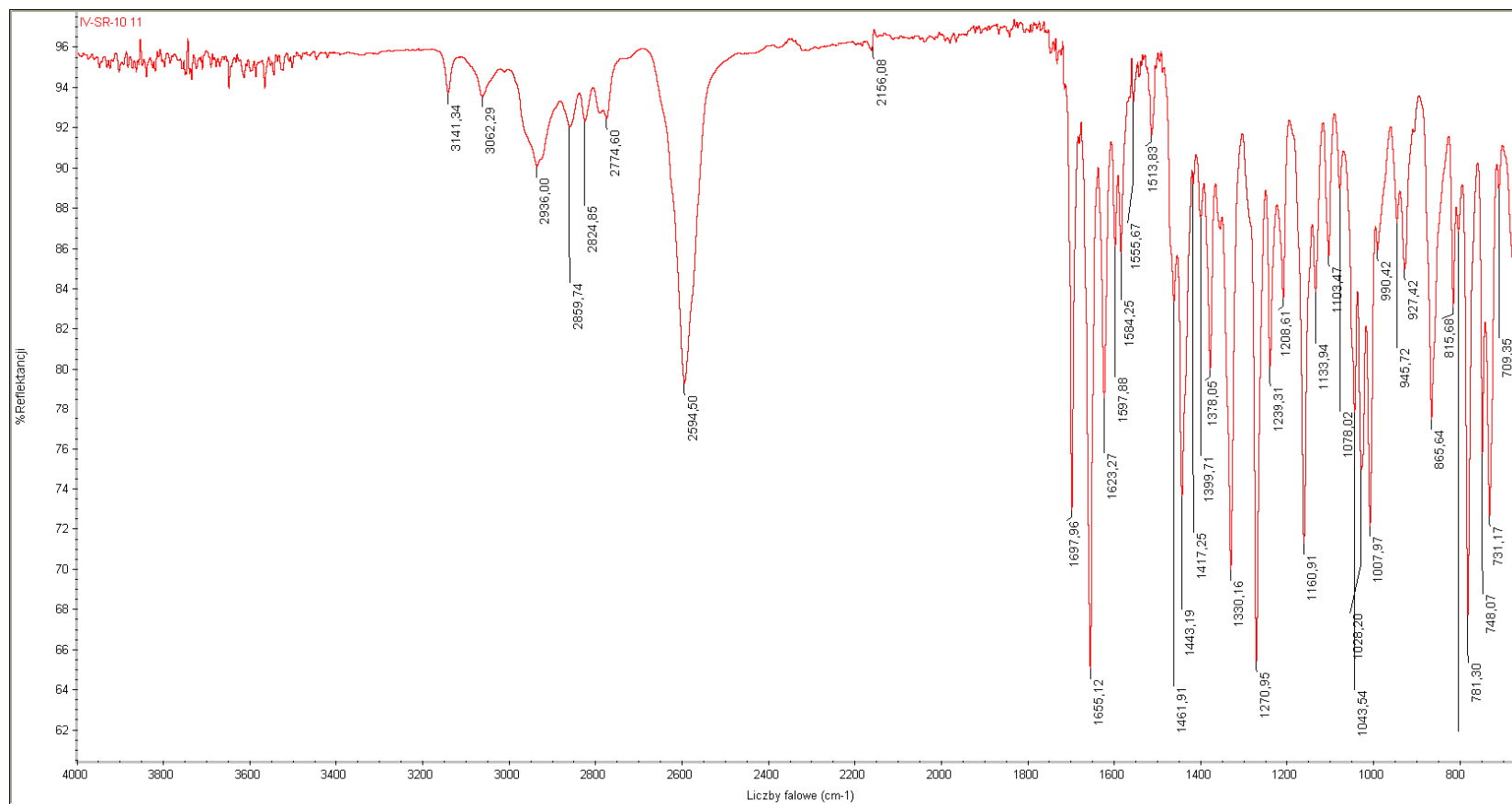
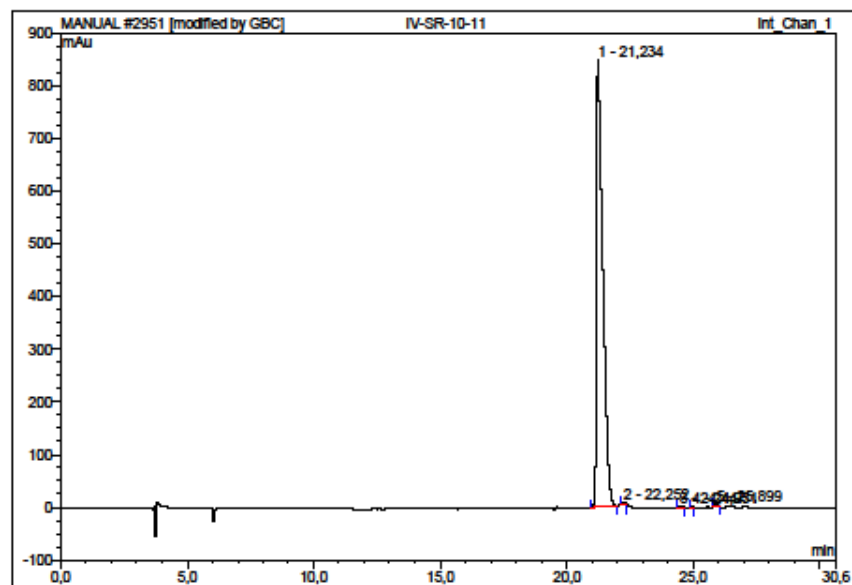


Figure S76. IR spectrum of 19.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	21,23	n.a.	849,952	248,891	99,30	n.a.	BMB
2	22,25	n.a.	4,583	0,672	0,27	n.a.	BM *
3	24,45	n.a.	1,821	0,243	0,10	n.a.	BMB*
4	24,95	n.a.	2,623	0,272	0,11	n.a.	BMB*
5	25,90	n.a.	4,032	0,565	0,23	n.a.	BMB*
Total:			863,010	250,642	100,00	0,000	

Figure S77. HPLC analysis of 19.

Spectrum Name: IV-SR-10_11_PT
Start Ion: 400
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

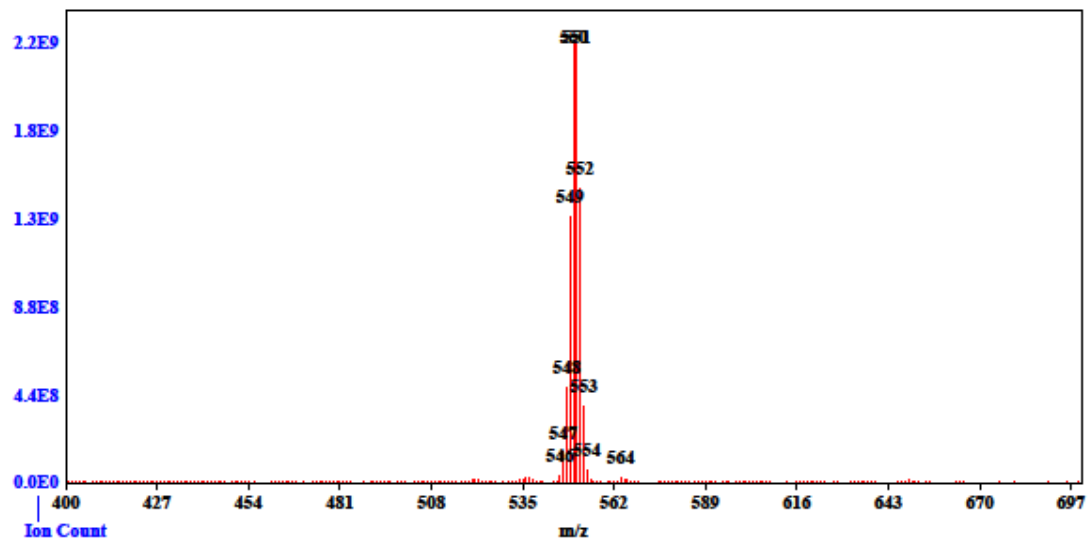


Figure S78. MS spectrum of 19.

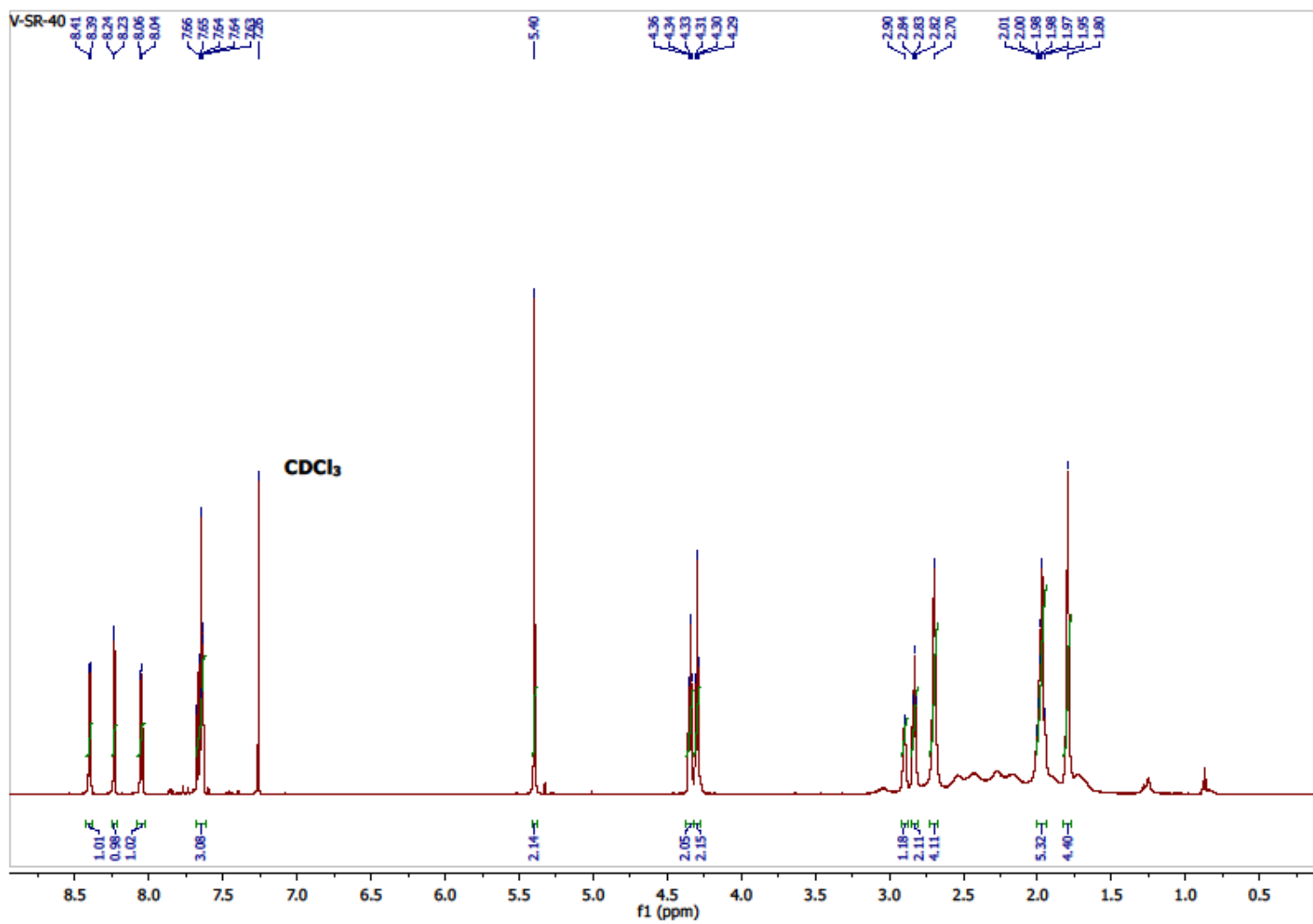


Figure S79. ¹H NMR spectrum of 20.

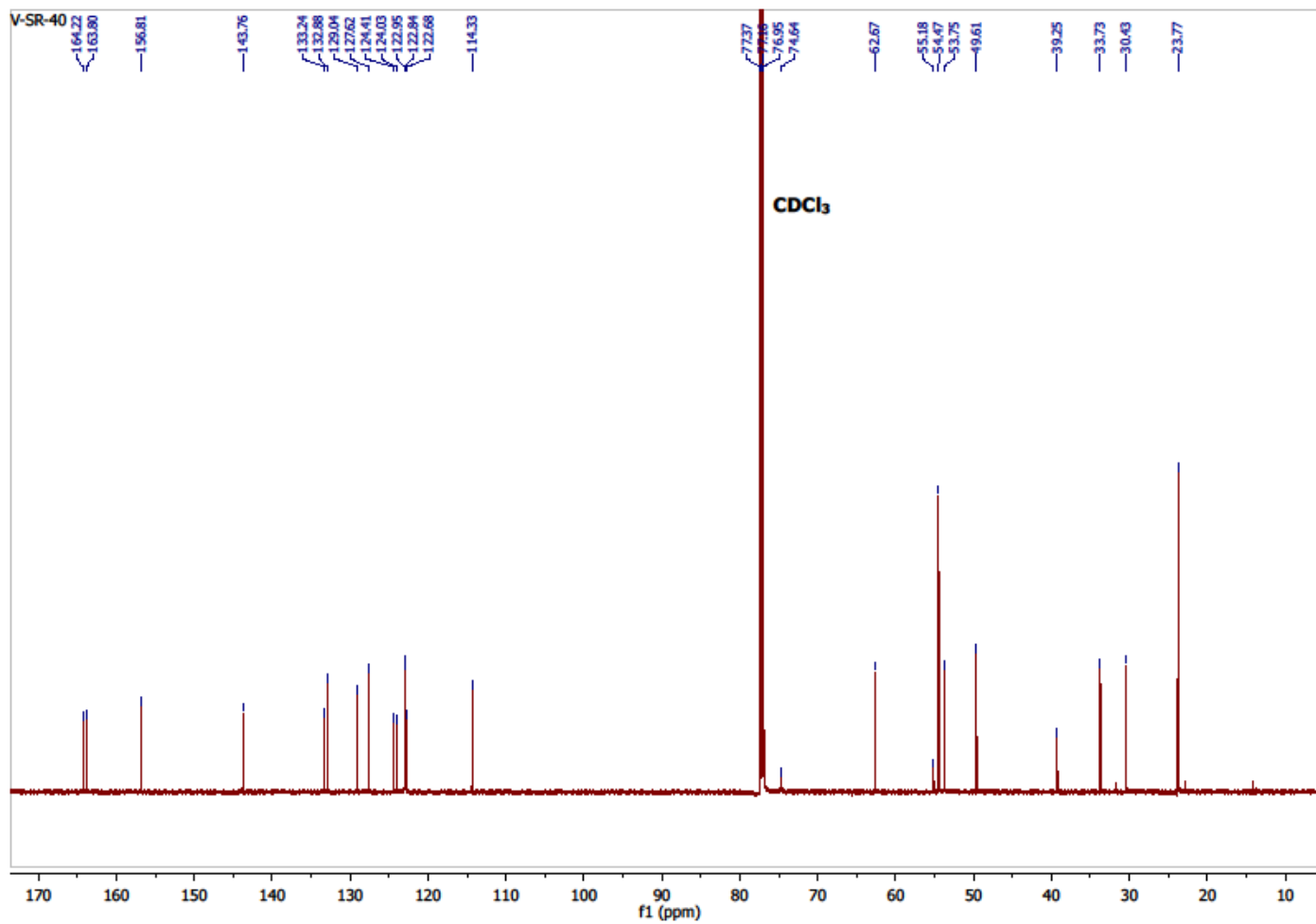


Figure S80. ¹³C NMR spectrum of 20.

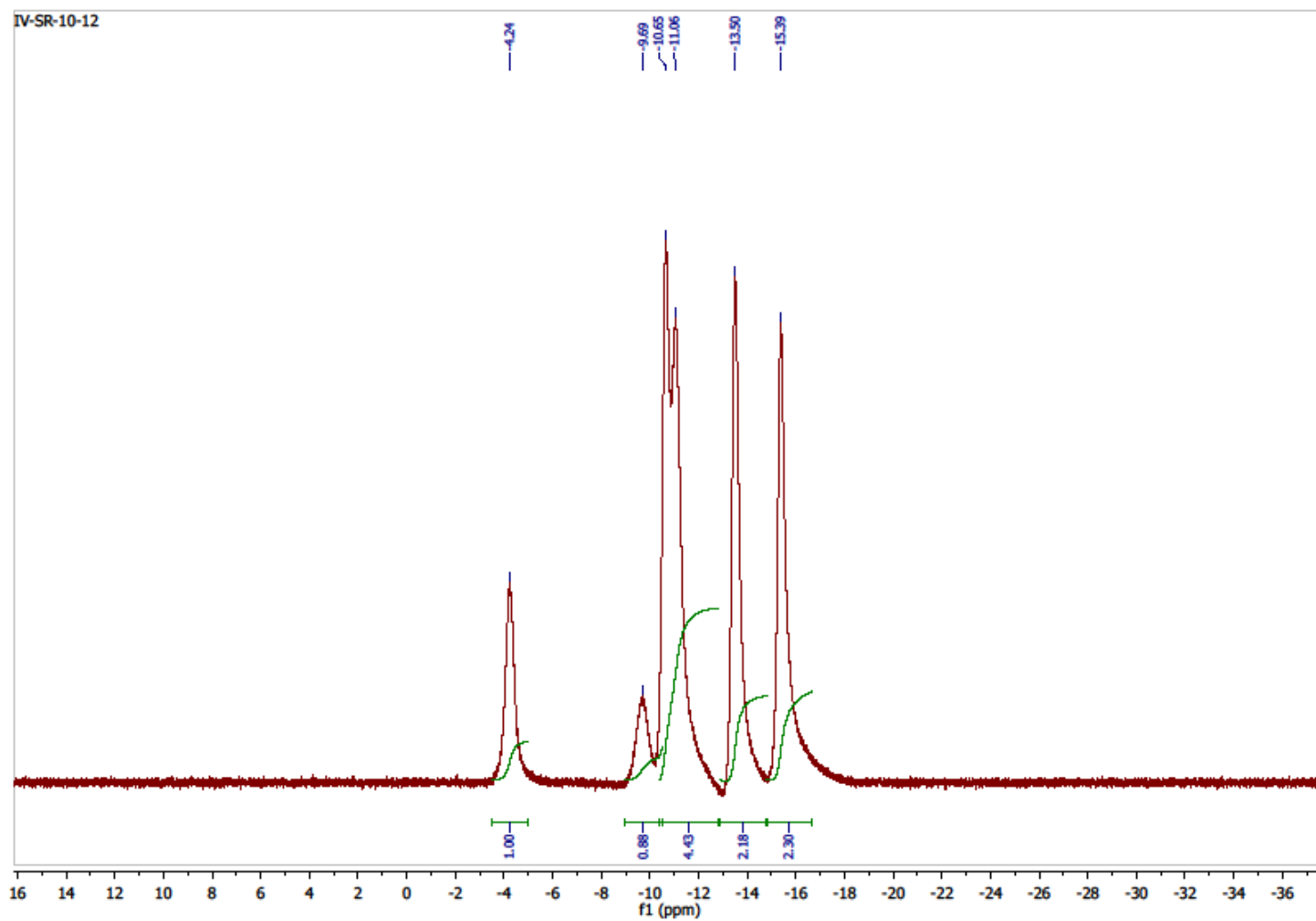


Figure S81. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 20.

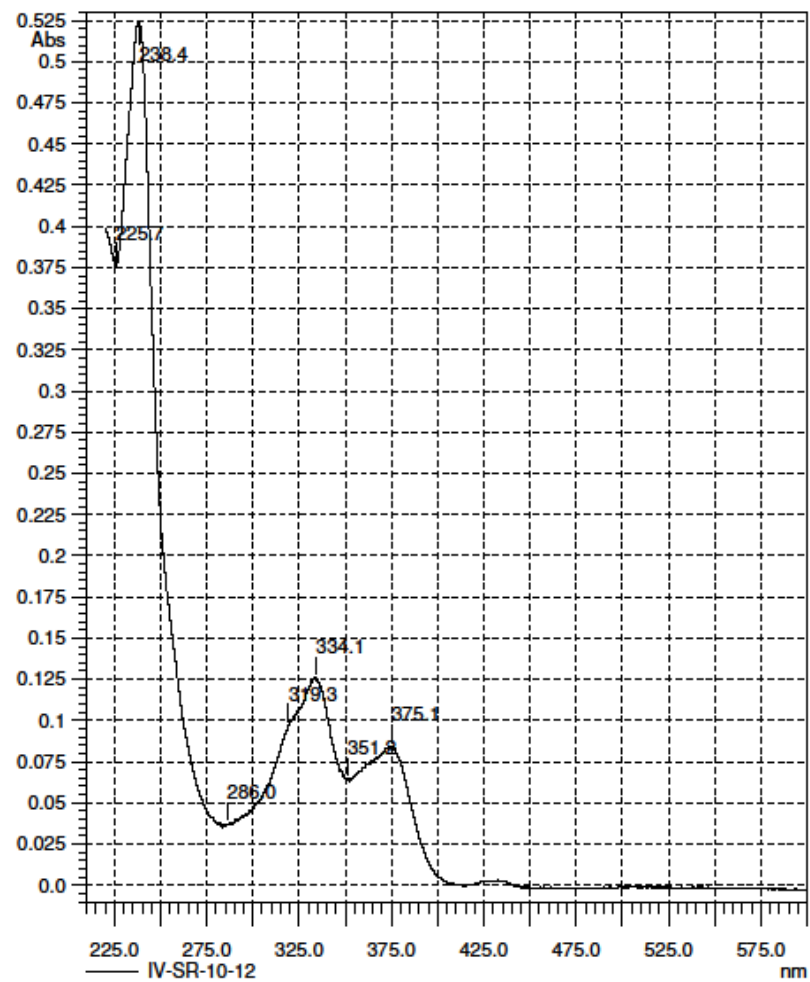


Figure S82. UV spectrum of 20.

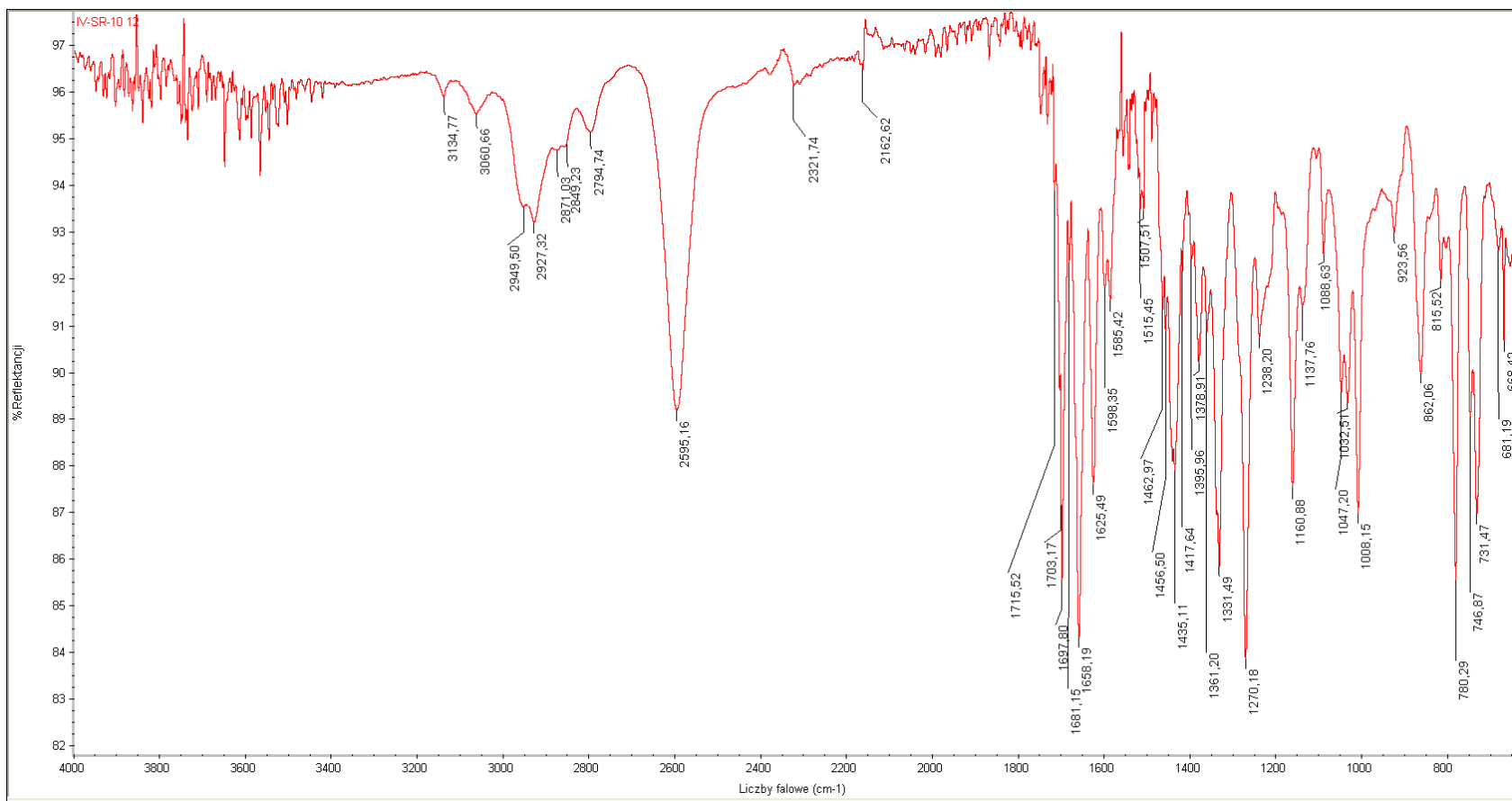
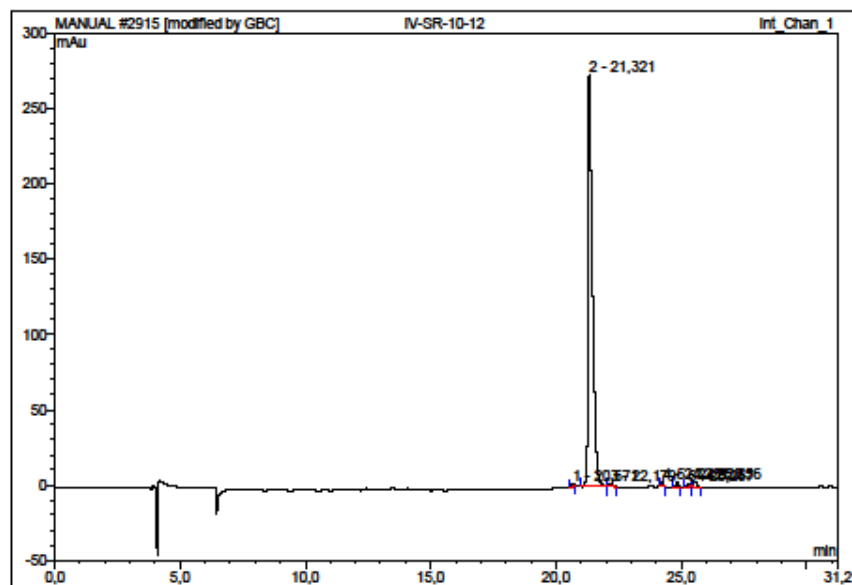


Figure S83. IR spectrum of 20.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	20,67	n.a.	2,378	0,234	0,40	n.a.	BMB*
2	21,32	n.a.	272,962	56,512	96,19	n.a.	BMB*
3	22,18	n.a.	1,980	0,368	0,62	n.a.	BMB*
4	24,25	n.a.	2,976	0,288	0,49	n.a.	BMB*
5	24,82	n.a.	2,954	0,408	0,69	n.a.	BMB*
6	25,27	n.a.	2,065	0,283	0,48	n.a.	BMB*
7	25,56	n.a.	3,923	0,659	1,12	n.a.	bMB*
Total:			289,235	58,748	100,00	0,000	

Figure S84. HPLC analysis of 20.

Spectrum Name: IV-SR-10_12_PT
Start Ion: 500
End Ion: 700
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

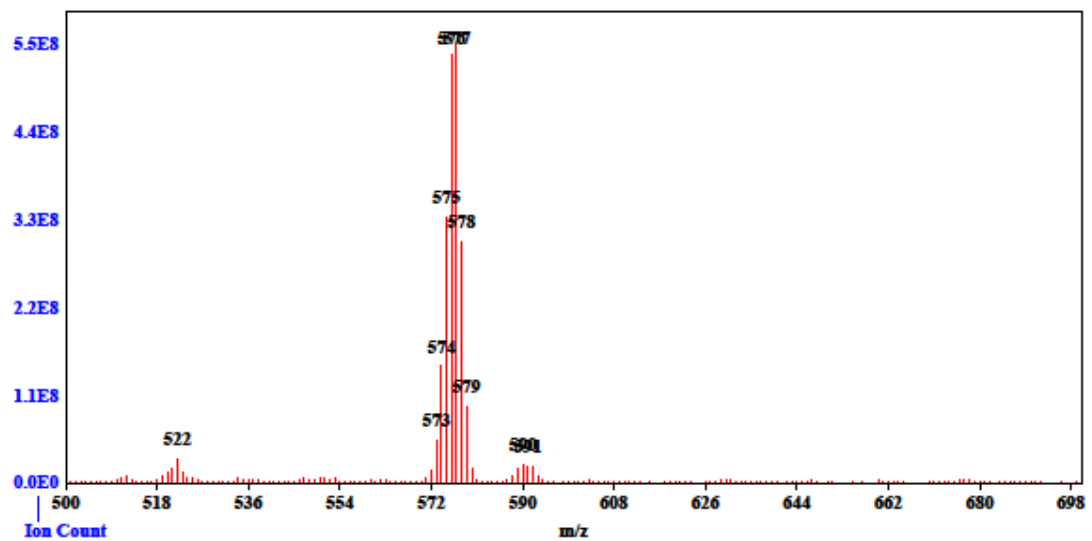


Figure S85. MS spectrum of 20.

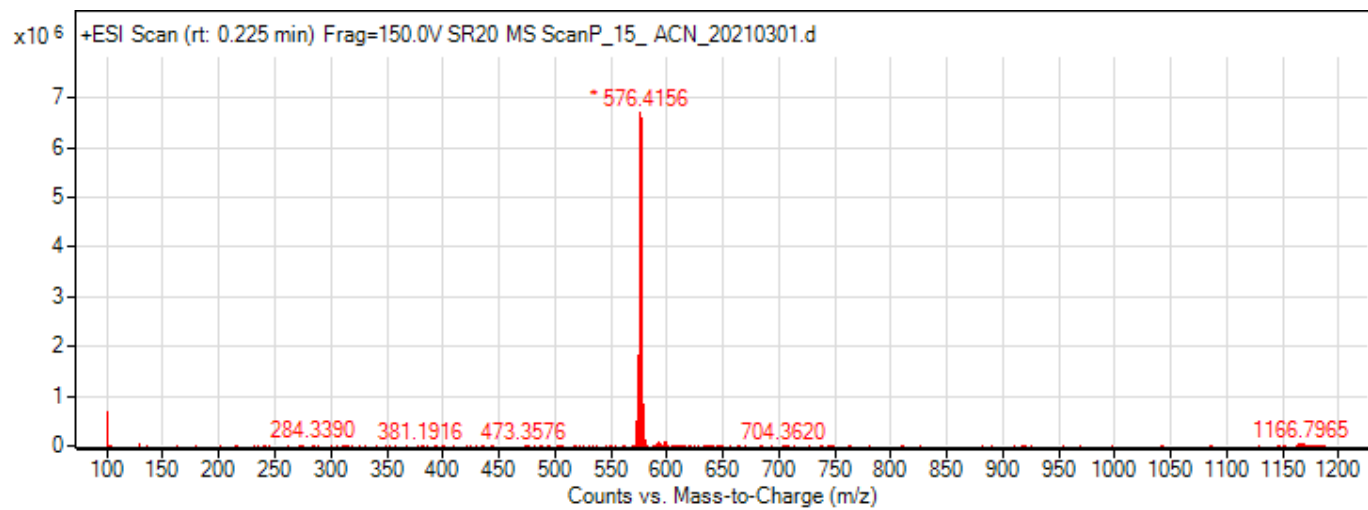


Figure S86. HRMS spectrum of 20.

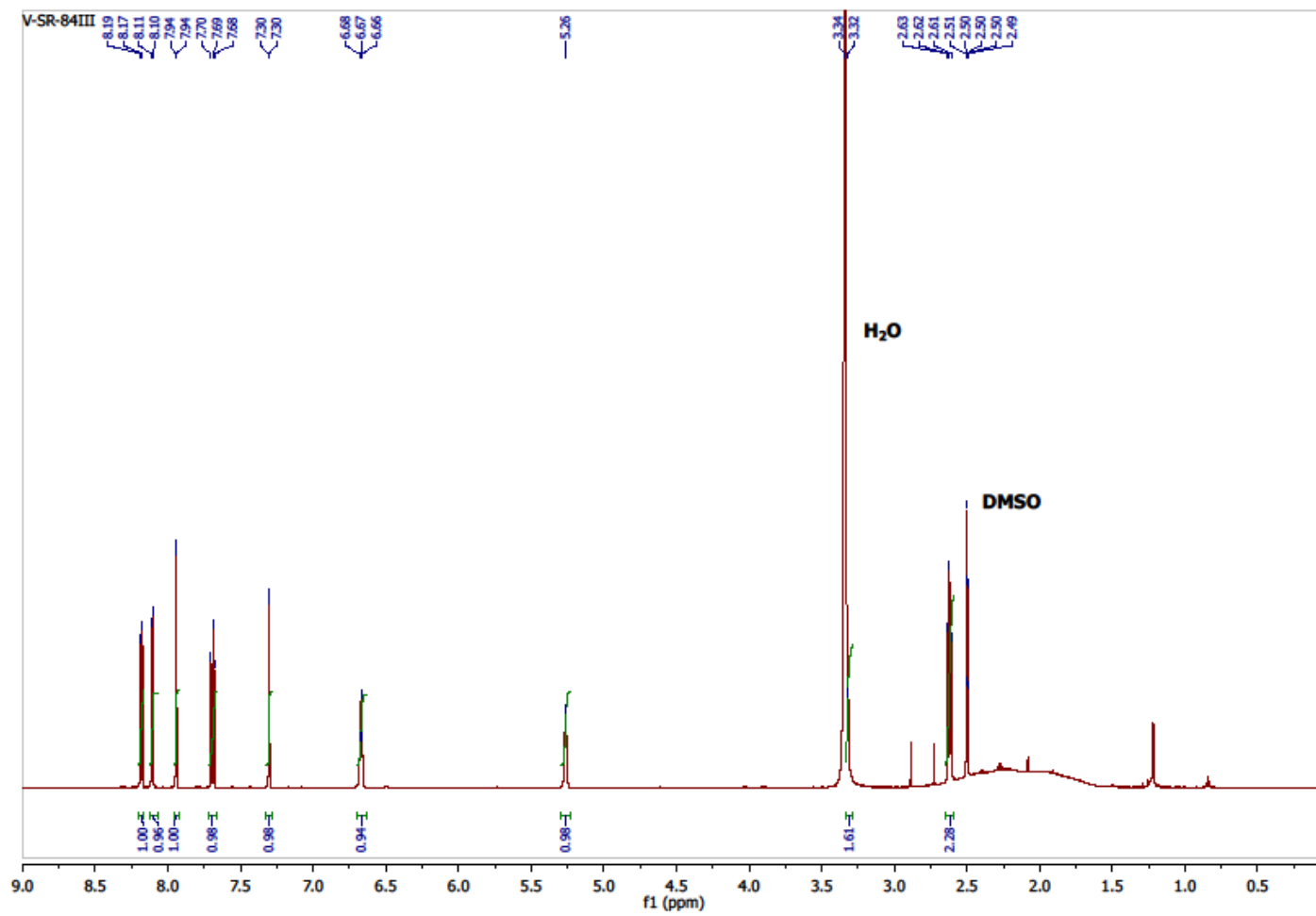


Figure S87. ¹H NMR spectrum of 31.

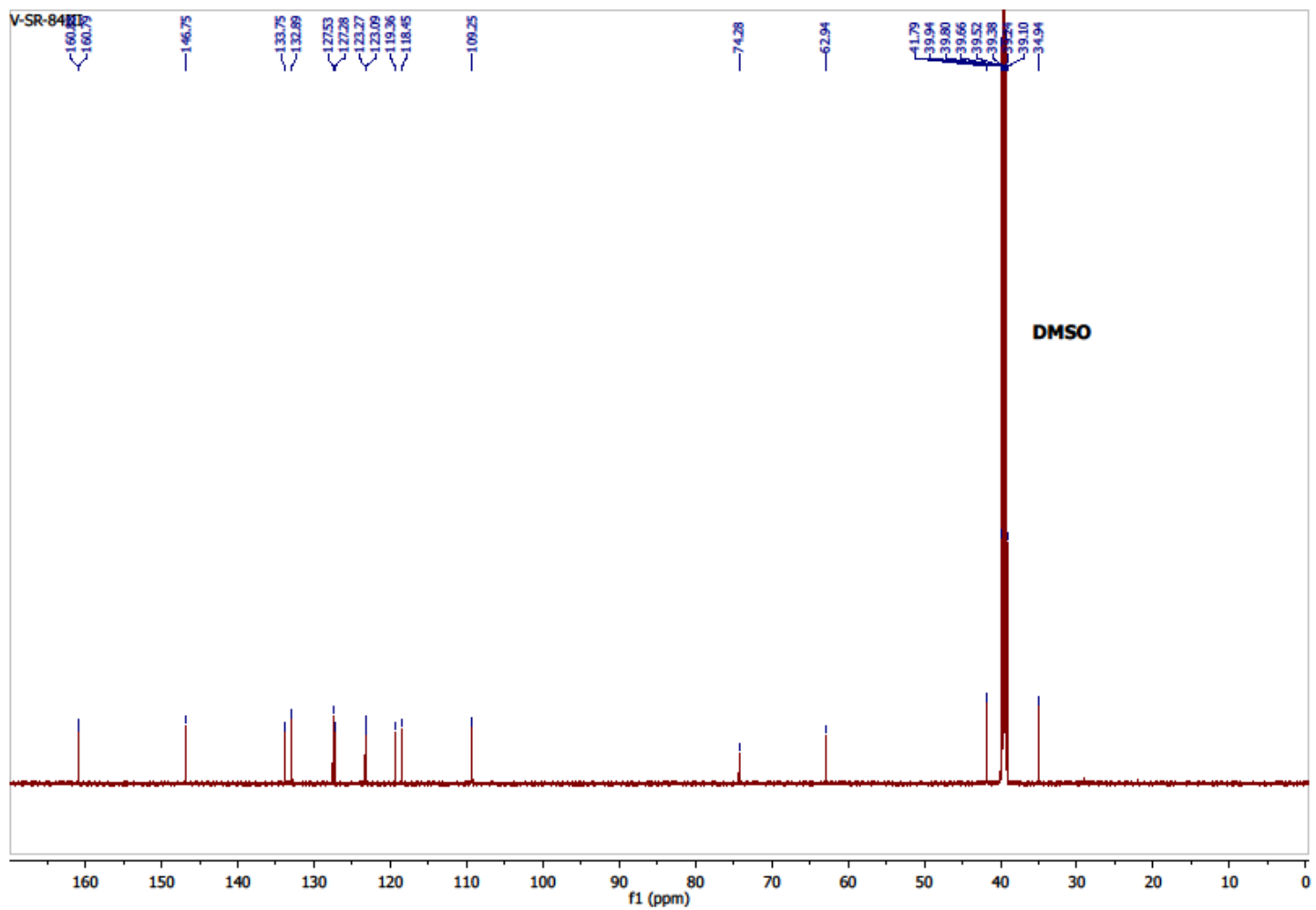


Figure S88. ^{13}C NMR spectrum of 31.

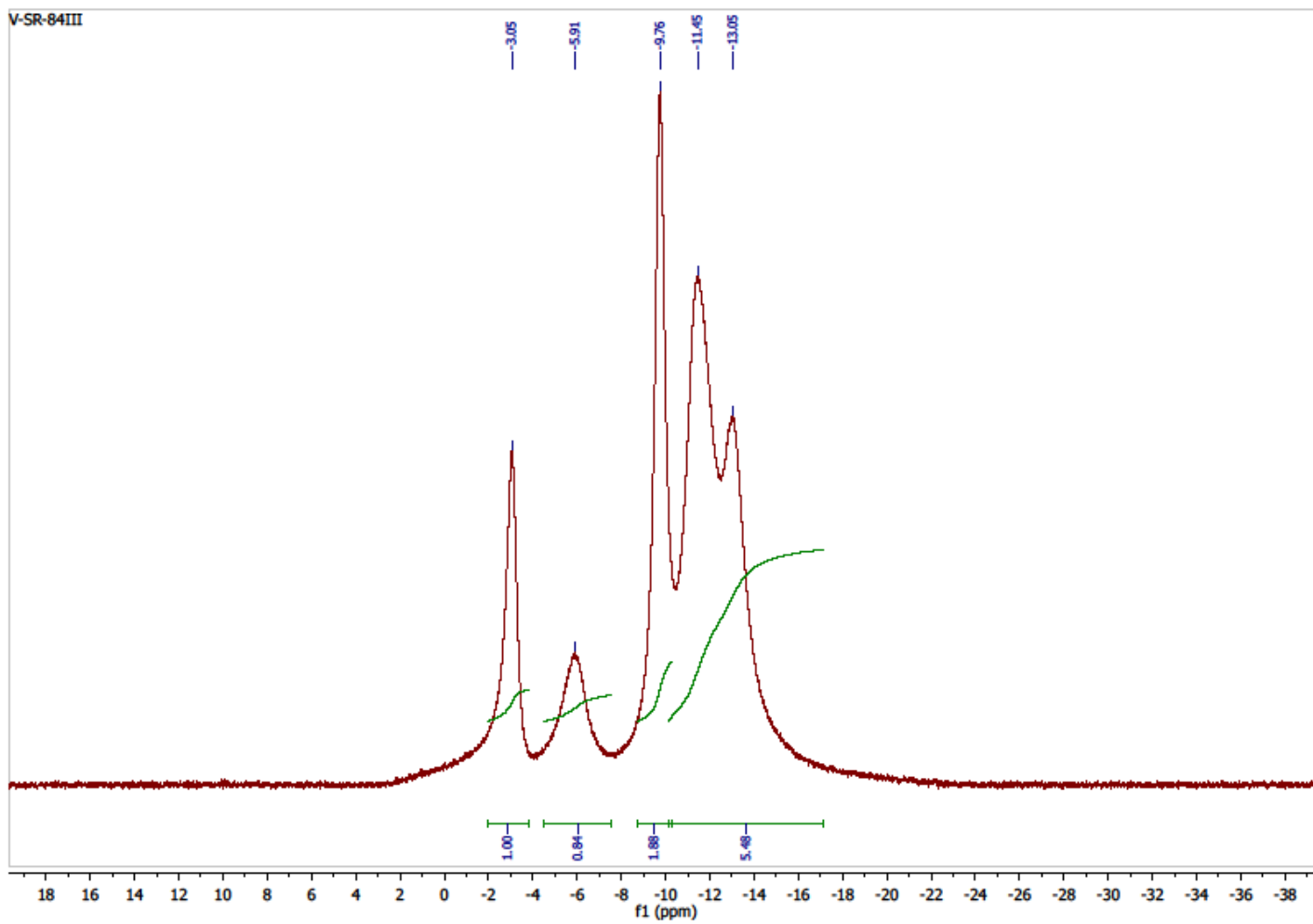


Figure S89. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 31.

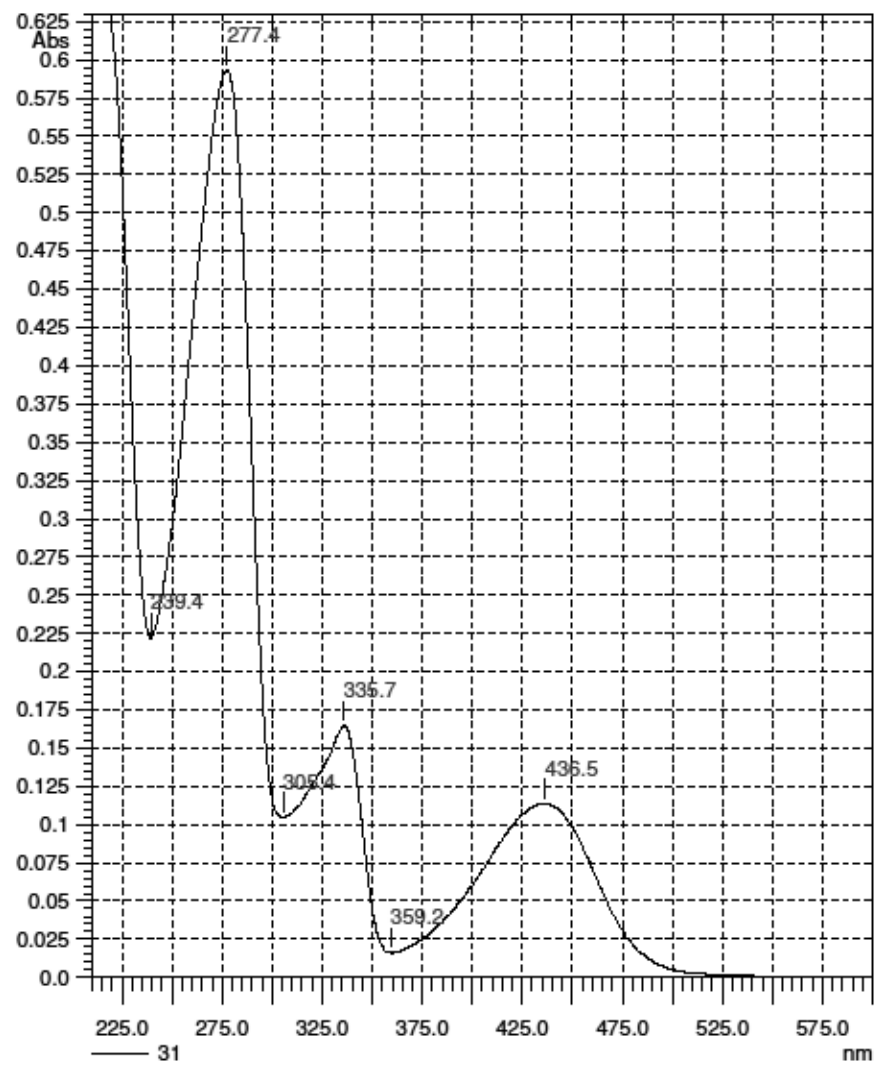


Figure S90. UV spectrum of 31.

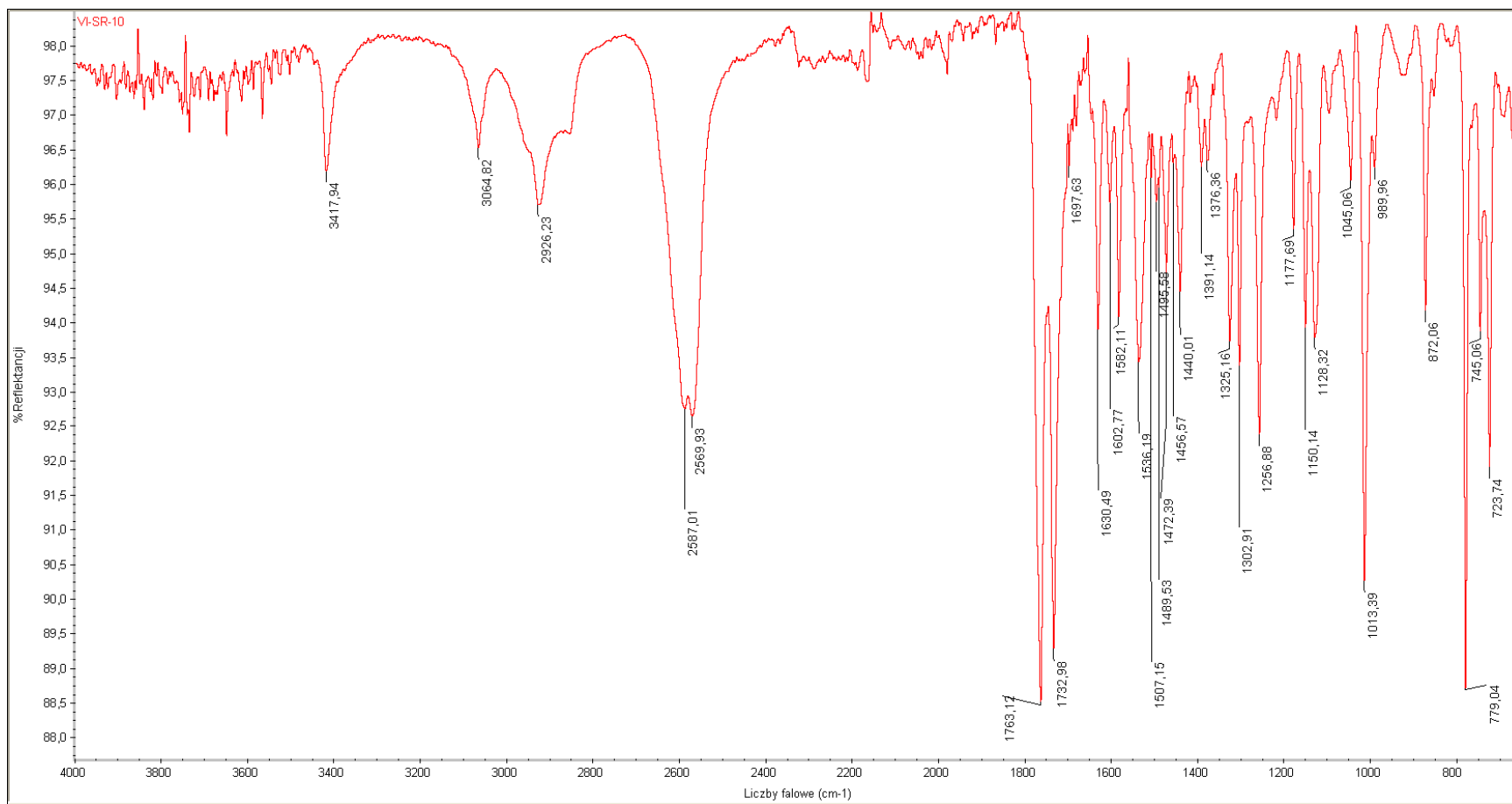
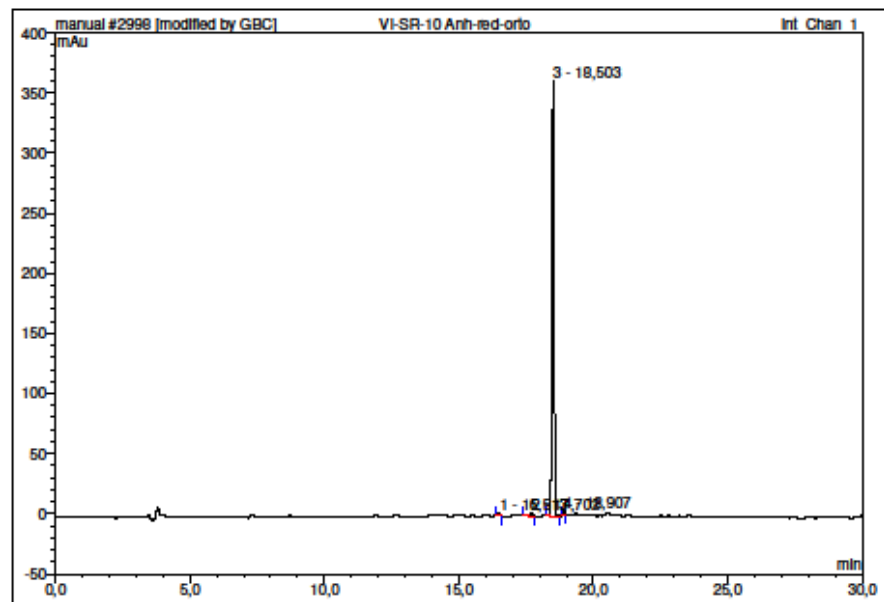


Figure S91. IR spectrum of 31.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	16,51	n.a.	1,476	0,158	0,49	n.a.	BMB*
2	17,70	n.a.	1,962	0,465	1,44	n.a.	BMB*
3	18,50	n.a.	361,479	31,441	97,33	n.a.	BMB
4	18,91	n.a.	3,089	0,240	0,74	n.a.	BMB*
Total:			368,005	32,304	100,00	0,000	

Figure S92. HPLC analysis of 31.

Spectrum Name: VI-SR-10_pr
Start Ion: 300
End Ion: 500
Source: APCI + 10.0µA 400C
Capillary: 180V 300C Offset: 30V Span: 20V

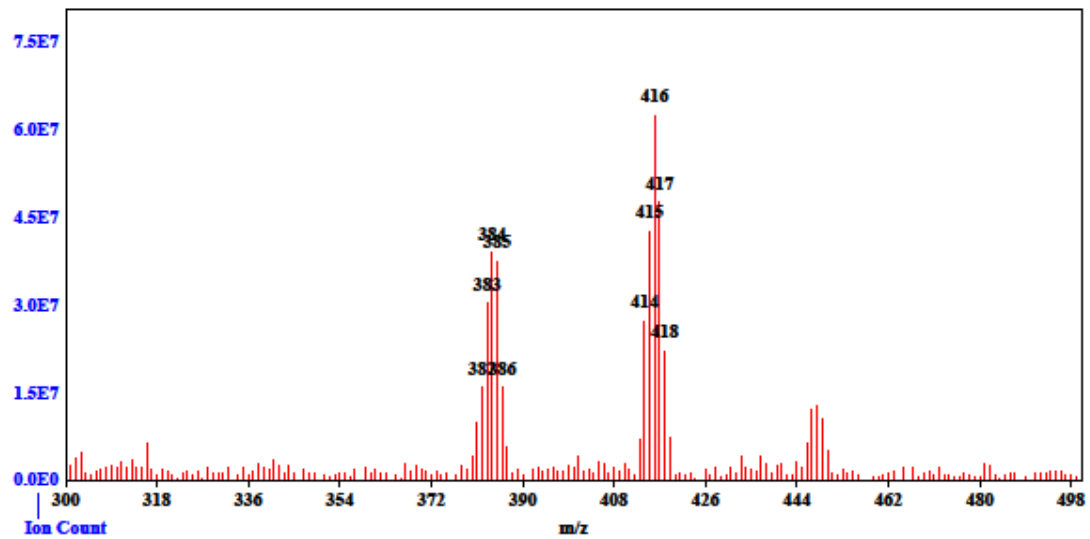


Figure S93. MS spectrum of 31.

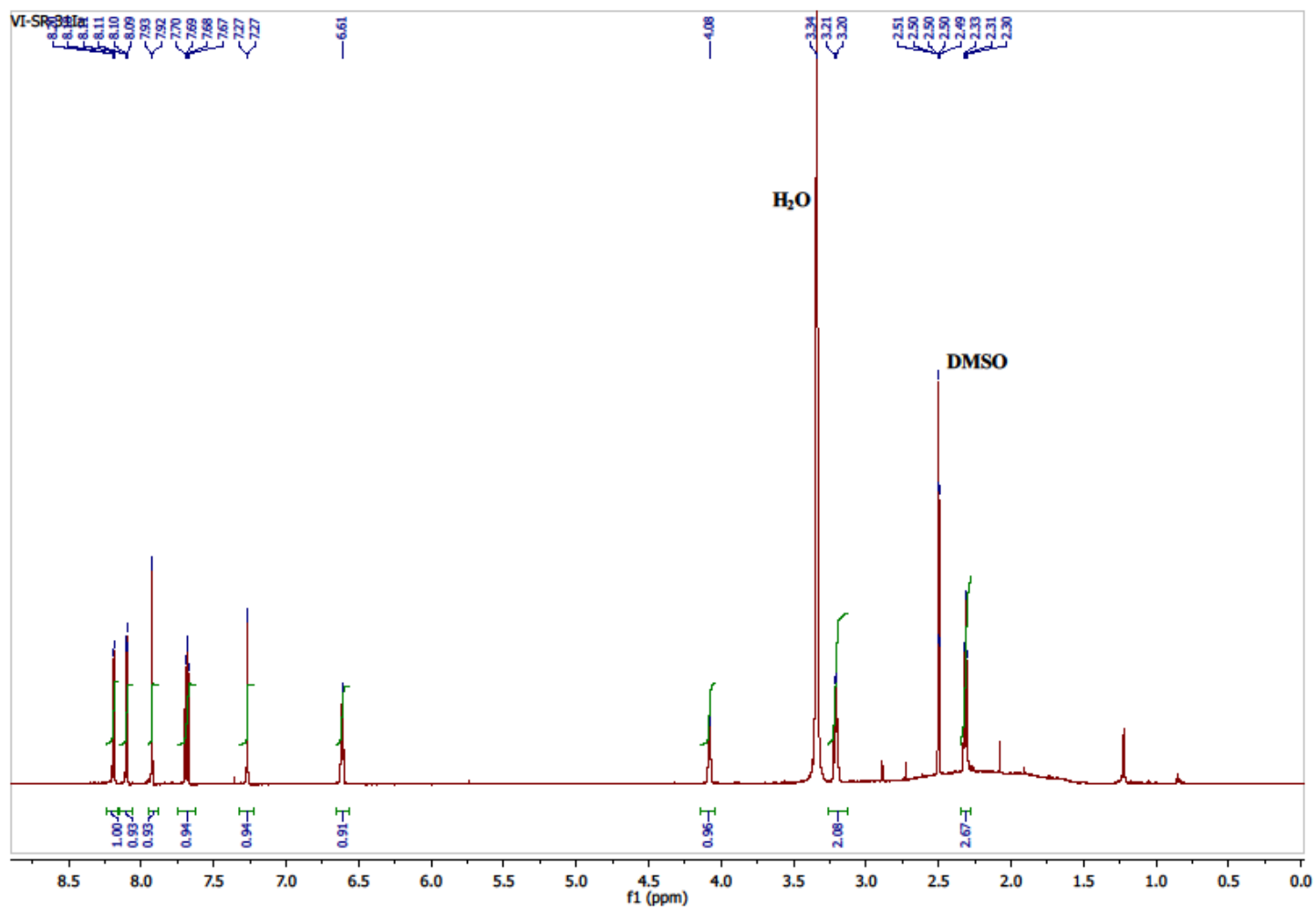


Figure S94. ¹H NMR spectrum of 32.

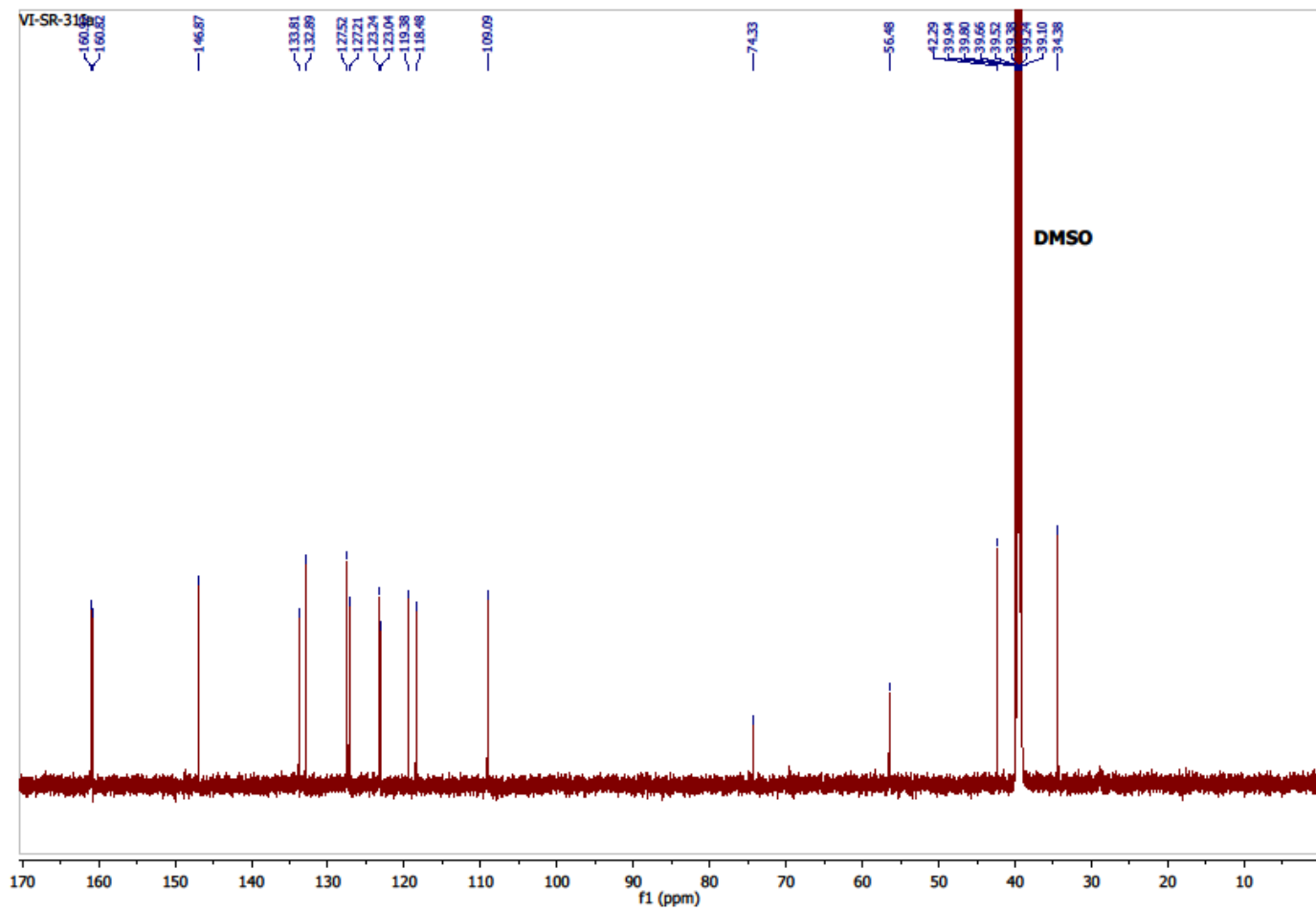


Figure S95. ^{13}C NMR spectrum of 32.

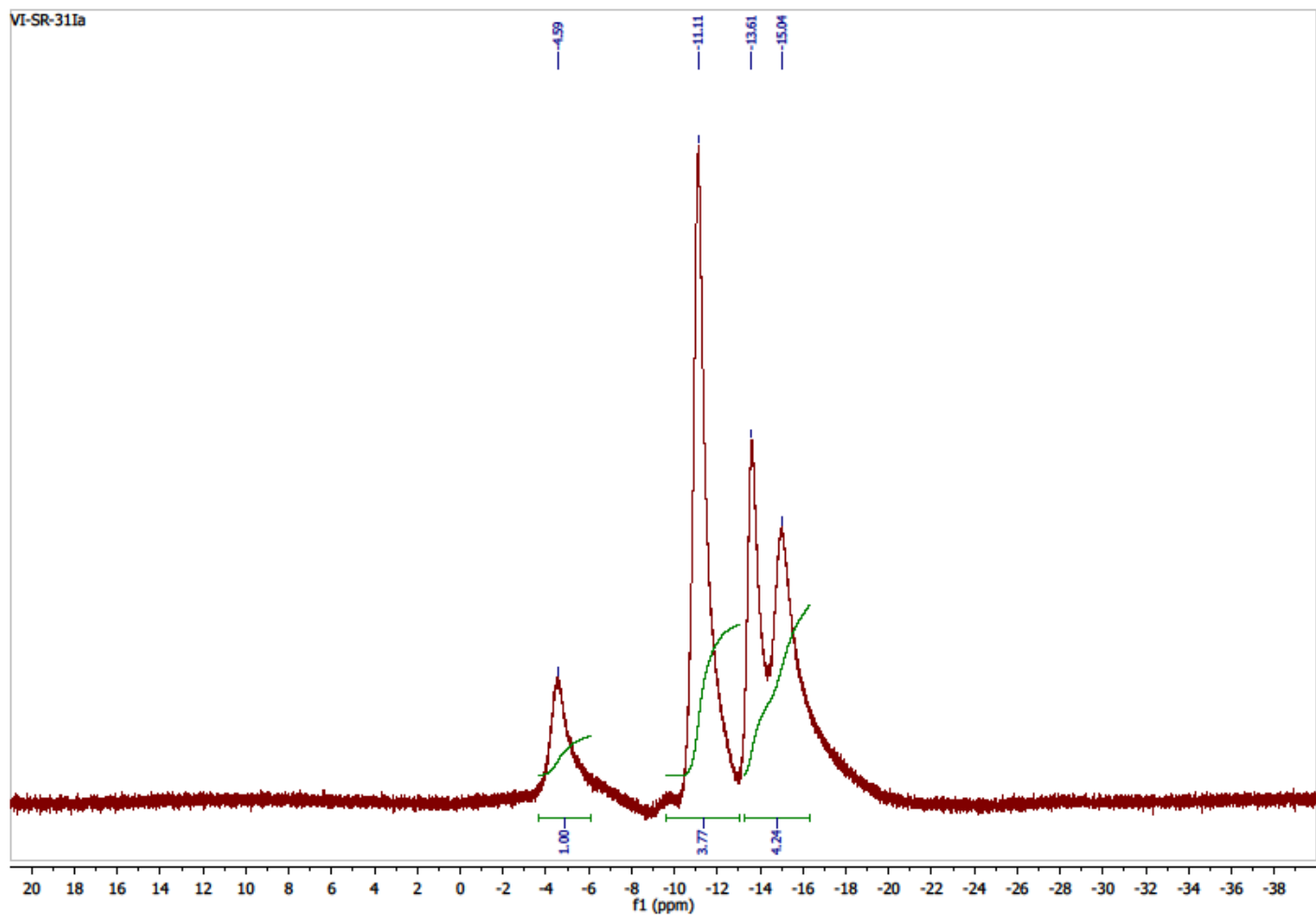


Figure S96. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 32.

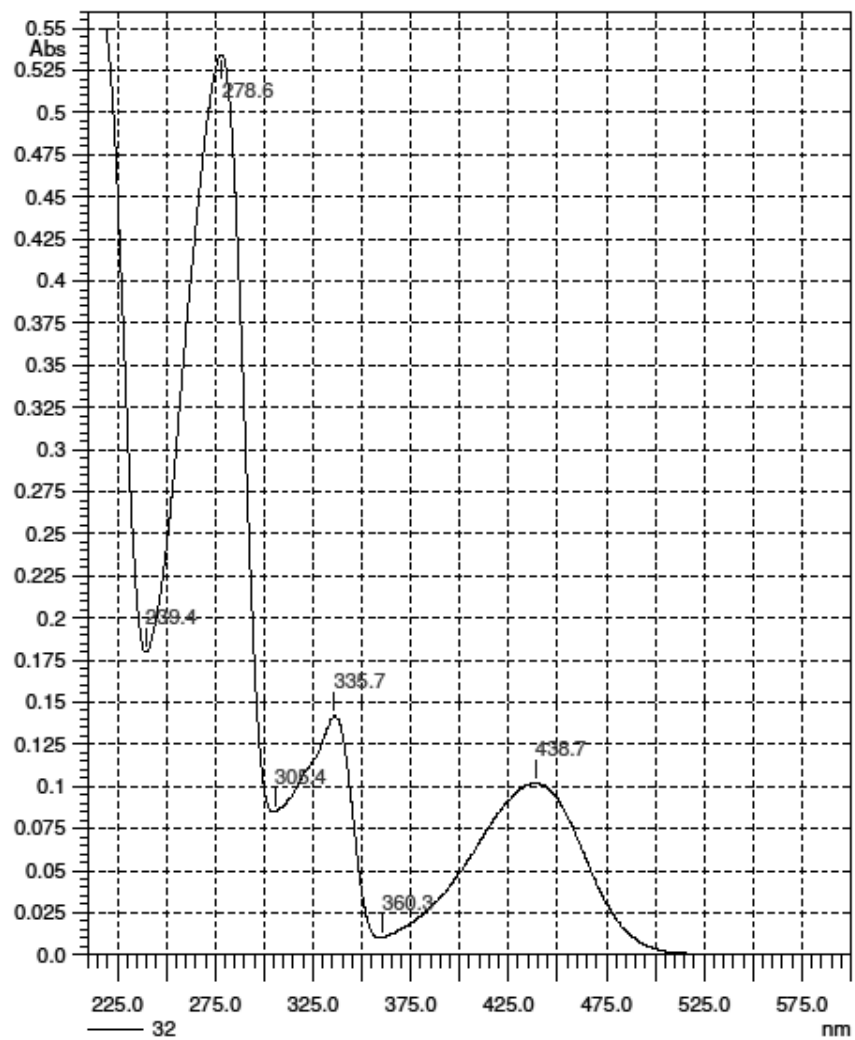


Figure S97. UV spectrum of 32.

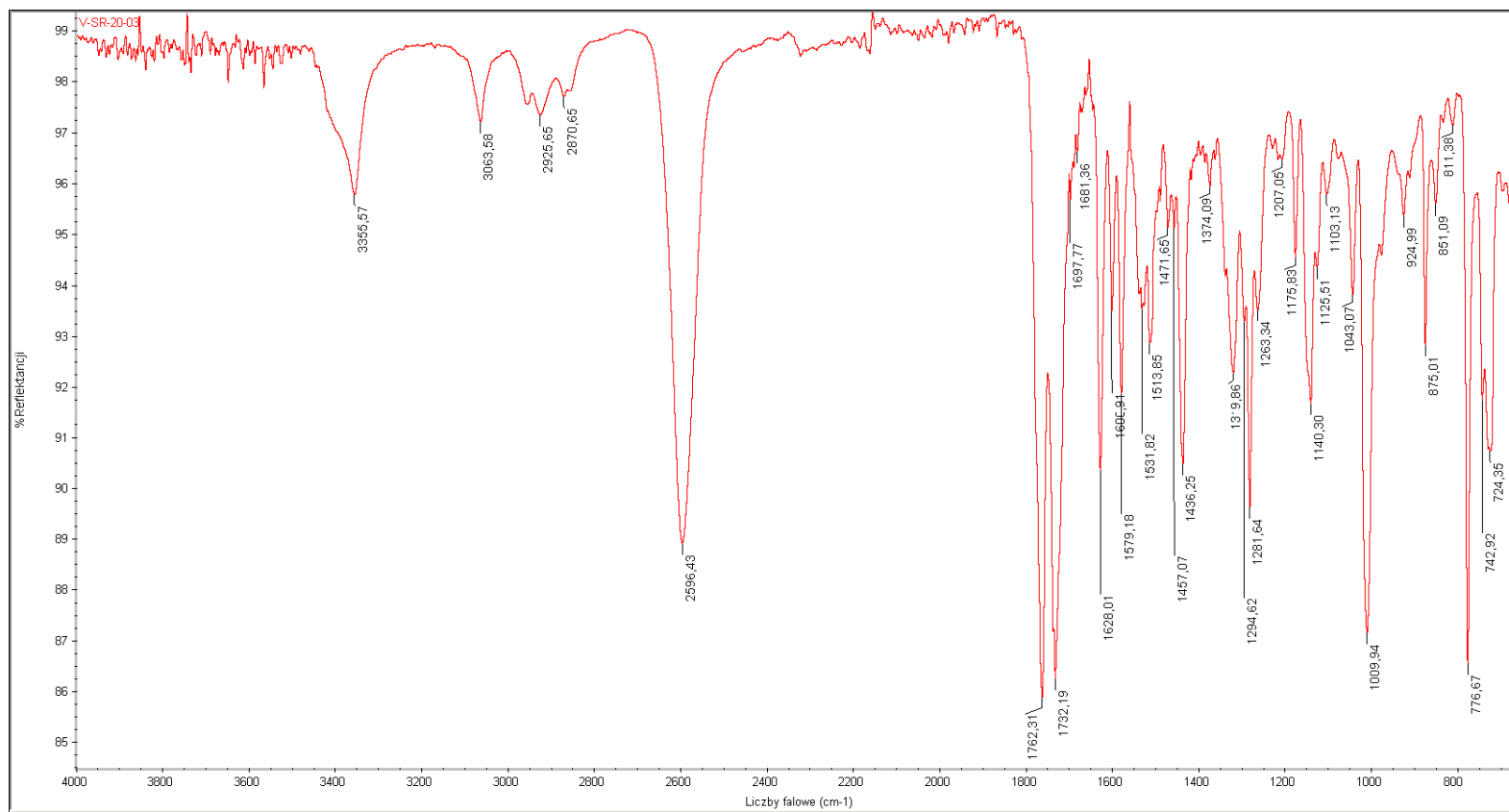


Figure S98. IR spectrum of 32.

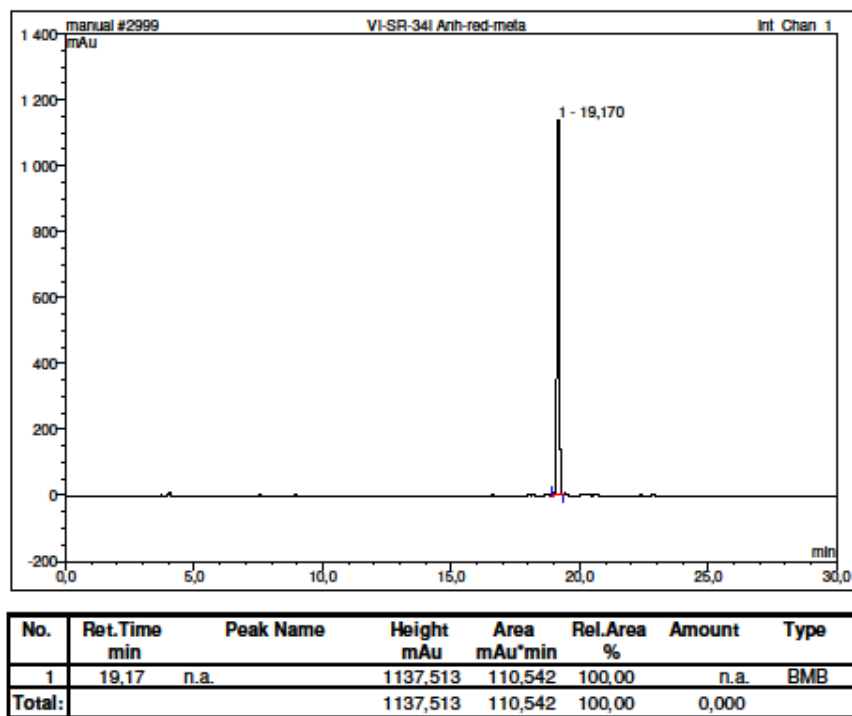


Figure S99. HPLC analysis of 32.

Spectrum Name: V-SR-20-03_PT
Start Ion: 300
End Ion: 500
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

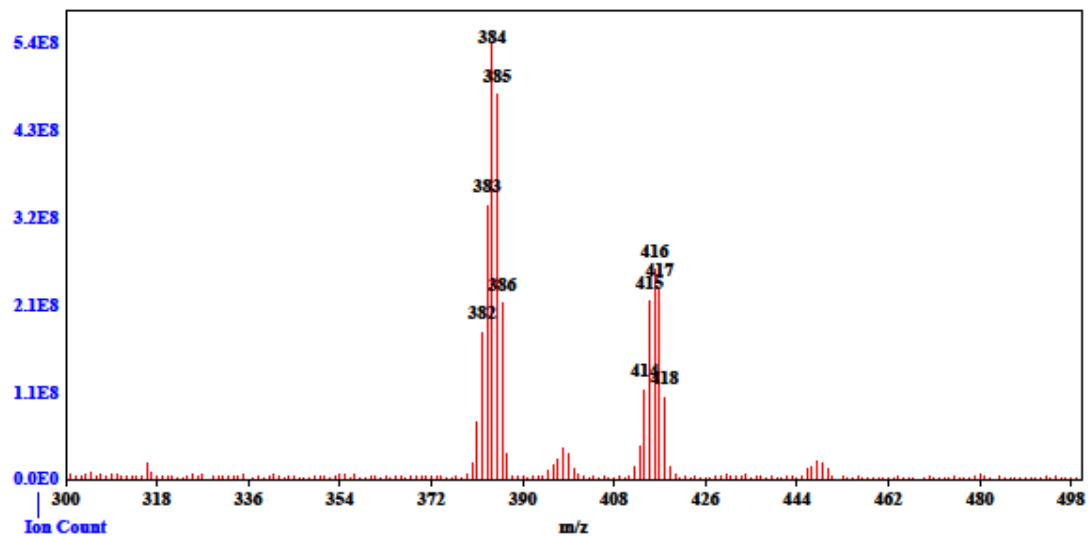


Figure S100. MS spectrum of 32.

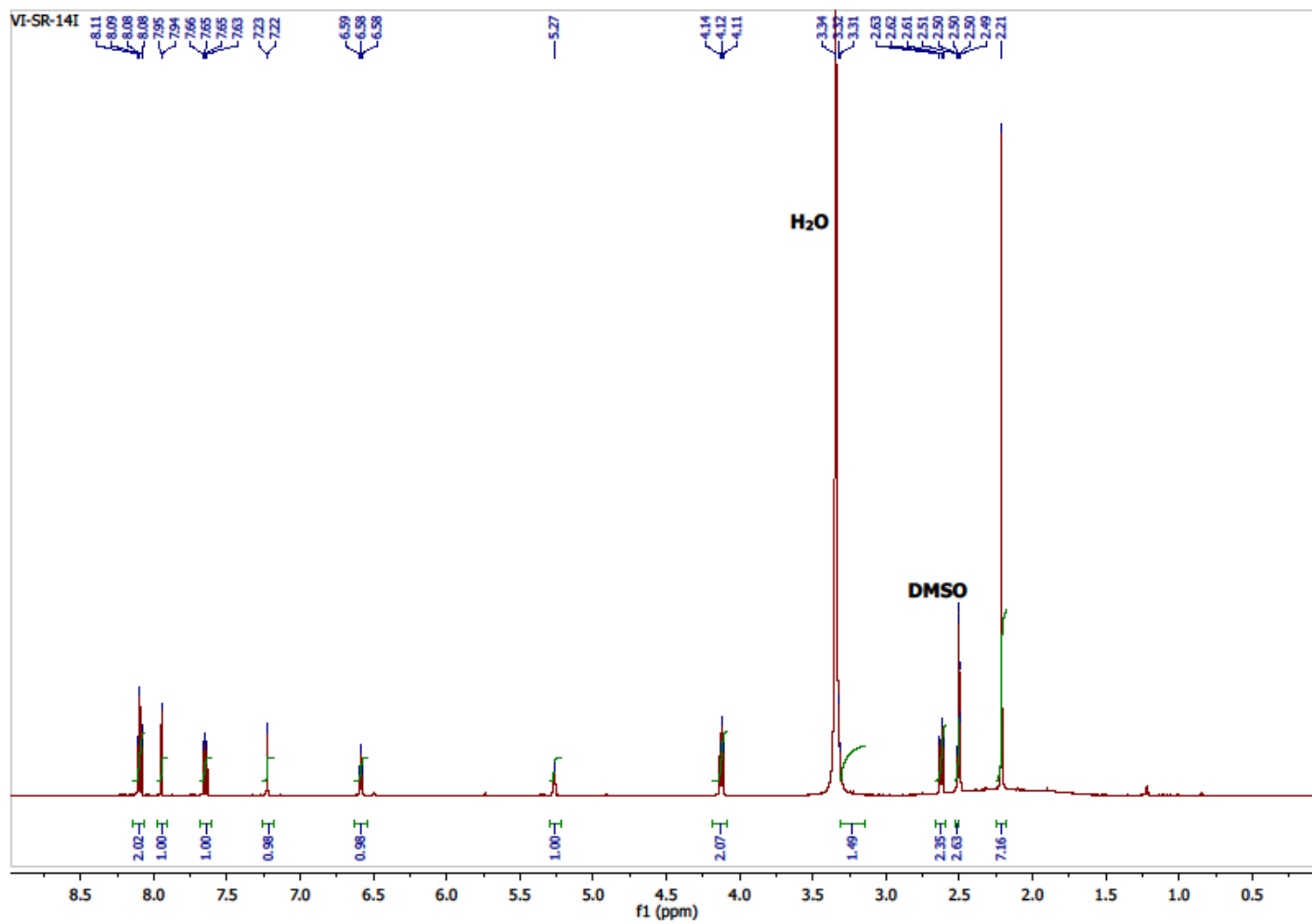


Figure S101. ¹H NMR spectrum of 33.

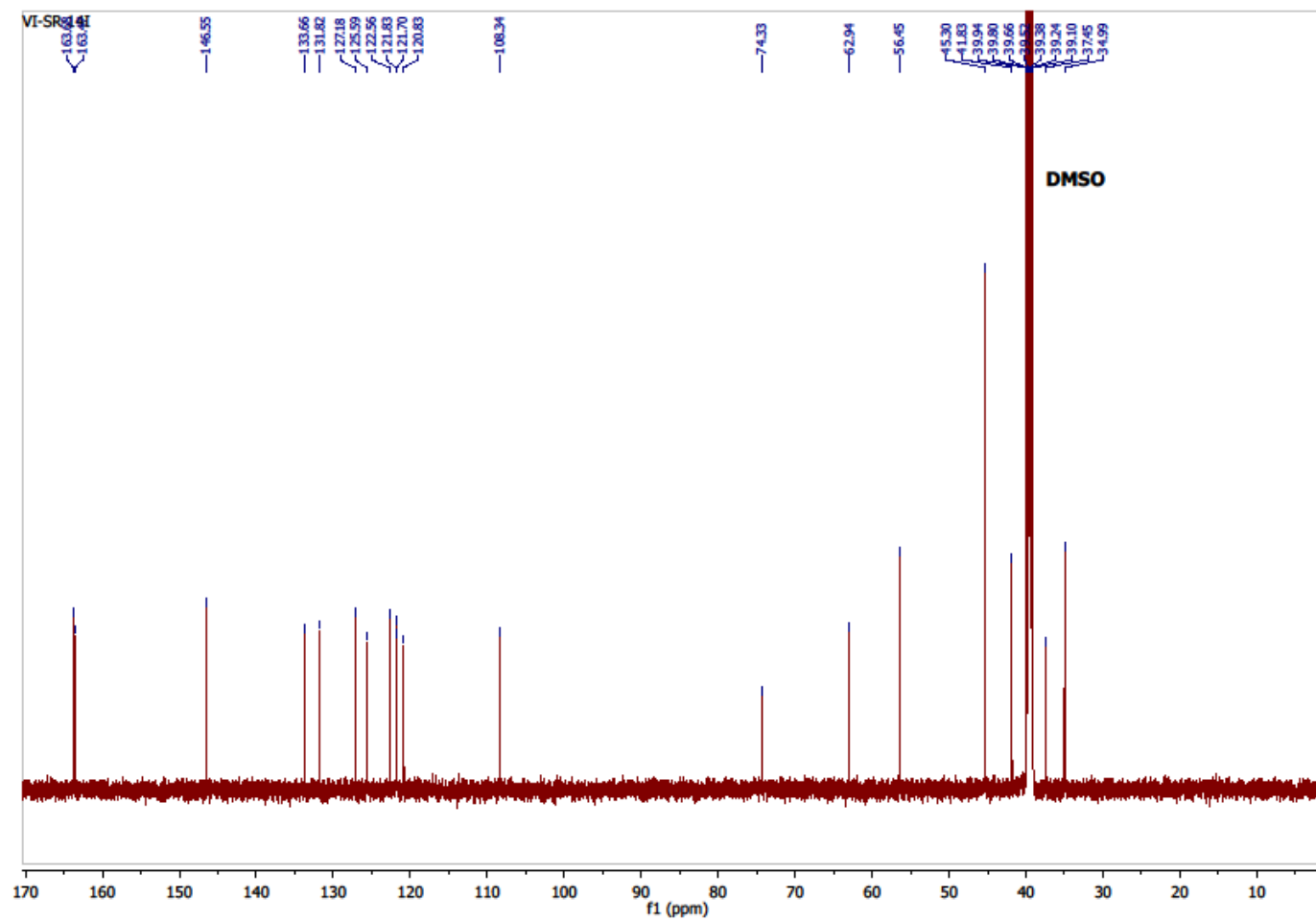


Figure S102. ^{13}C NMR spectrum of 33.

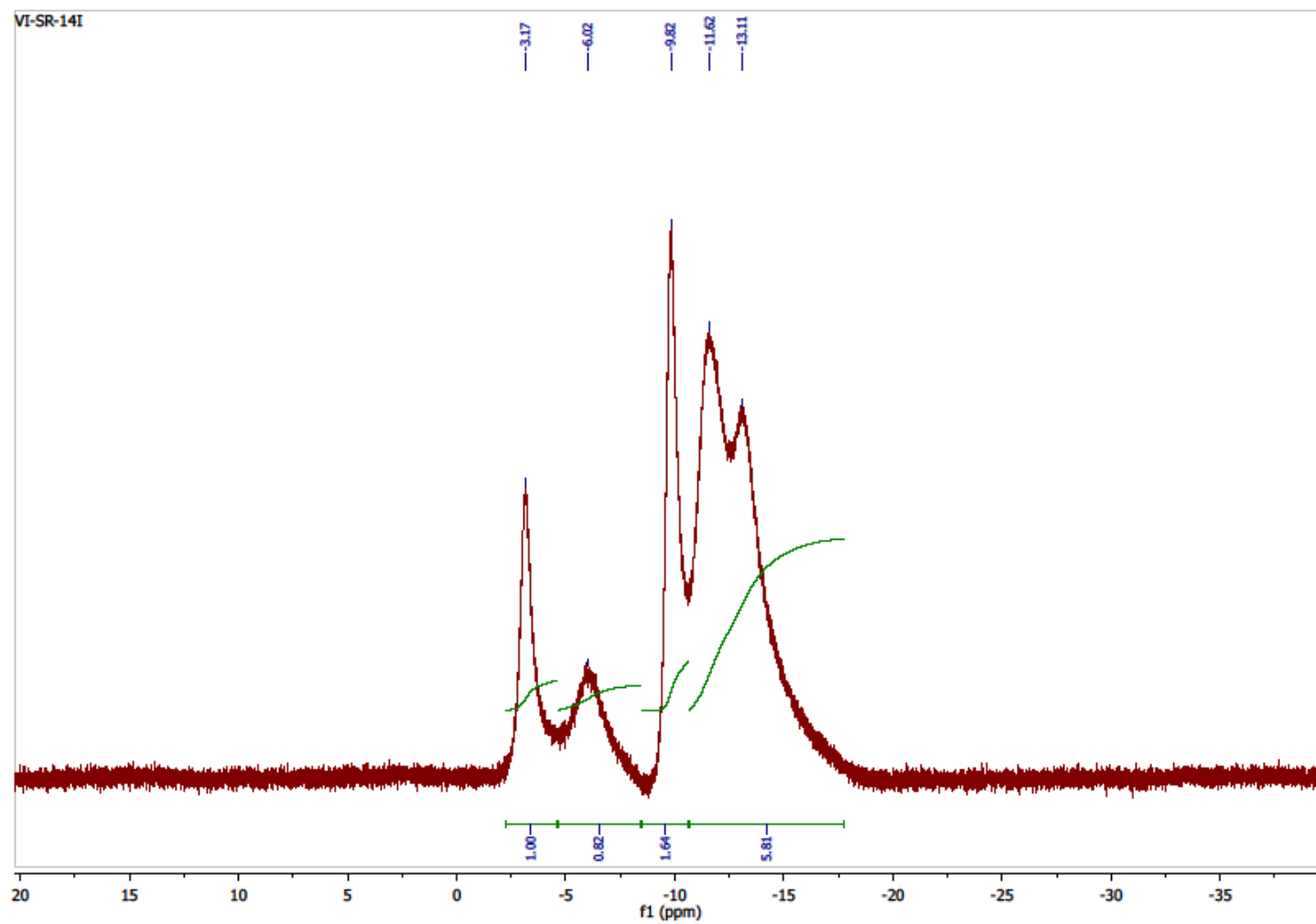


Figure S103. ^{11}B NMR (^1H BB) spectrum of 33.

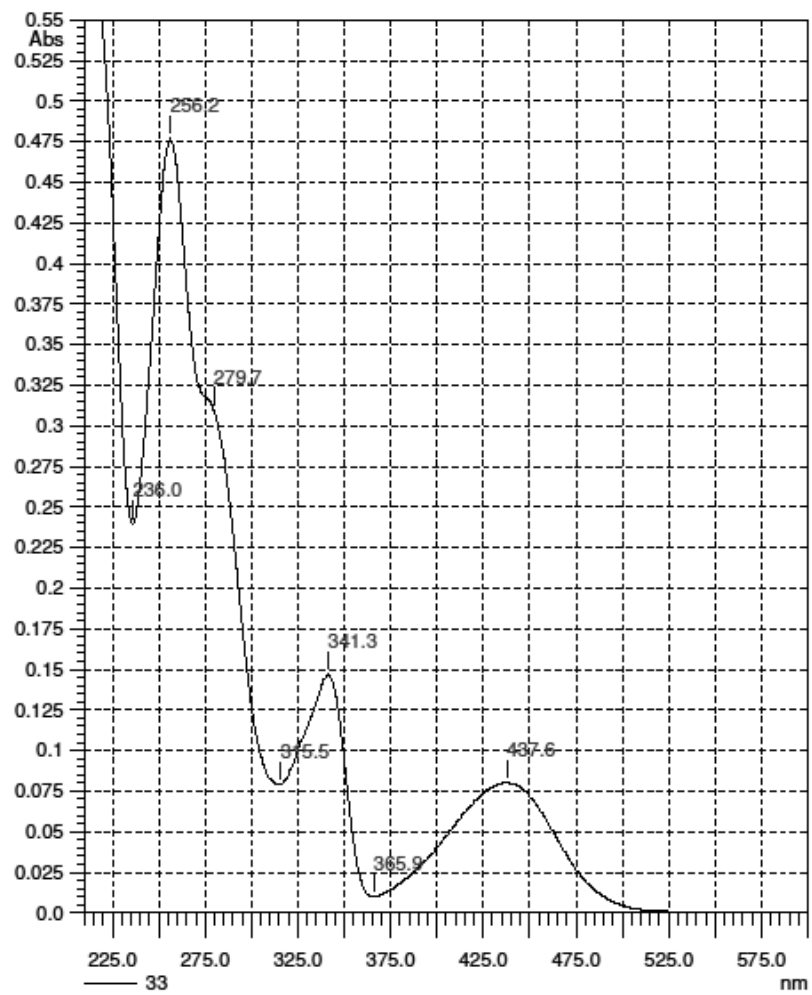


Figure S104. UV spectrum of 33.

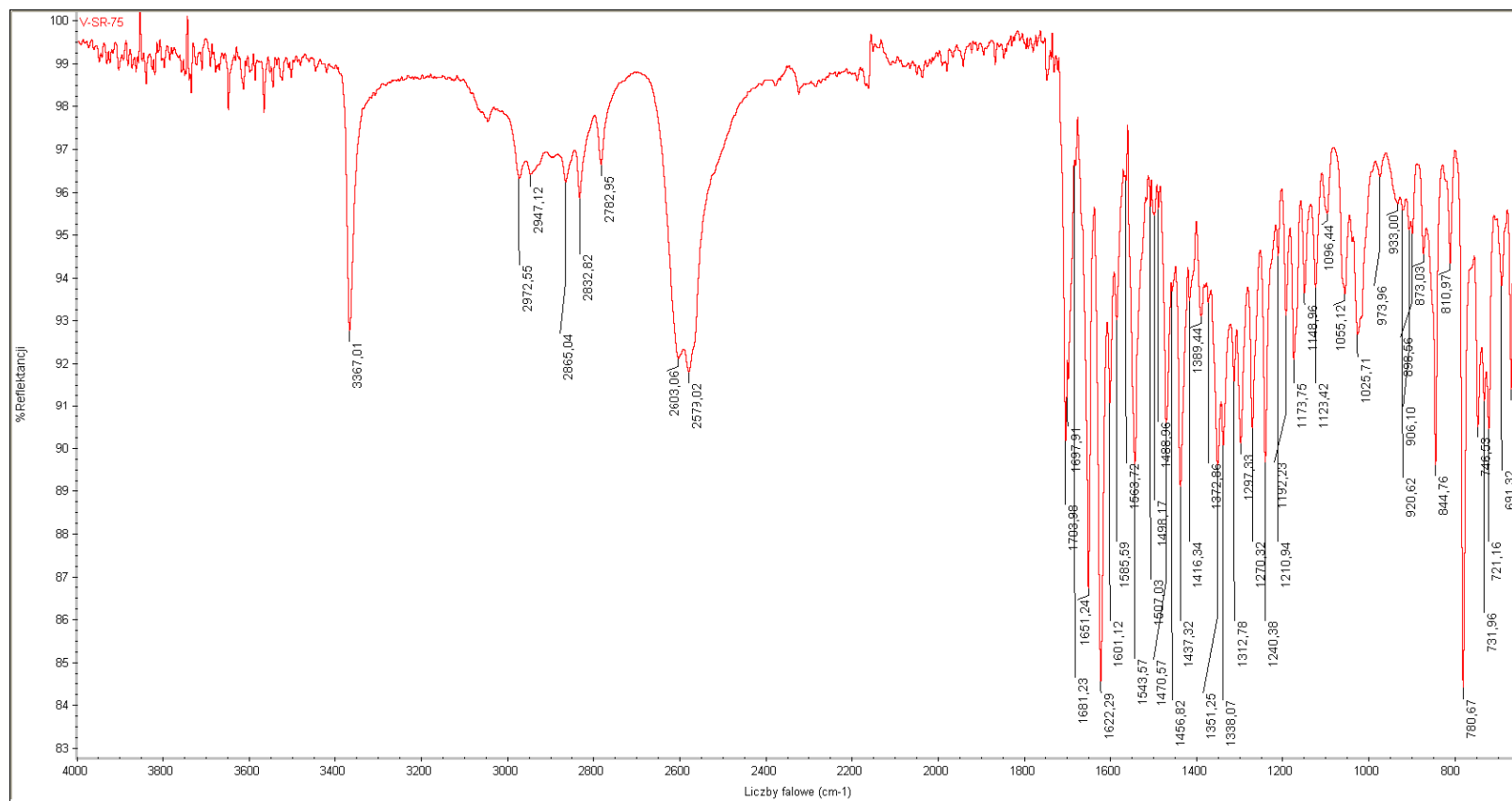
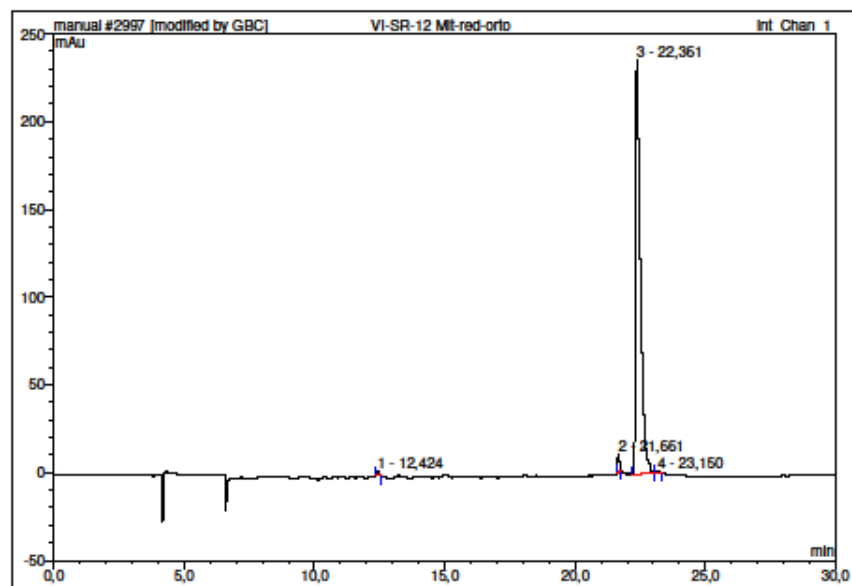


Figure S105. IR spectrum of 33.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	12,42	n.a.	2,295	0,298	0,58	n.a.	BMB*
2	21,66	n.a.	10,037	0,950	1,85	n.a.	BMB*
3	22,36	n.a.	235,948	49,811	97,15	n.a.	BMB*
4	23,15	n.a.	1,591	0,215	0,42	n.a.	BMB*
Total:			249,872	51,275	100,00	0,000	

Figure S106. HPLC analysis of 33.

Spectrum Name: V-SR-75
Start Ion: 400
End Ion: 520
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

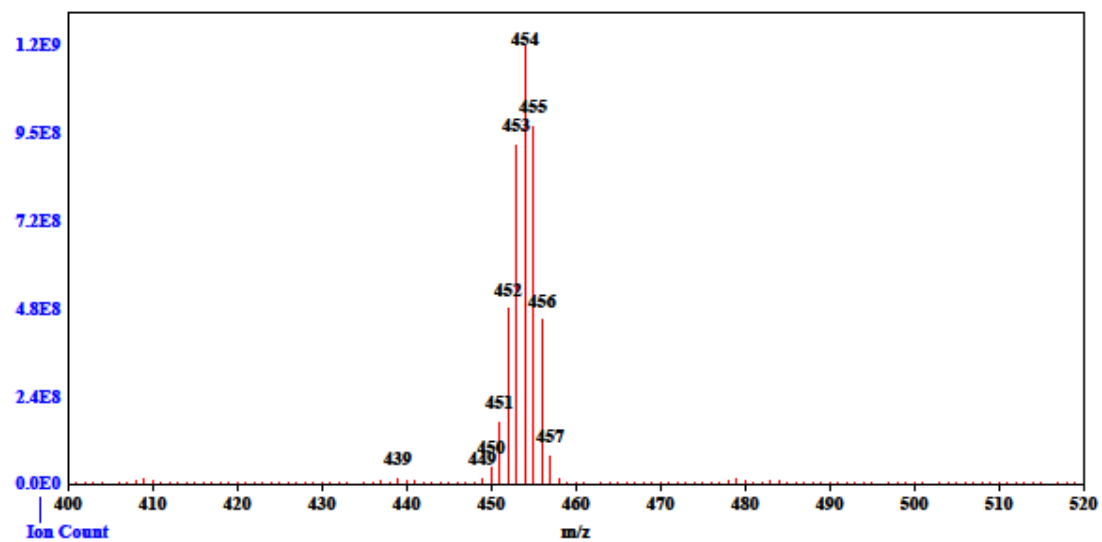


Figure S107. MS spectrum of 33.

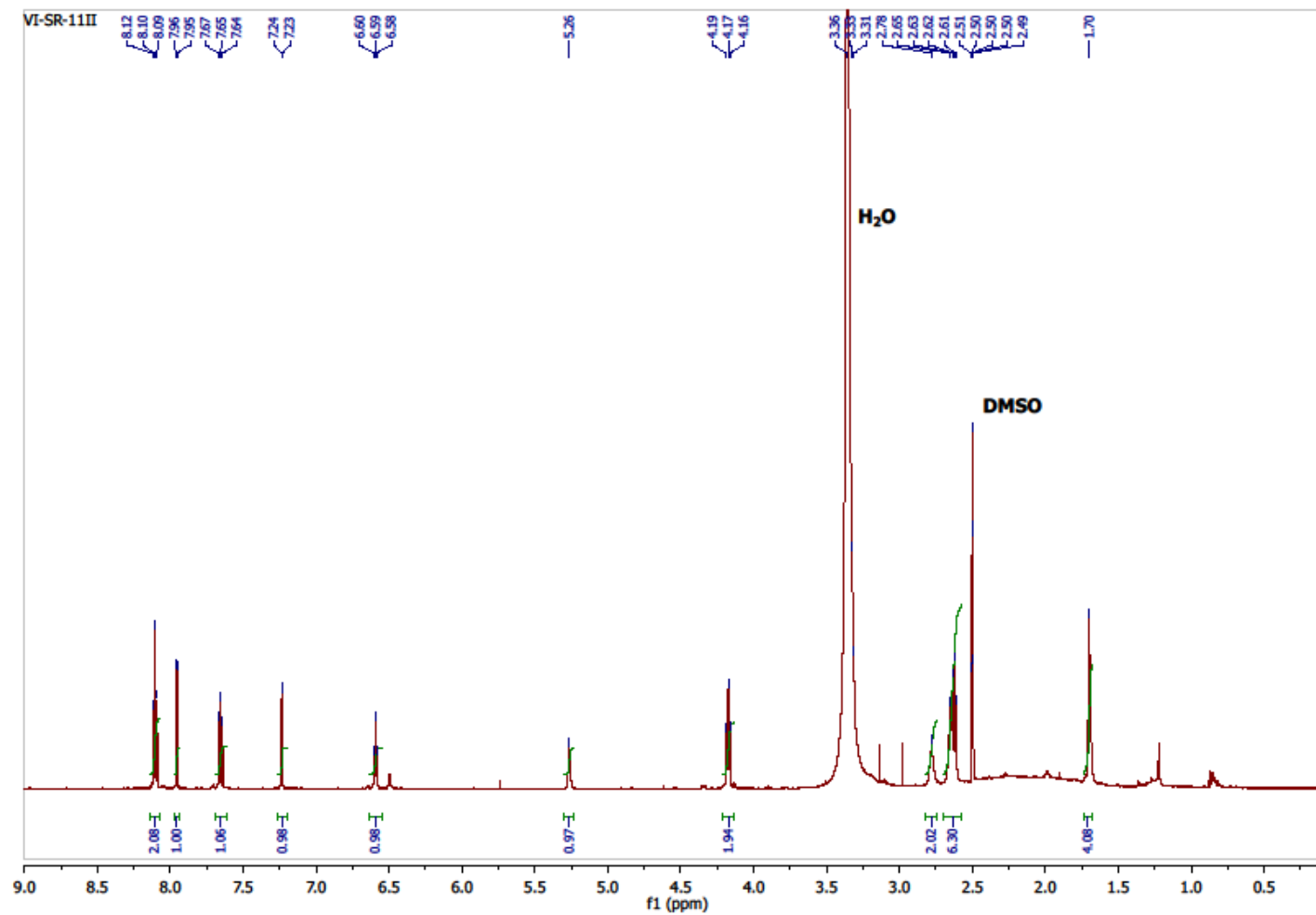


Figure S108. ¹H NMR spectrum of 34.

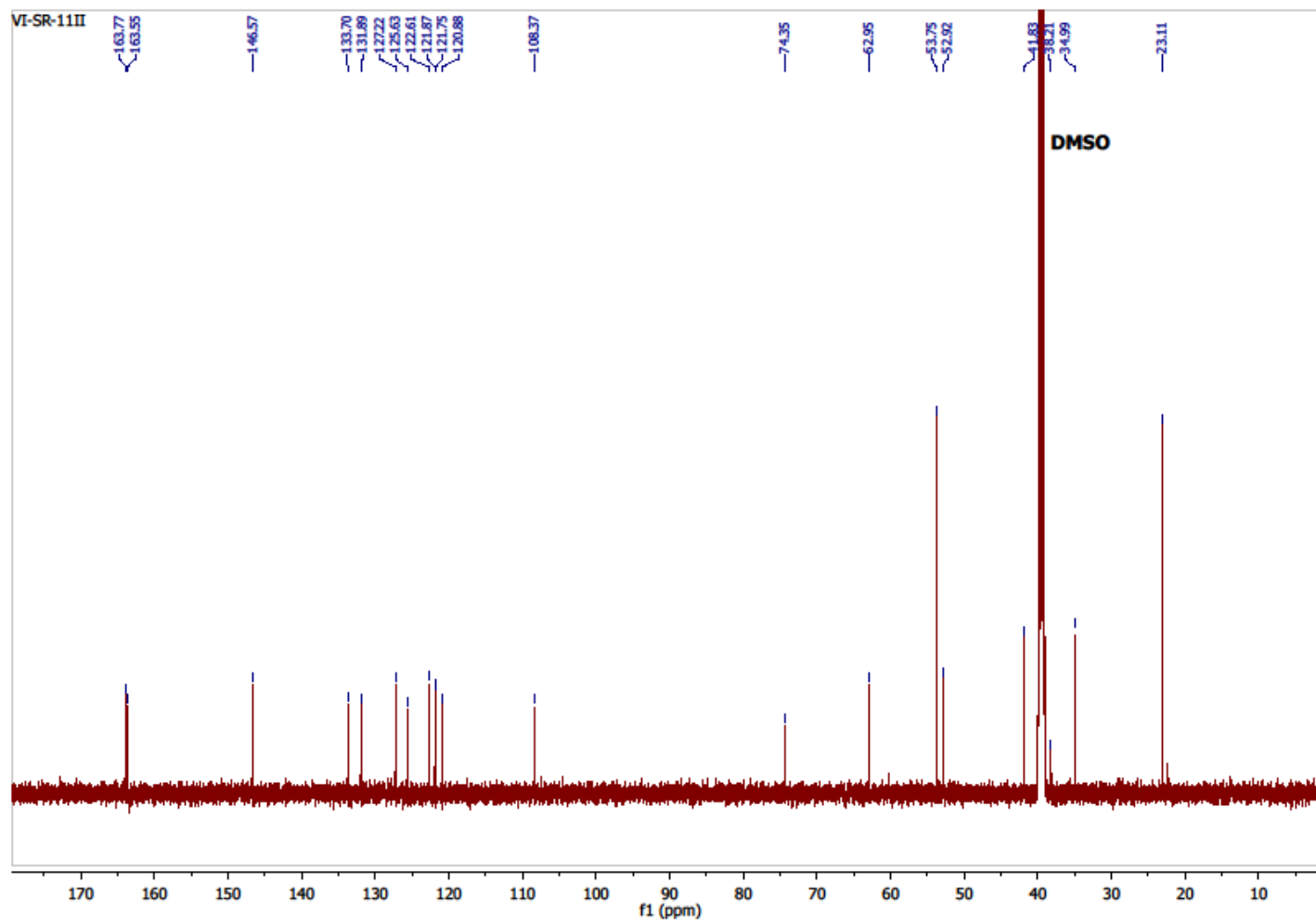


Figure S109. ^{13}C NMR spectrum of 34.

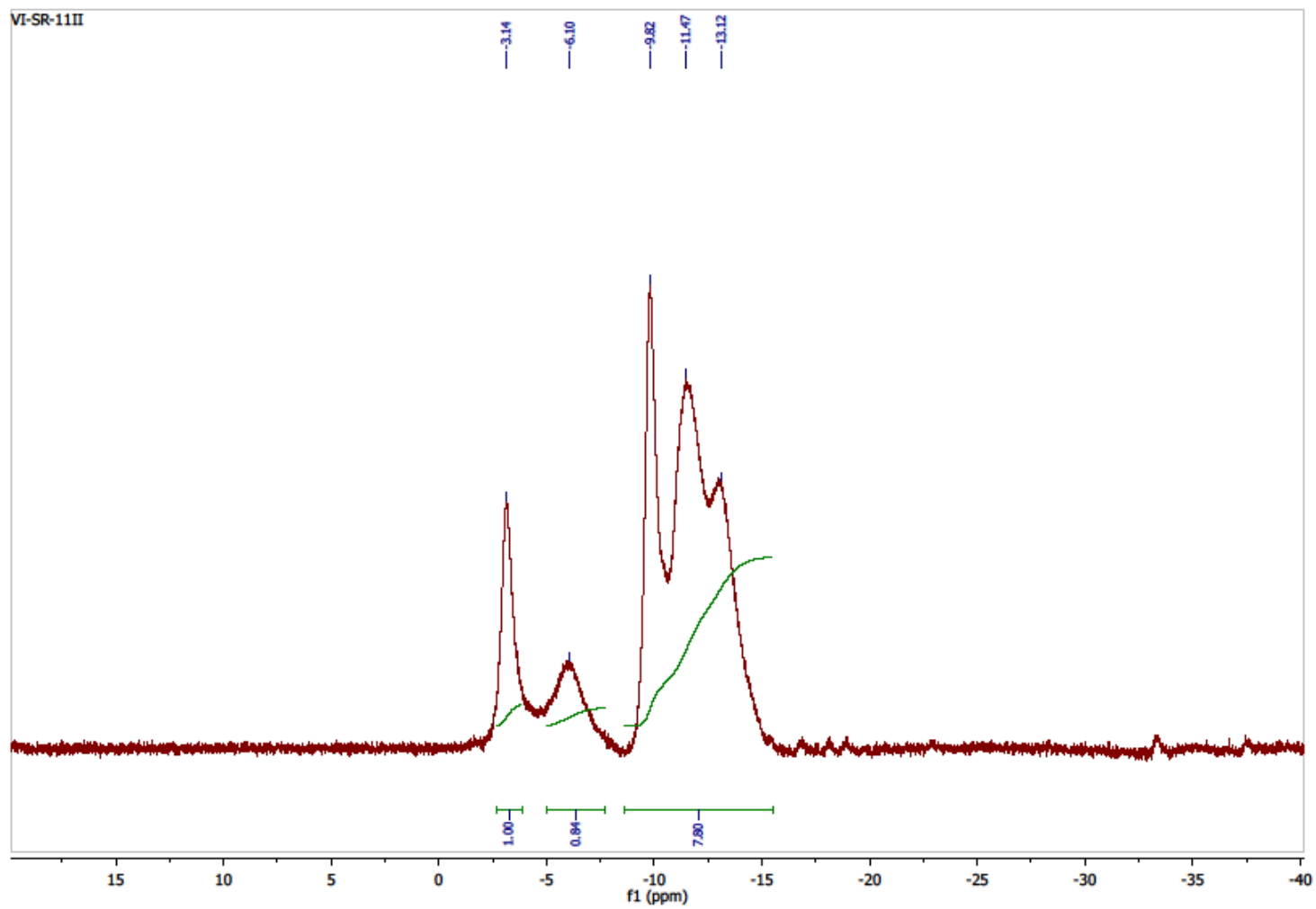


Figure S110. ^{11}B NMR (^1H BB) spectrum of 34.

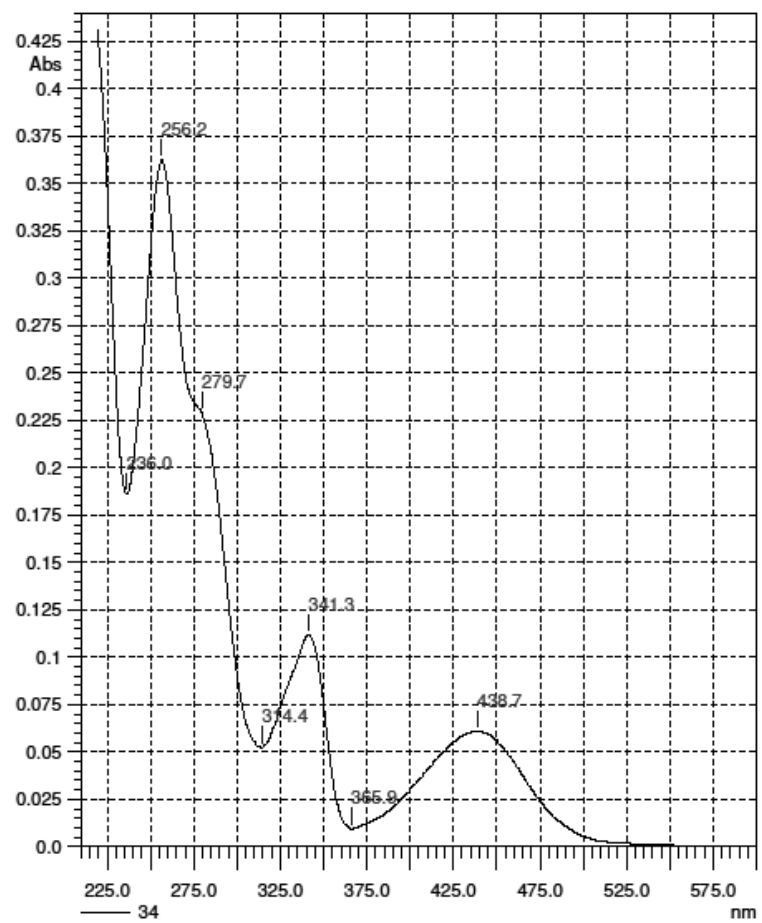


Figure S111. UV spectrum of 34.

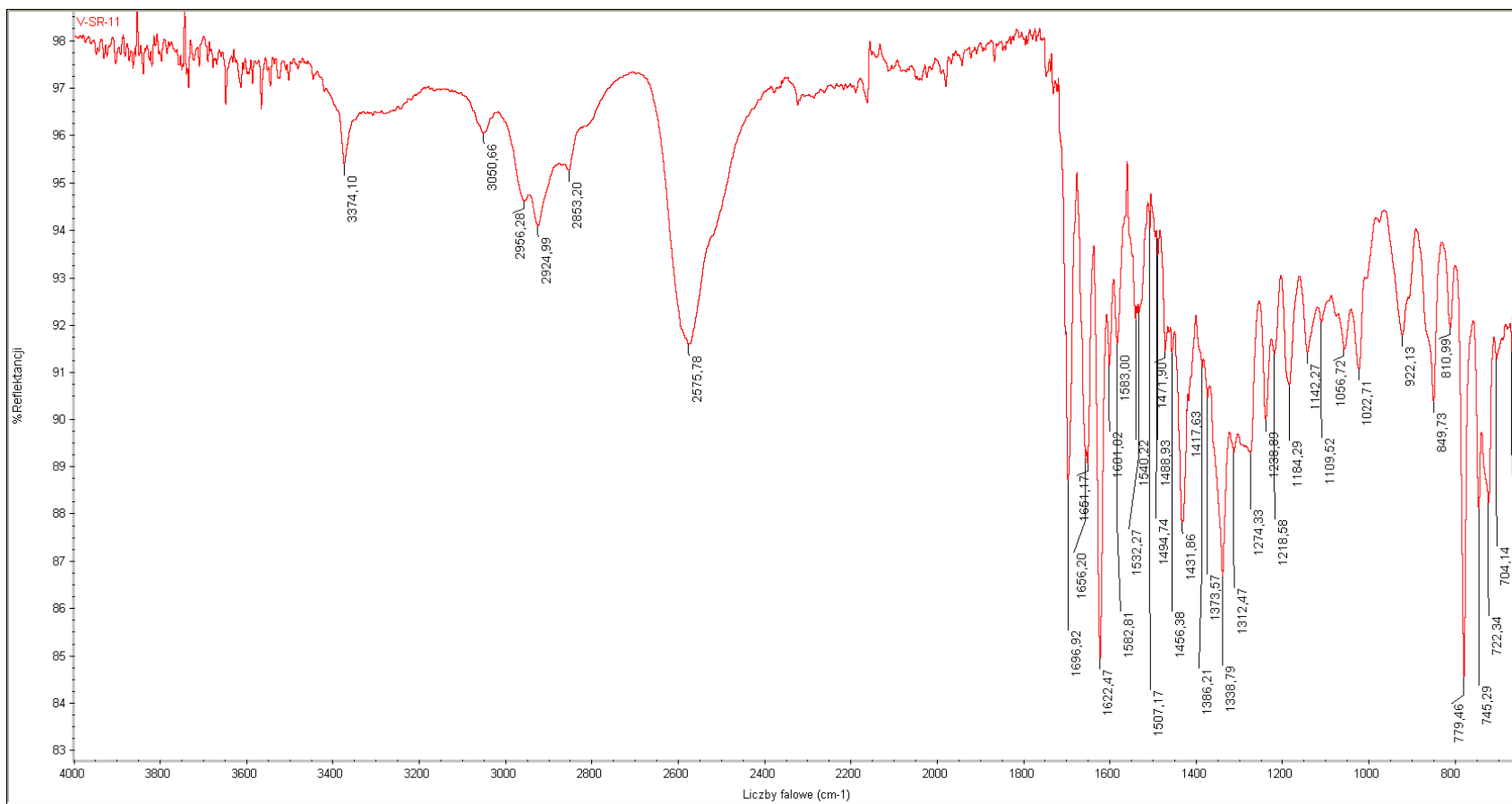
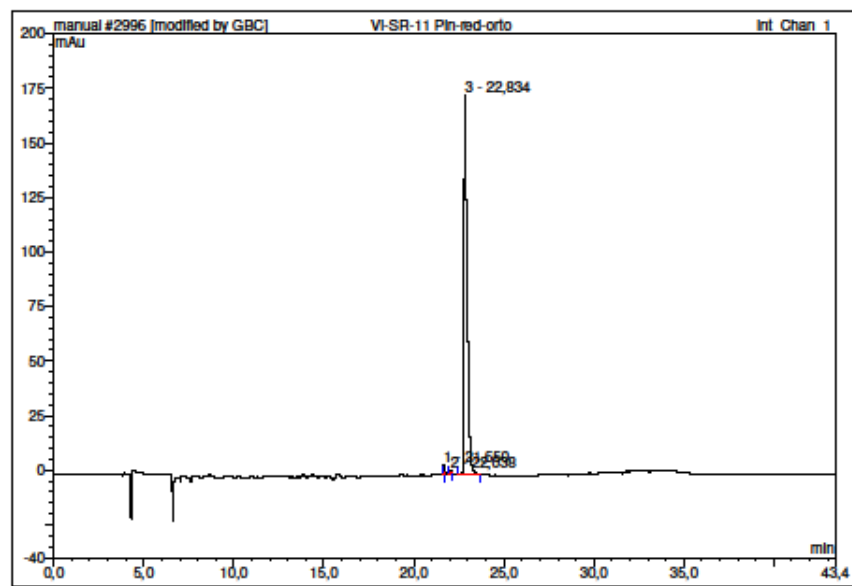


Figure S112. IR spectrum of 34.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	21,65	n.a.	3,876	0,366	1,01	n.a.	BMB*
2	22,04	n.a.	1,402	0,149	0,41	n.a.	BMB*
3	22,83	n.a.	173,815	35,568	98,57	n.a.	BMB
Total:			179,093	36,083	100,00	0,000	

Figure S113. HPLC analysis of 34.

Spectrum Name: V-SR-11
Start Ion: 400
End Ion: 550
Source: APCI + 10.0μA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

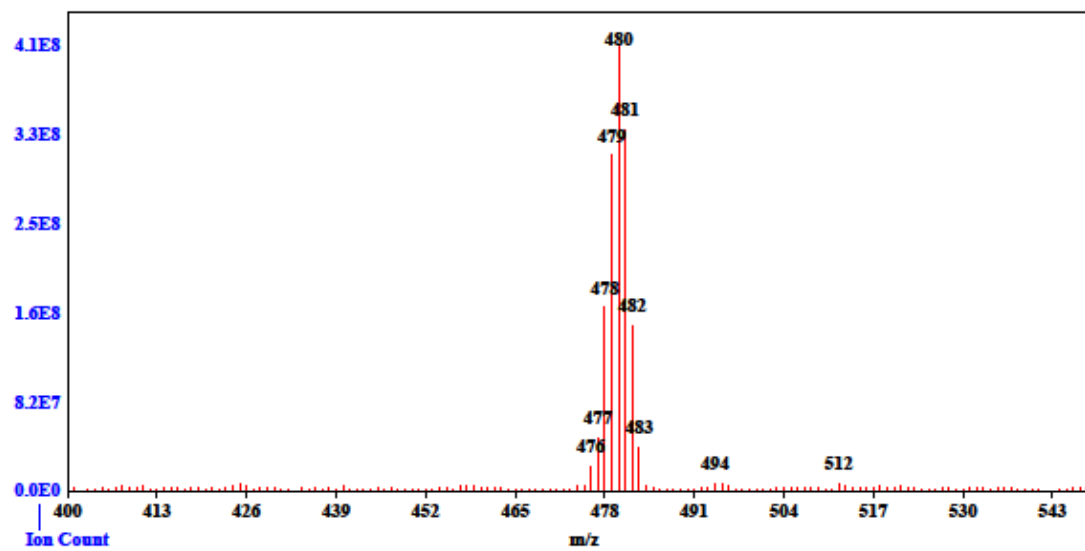


Figure S114. MS spectrum of 34.

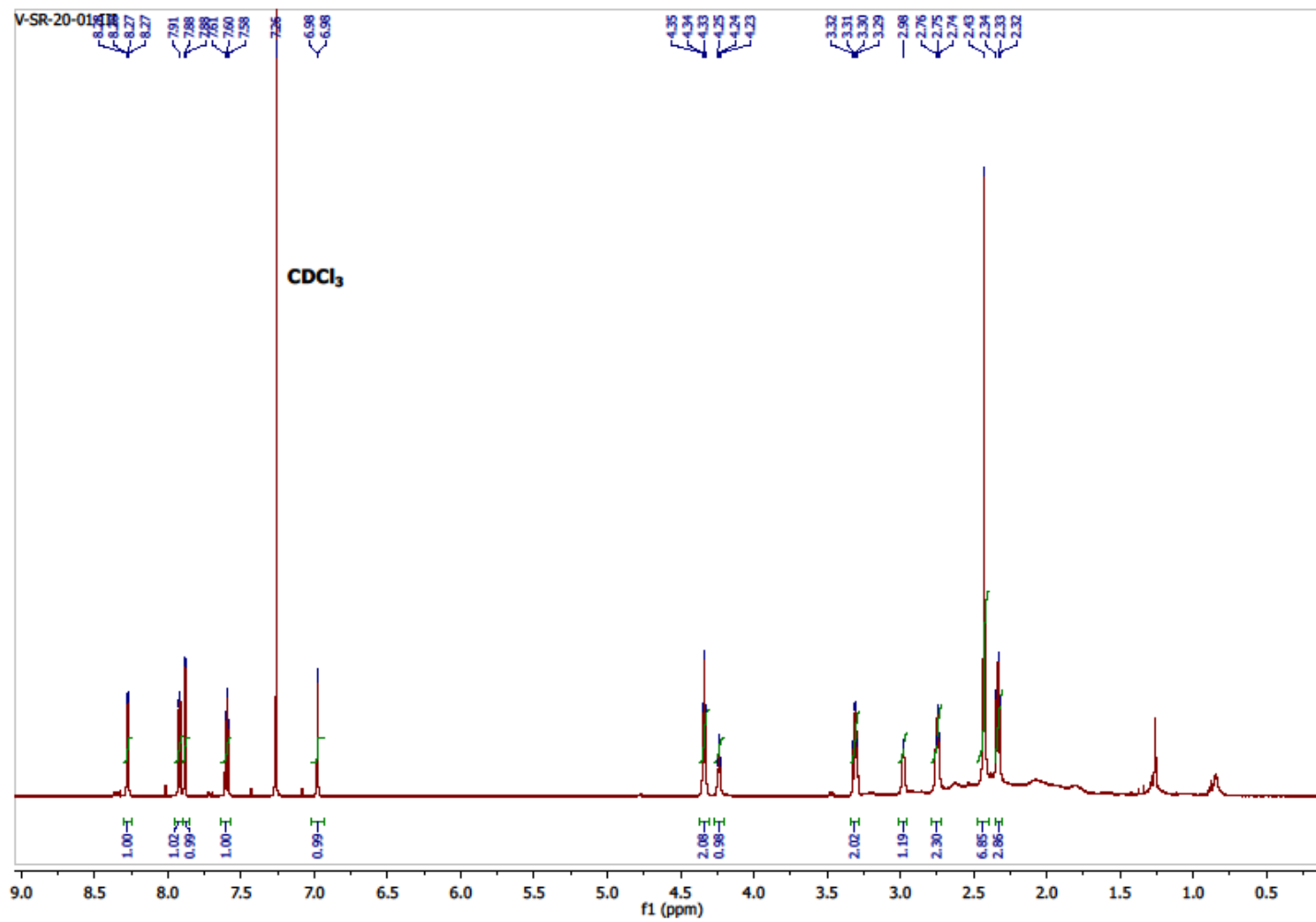


Figure S115. ¹H NMR spectrum of 35.

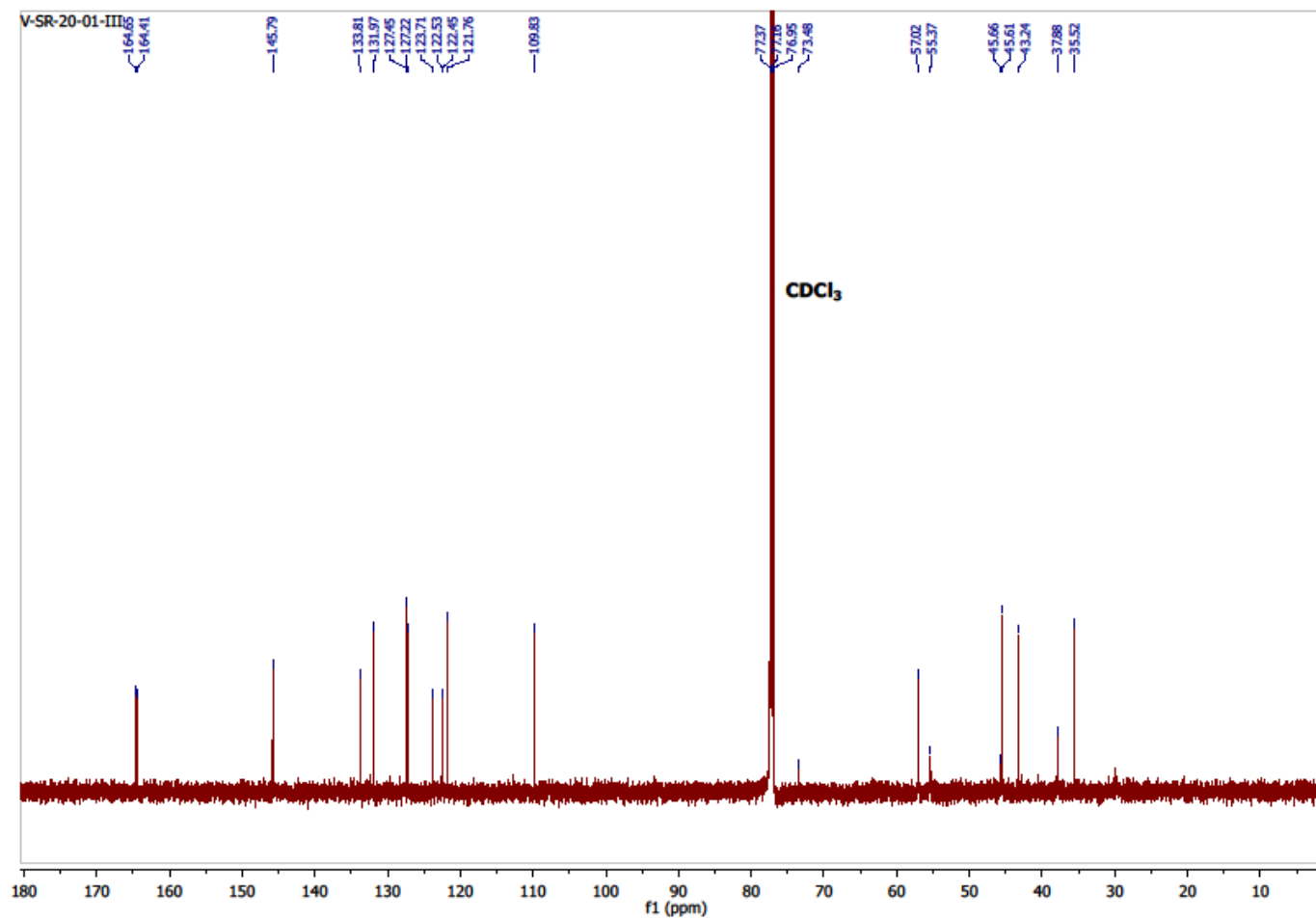


Figure S116. ¹³C NMR spectrum of 35.

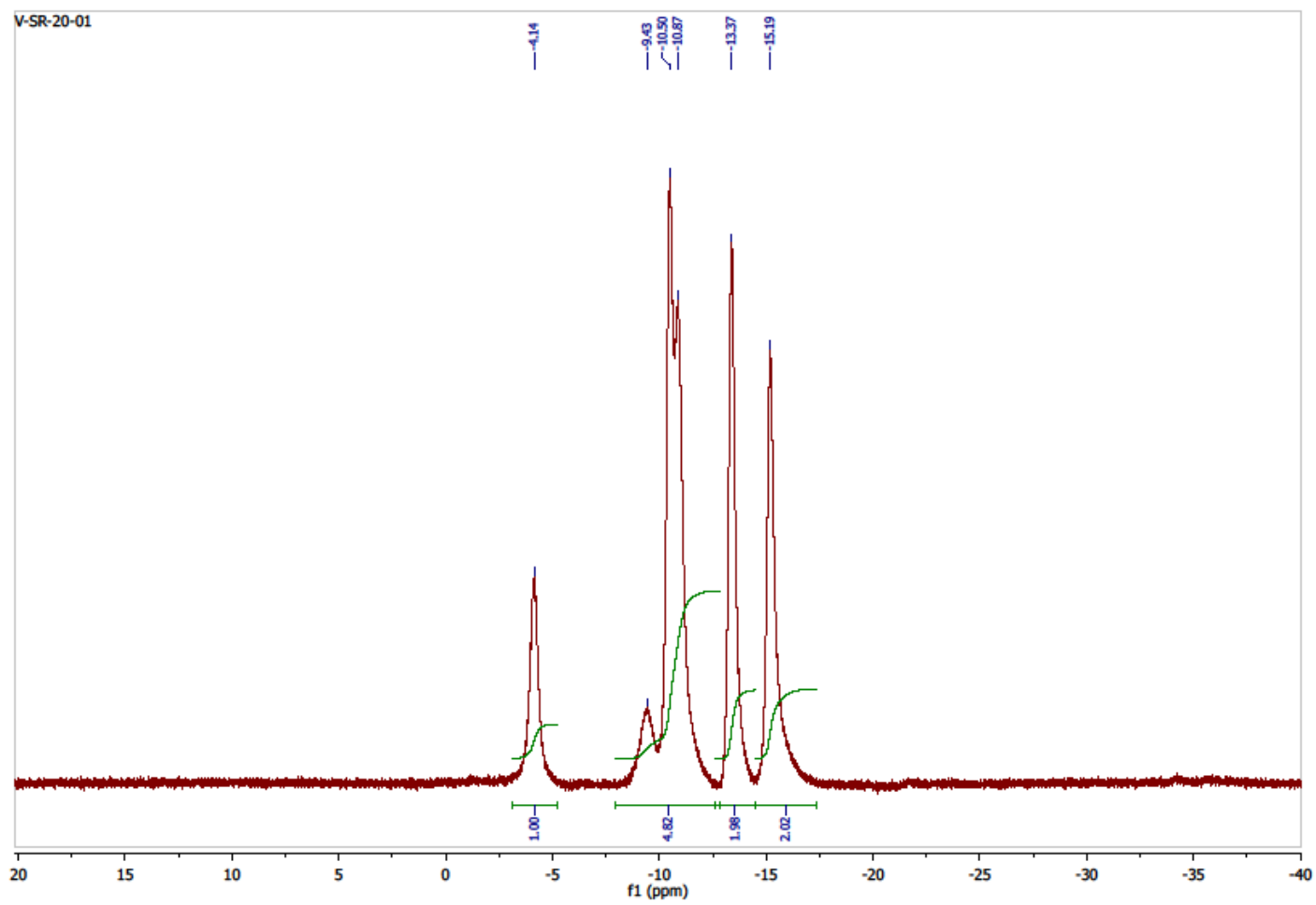


Figure S117. ^{11}B NMR (^1H BB) spectrum of 35.

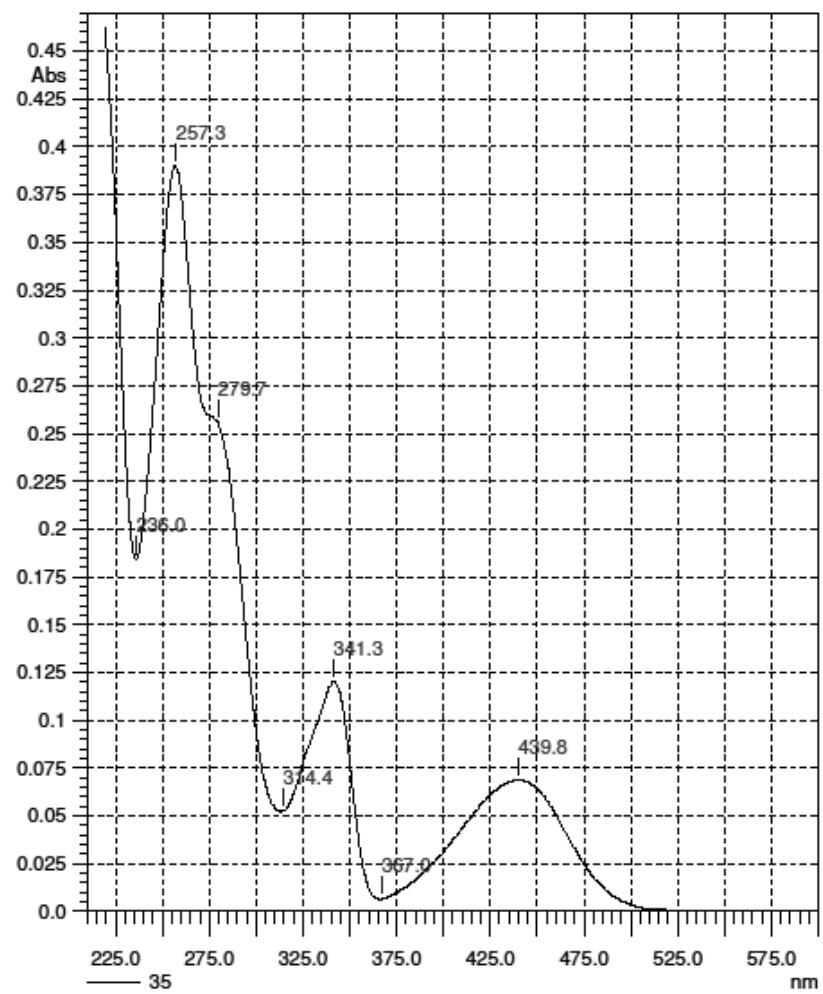


Figure S118. UV spectrum of 35.

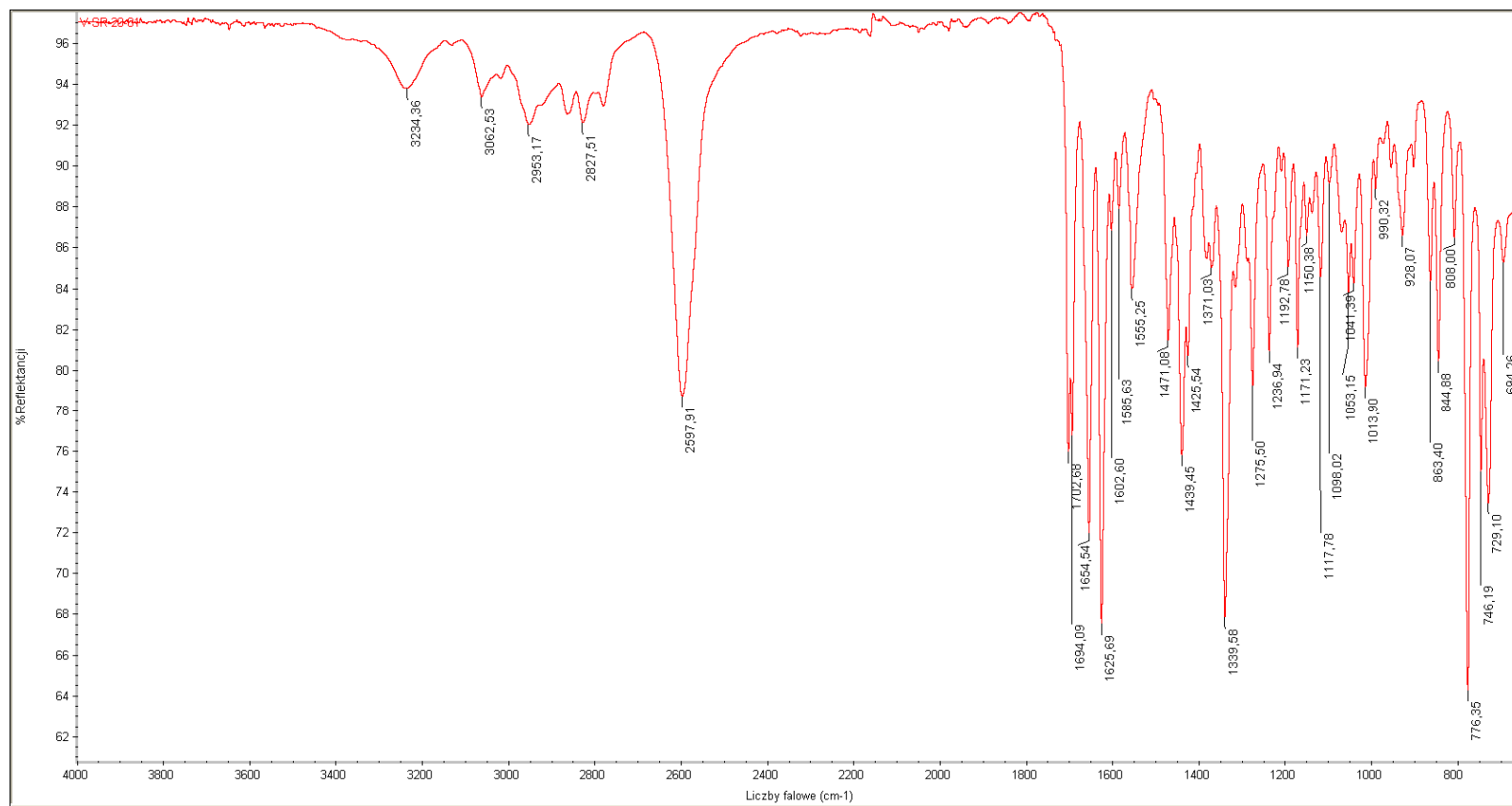


Figure S119. IR spectrum of 35.

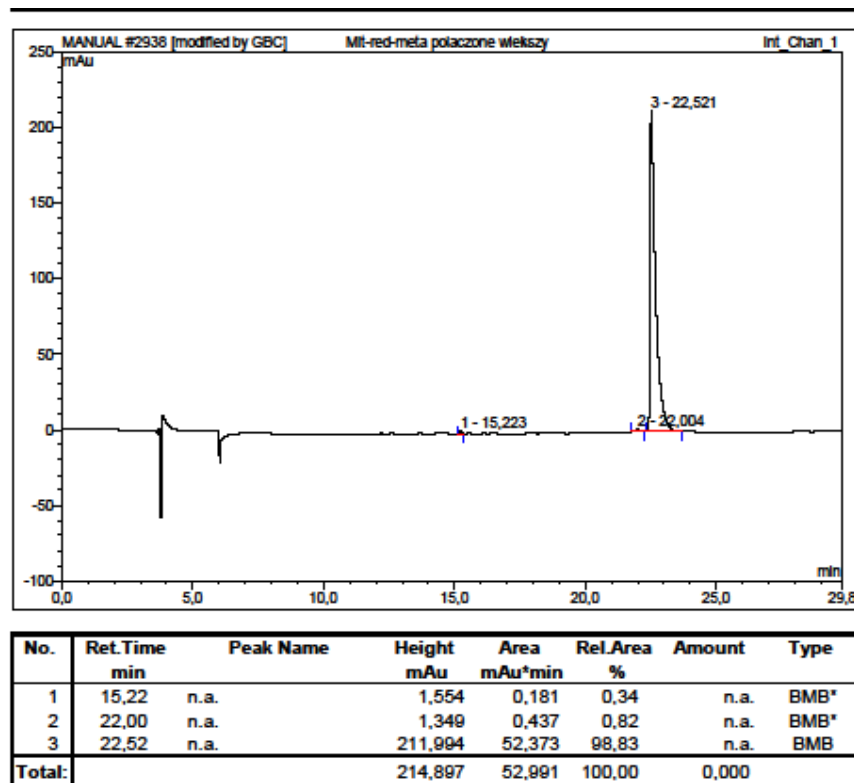


Figure S120. HPLC analysis of 35.

Spectrum Name: V-SR-20-01
Start Ion: 350
End Ion: 550
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

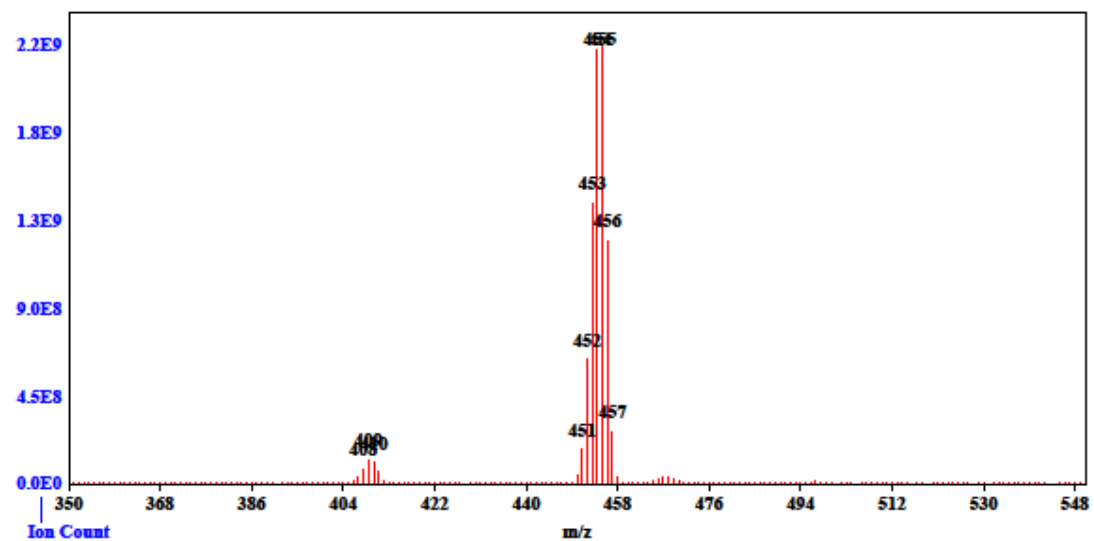


Figure S121. MS spectrum of 35.

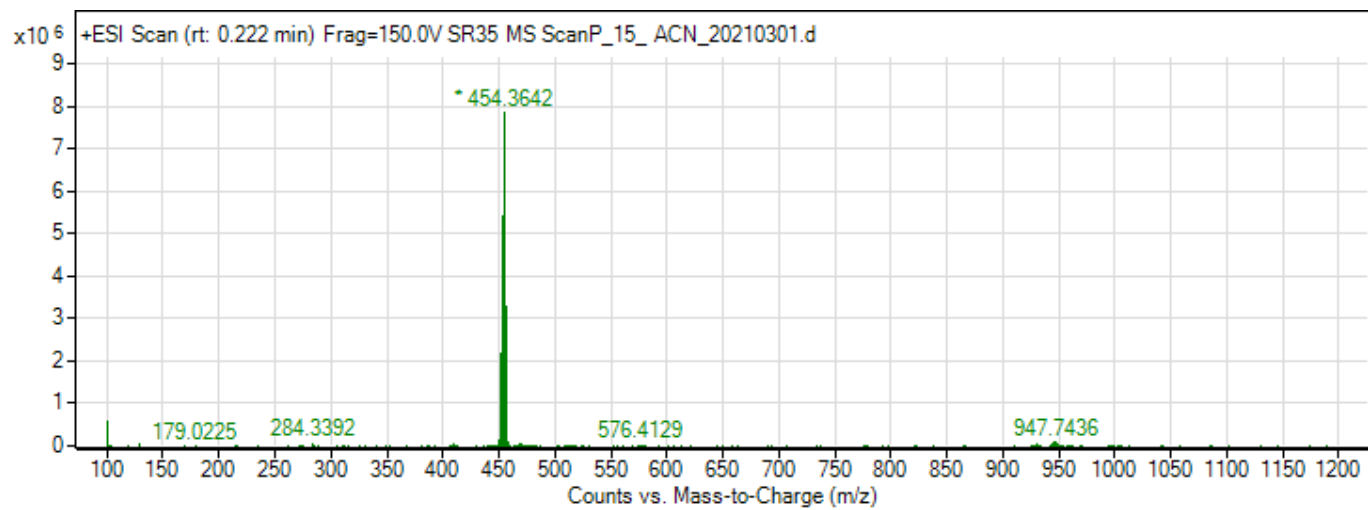


Figure S122. HRMS spectrum of 35.

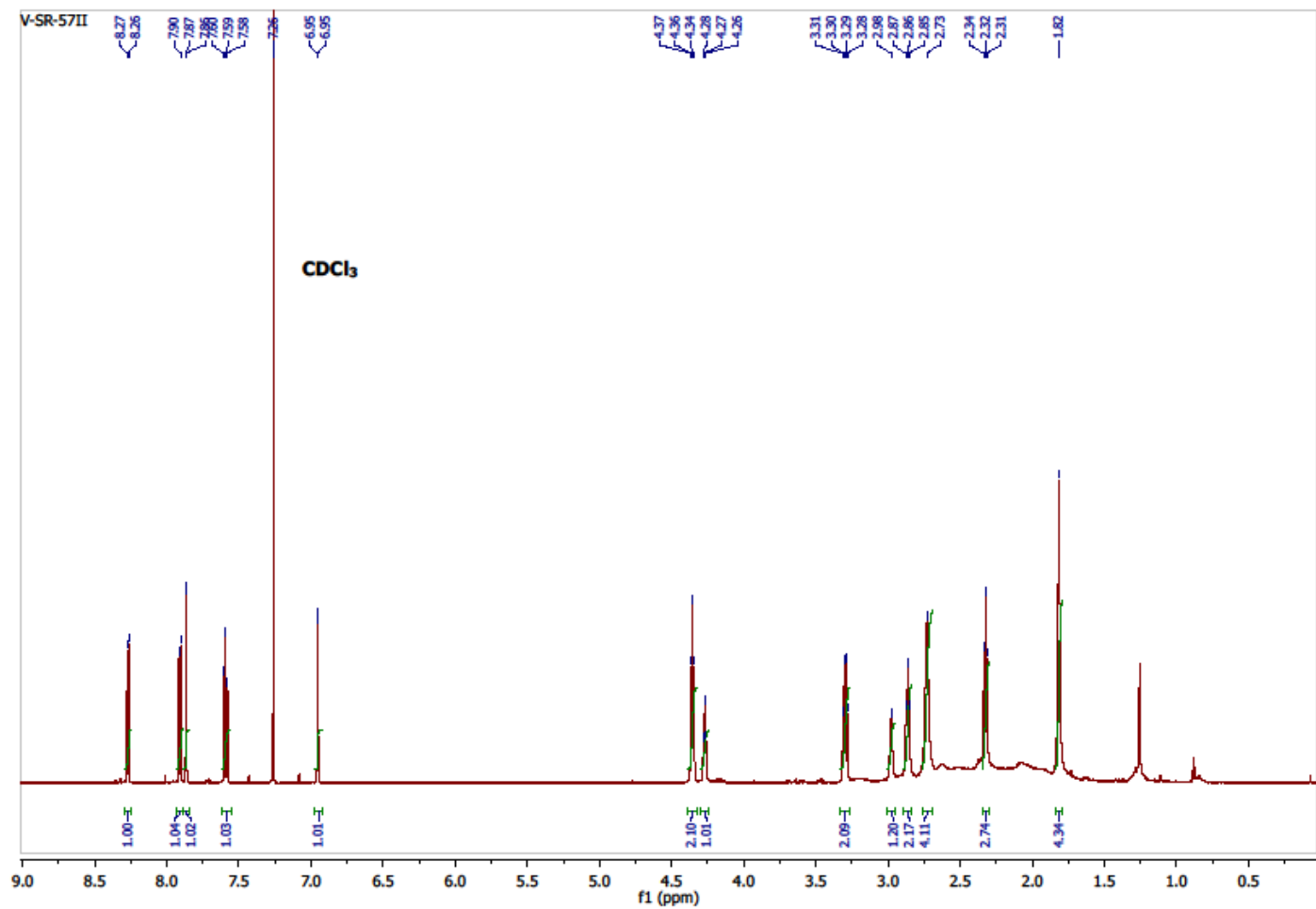


Figure S123. ¹H NMR spectrum of 36.

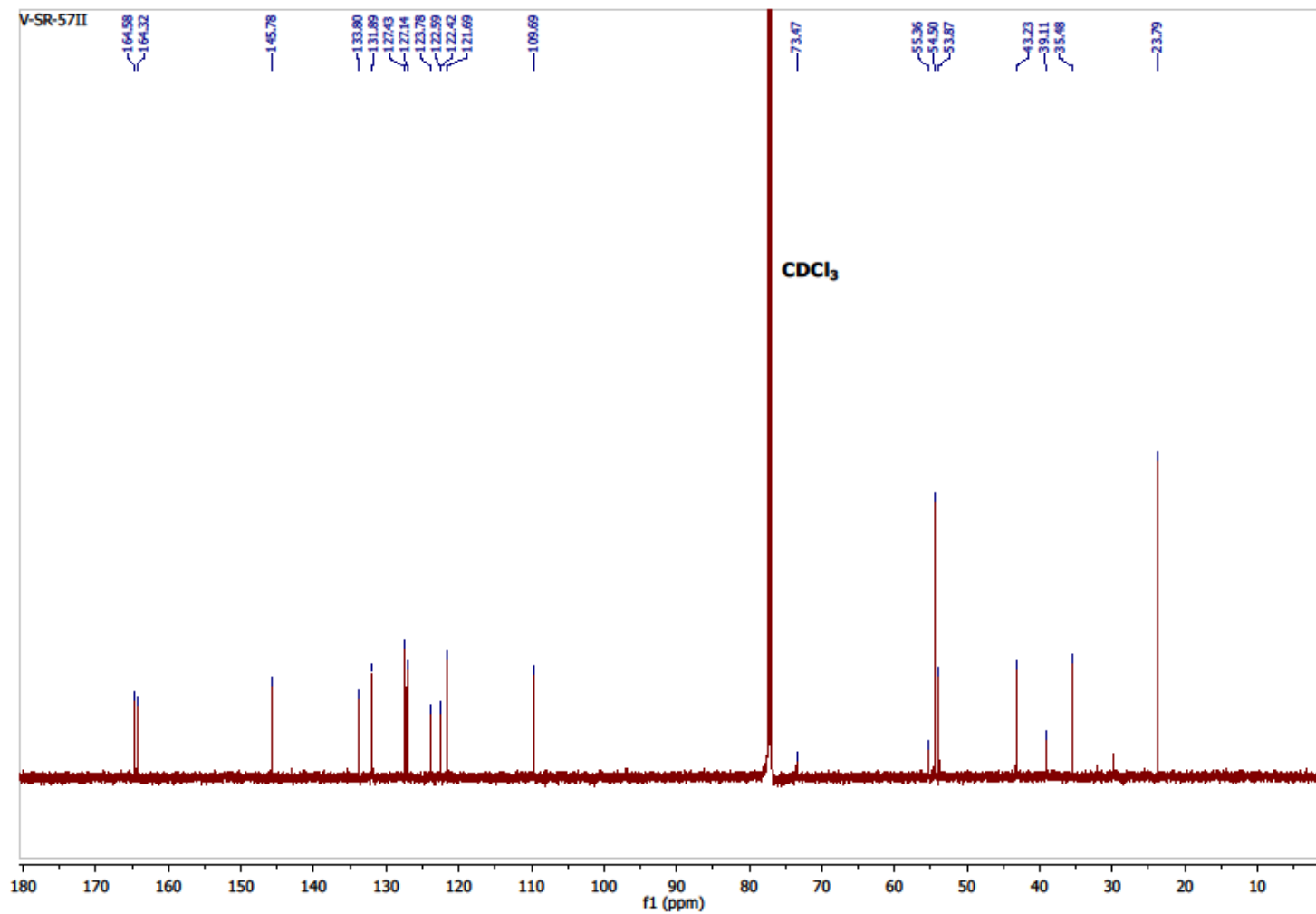


Figure S124. ¹³C NMR spectrum of 36.

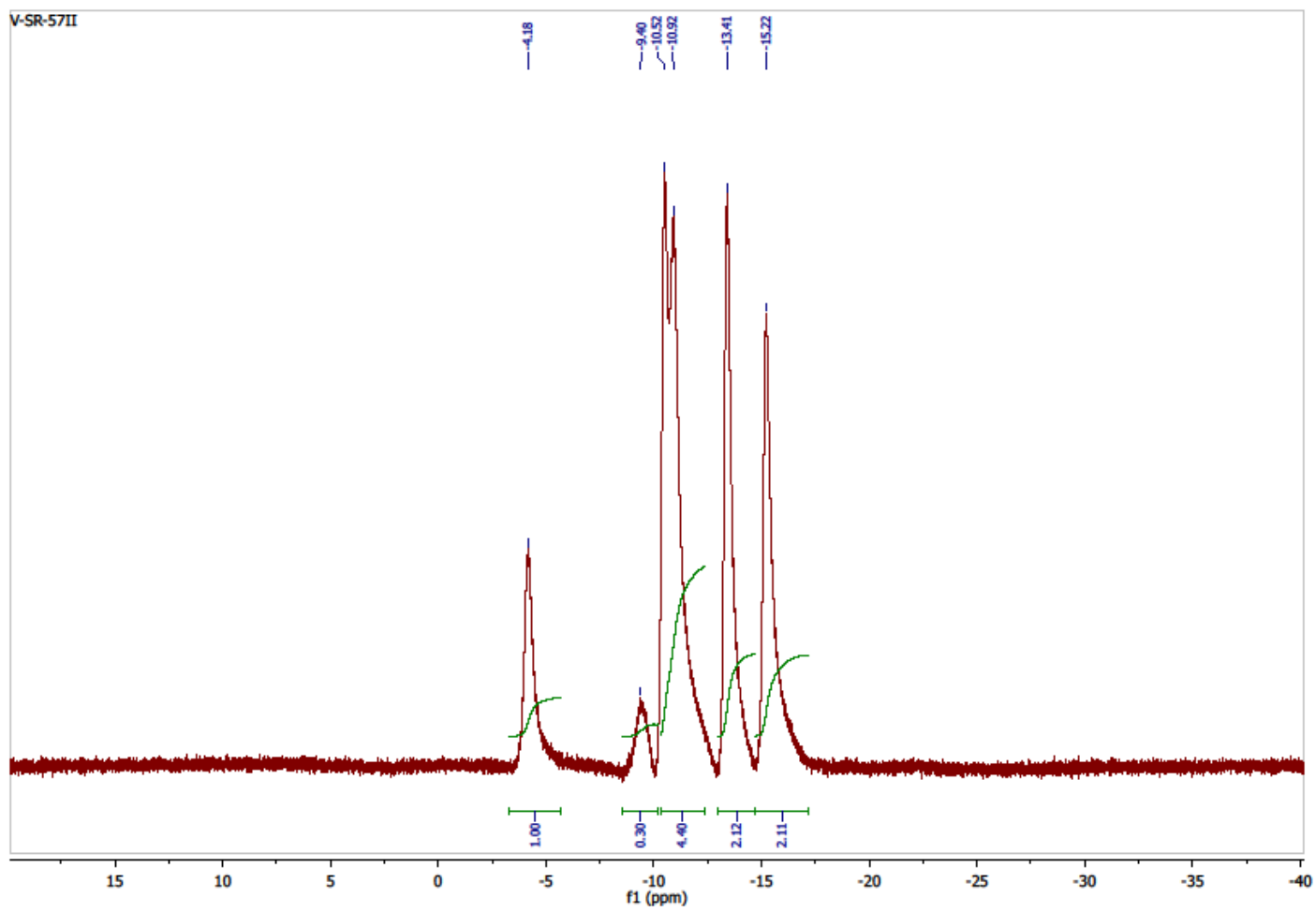


Figure S125. ^{11}B NMR (^1H BB) spectrum of **36**.

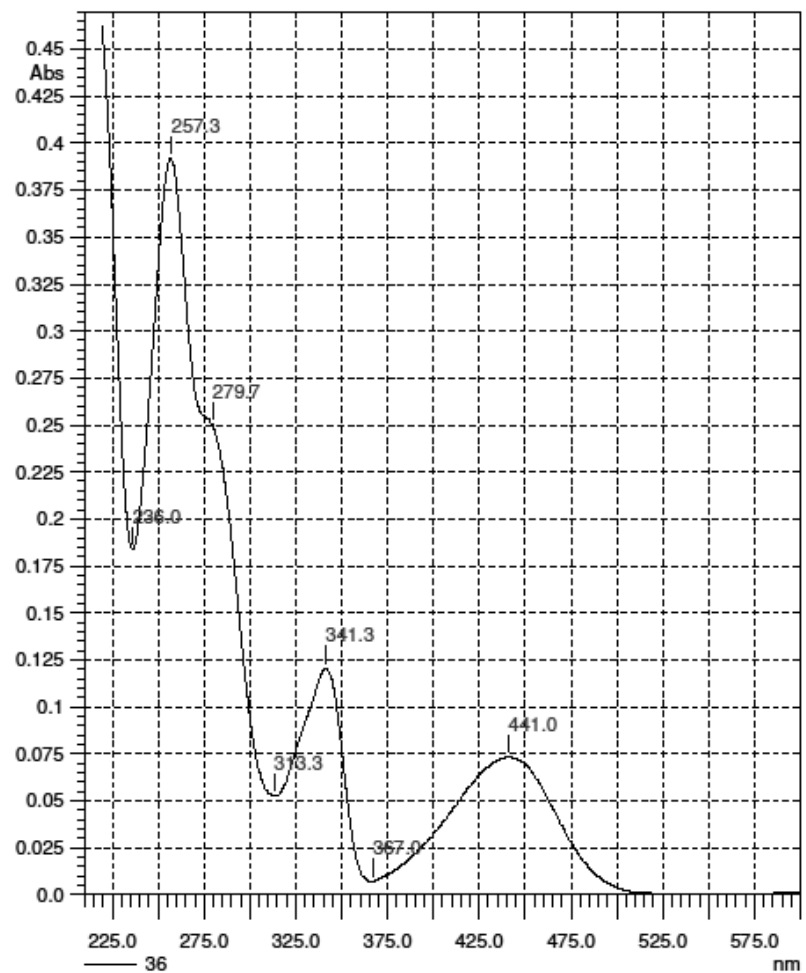


Figure S126. UV spectrum of 36.

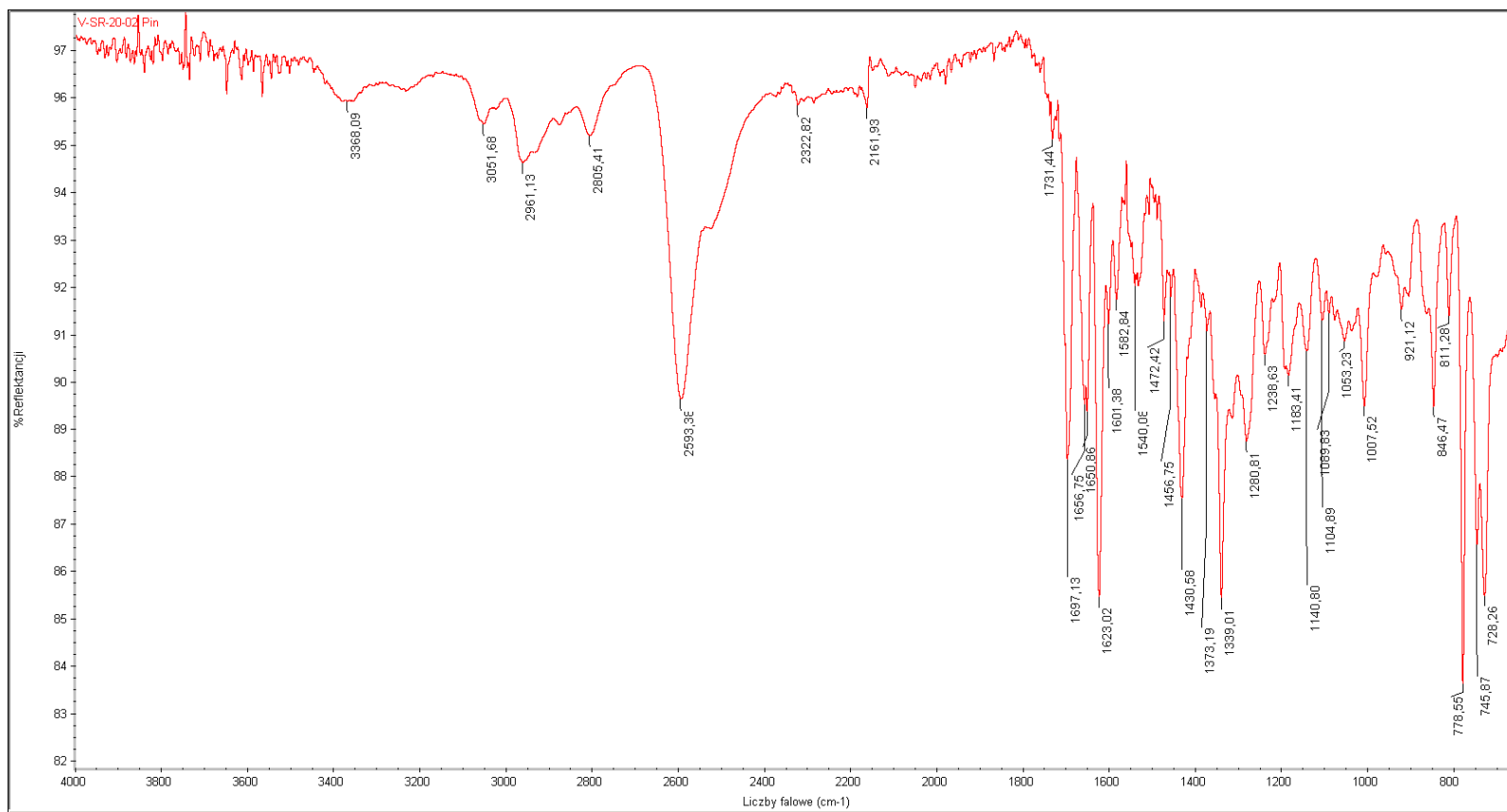


Figure S127. IR spectrum of 36.

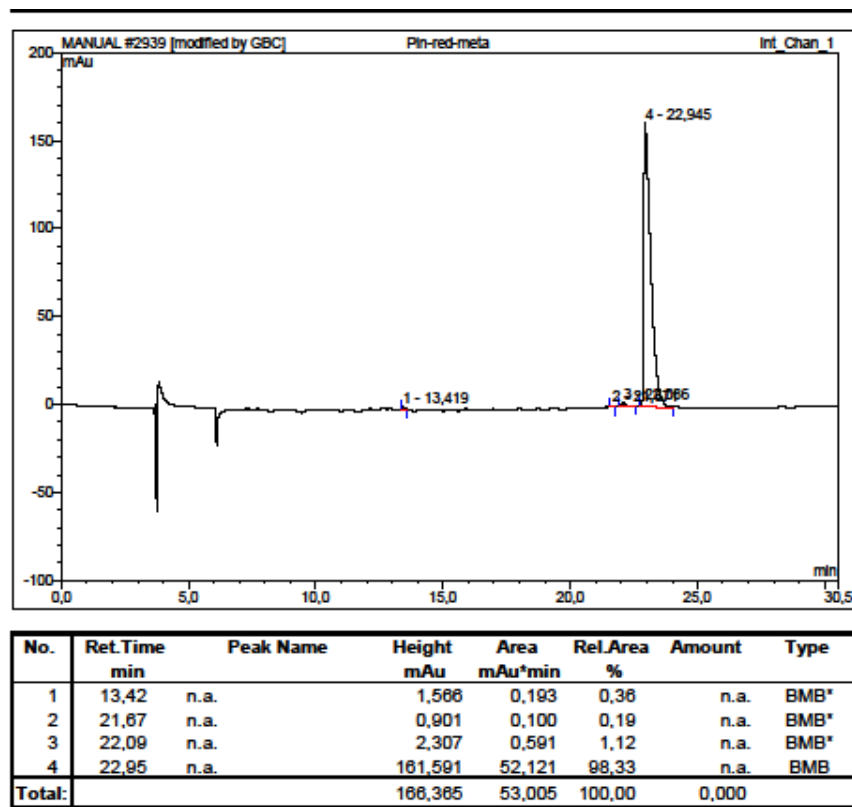


Figure S128. HPLC analysis of 36.

Spectrum Name: V-SR-57
Start Ion: 400
End Ion: 600
Source: APCI + 10.0 μ A 400C
Capillary: 150V 300C Offset: 25V Span: 0V

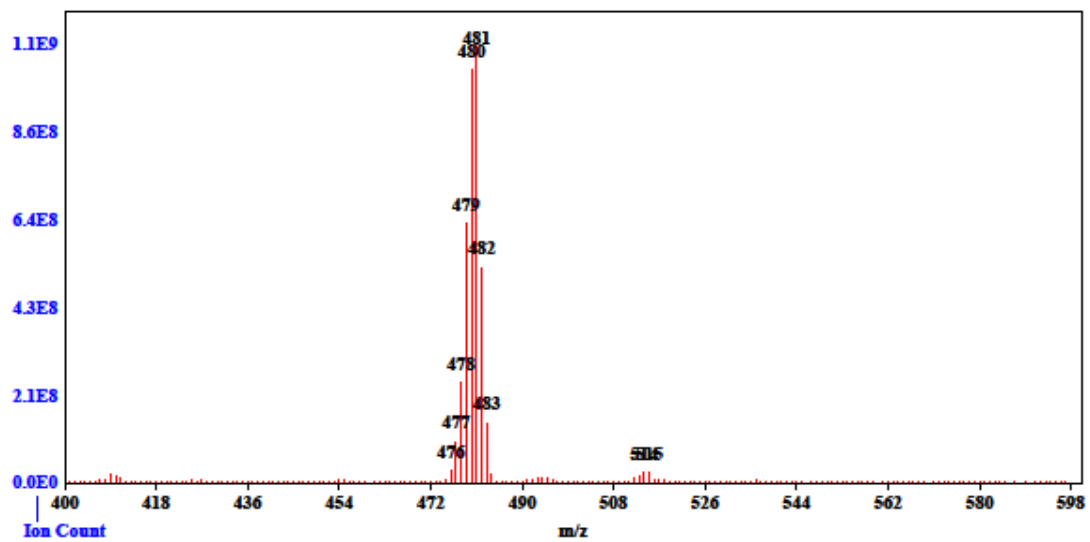


Figure S129. MS spectrum of 36.

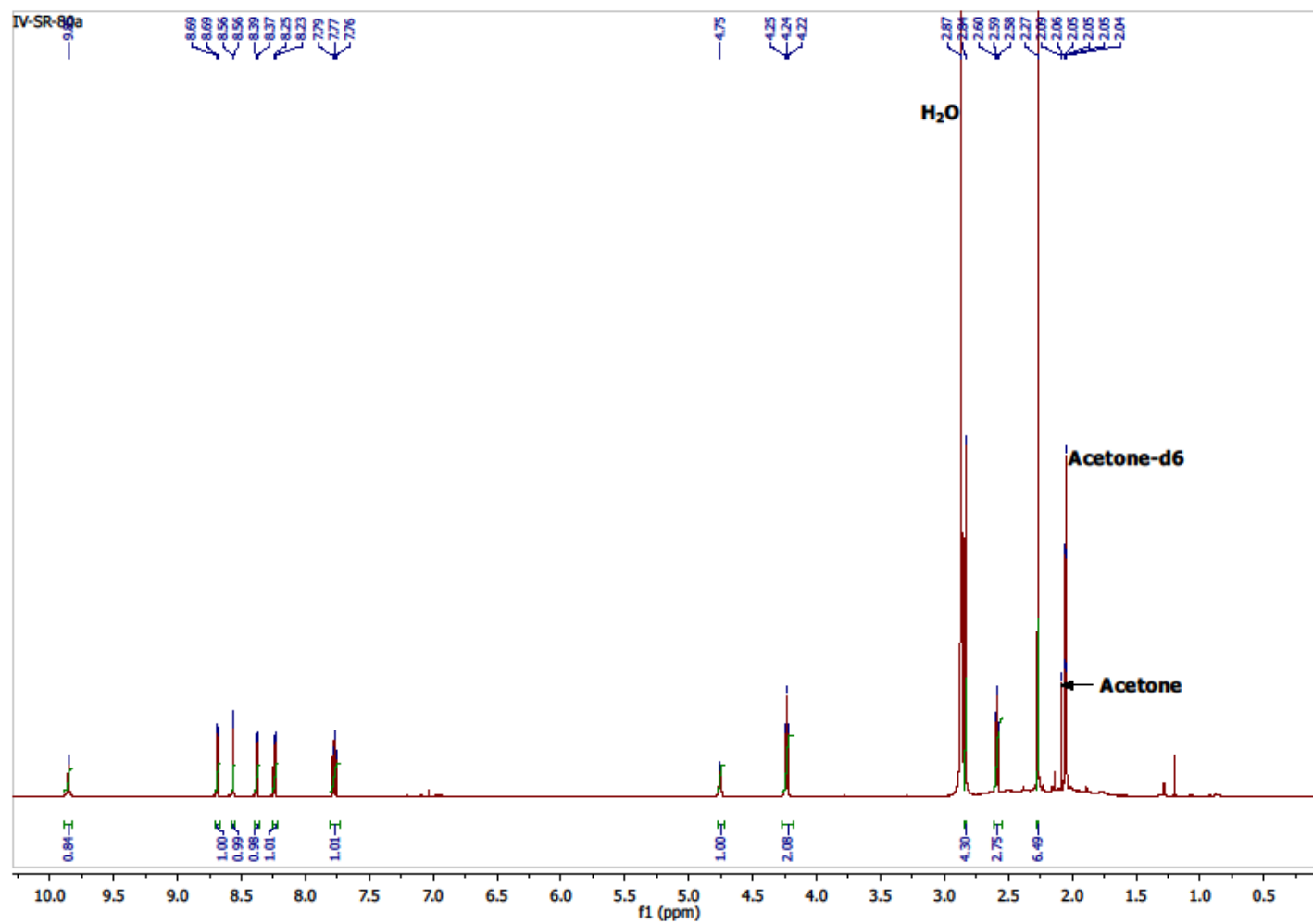


Figure S130. ¹H NMR spectrum of 39.

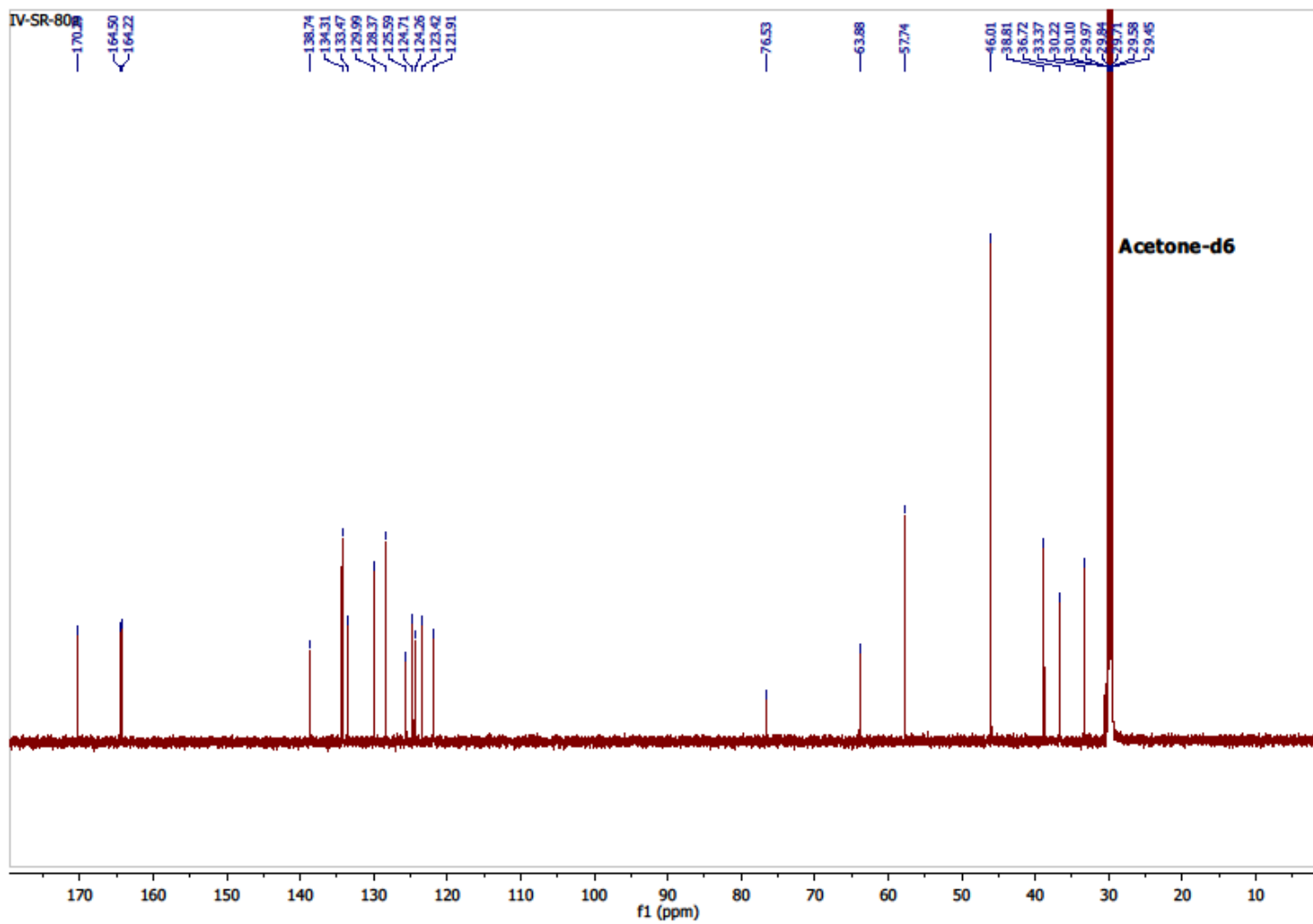


Figure S131. ^{13}C NMR spectrum of 39.

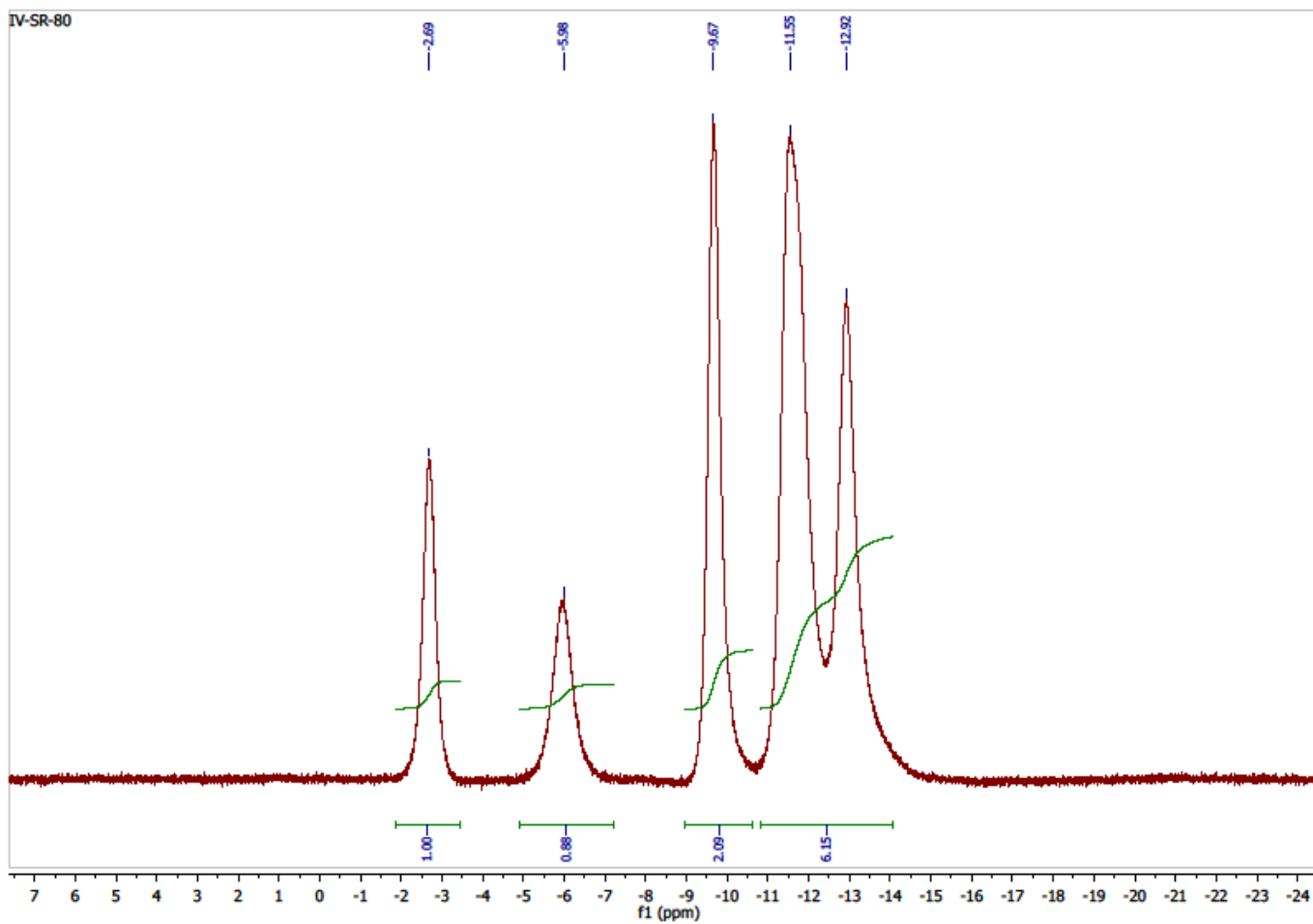


Figure S132. ^{11}B NMR (^1H BB) spectrum of 39.

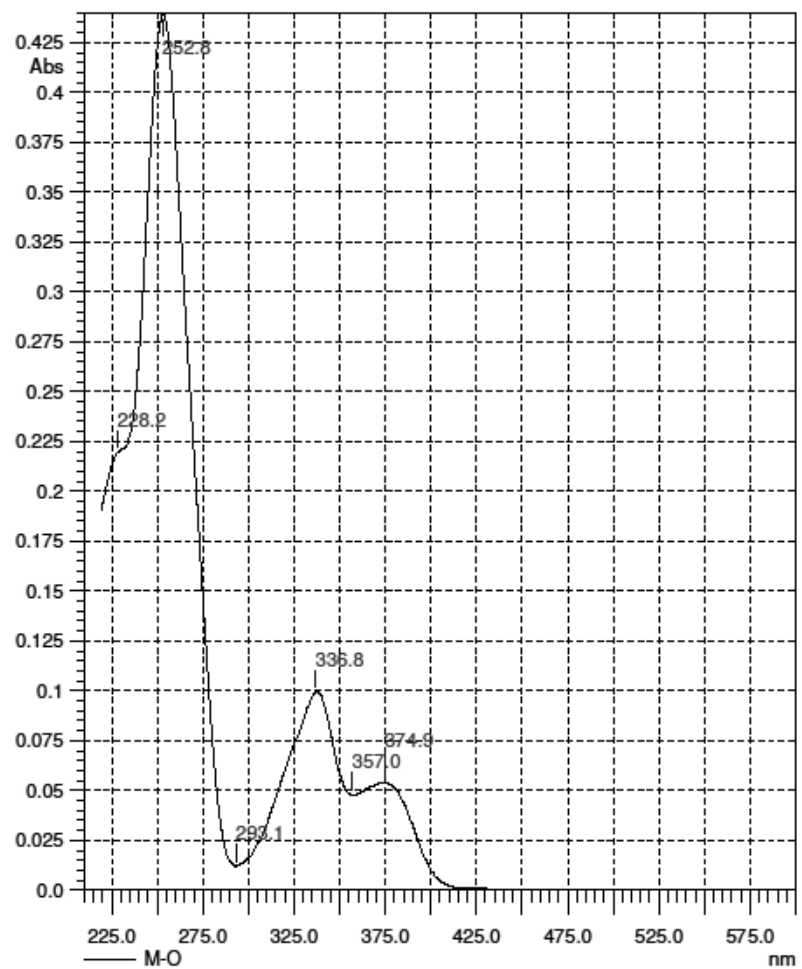


Figure S133. UV spectrum of 39.

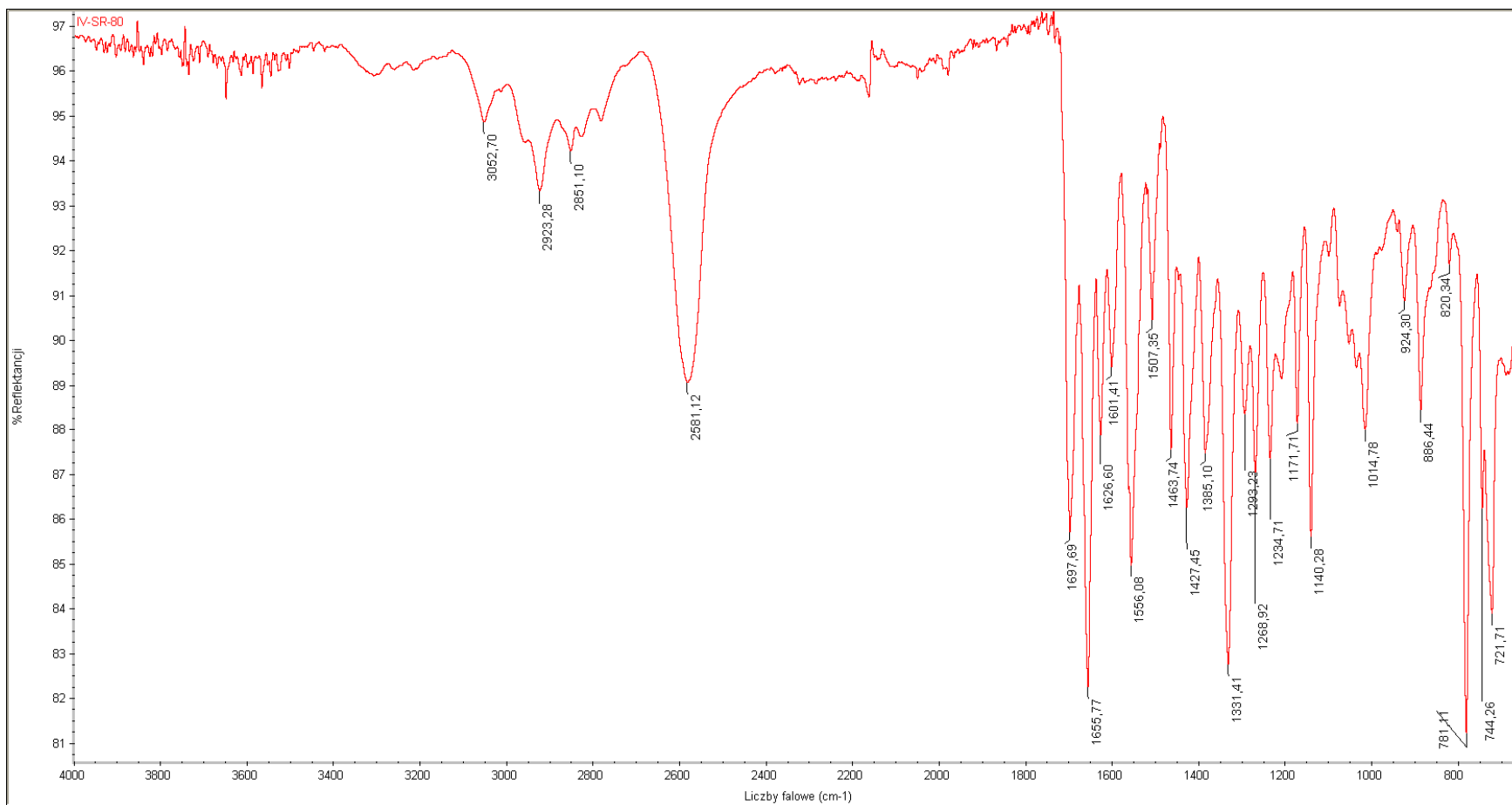
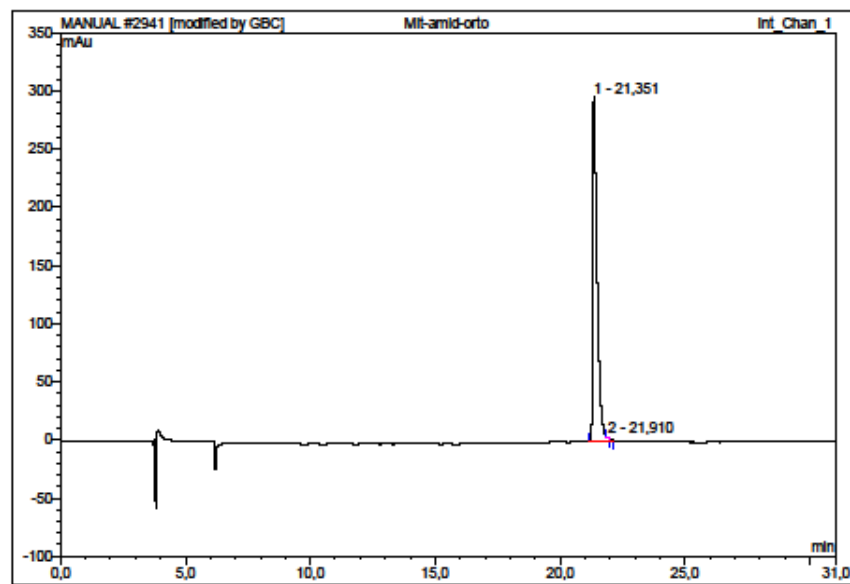


Figure S134. IR spectrum of 39.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	21,35	n.a.	296,387	60,775	99,89	n.a.	BMB*
2	21,91	n.a.	0,740	0,068	0,11	n.a.	Rd*
Total:			297,127	60,843	100,00	0,000	

Figure S135. HPLC analysis of 39.

Spectrum Name: IV-SR-80
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

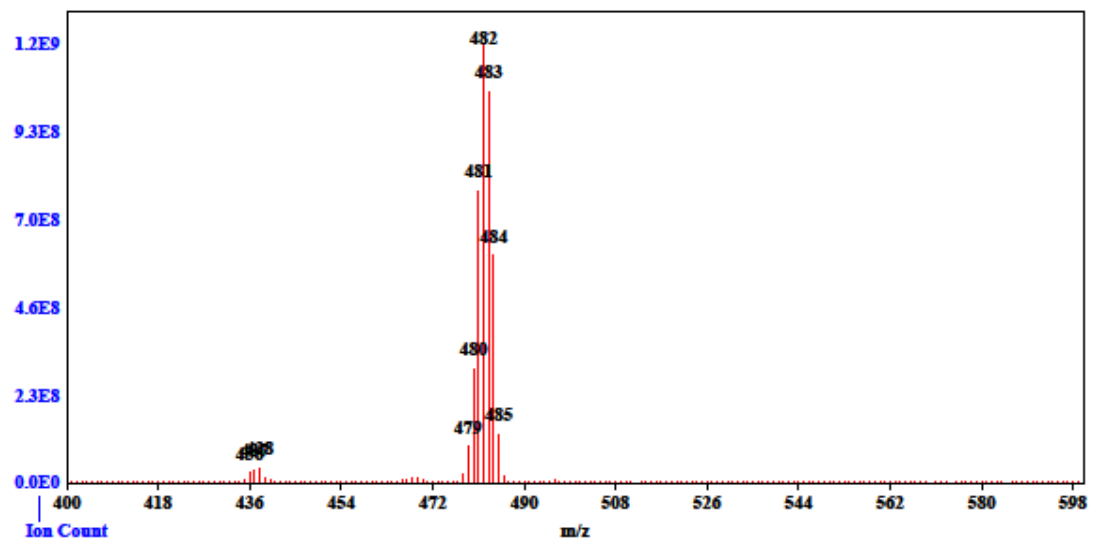


Figure S136. MS spectrum of 39.

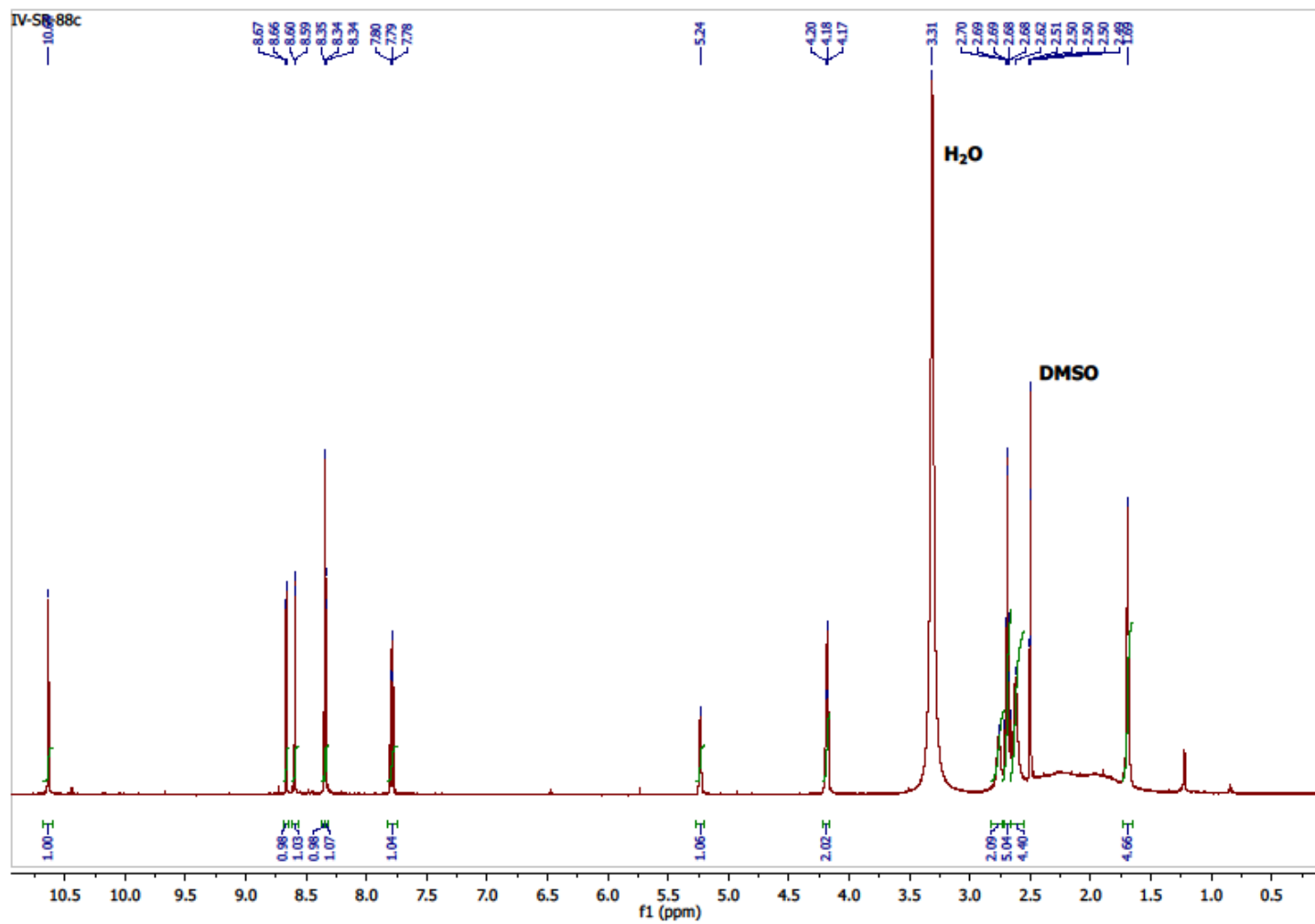


Figure S137. ¹H NMR spectrum of 40.

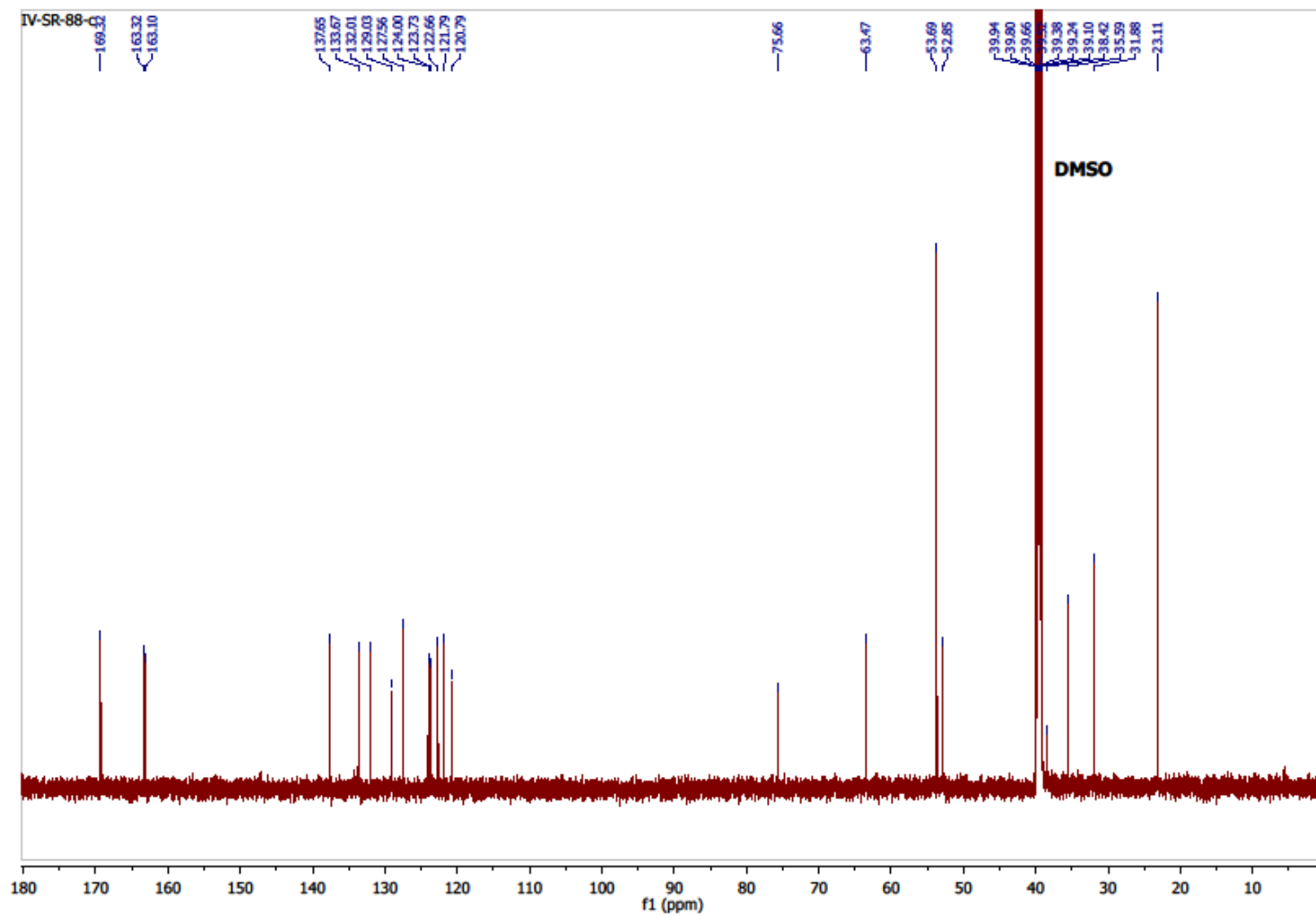


Figure S138. ^{13}C NMR spectrum of 40.

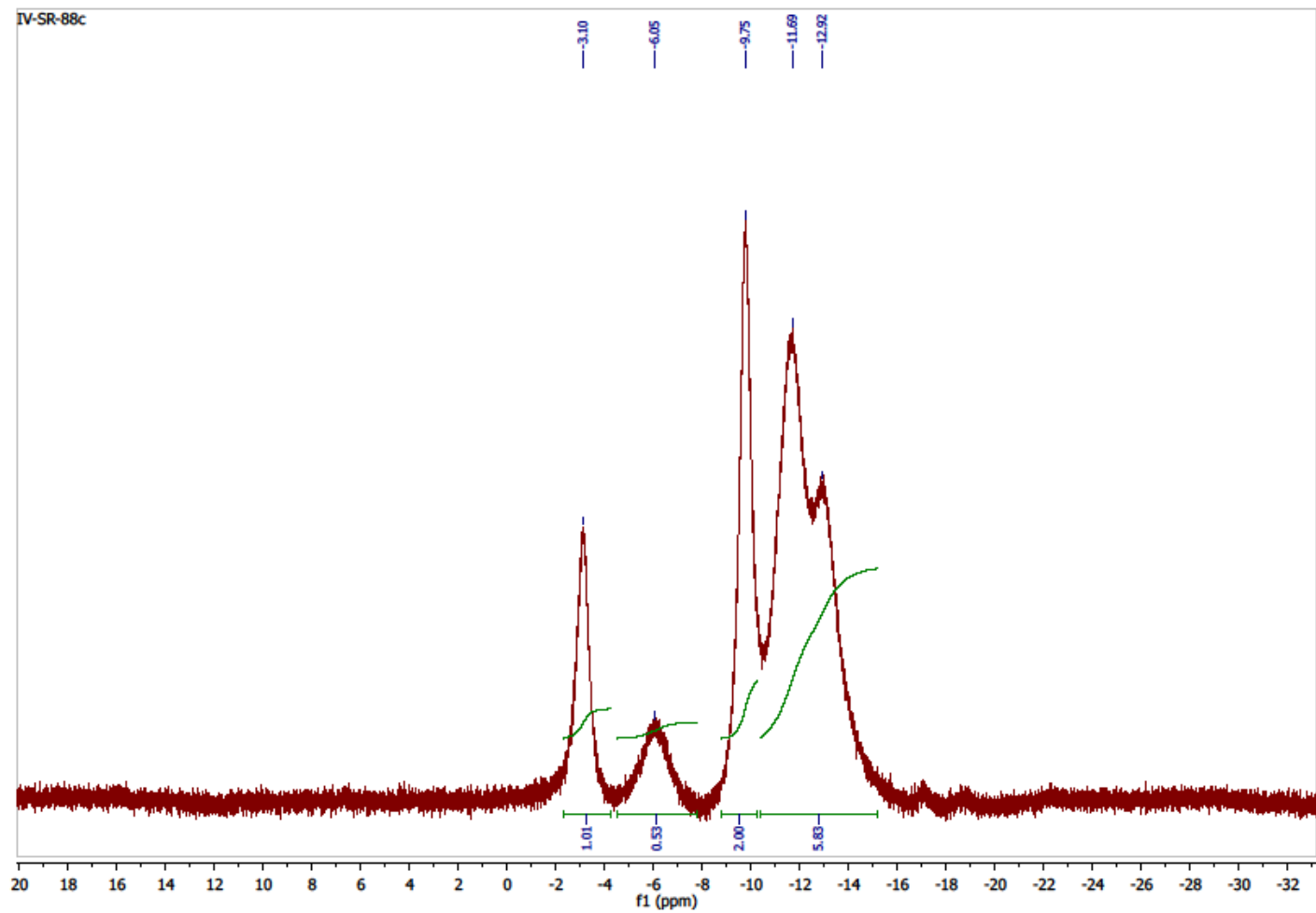


Figure S139. ^{11}B NMR $\{^1\text{H BB}\}$ spectrum of 40.

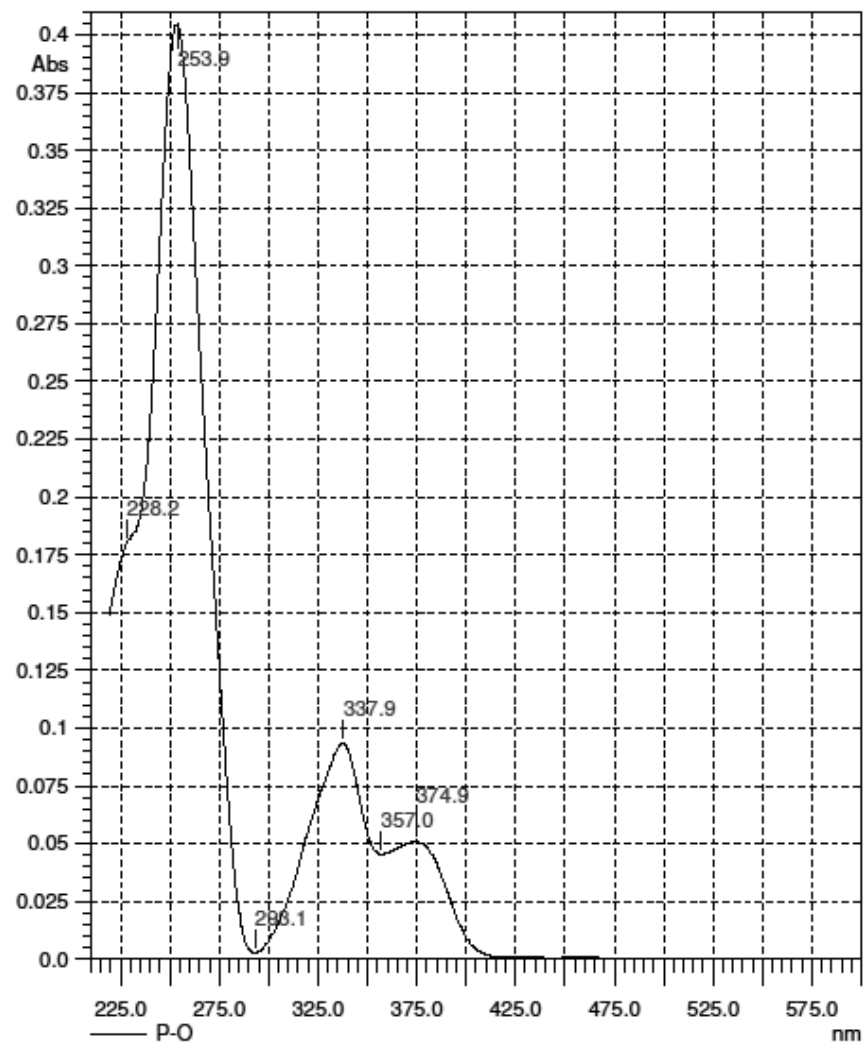


Figure S140. UV spectrum of 40.

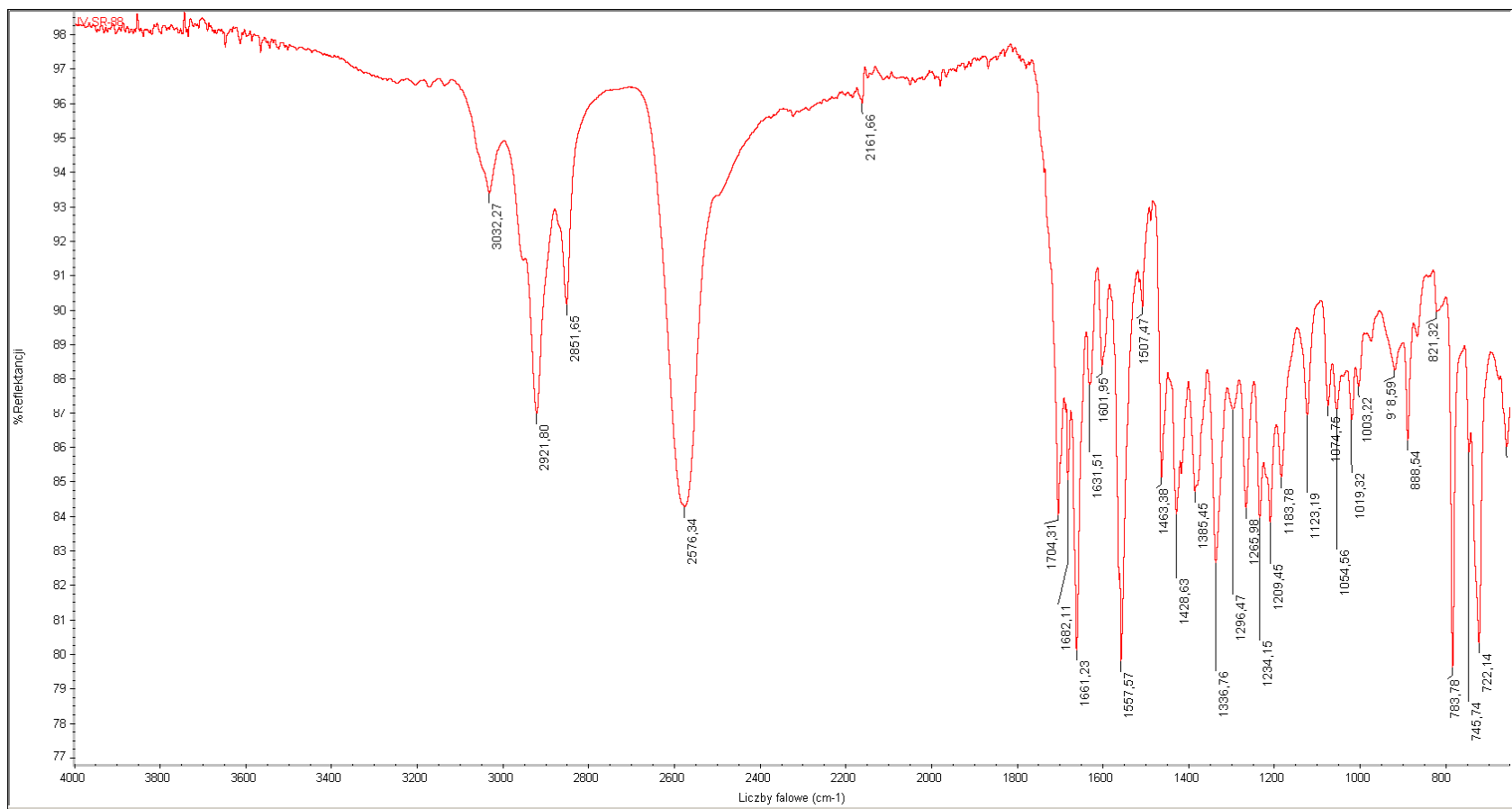
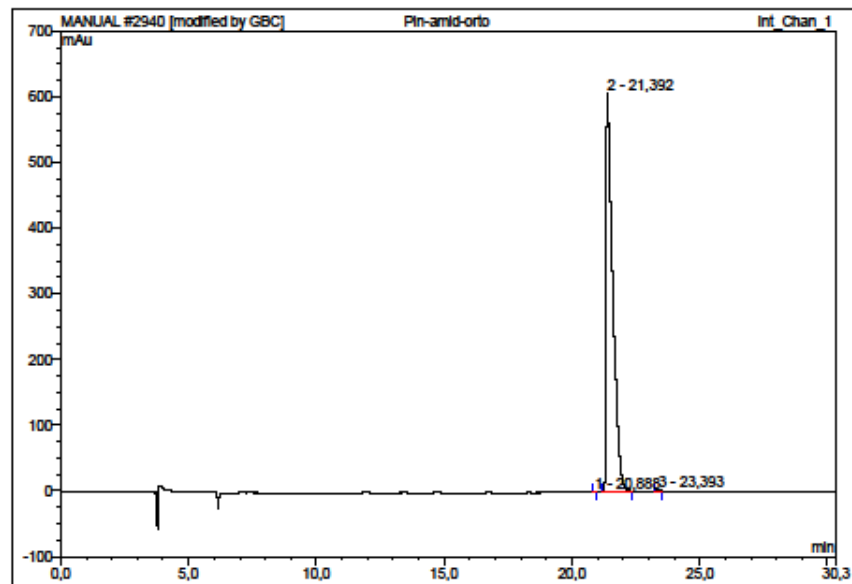


Figure S141. IR spectrum of 40.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	20,89	n.a.	0,743	0,064	0,03	n.a.	BMB*
2	21,39	n.a.	606,469	181,277	99,65	n.a.	BMB
3	23,39	n.a.	3,461	0,571	0,31	n.a.	BMB*
Total:			610,674	181,911	100,00	0,000	

Figure S142. HPLC analysis of 40.

Spectrum Name: IV-SR-88
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

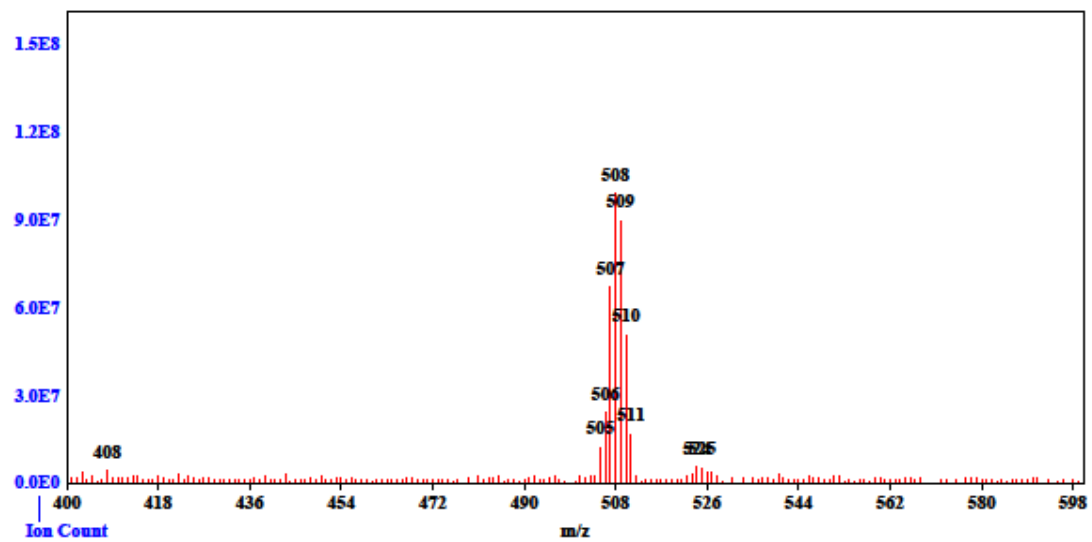


Figure S143. MS spectrum of 40.

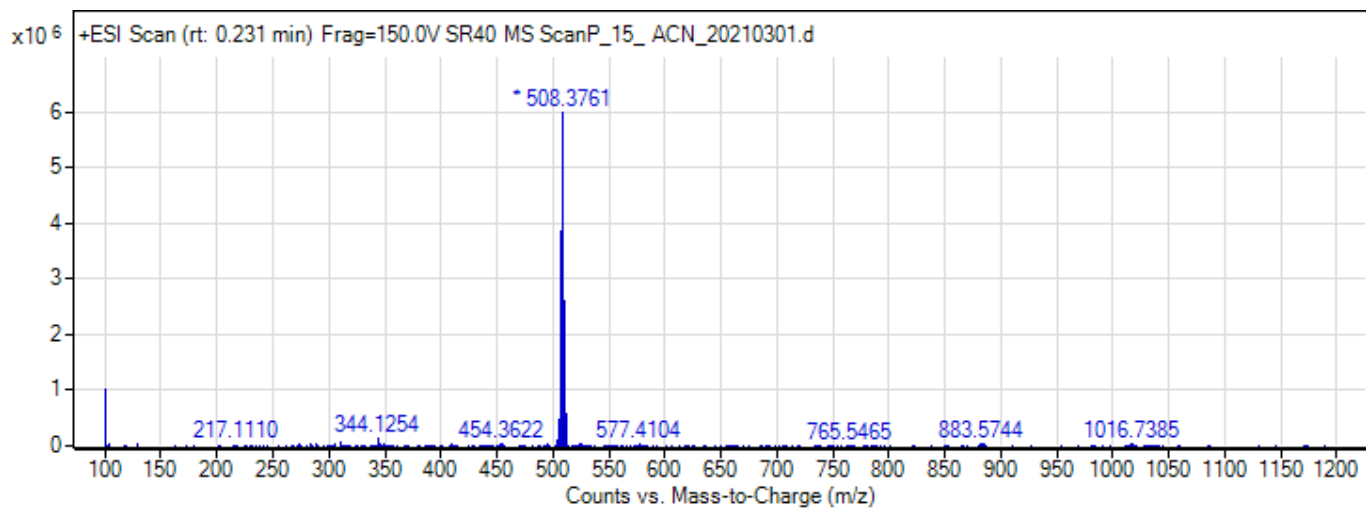


Figure S144. HRMS spectrum of 40.

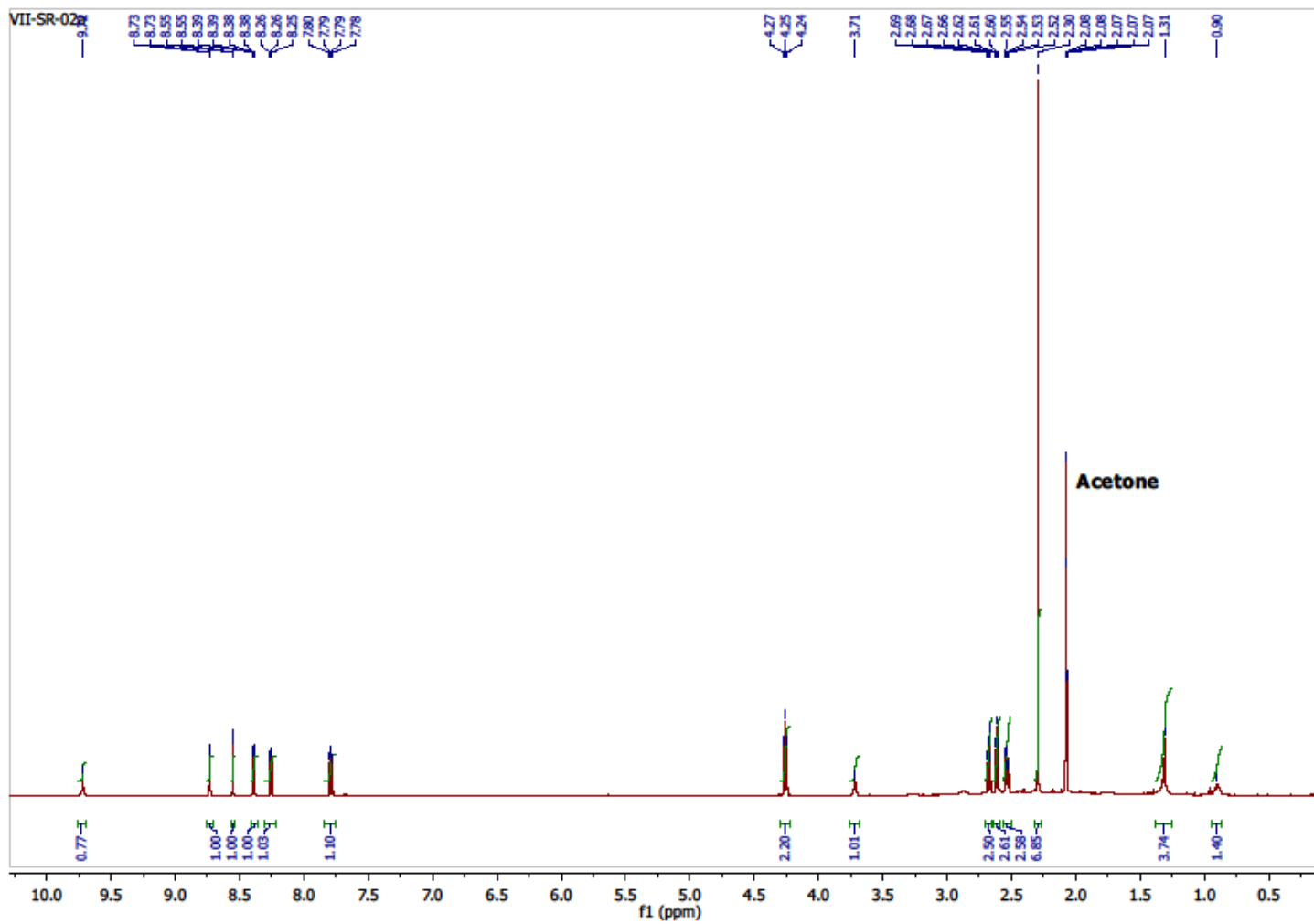


Figure S145. ^1H NMR spectrum of **41**.

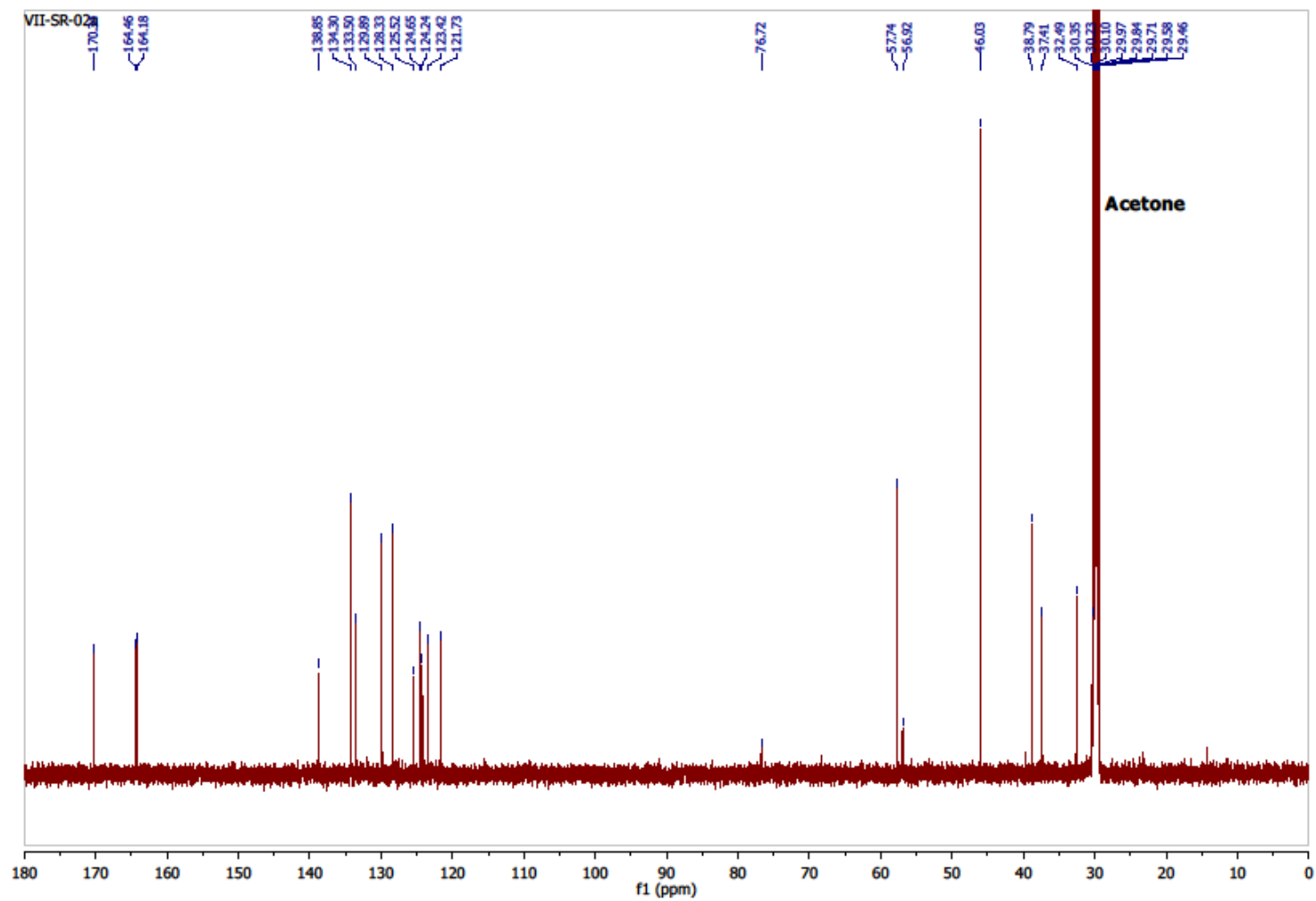


Figure S146. ^{13}C NMR spectrum of 41.

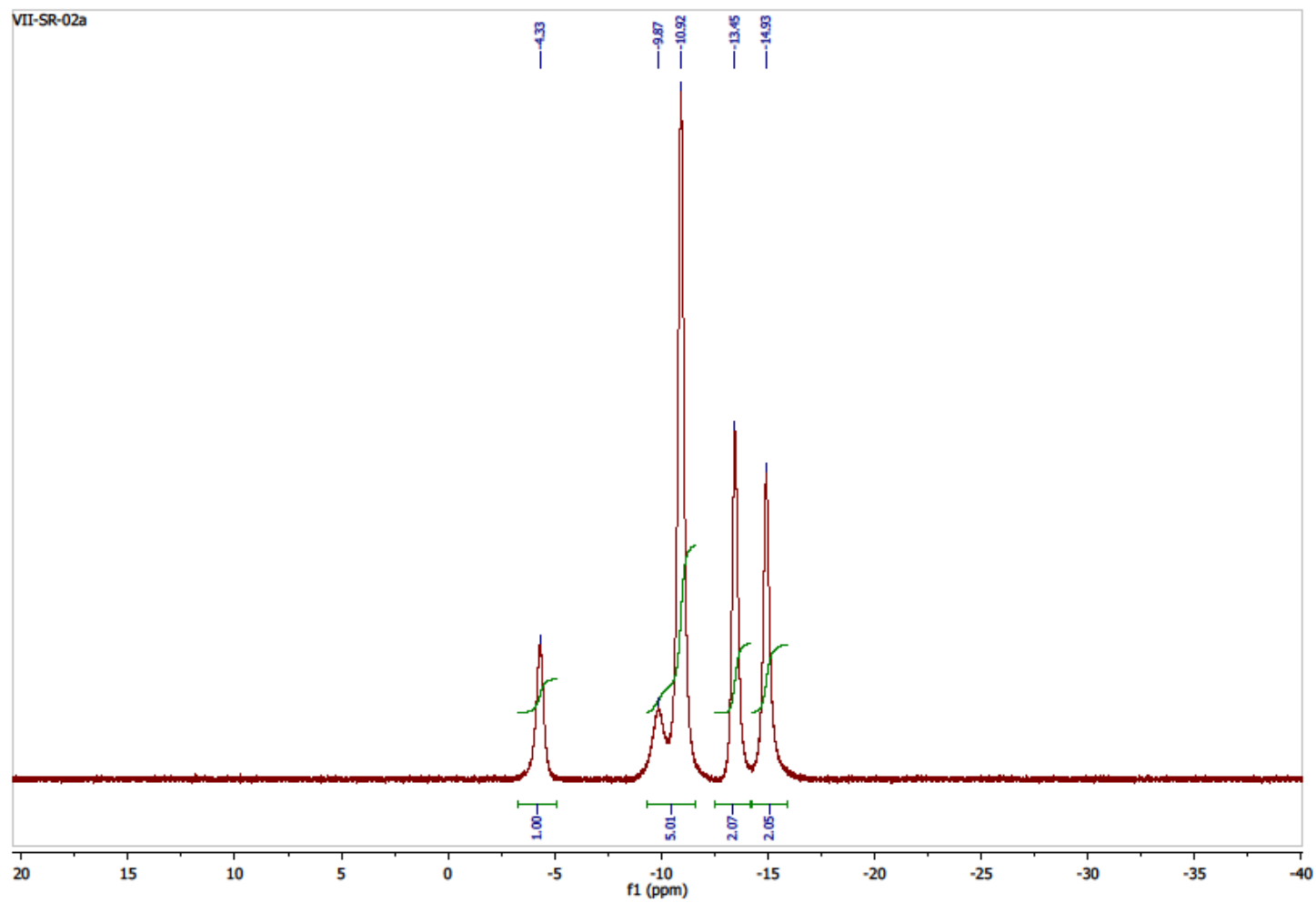


Figure S147. IR spectrum of 41.

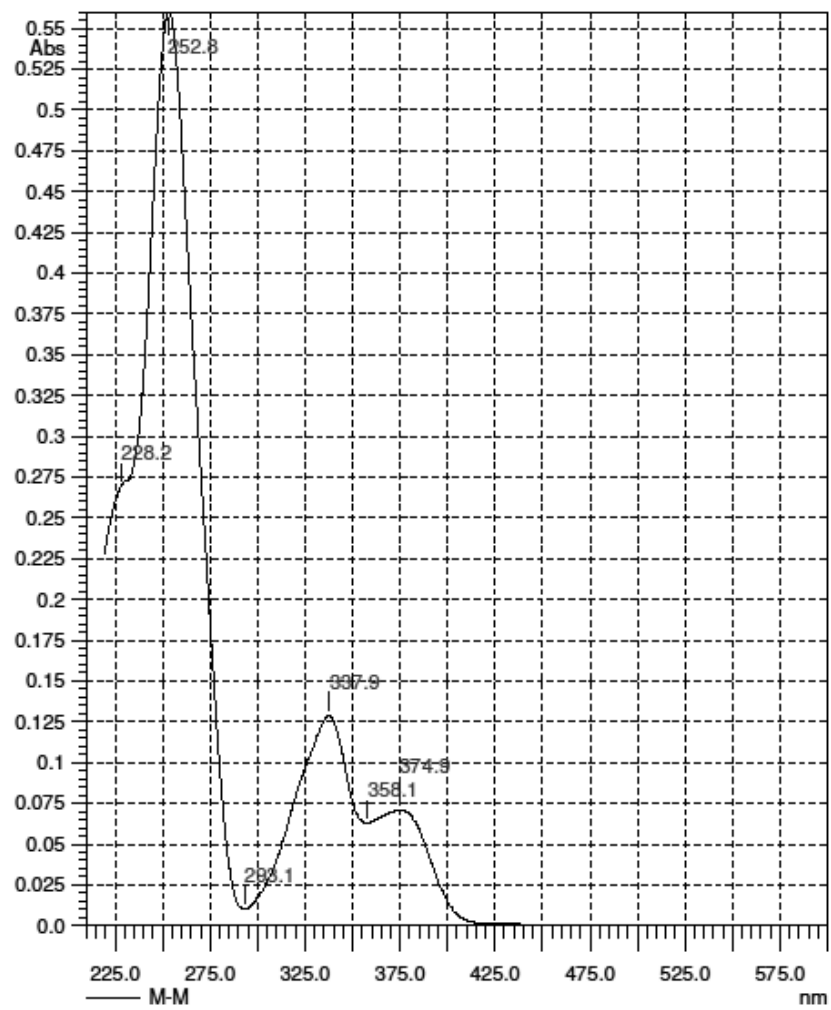


Figure S148. UV spectrum of 41.

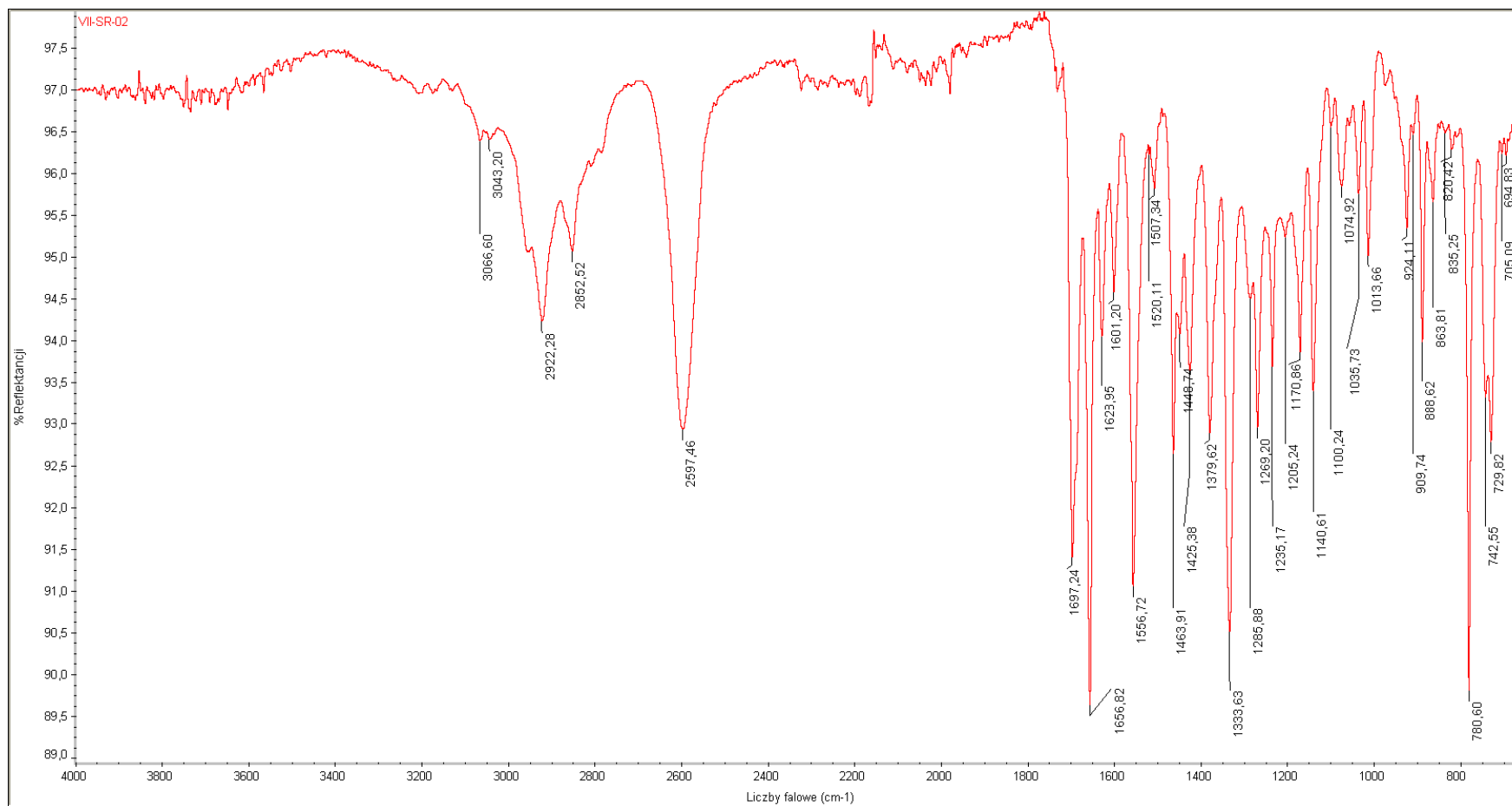
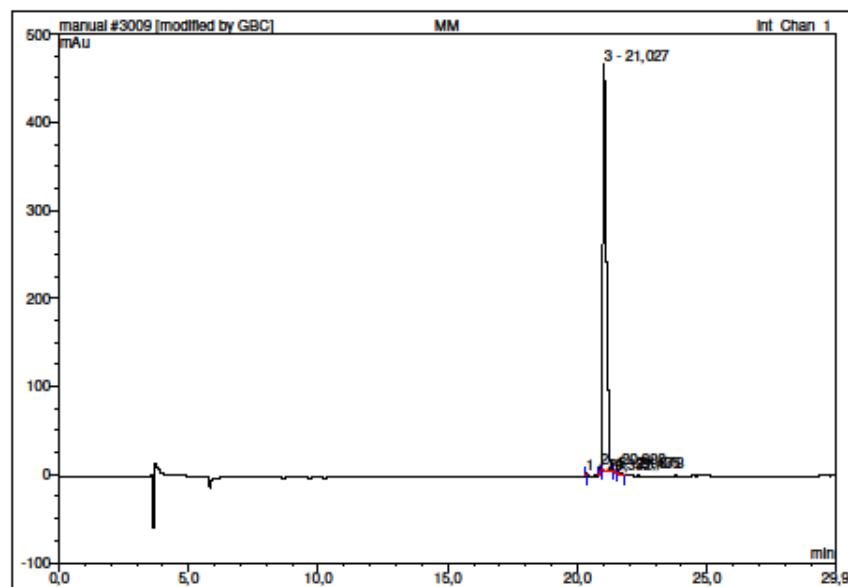


Figure S149. IR spectrum of 41.



No.	Ret.Time min	Peak Name	Height mAu	Area mAu*min	Rel.Area %	Amount	Type
1	20,33	n.a.	3,809	0,284	0,39	n.a.	BMB*
2	20,88	n.a.	6,404	0,384	0,52	n.a.	BMB*
3	21,03	n.a.	460,312	72,780	98,54	n.a.	bMB*
4	21,44	n.a.	1,057	0,068	0,09	n.a.	BMB*
5	21,58	n.a.	2,437	0,339	0,46	n.a.	BMB*
Total:			474,019	73,856	100,00	0,000	

Figure S150. HPLC analysis of 41.

Spectrum Name: VII-SR-02
Start Ion: 400
End Ion: 570
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

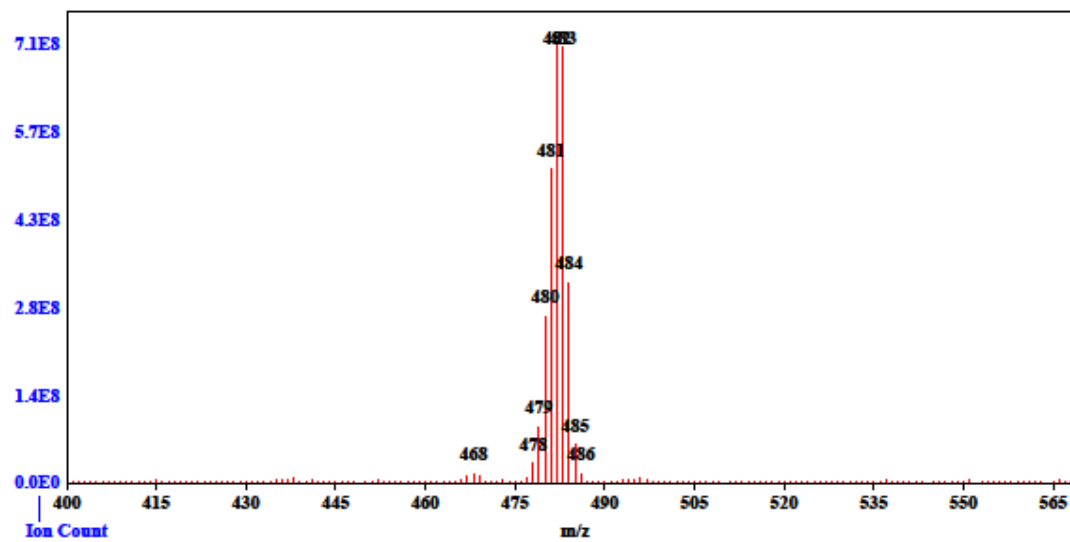


Figure S151. MS spectrum of 41.

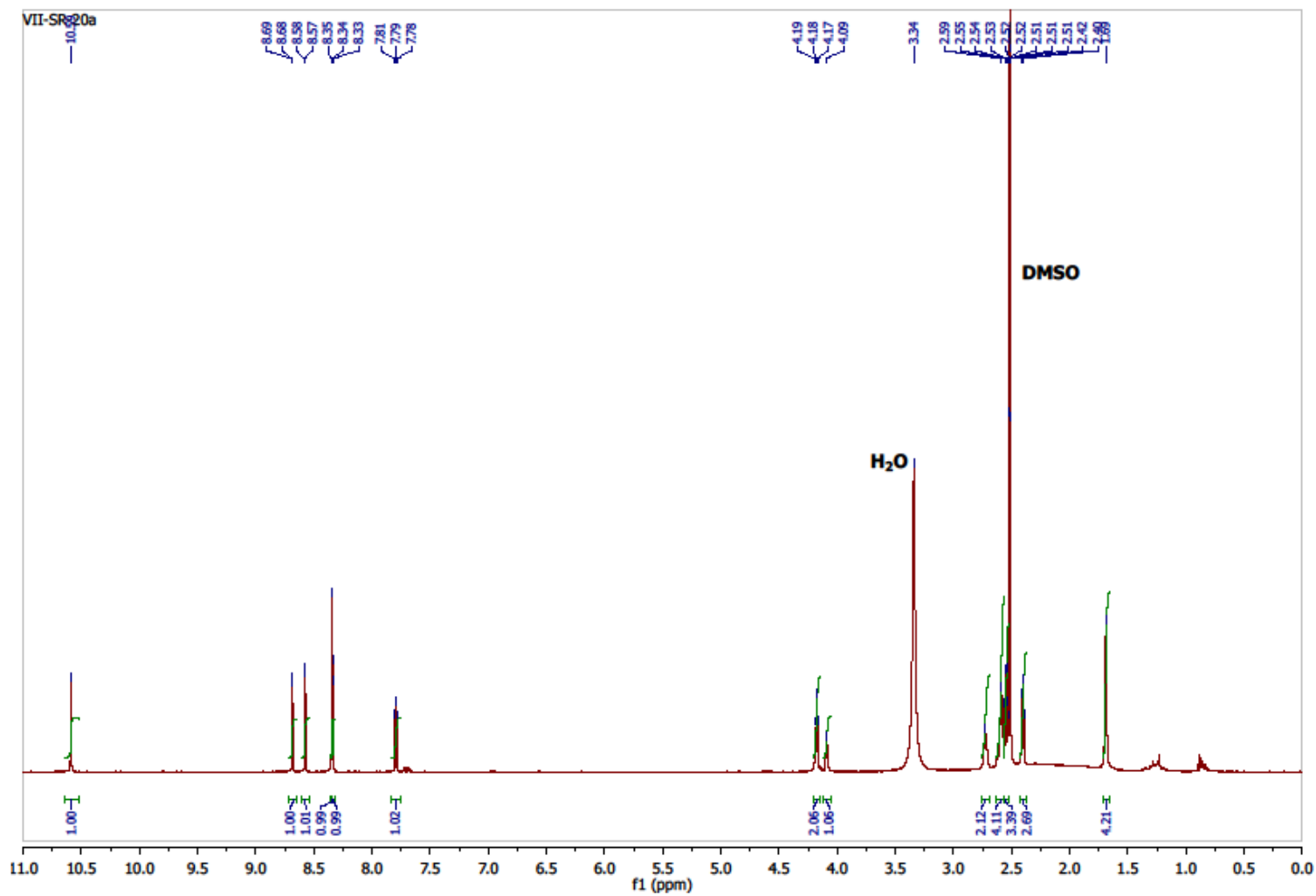


Figure S152. ¹H NMR spectrum of 42.

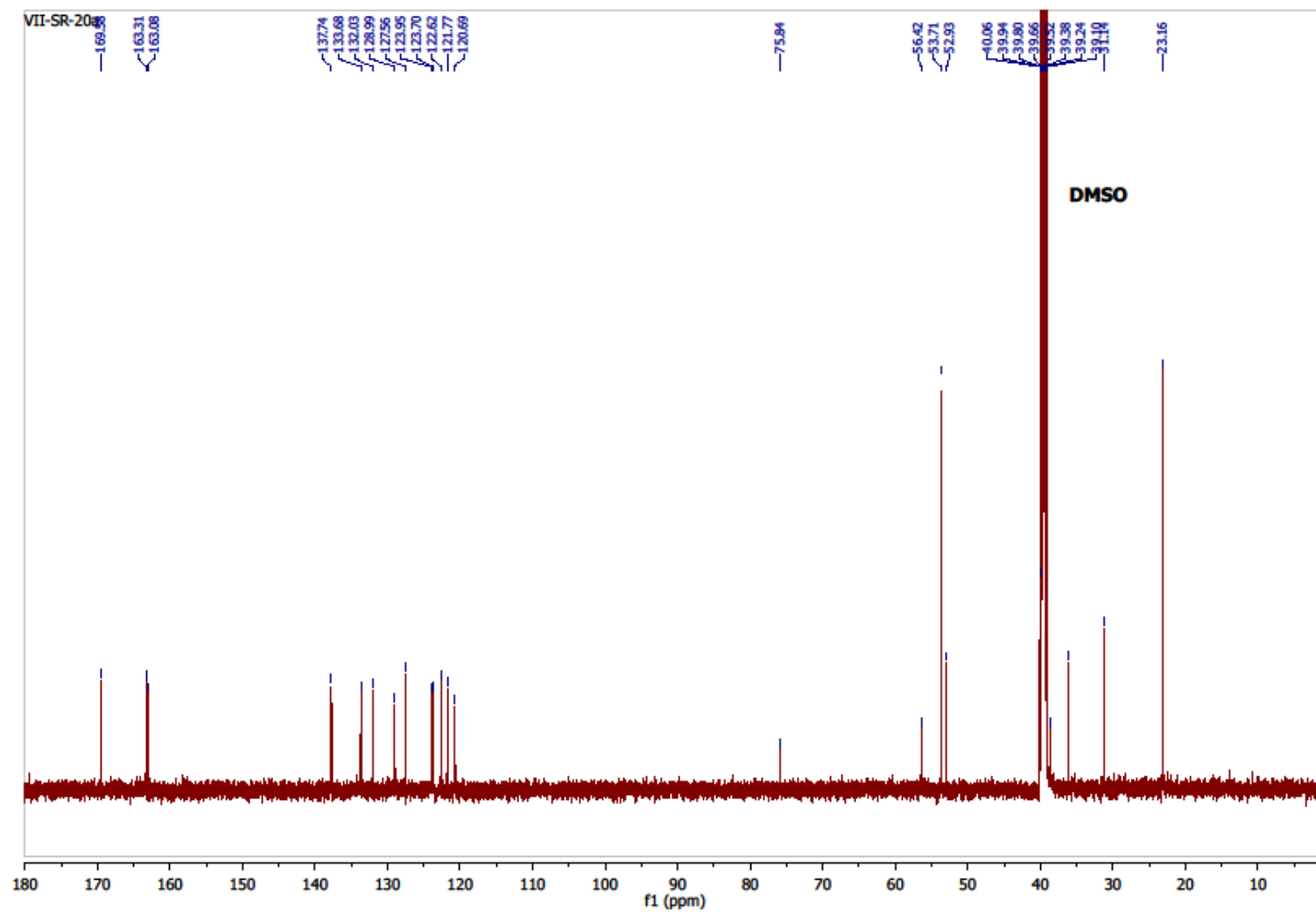


Figure S153. ¹³C NMR spectrum of 42.

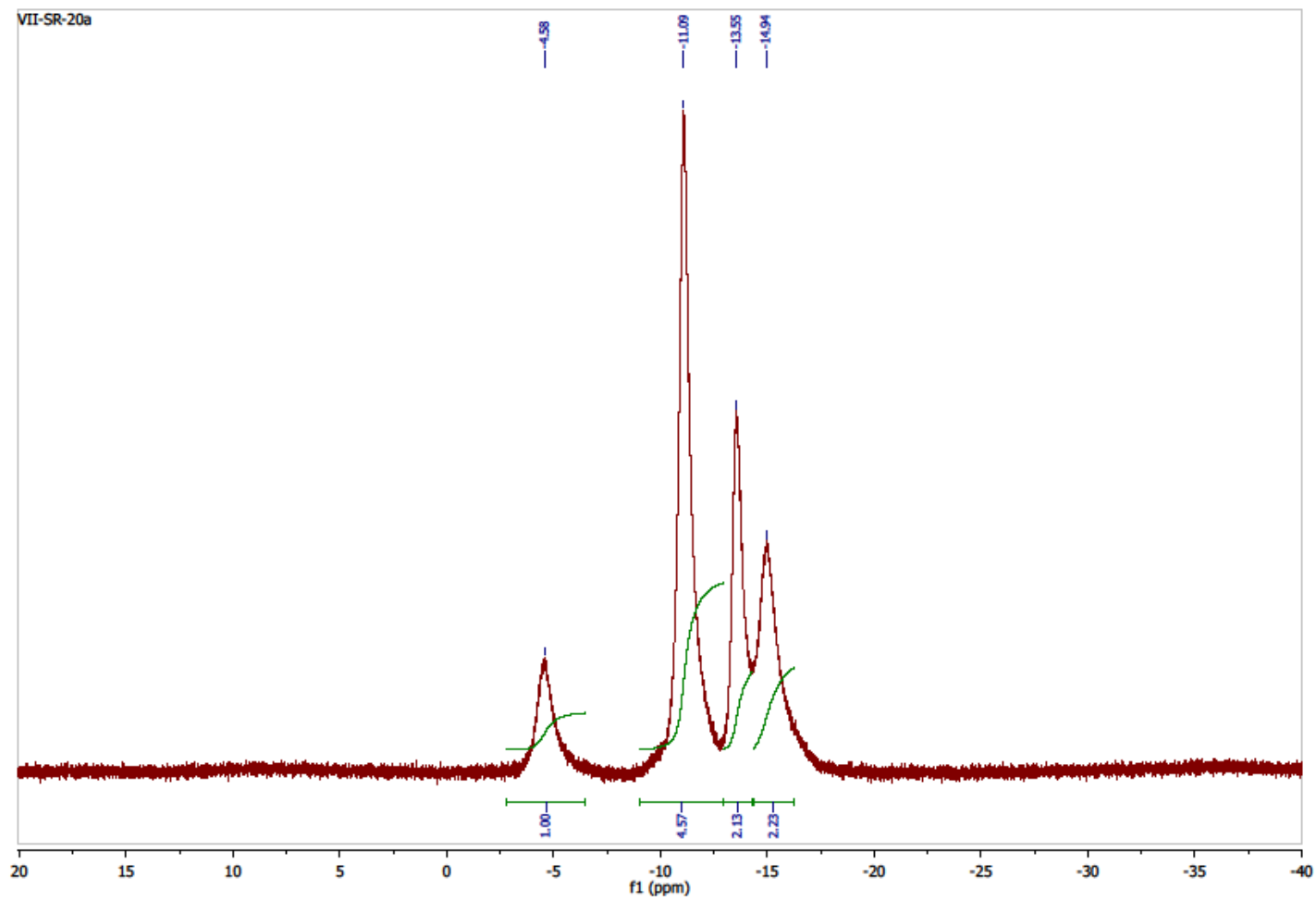


Figure S154. IR spectrum of 42.

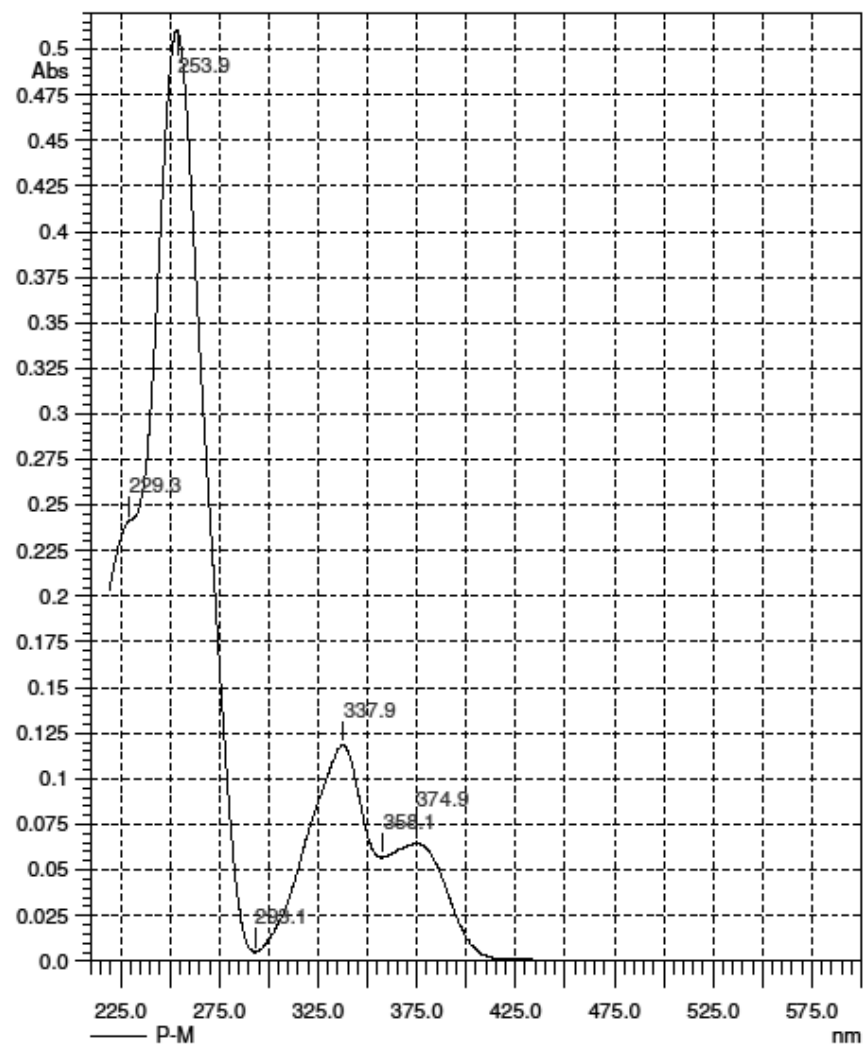


Figure S155. UV spectrum of 42.

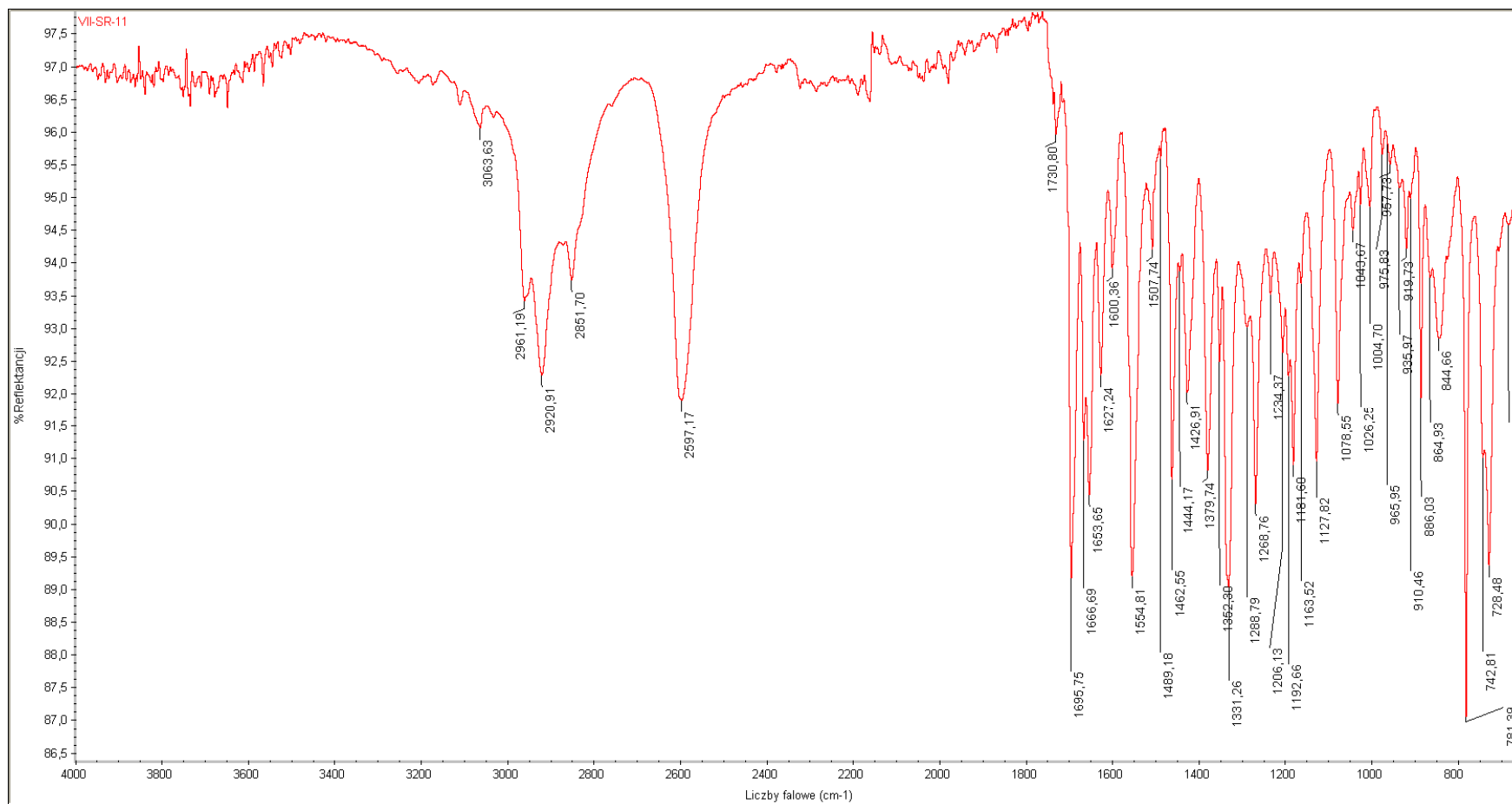
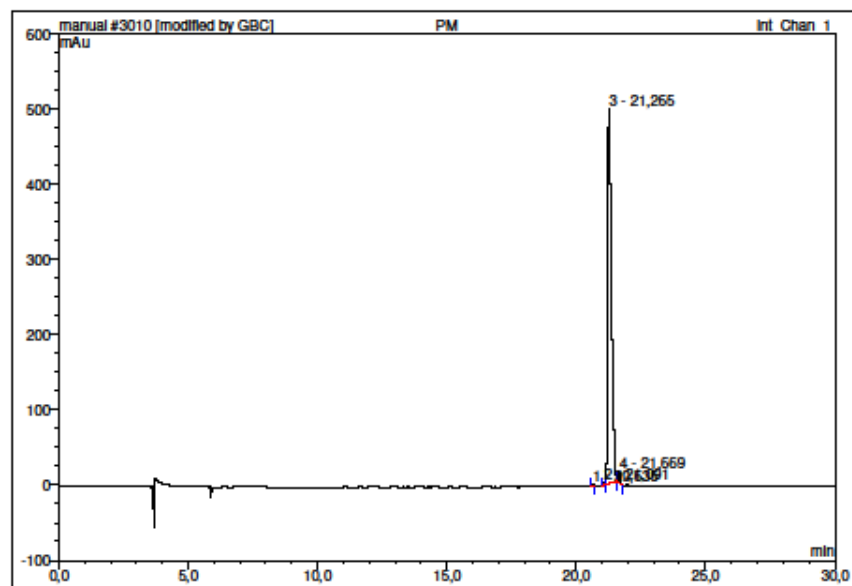


Figure S156. IR spectrum of 42.



No.	Ret. Time min	Peak Name	Height mAu	Area mAu*min	Rel. Area %	Amount	Type
1	20,63	n.a.	2,620	0,196	0,23	n.a.	BMB*
2	21,09	n.a.	2,455	0,155	0,18	n.a.	BMB*
3	21,27	n.a.	499,429	85,637	98,17	n.a.	BMB
4	21,67	n.a.	14,407	1,245	1,43	n.a.	BMB*
Total:			518,910	87,233	100,00	0,000	

Figure S157. HPLC analysis of 42.

Spectrum Name: VII-SR-11
Start Ion: 400
End Ion: 600
Source: APCI + 10.0µA 400C
Capillary: 150V 300C Offset: 25V Span: 0V

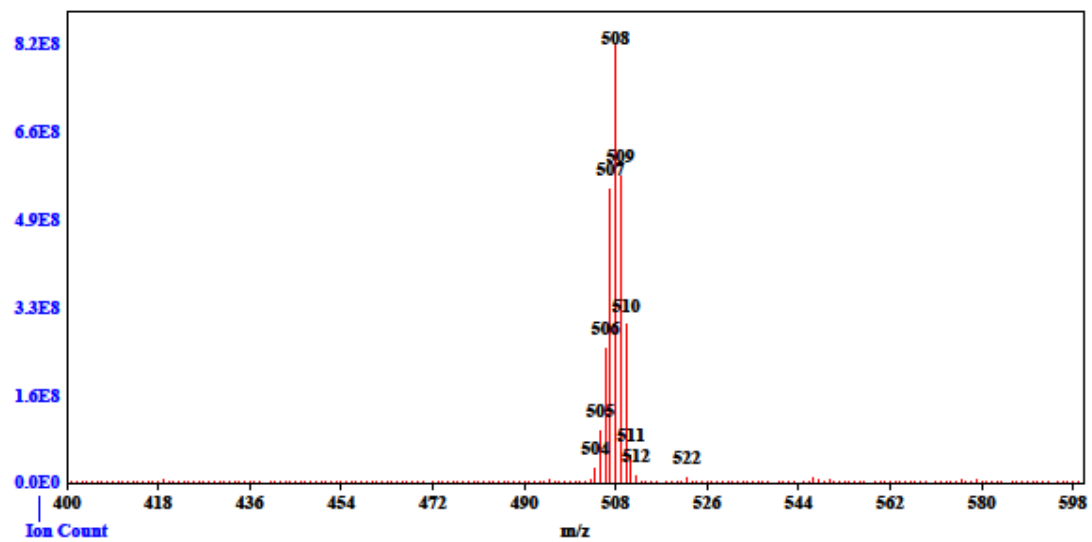


Figure S158. MS spectrum of 42.

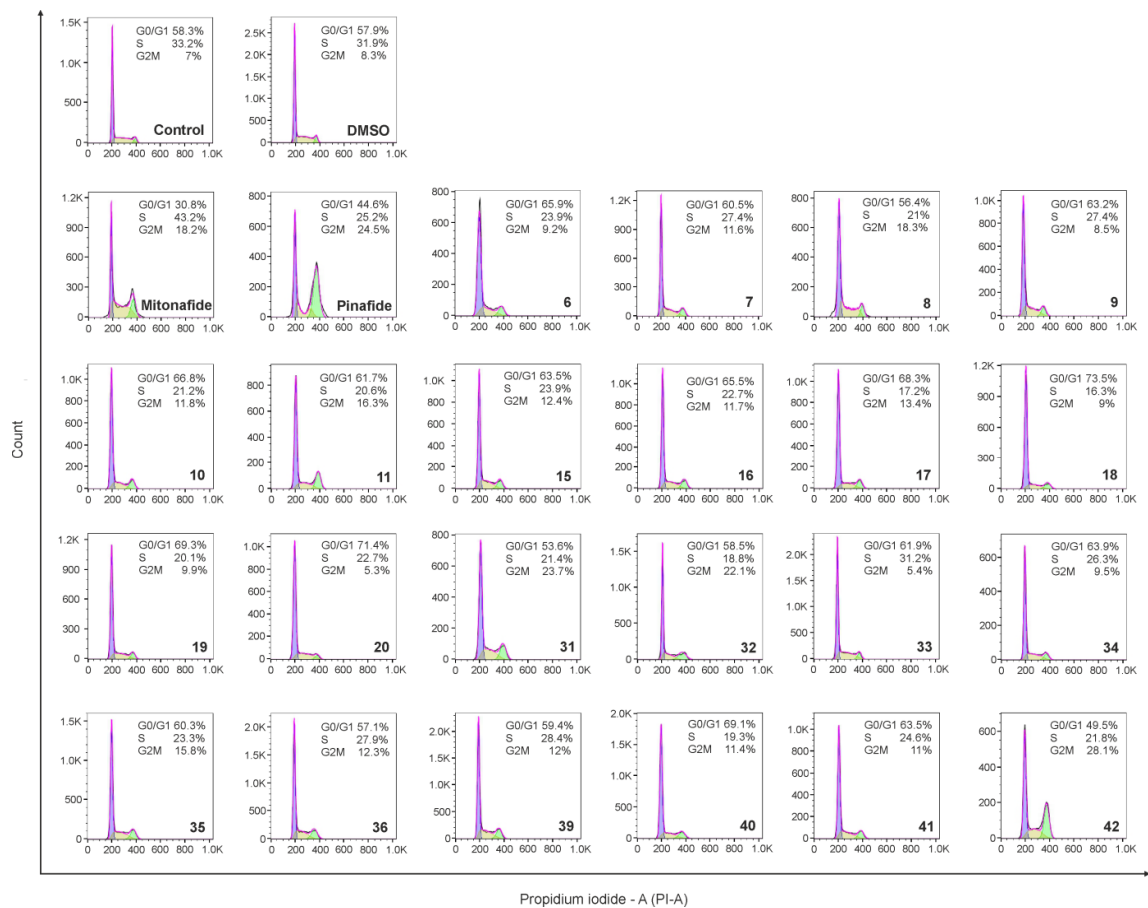


Figure S159. Influence of compound 6 (115 μ M), 7 (104 μ M), 8 (4 μ M), 9 (3 μ M), 10 (8 μ M), 11 (5 μ M), 15 (68 μ M), 16 (61 μ M), 17 (10 μ M), 18 (15 μ M), 19 (14 μ M), 20 (12 μ M), 31, (53 μ M), 32 (42 μ M), 33 (5 μ M), 34 (8 μ M), 35 (9 μ M), 36 (6 μ M), 39 (11 μ M), 40 (13 μ M), 41 (10 μ M), 42 (6 μ M) on cell cycle distribution in HepG2 cells. Flow cytometry analysis of cells treated for 24 h with tested compounds. One representative experiment of three is shown.

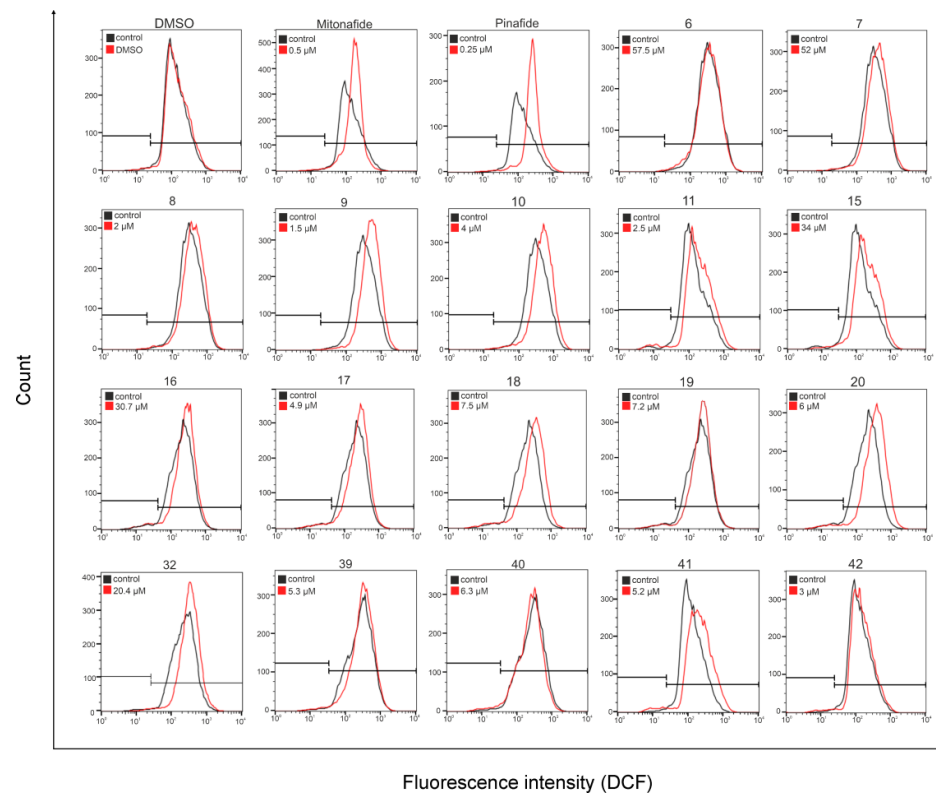


Figure S160. ROS production in HepG2 cells after 24 h incubation with compound **6** (57.5 μM), **7** (52 μM), **8** (2 μM), **9** (1.5 μM), **10** (4 μM), **11** (2.5 μM), **15** (34 μM), **16** (30.7 μM), **17** (4.9 μM), **18** (7.5 μM), **19** (7.2 μM), **20** (6 μM), **32** (20.4 μM), **39** (5.3 μM), **40** (6.3 μM), **41** (5.2 μM), **42** (3 μM). Intracellular production of ROS was measured using dual H₂DCFDA/PI staining. The intensity of DCF fluorescence corresponds to intracellular ROS level in HepG2 cells. The flow cytometric analysis indicated DCF fluorescence shift, which is correlated with higher ROS production after 24 h incubation with the tested compounds compared to control.

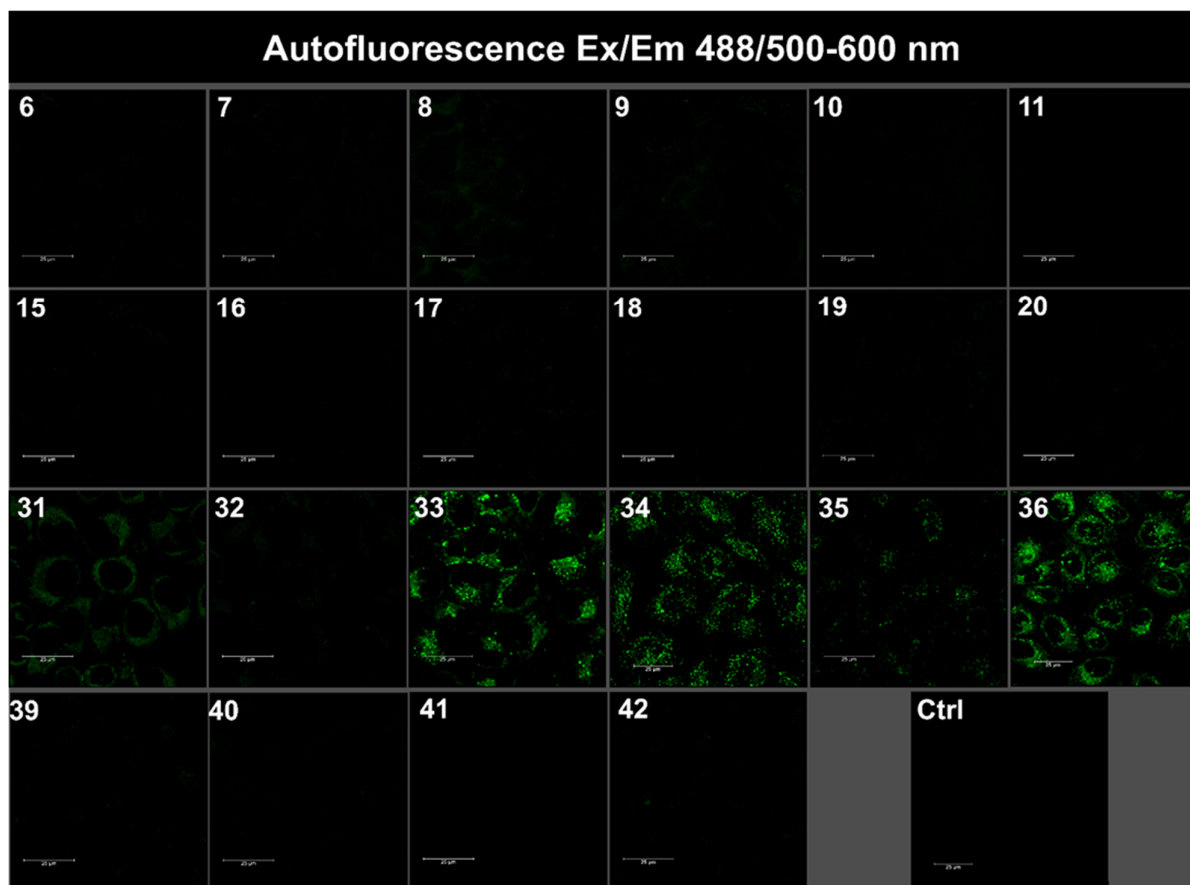


Figure S161. Autofluorescence analysis of the tested compounds in HepG2 cells. Confocal microscopy analysis was performed 8 h after treatment with the compounds in the final concentration corresponding to IC_{50} . The number of each compound is placed in the left corner of the picture. The intensity of the autofluorescence was analyzed at Ex/Em 488/500-600 nm.

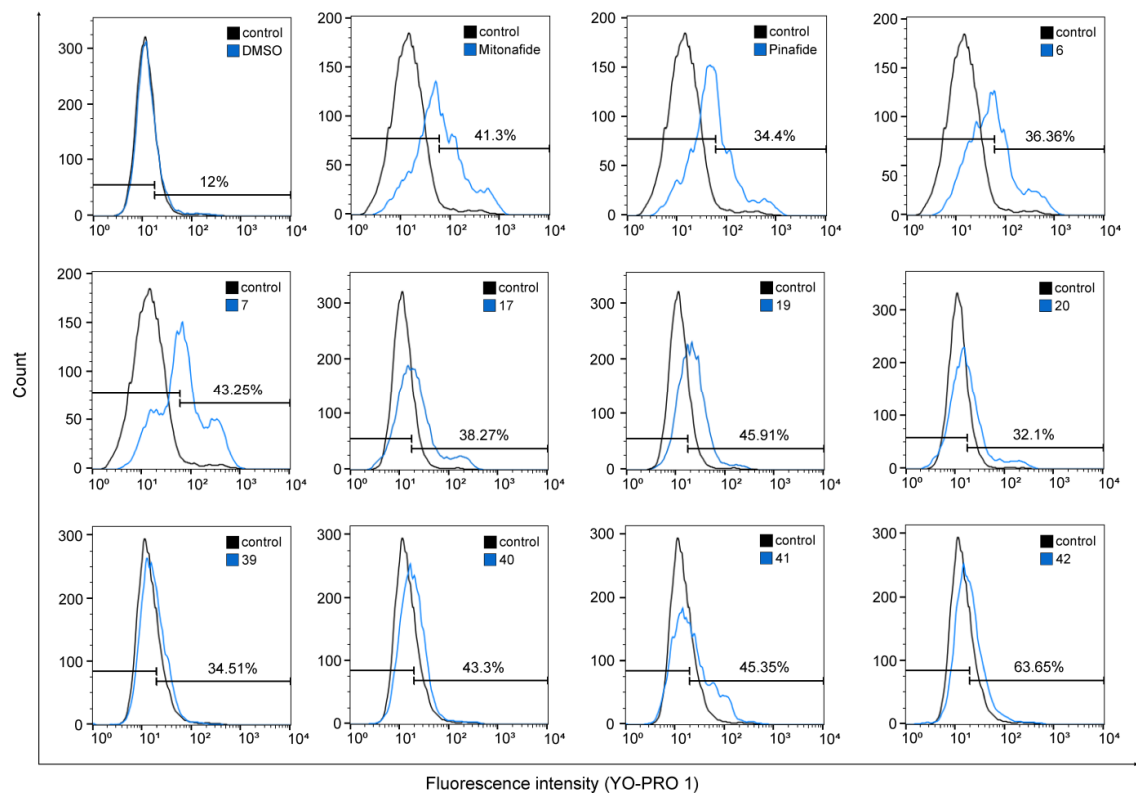


Figure S162. Flow cytometry analysis of apoptosis/necrosis in HepG2 cells after cell toxicity induction with compound 6 (115 μ M), 7 (104 μ M), 8 (4 μ M), 9 (3 μ M), 10 (8 μ M), 11 (5 μ M), 15 (68 μ M), 16 (61 μ M), 17 (10 μ M), 18 (15 μ M), 19 (14 μ M), 20 (12 μ M), 31 (53 μ M), 32 (42 μ M), 33 (5 μ M), 34 (8 μ M), 35 (9 μ M), 36 (6 μ M), 39 (11 μ M), 40 (13 μ M), 41 (10 μ M), 42 (6 μ M). The chosen concentration of each compound corresponded to whole IC₅₀ values. The number of apoptotic cells for each compound is indicated on histogram. Level of apoptosis was evaluated with dual staining with YO-PRO-1/PI.

Table 1S. Percentage distribution of early and late apoptotic and necrotic cells assessed by flow cytometry.

compound	live cells [%]	early apoptosis [%]	late apoptosis [%]	necrosis [%]
6	47.75 ± 4.78	1.56 ± 0.26	28.80 ± 3.72	21.85 ± 1.12
7	25.90 ± 0.34	4.55 ± 0.67	38.70 ± 1.72	30.85 ± 2.14
17	60.75 ± 4.49	30.70 ± 4.76	7.57 ± 0.98	0.98 ± 0.33
19	53.40 ± 3.59	39.25 ± 6.30	6.66 ± 2.55	0.72 ± 0.35
20	66.70 ± 2.86	18.75 ± 2.5	13.35 ± 2.69	1.23 ± 0.41
39	65.40 ± 0.88	31.65 ± 1.52	2.86 ± 1.05	0.08 ± 0.02
40	57.40 ± 1.9	32.35 ± 2.49	9.95 ± 2.17	0.35 ± 0.21
41	54.35 ± 3.82	26.75 ± 2.17	18.60 ± 3.01	0.34 ± 0.07
42	36.10 ± 3.8	24.65 ± 1.78	39.00 ± 5.33	0.24 ± 0.04
Mitonafide	37.25 ± 1.09	1.90 ± 0.19	39.40 ± 1.94	21.40 ± 3.13
Pinafide	47.10 ± 1.01	1.40 ± 0.57	33.00 ± 1.19	18.50 ± 1.72

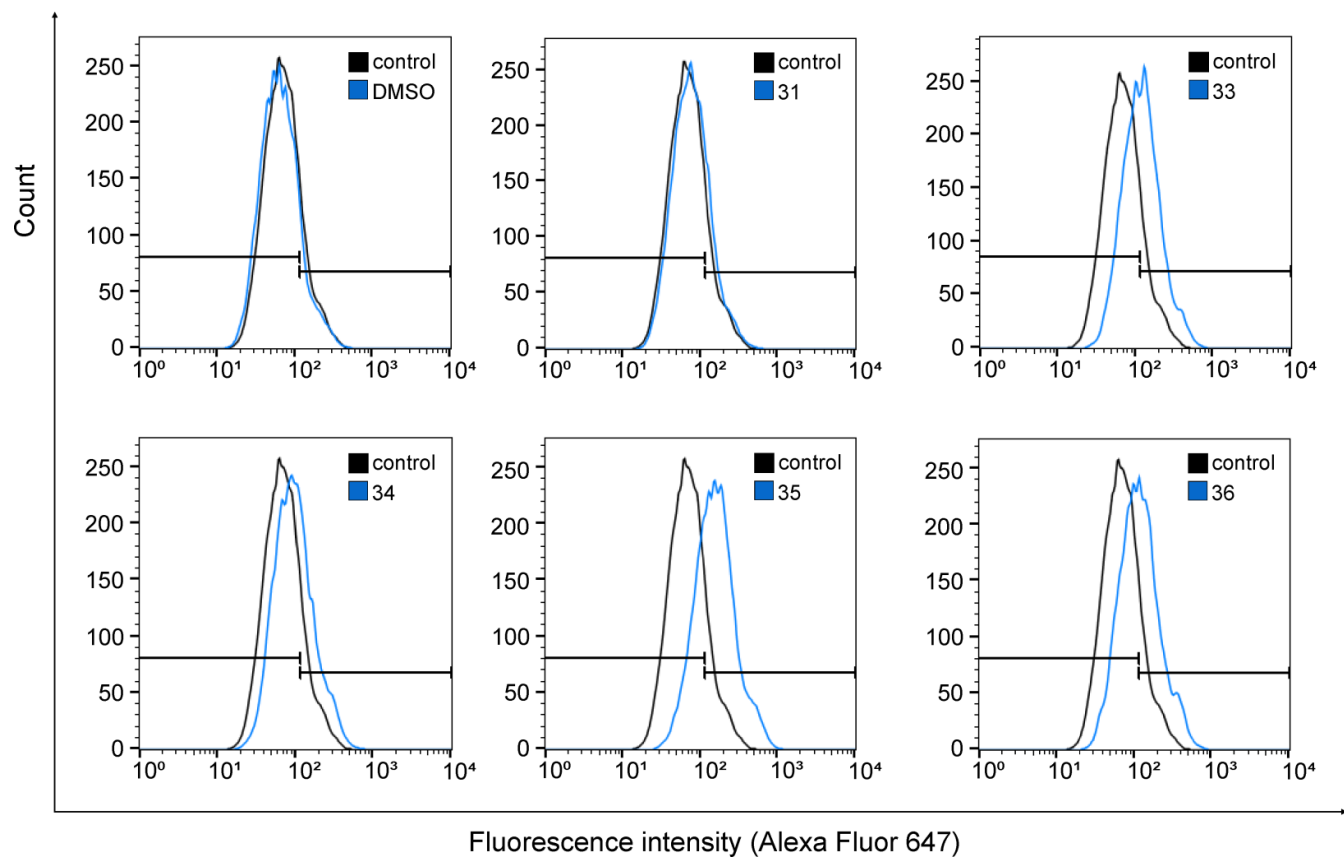


Figure S163. Flow cytometry analysis of apoptosis/necrosis in HepG2 cells after cell toxicity induction with compound **31** (53 μM), **33** (5 μM), **34** (8 μM), **35** (9 μM), **36** (6 μM). The chosen concentration of each compound corresponded to whole IC_{50} values. The number of apoptotic cells for each compound is indicated on histogram. Level of apoptosis was evaluated with Annexin V Alexa Fluor 647 conjugate.

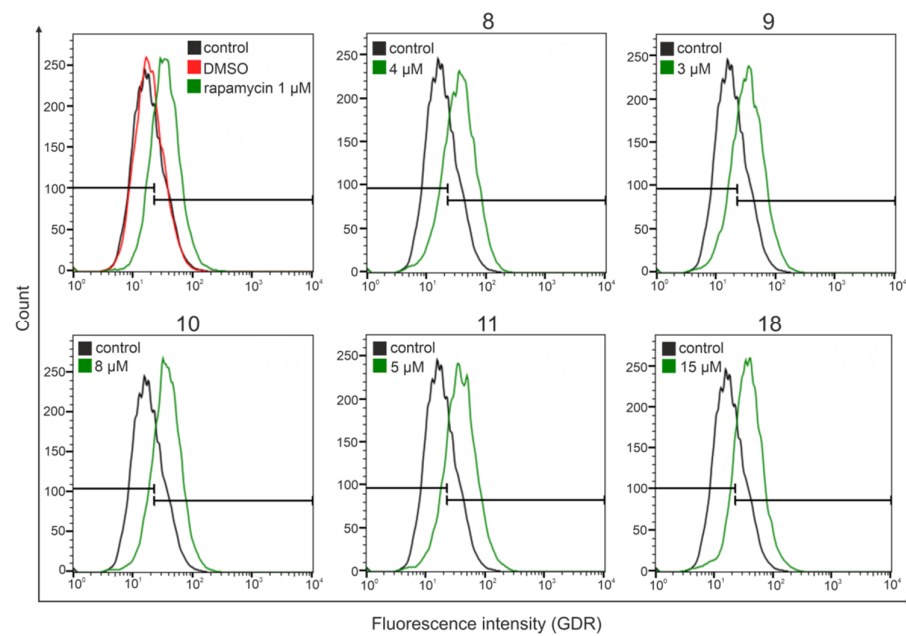


Figure S164. Flow cytometry analysis of autophagy in HepG2 cells after cell toxicity induction with compound **8** (4 μM), **9** (3 μM), **10** (8 μM), **11** (5 μM), **18** (15 μM). The chosen concentration of each compound corresponded to whole IC_{50} values. Level of autophagy was evaluated with Green Detection Reagent. Rapamycin was used as positive control. One representative experiment of three is shown.

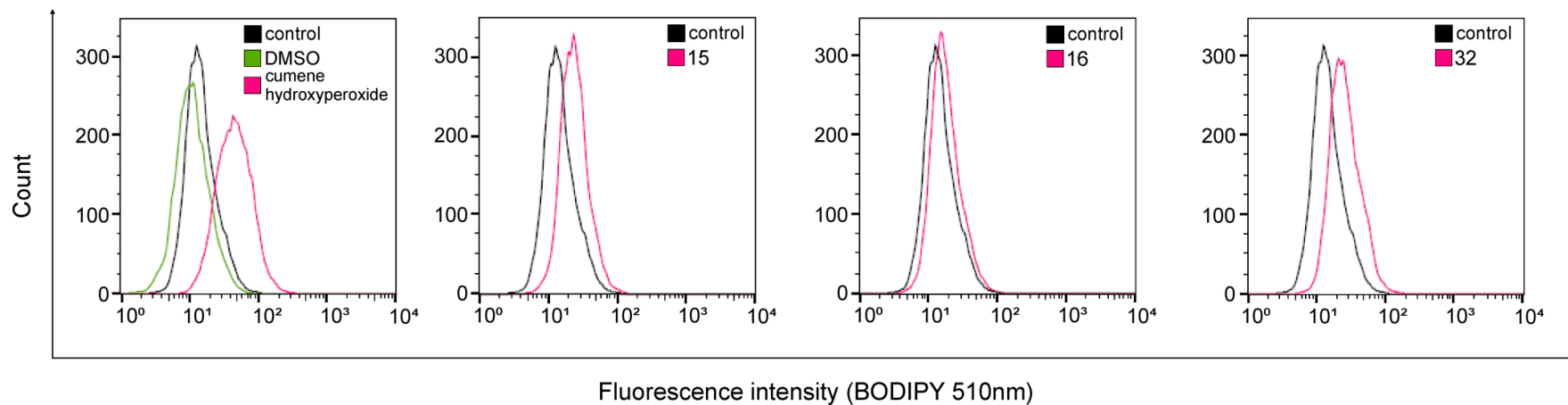


Figure S165. Flow cytometry analysis of lipid peroxidation in HepG2 cells after cell toxicity induction with compound **15** (68 μM), **16** (61 μM), **32** (42 μM). The chosen concentration of each compound corresponded to whole IC_{50} values. Level of lipid peroxidation was evaluated with 581/591 C11 reagent. To induce strong positive signal the cells were incubated with cumene peroxide. One representative experiment of three is shown.

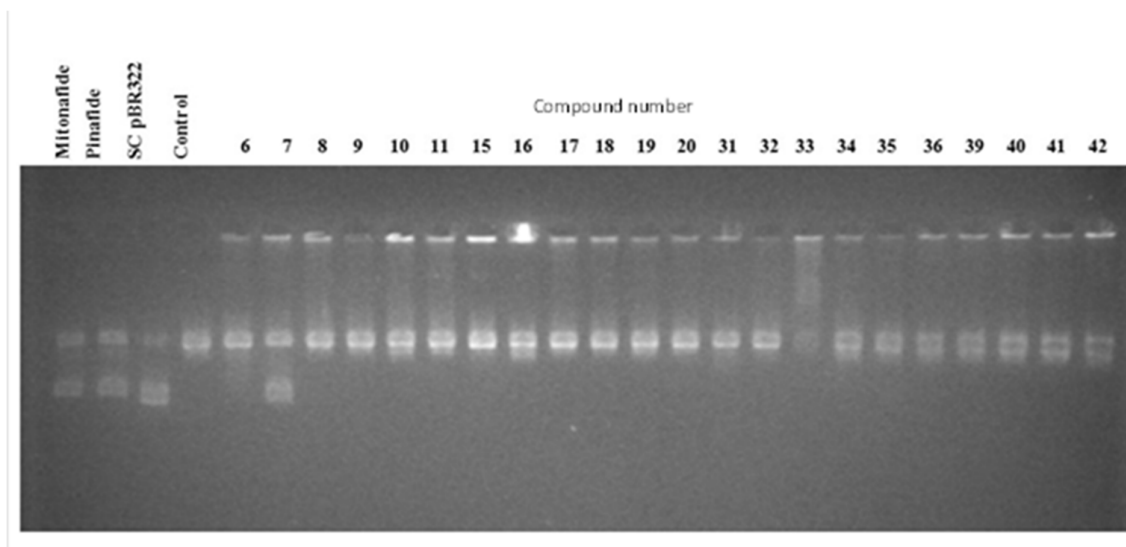


Figure S166. Human Topoisomerase II α relaxation assay in the presence of modified with carborane cluster naphthalic anhydrides (6, 7, 15, 16, 31, 32), naphthalimides (8-11, 17-20, 33-36, 39-42), and the control drugs mitonafide and pinafide at a concentration of 100 μ M.

SC – supercoiled DNA.

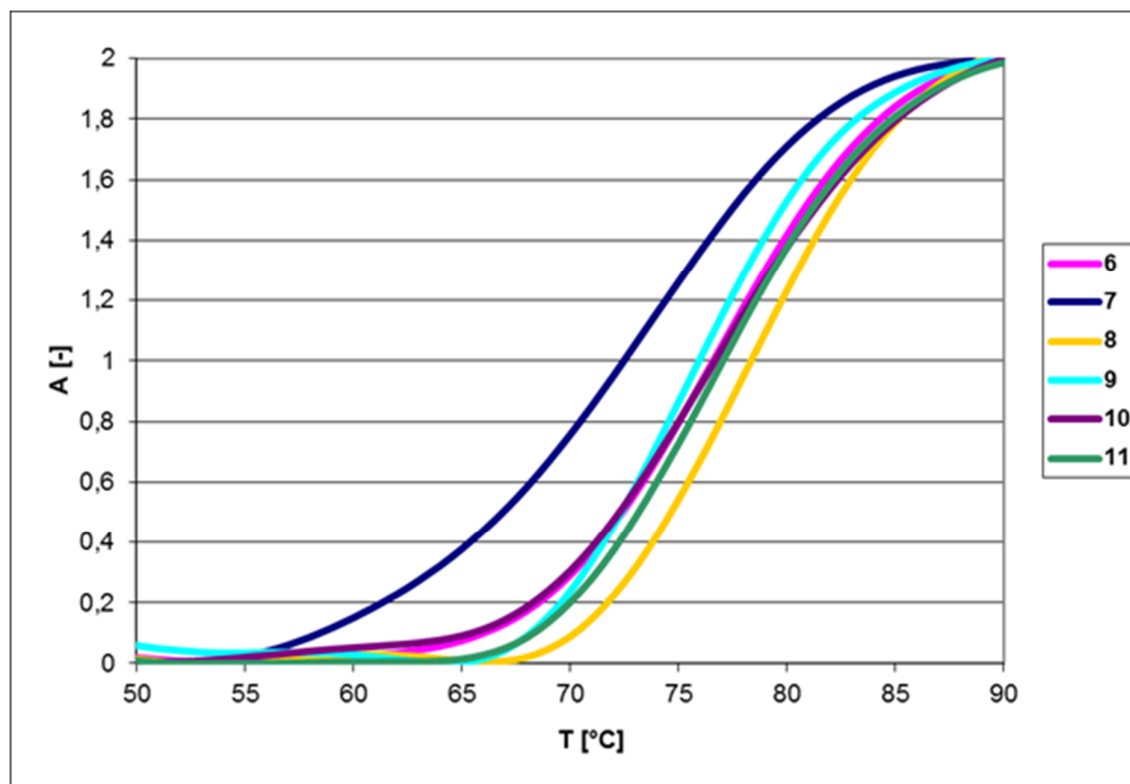


Figure S167. Melting curves of ct-DNA upon addition of **6-11** ($c(\text{ct-DNA}) = 2 \times 10^{-5} \text{ mol dm}^{-3}$) at molar ratio $r = 0.3$ ($r = [\text{compound}]/[\text{ct-DNA}]$), sodium cacodylate buffer (pH 7.0, 20 mM).

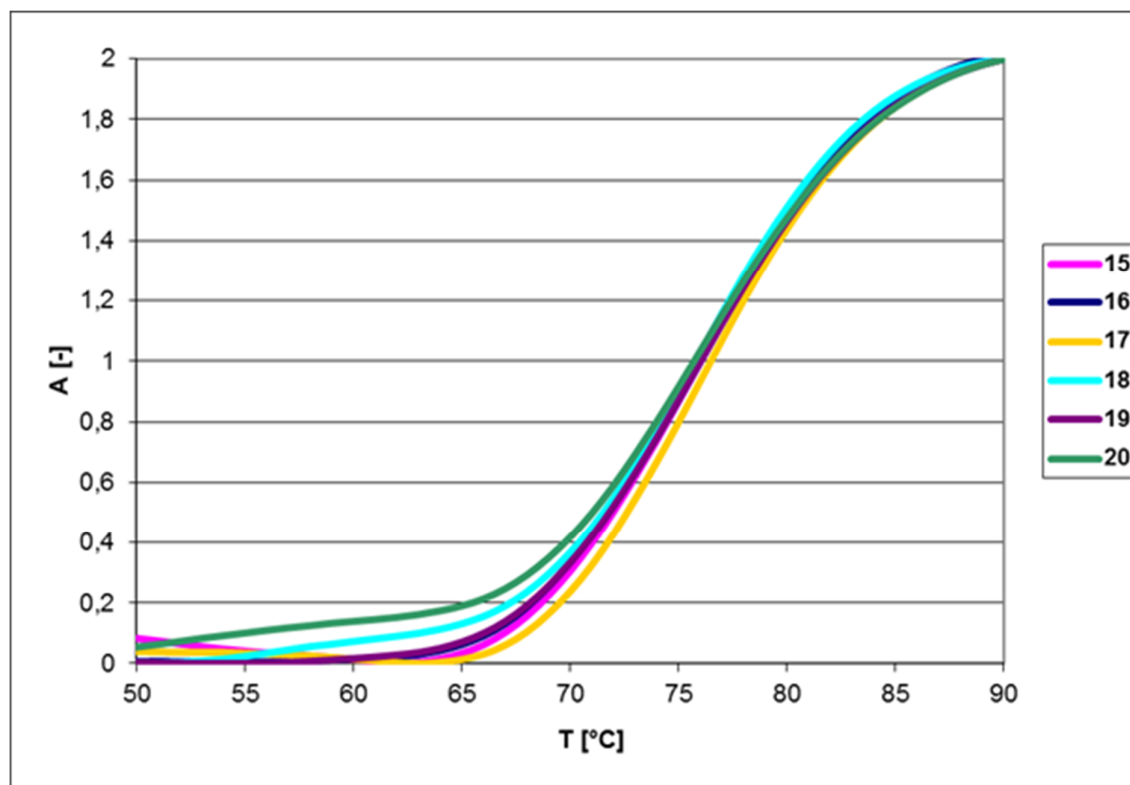


Figure S168. Melting curves of ct-DNA upon addition of **15-20** ($c(\text{ct-DNA}) = 2 \times 10^{-5} \text{ mol dm}^{-3}$) at molar ratio $r = 0.3$ ($r = [\text{compound}]/[\text{ct-DNA}]$), sodium cacodylate buffer (pH 7.0, 20 mM).

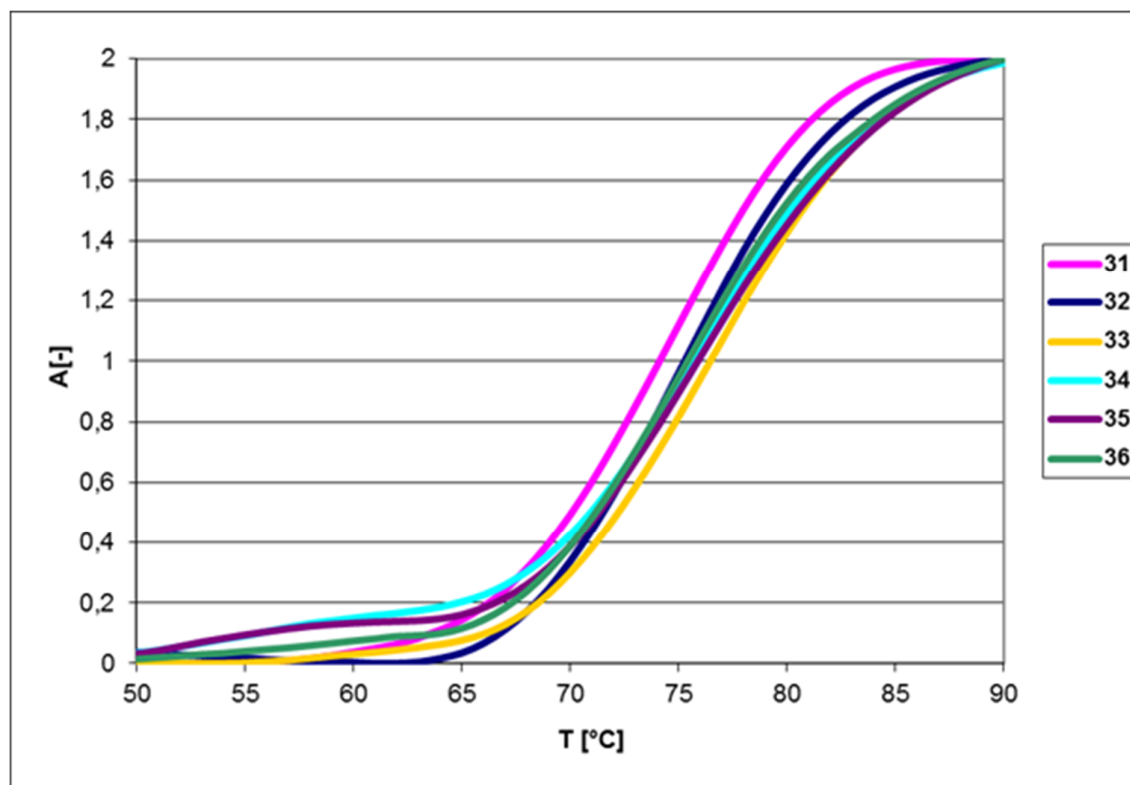


Figure S169. Melting curves of ct-DNA upon addition of **31-36** ($c(\text{ct-DNA}) = 2 \times 10^{-5} \text{ mol dm}^{-3}$) at molar ratio $r = 0.3$ ($r = [\text{compound}]/[\text{ct-DNA}]$), sodium cacodylate buffer (pH 7.0, 20 mM).

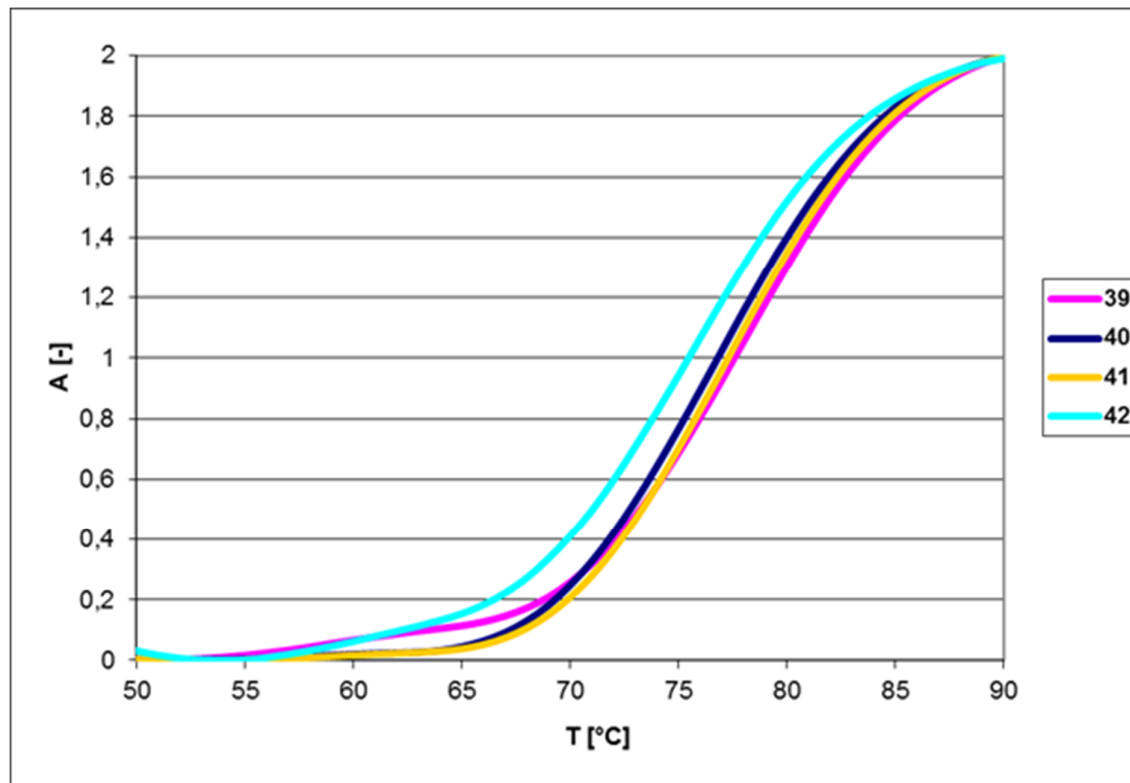


Figure S170. Melting curves of ct-DNA upon addition of **39-42** ($c(\text{ct-DNA}) = 2 \times 10^{-5} \text{ mol dm}^{-3}$) at molar ratio $r = 0.3$ ($r = [\text{compound}]/[\text{ct-DNA}]$), sodium cacodylate buffer (pH 7.0, 20 mM).

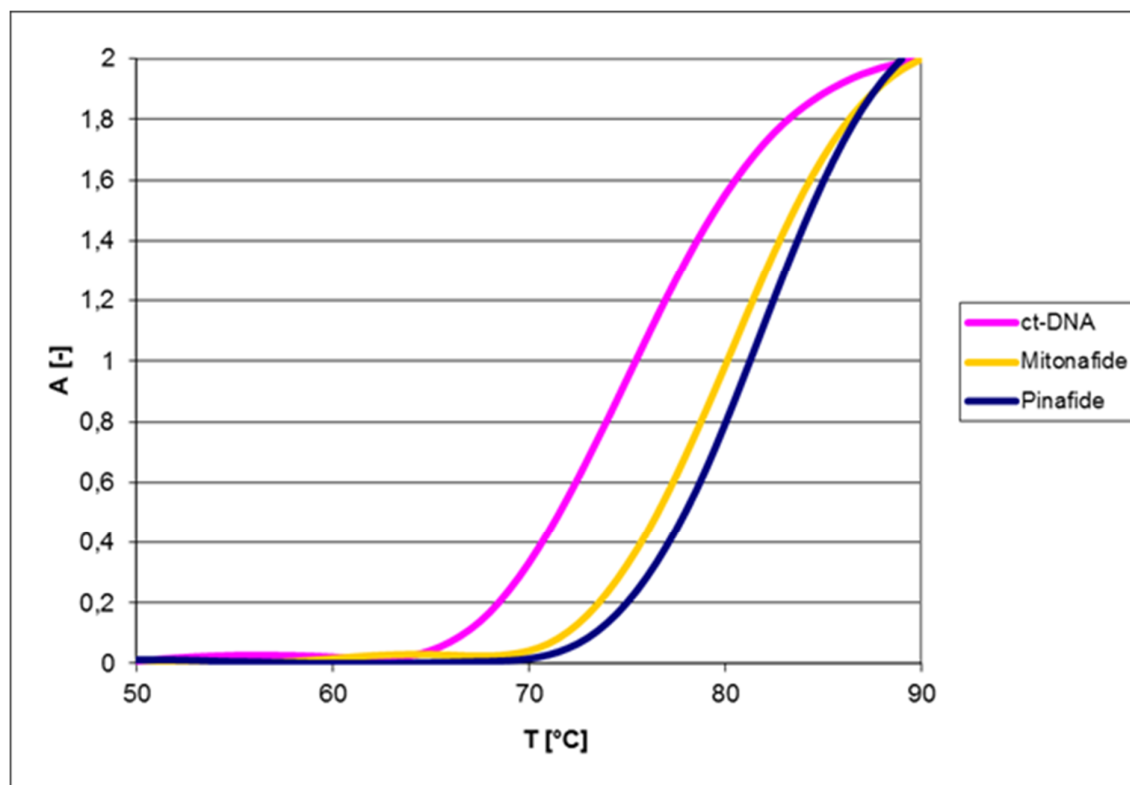


Figure S171. Melting curves of ct-DNA upon addition of mitonafide and pinafide ($c(\text{ct-DNA}) = 2 \times 10^{-5} \text{ mol dm}^{-3}$) at molar ratio $r = 0.3$ ($r = [\text{compound}]/[\text{ct-DNA}]$), sodium cacodylate buffer (pH 7.0, 20 mM).

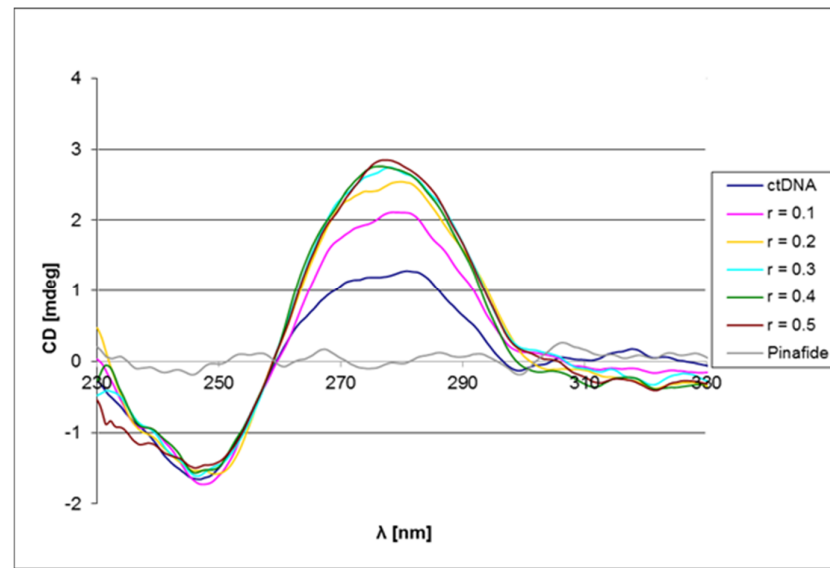
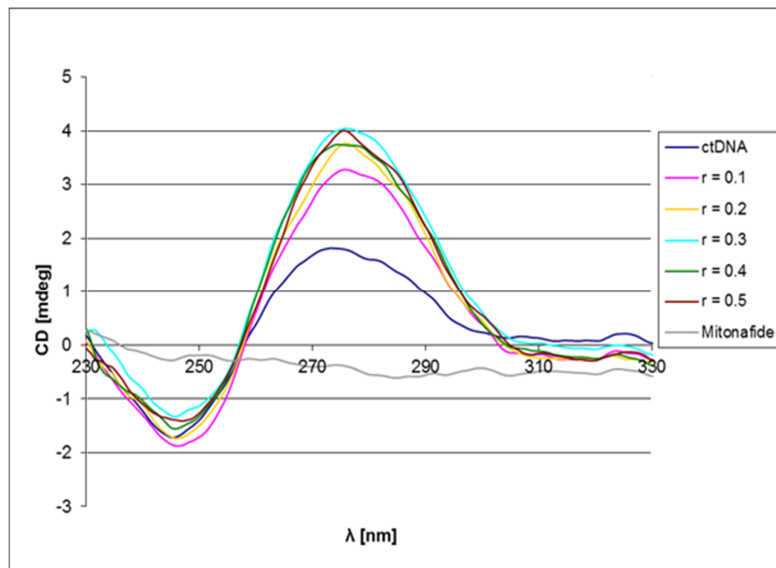


Figure S172. Changes in the CD spectrum of ct-DNA upon addition of mitonafide (left) and pinafide (right) ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

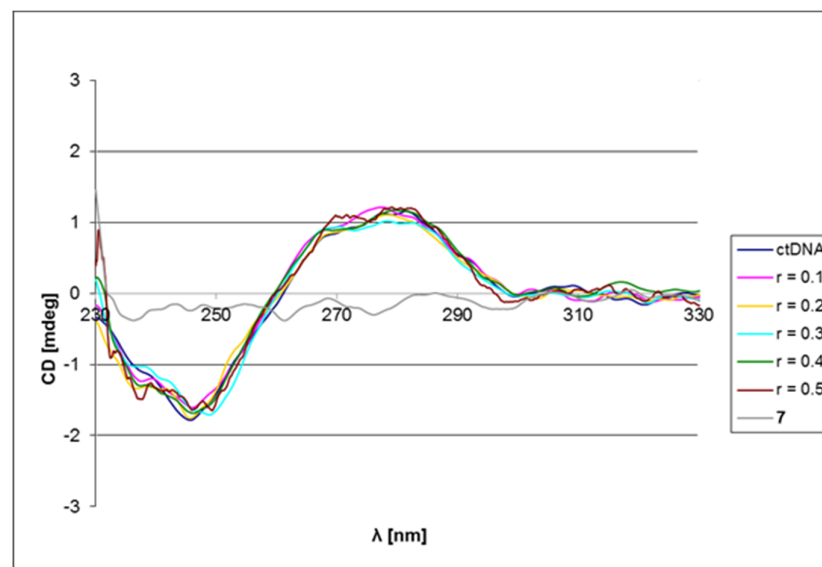
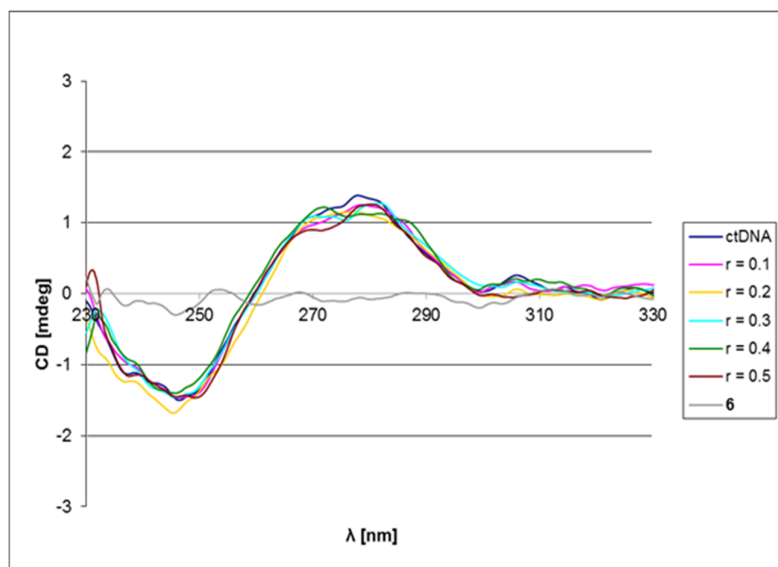


Figure S173. Changes in the CD spectrum of ct-DNA upon addition of **6** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **7** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

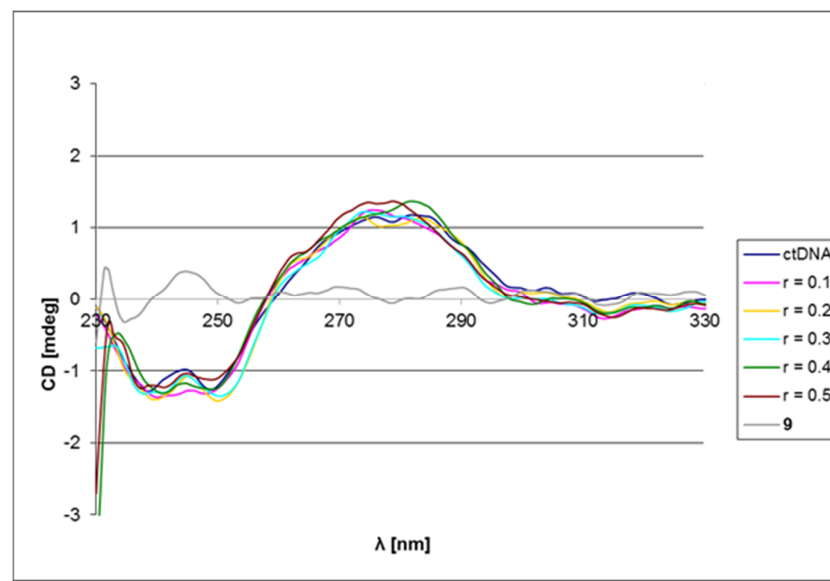
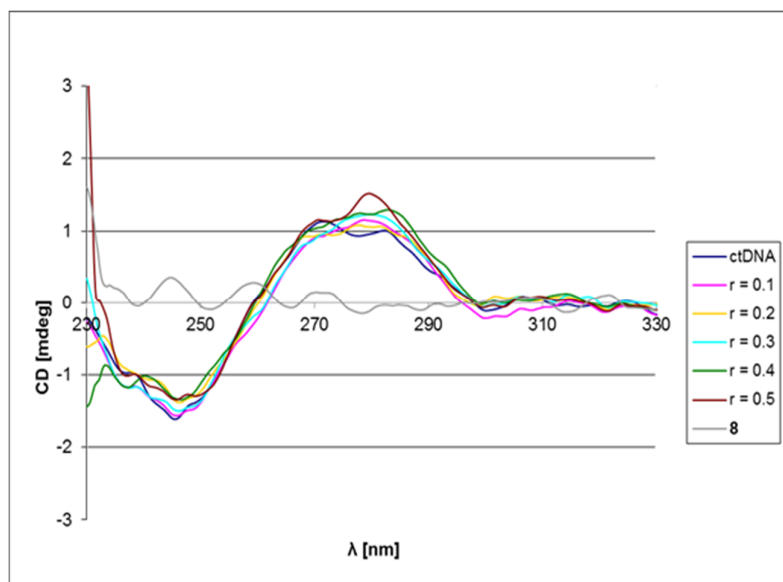


Figure S174. Changes in the CD spectrum of ct-DNA upon addition of **8** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **9** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

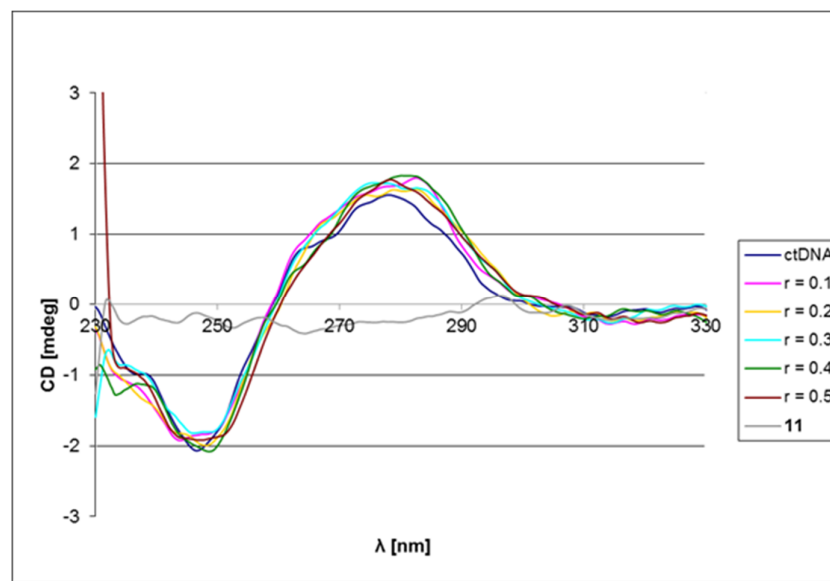
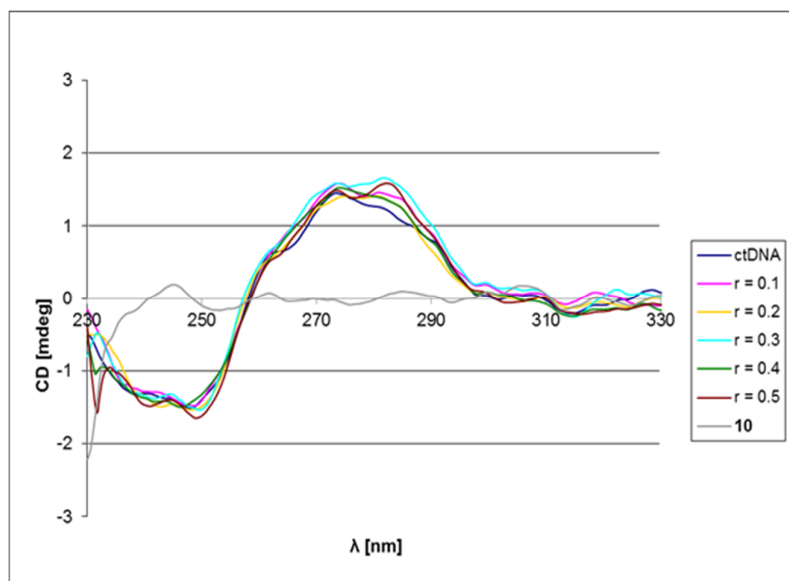


Figure S175. Changes in the CD spectrum of ct-DNA upon addition of **10** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **11** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

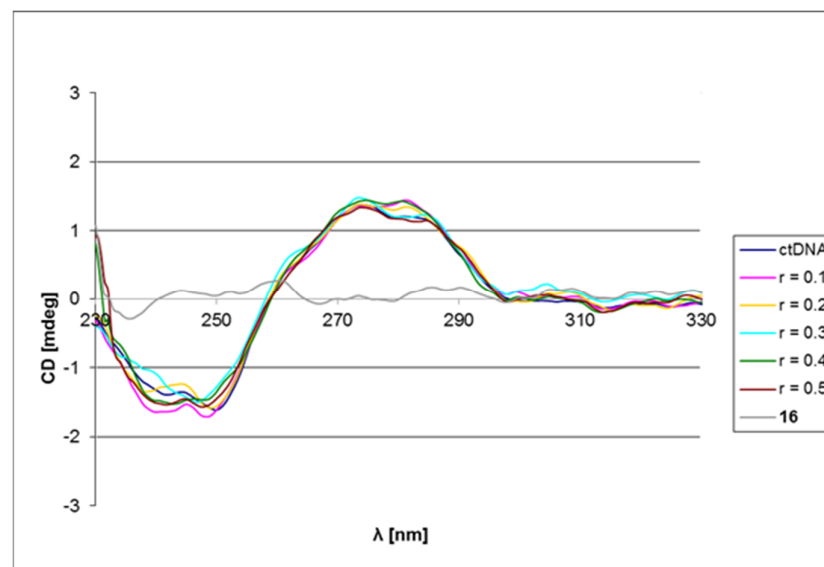
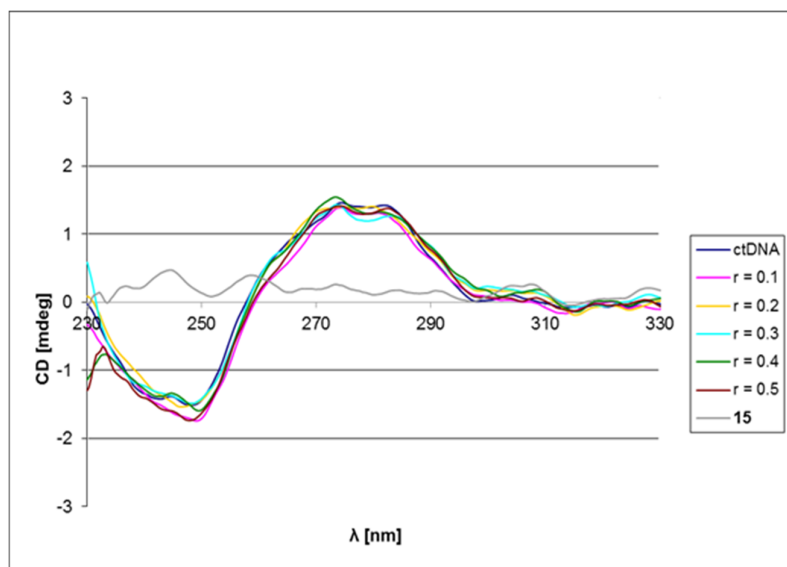


Figure S176. Changes in the CD spectrum of ct-DNA upon addition of **15** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **16** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

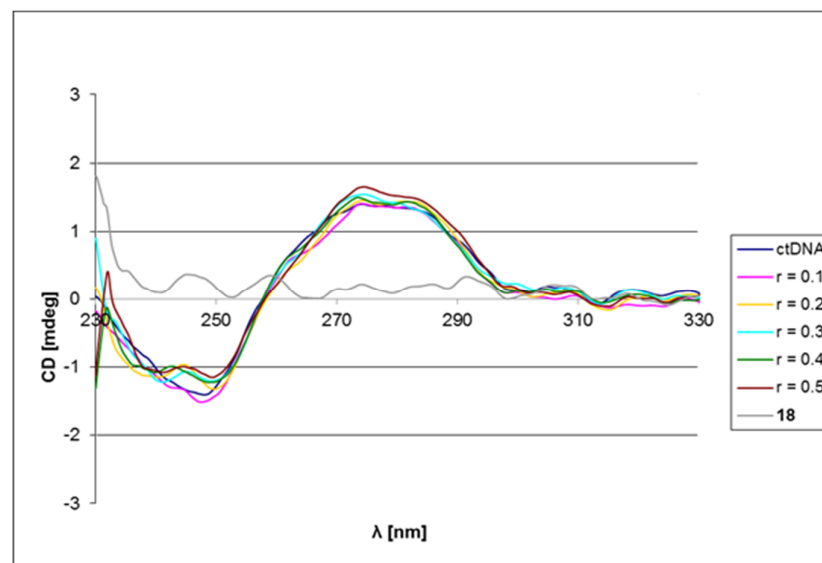
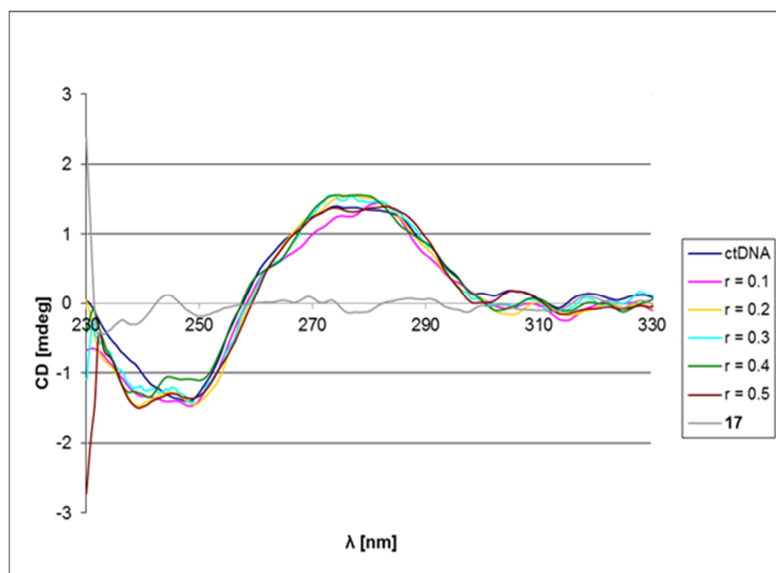


Figure S177. Changes in the CD spectrum of ct-DNA upon addition of **17** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **18** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

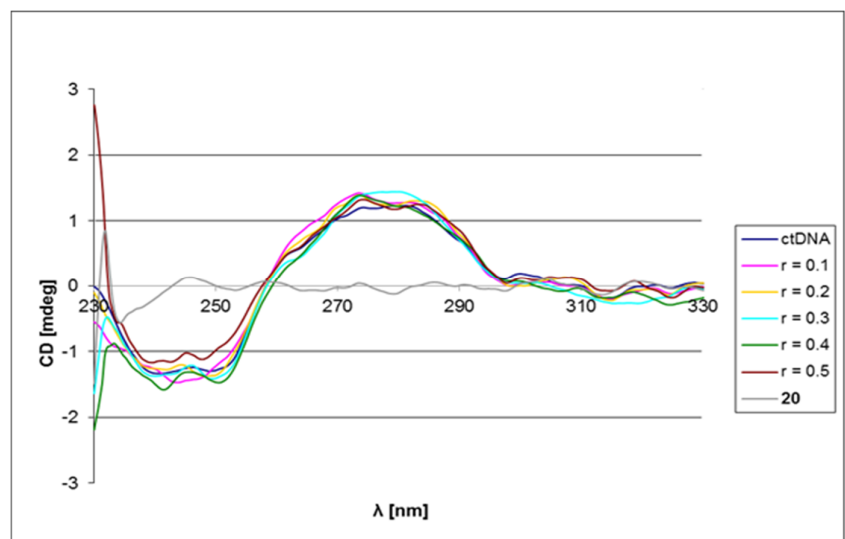
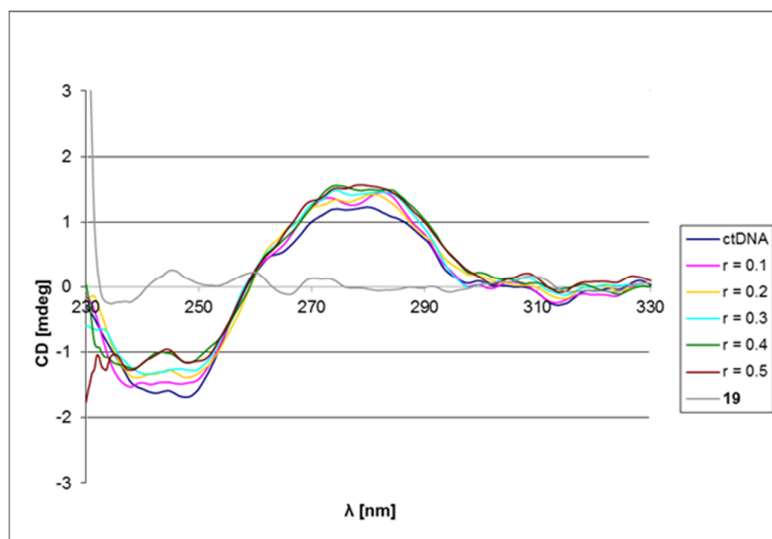


Figure S178. Changes in the CD spectrum of ct-DNA upon addition of **19** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **20** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

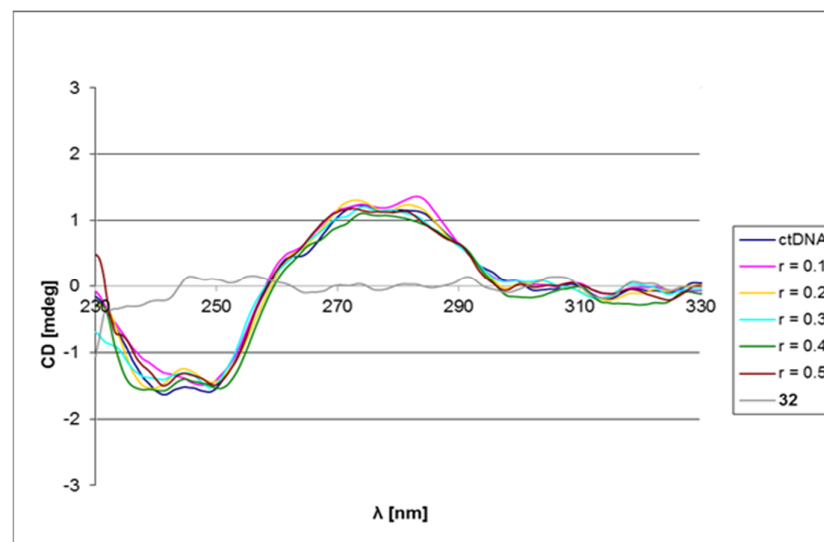
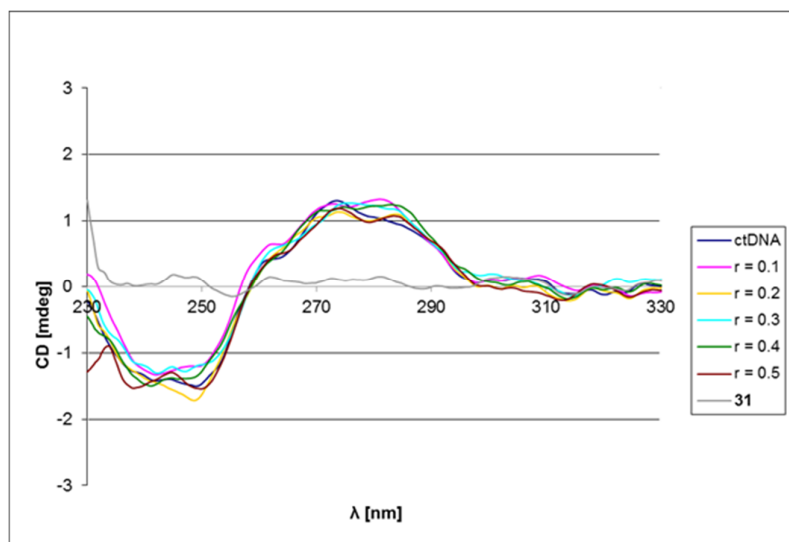


Figure S179. Changes in the CD spectrum of ct-DNA upon addition of **31** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **32** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

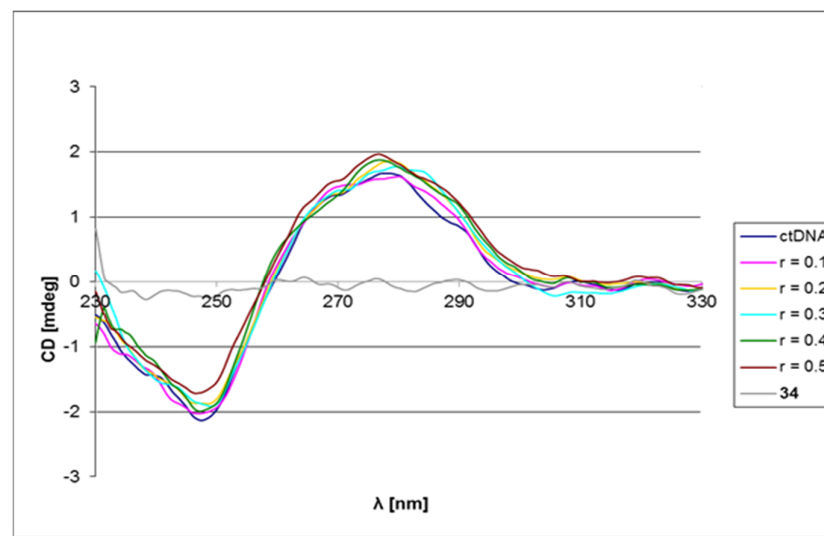
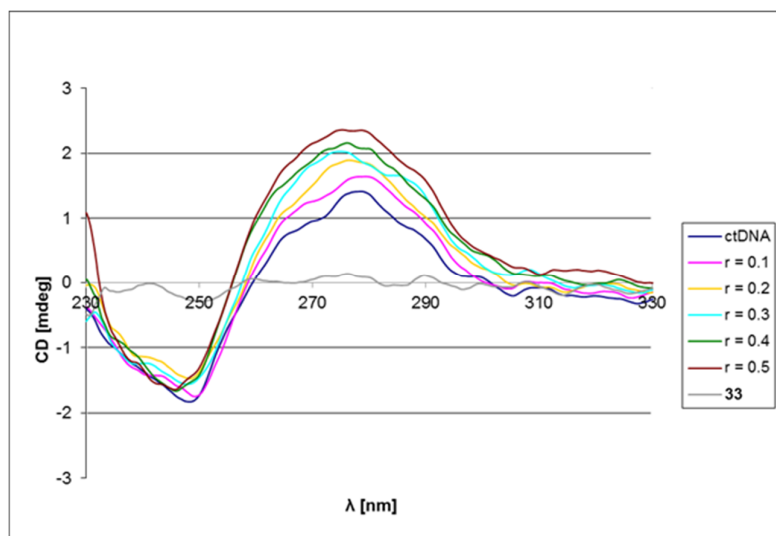


Figure S180. Changes in the CD spectrum of ct-DNA upon addition of **33** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **34** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

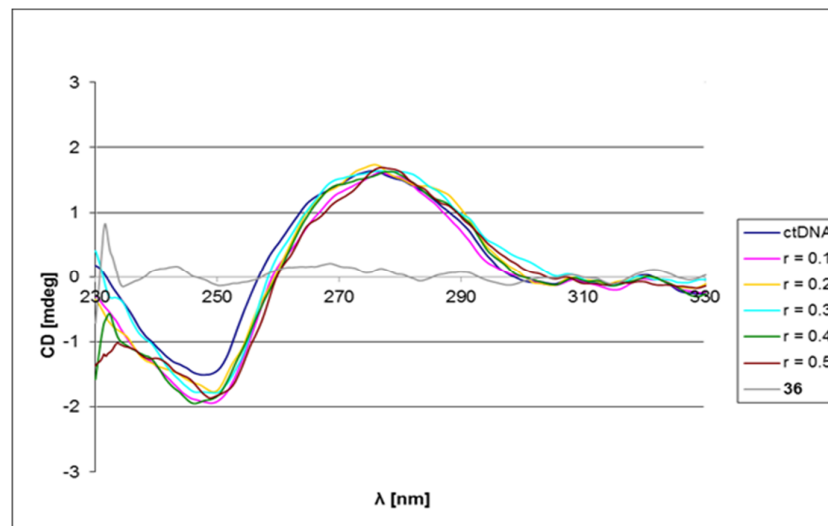
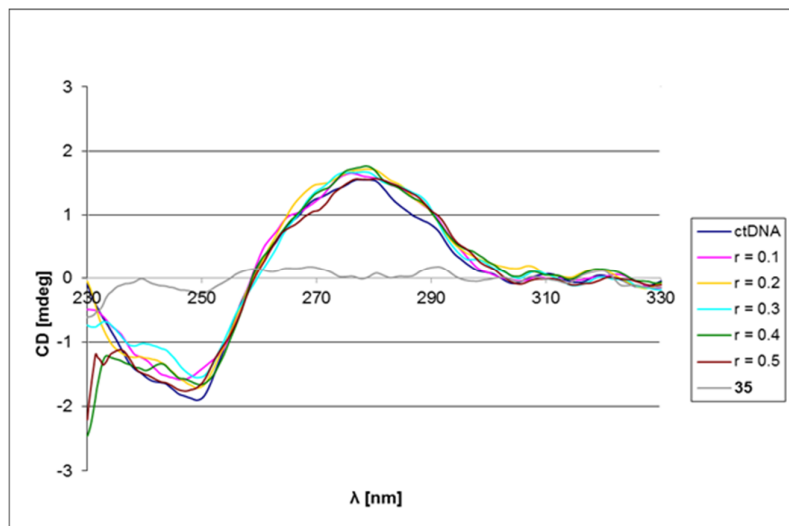


Figure S181. Changes in the CD spectrum of ct-DNA upon addition of **35** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **36** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

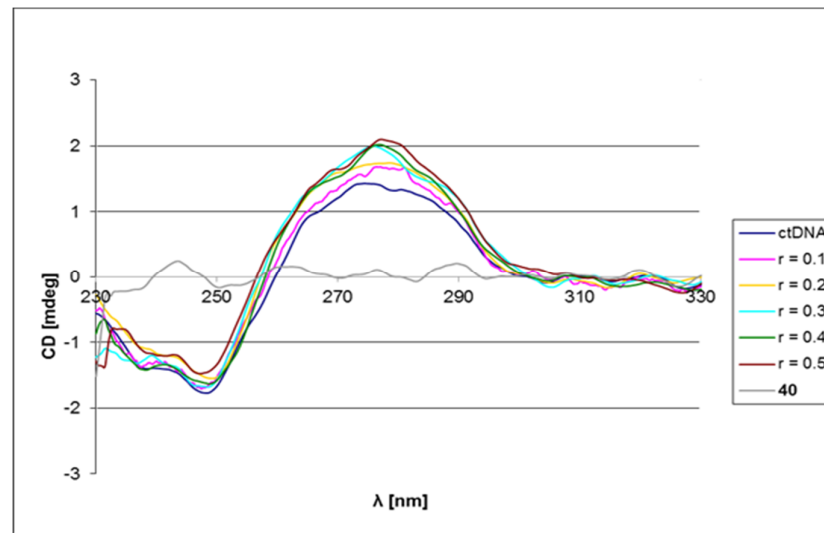
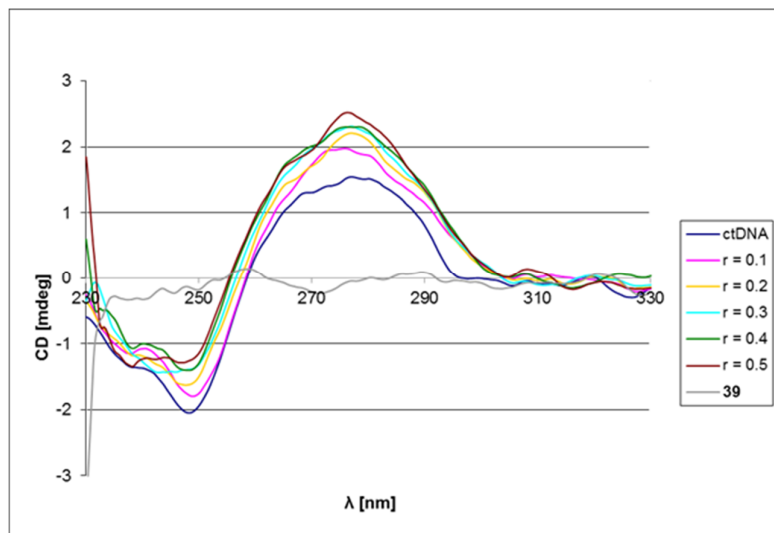


Figure S182. Changes in the CD spectrum of ct-DNA upon addition of **39** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **40** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

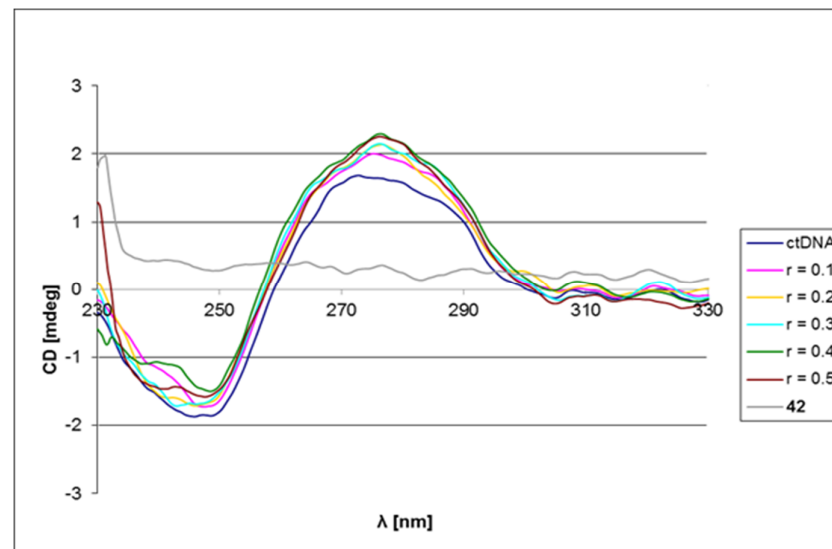
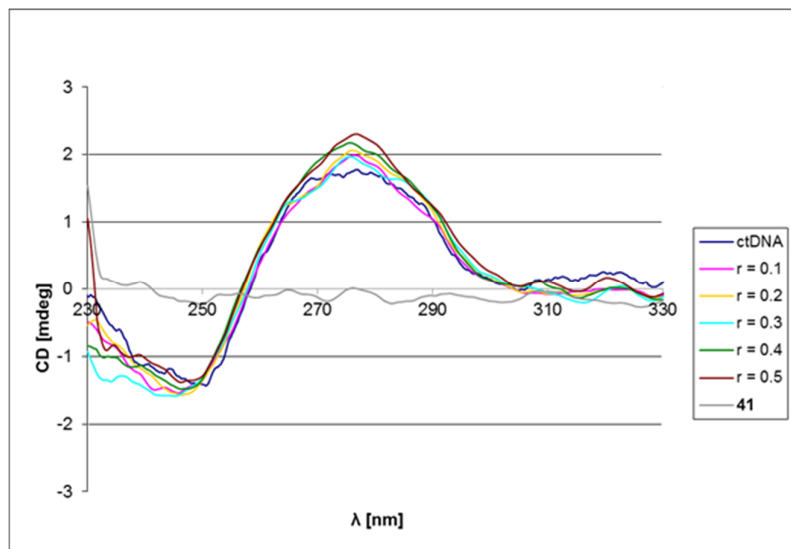


Figure S183. Changes in the CD spectrum of ct-DNA upon addition of **41** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (left) and **42** ($c(\text{ct-DNA}) = 4 \times 10^{-5} \text{ mol dm}^{-3}$) (right) at different molar ratios $r = [\text{compound}]/[\text{ct-DNA}]$, sodium cacodylate buffer (pH 7.0, 20 mM).

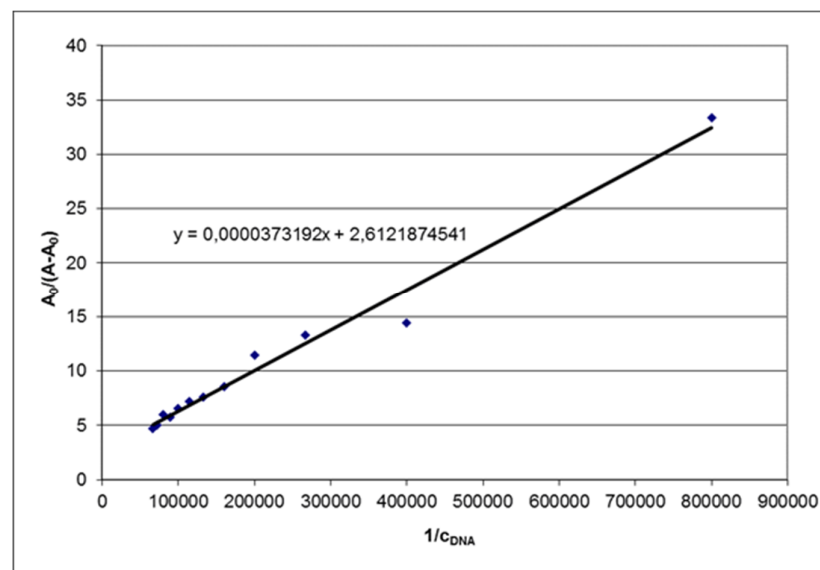
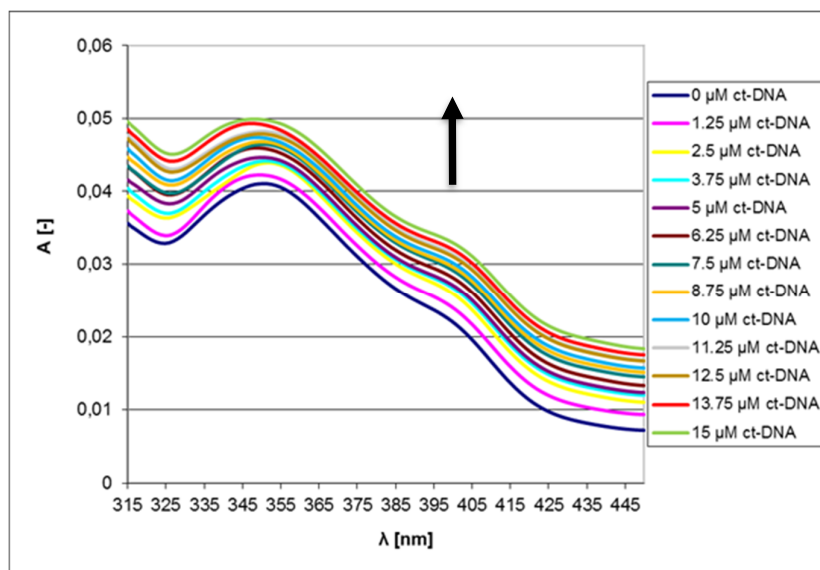


Figure S184. UV-vis absorption spectra of compound **6** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

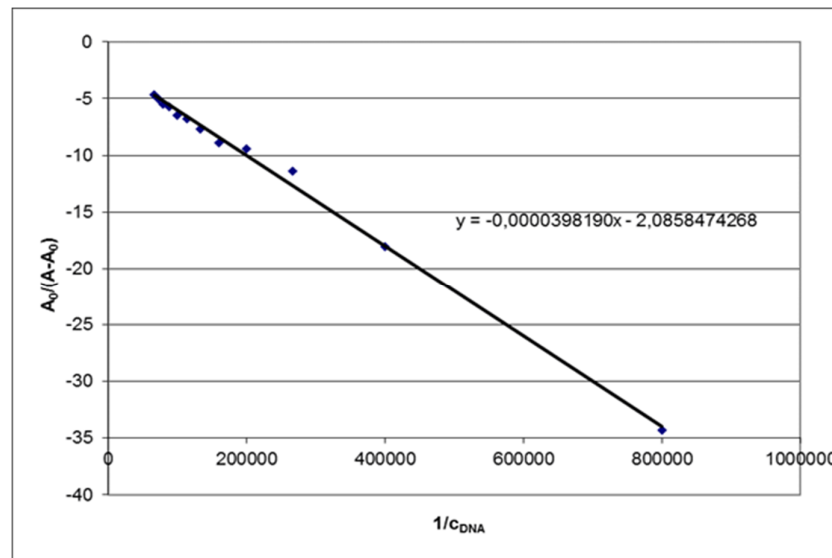
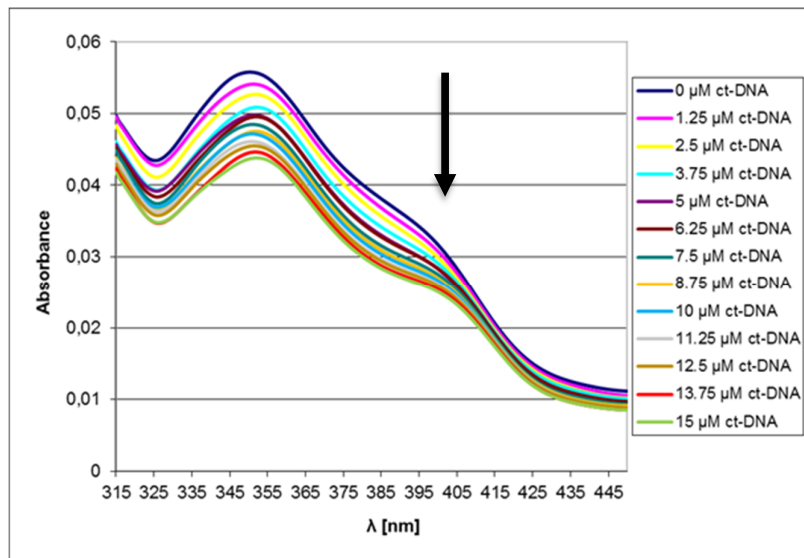


Figure S185. UV-vis absorption spectra of compound 7 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[DNA]$ yielded the binding constant (right).

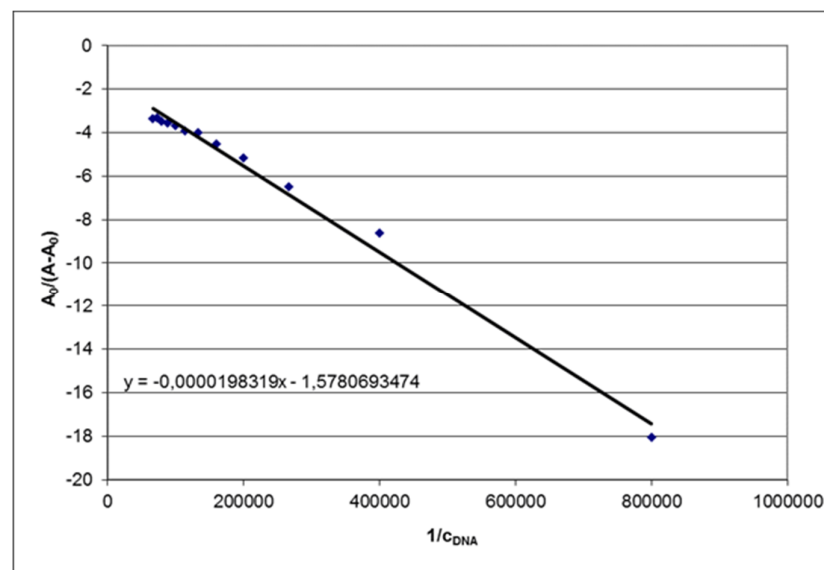
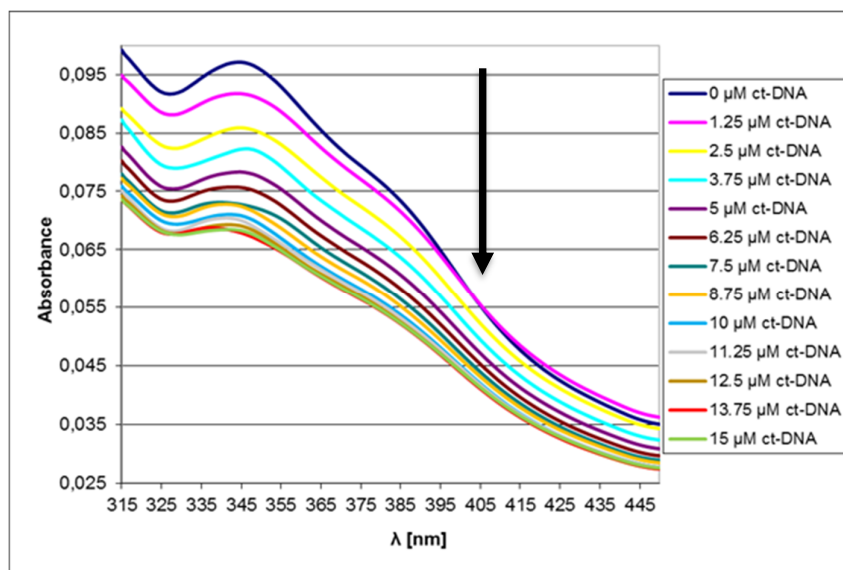


Figure S186. UV-vis absorption spectra of compound 8 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[DNA]$ yielded the binding constant (right).

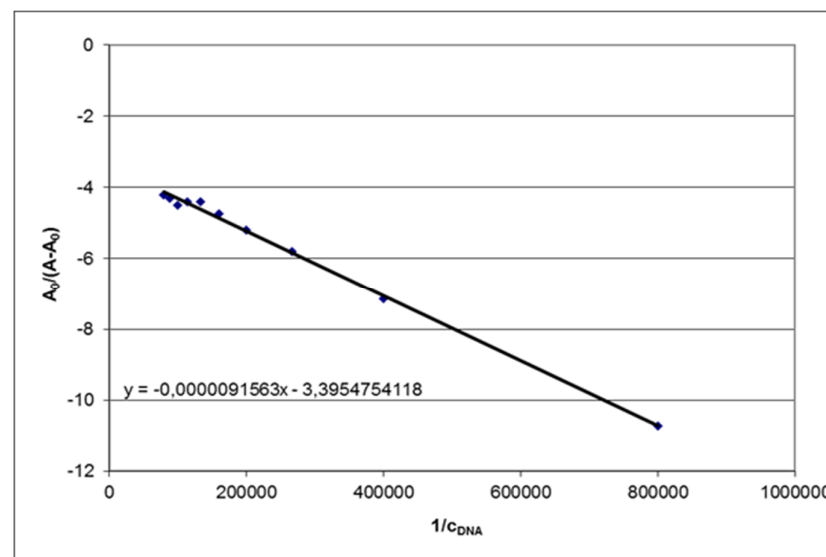
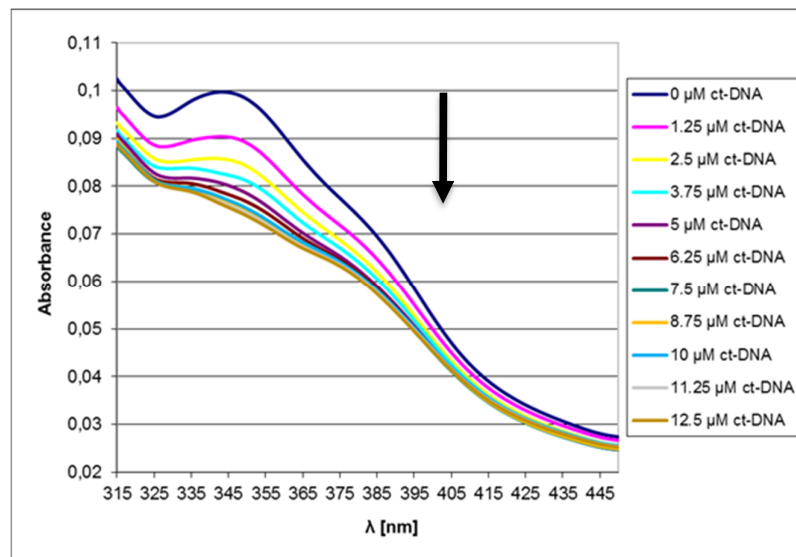


Figure S187. UV-vis absorption spectra of compound 9 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

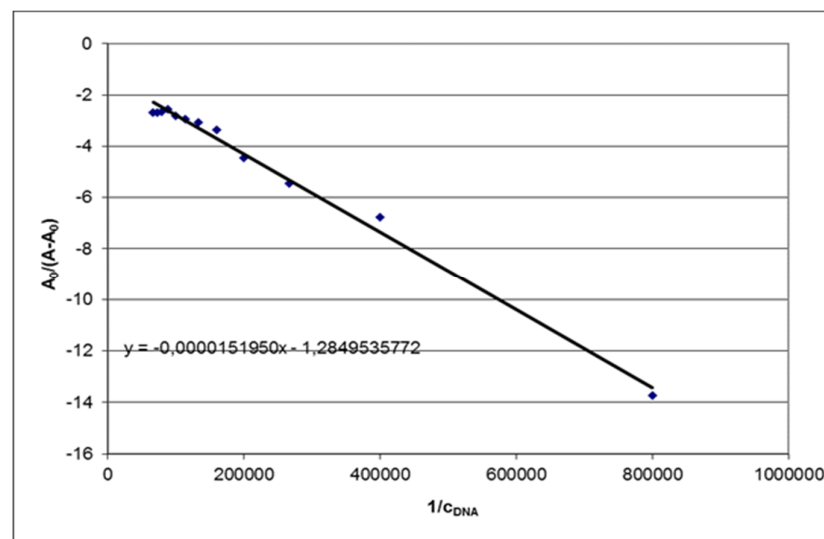
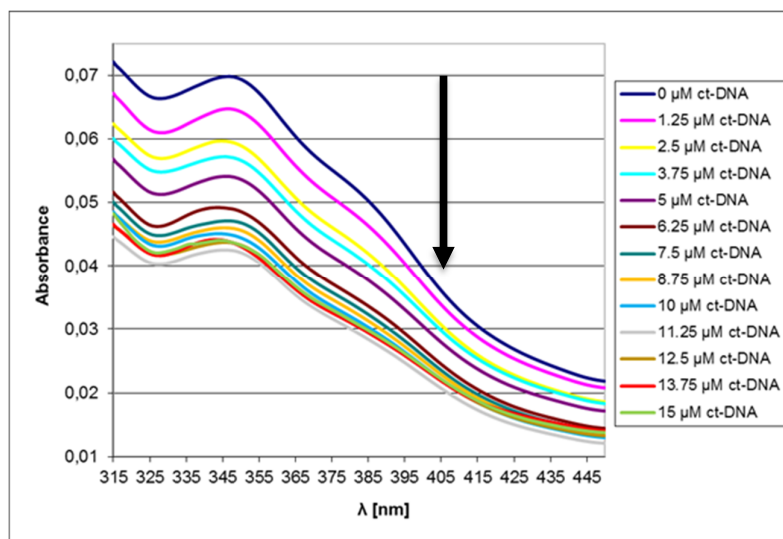


Figure S188. UV-vis absorption spectra of compound **10** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

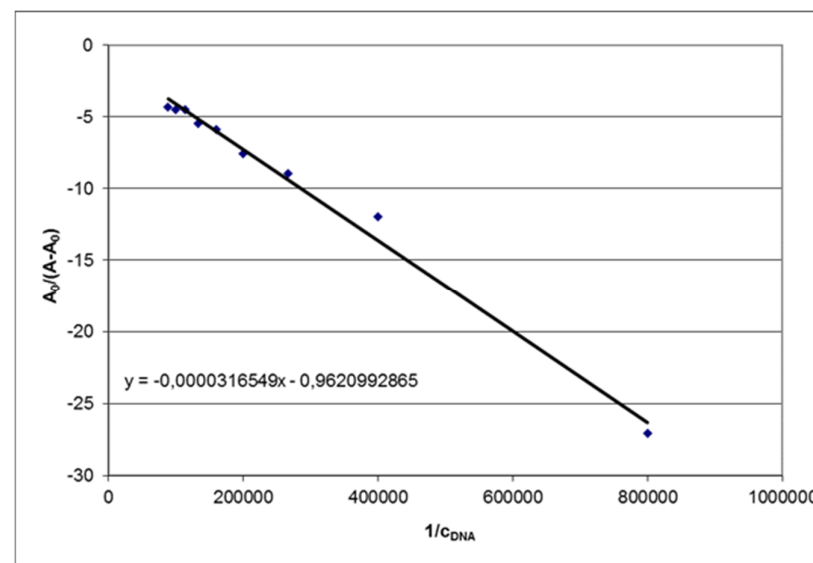
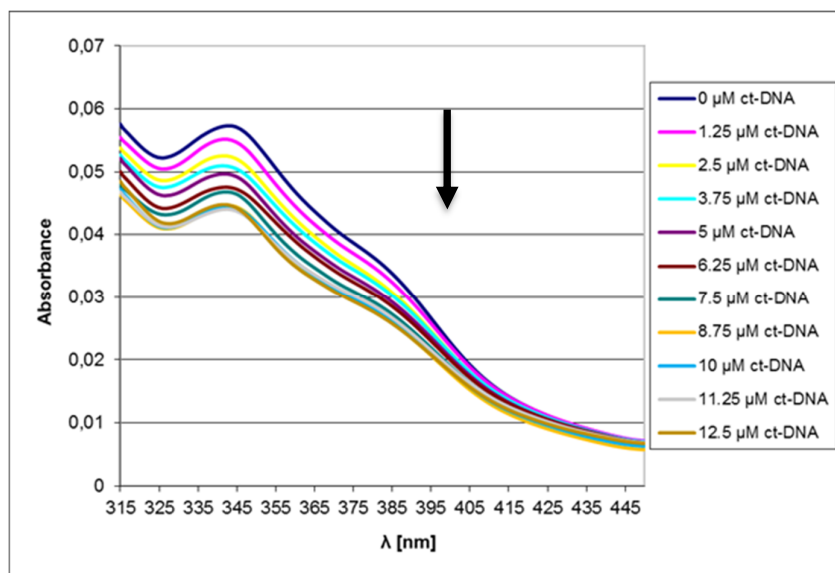


Figure S189. UV-vis absorption spectra of compound **11** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

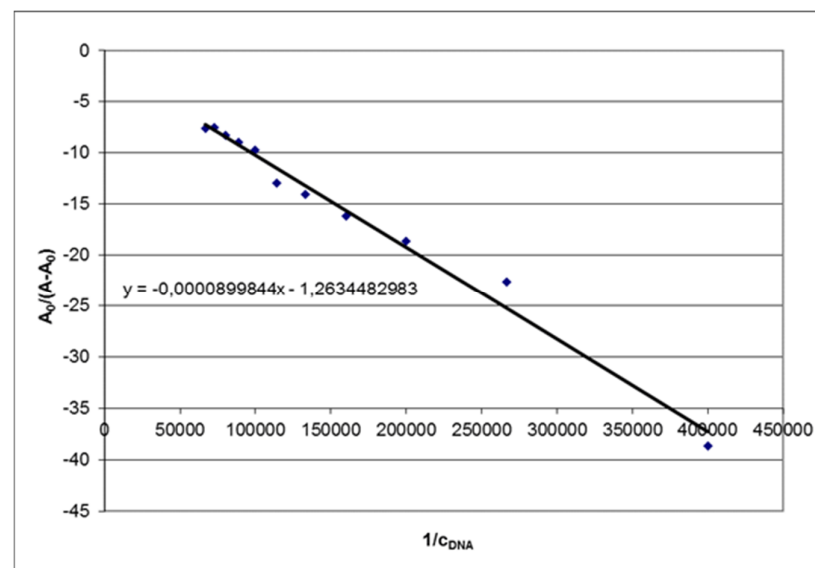
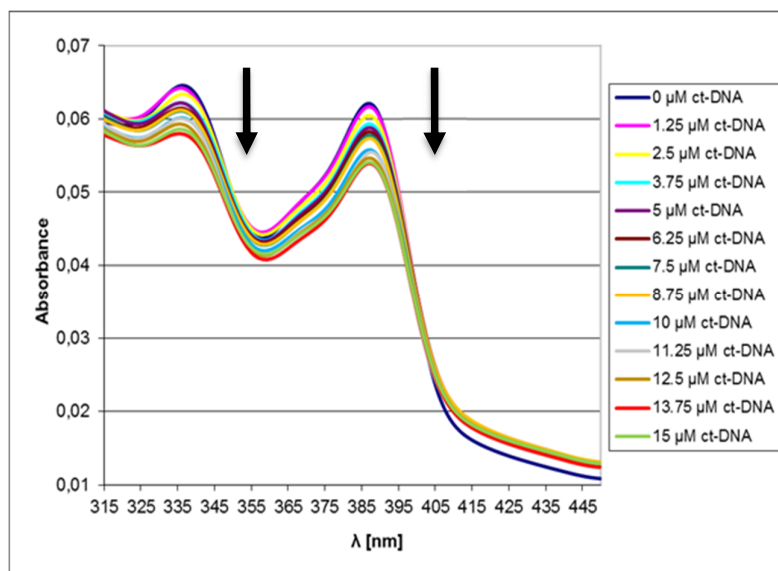


Figure S190. UV-vis absorption spectra of compound 15 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

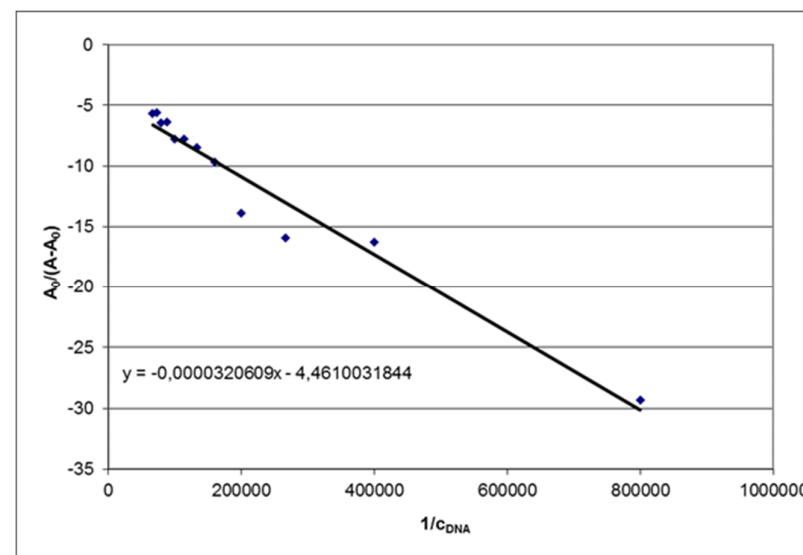
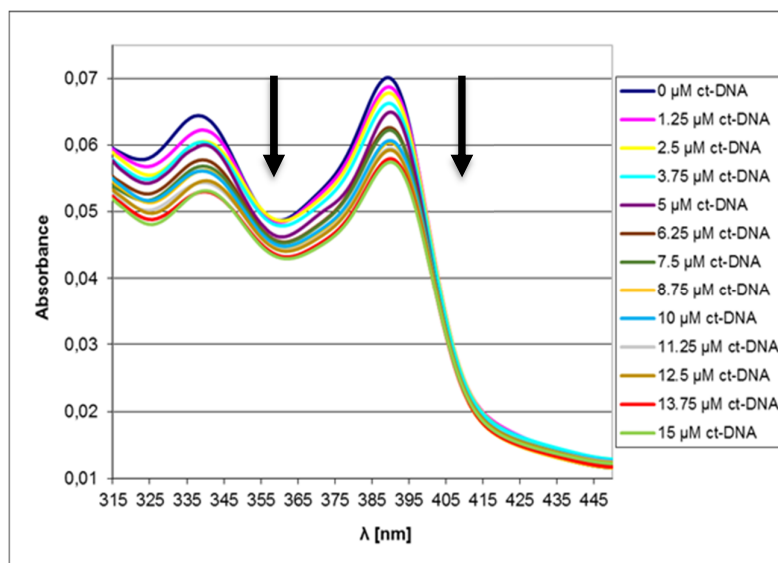


Figure S191. UV-vis absorption spectra of compound **16** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

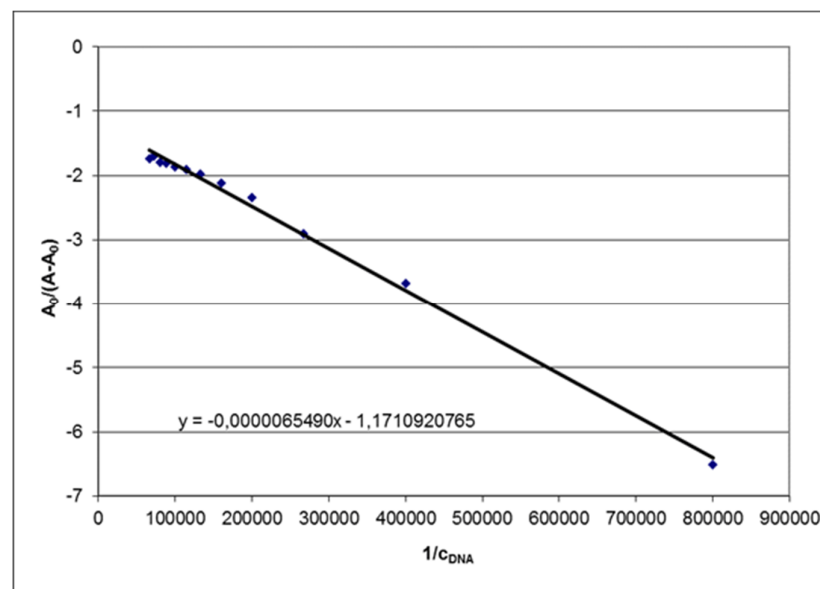
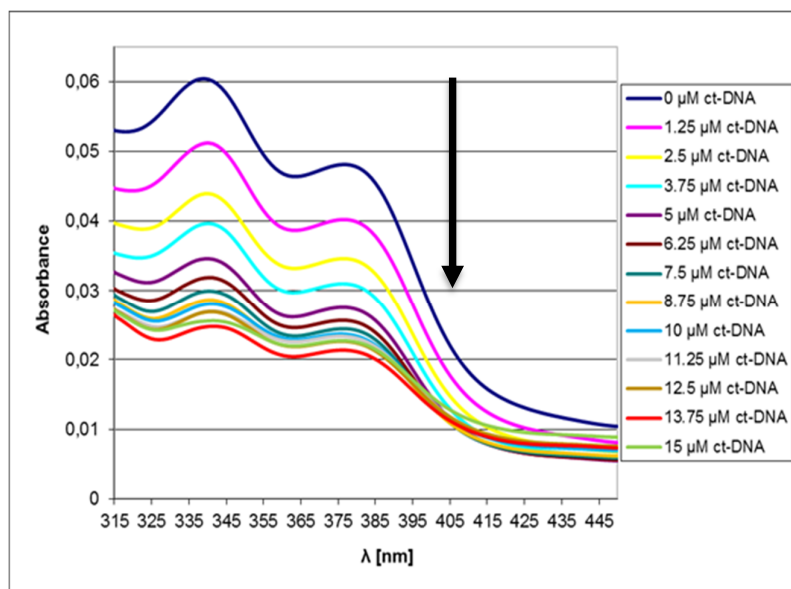


Figure S192. UV-vis absorption spectra of compound 17 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

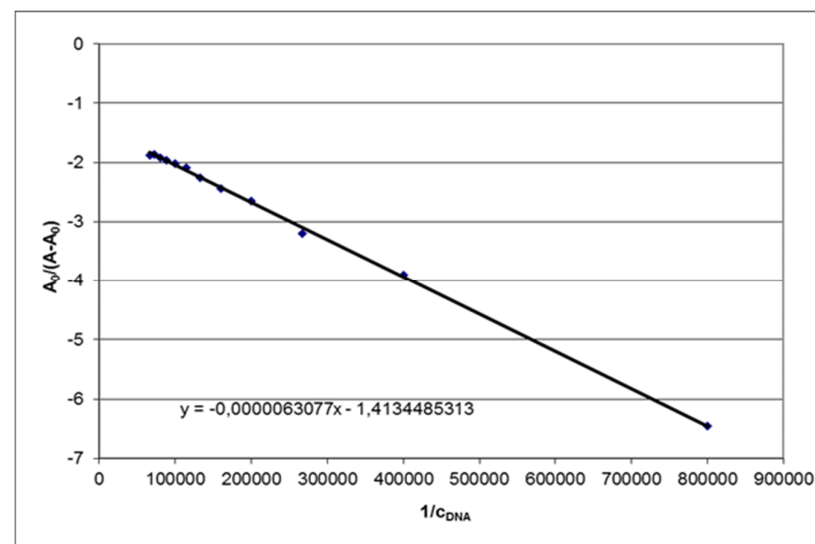
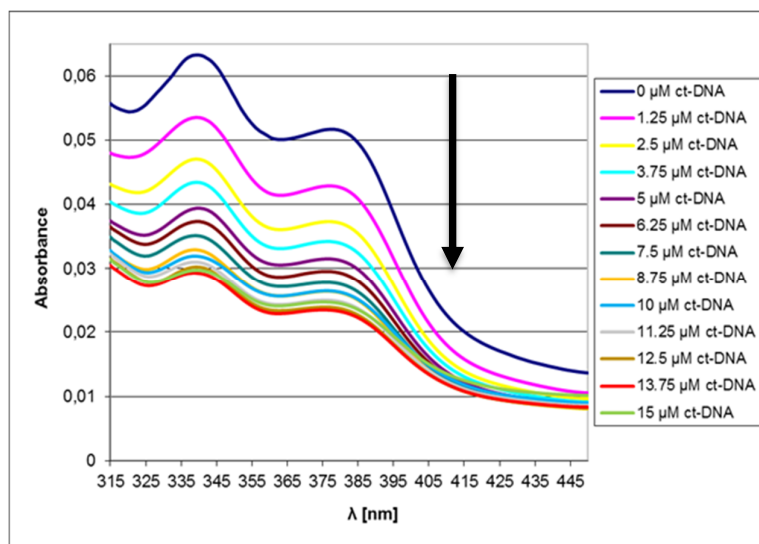


Figure S193. UV-vis absorption spectra of compound 18 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

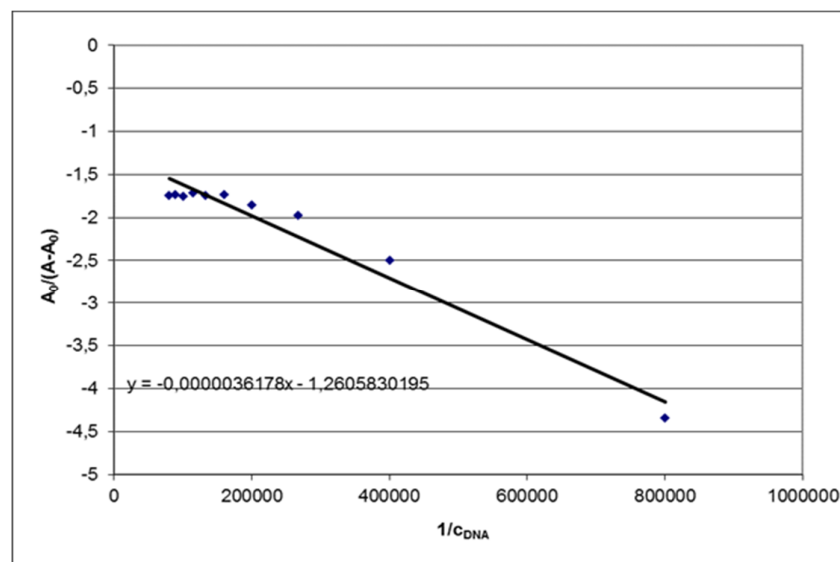
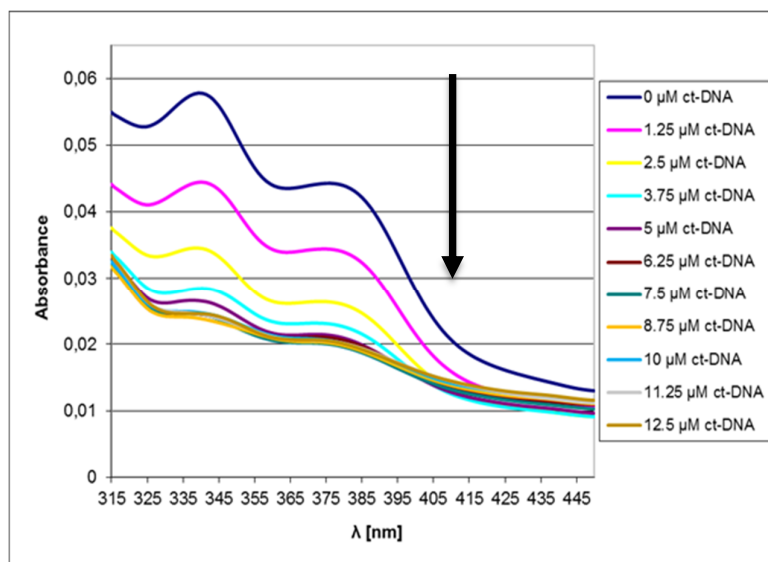


Figure S194. UV-vis absorption spectra of compound **19** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

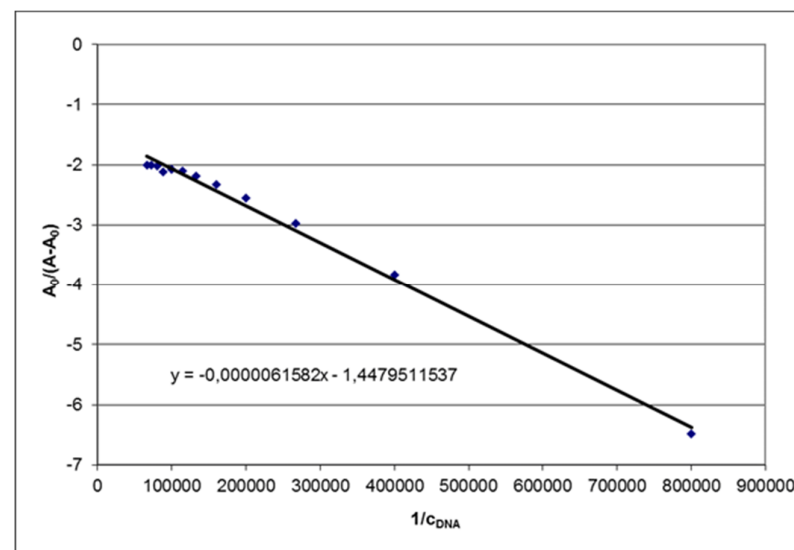
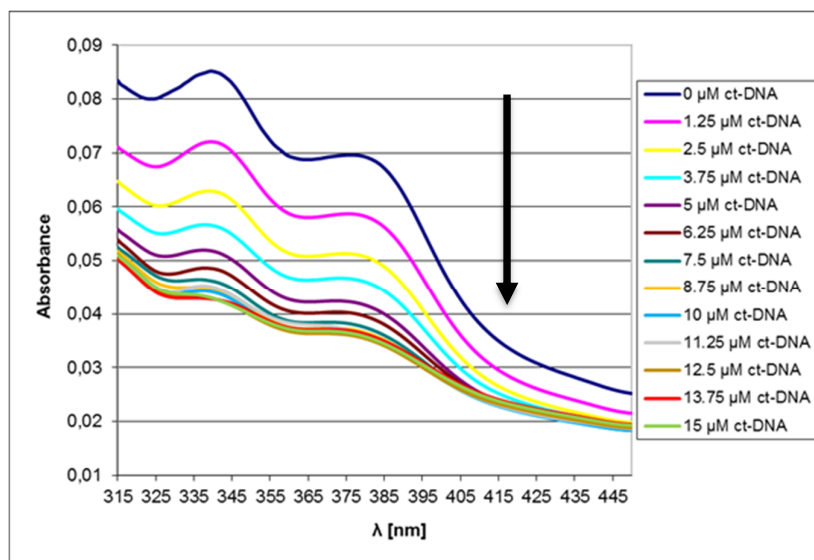


Figure S195. UV-vis absorption spectra of compound **20** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

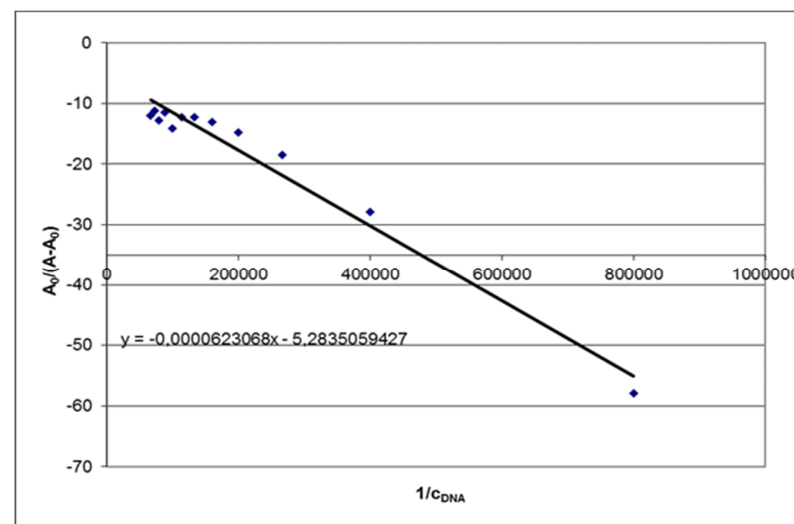
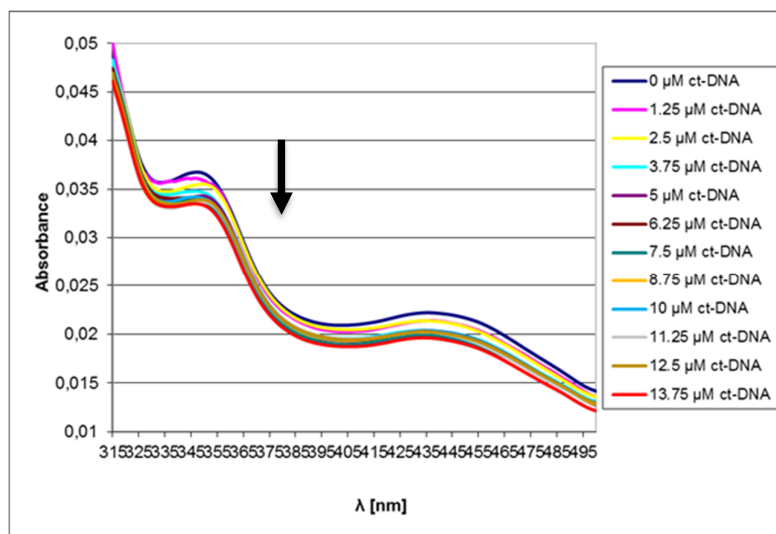


Figure S196. UV-vis absorption spectra of compound **33** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

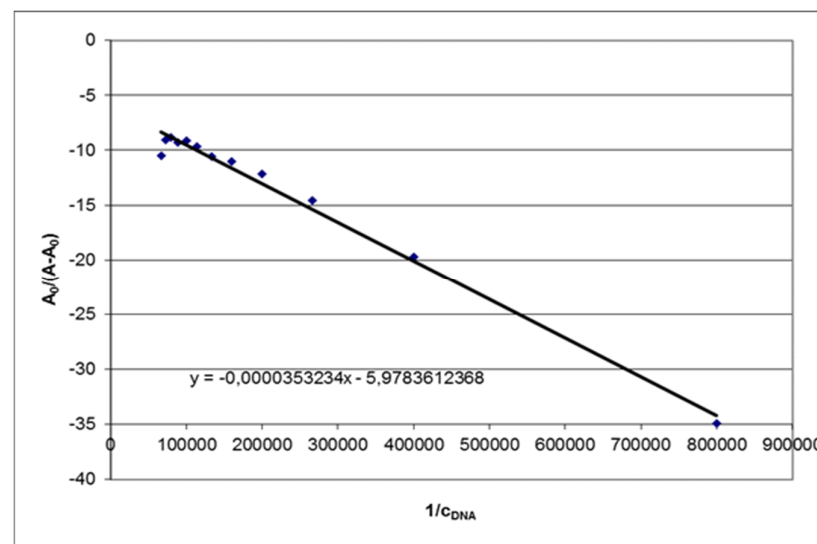
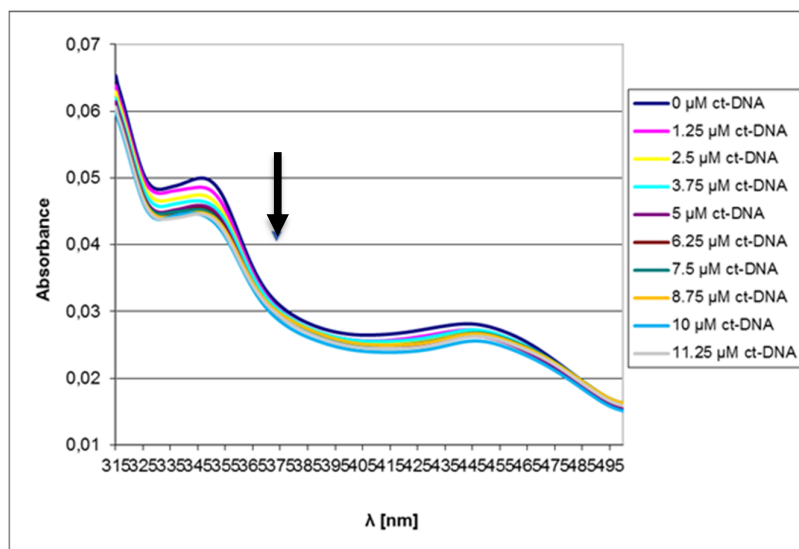


Figure S197. UV-vis absorption spectra of compound **34** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

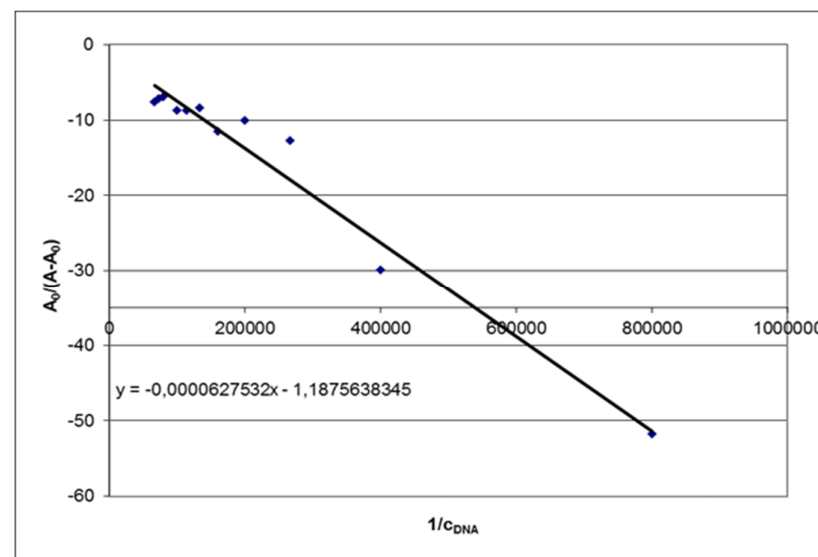
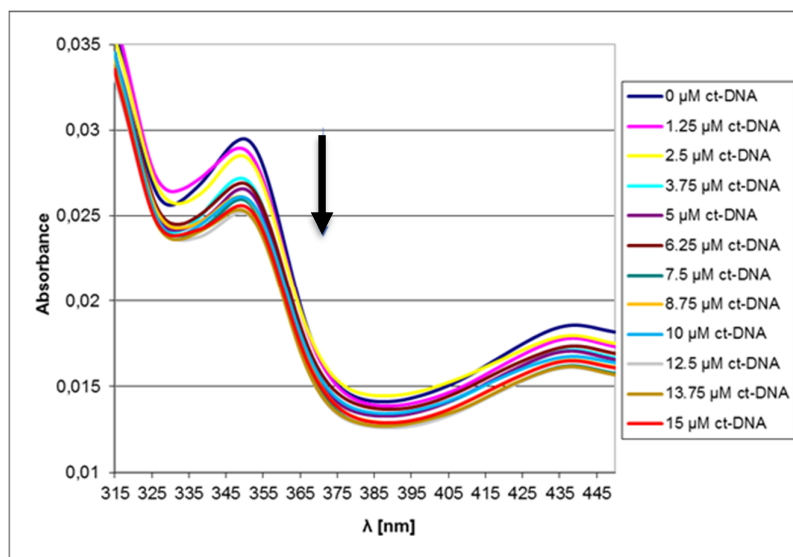


Figure S198. UV-vis absorption spectra of compound 35 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[DNA]$ yielded the binding constant (right).

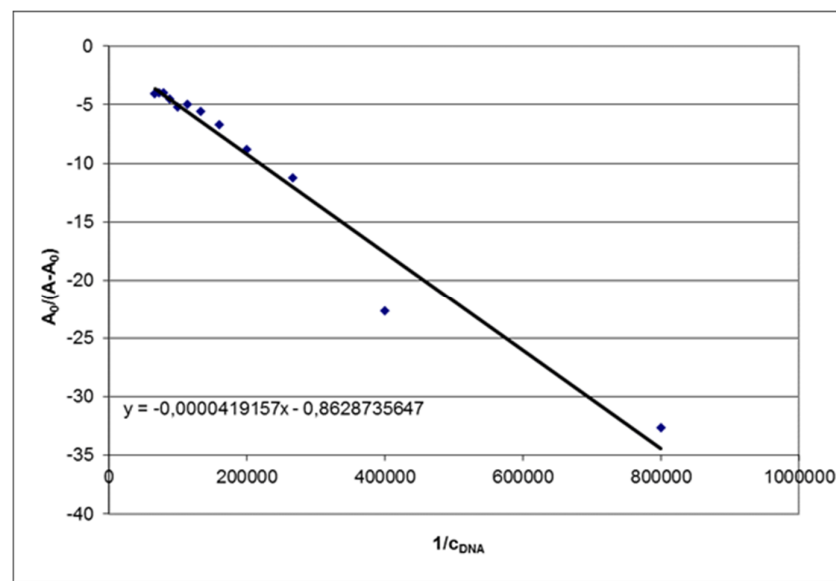
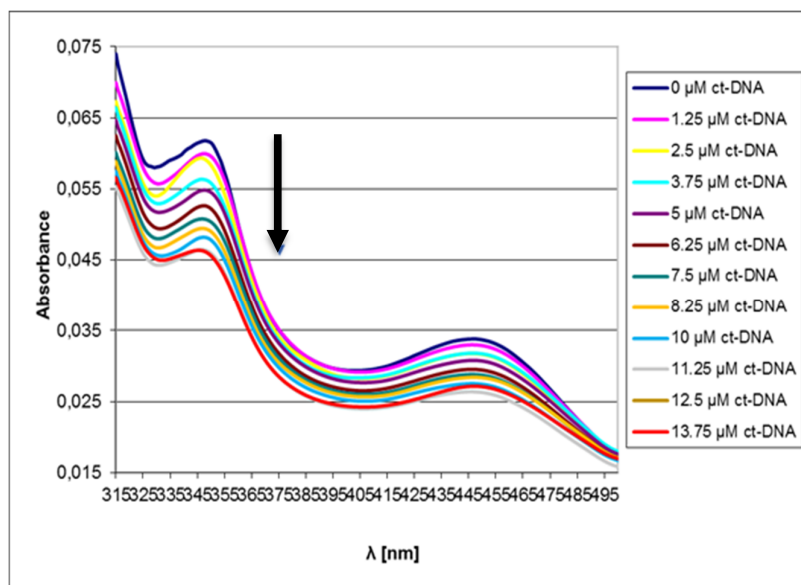


Figure S199. UV-vis absorption spectra of compound 36 (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/A-A_0$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

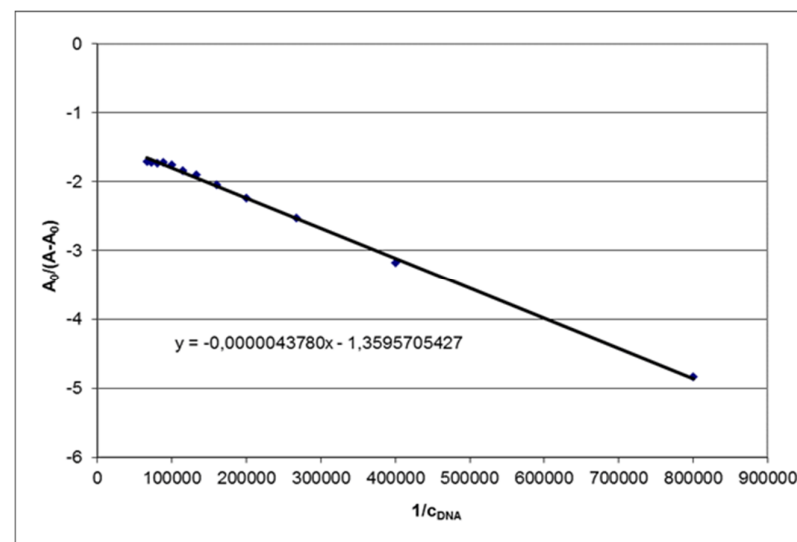
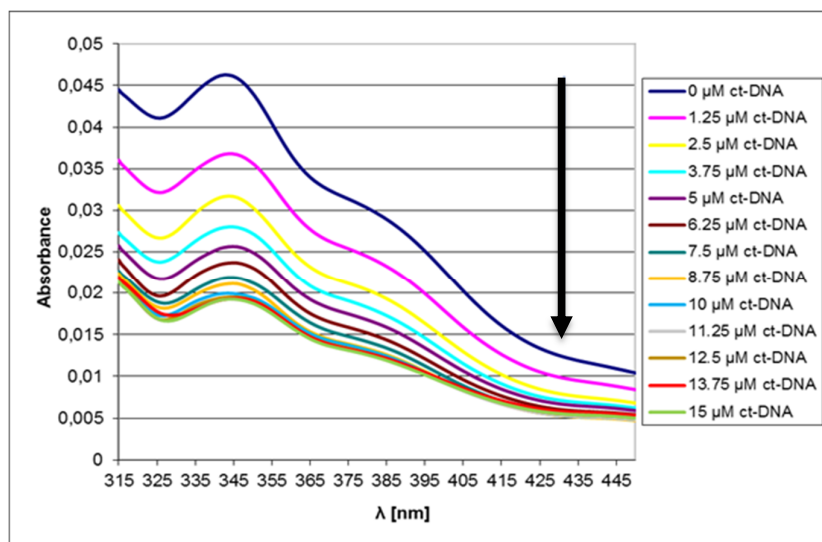


Figure S200. UV-vis absorption spectra of compound **39** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[\text{DNA}]$ yielded the binding constant (right).

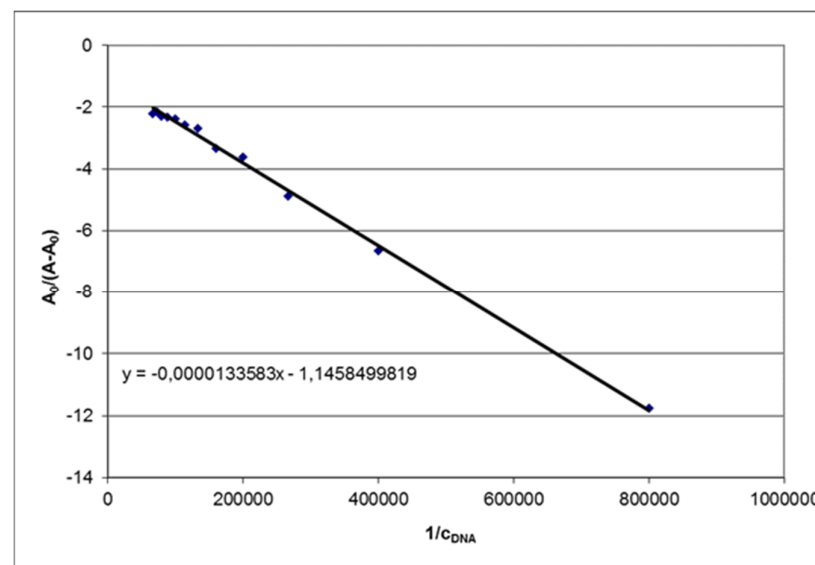
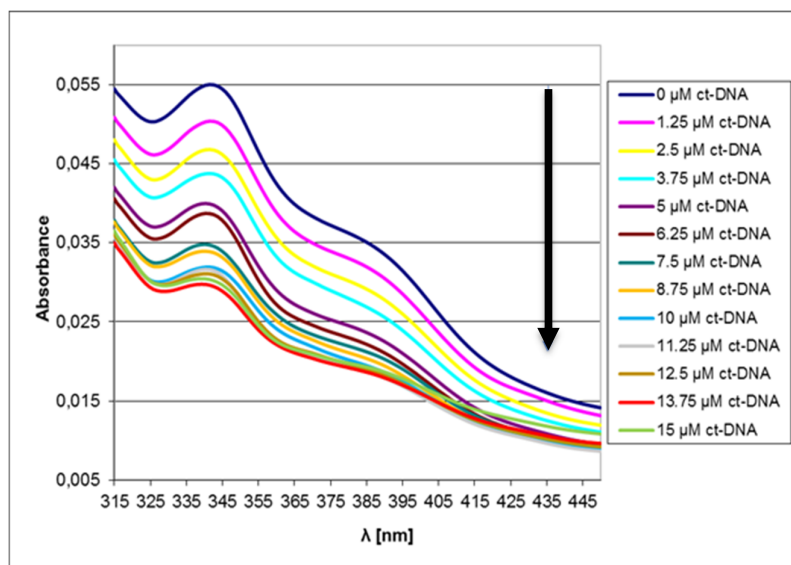


Figure S201. UV-vis absorption spectra of compound **40** (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[DNA]$ yielded the binding constant (right).

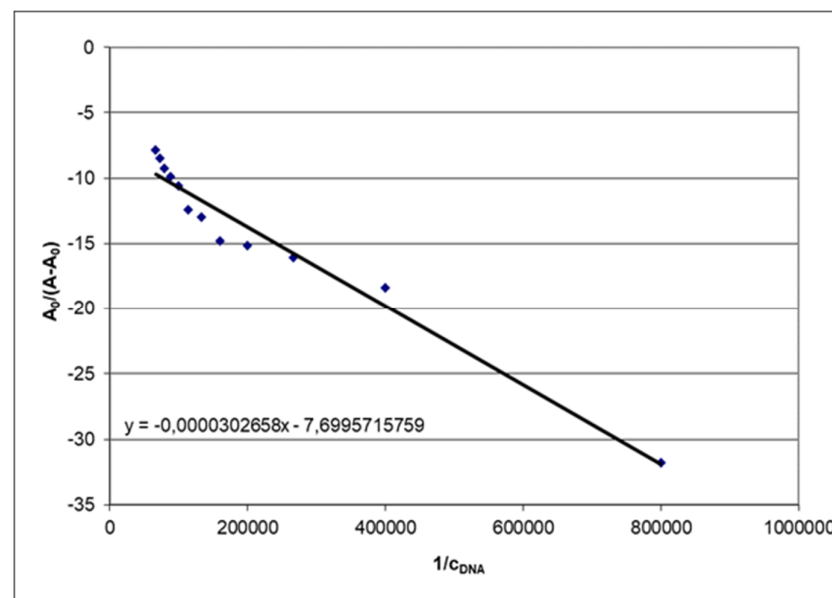
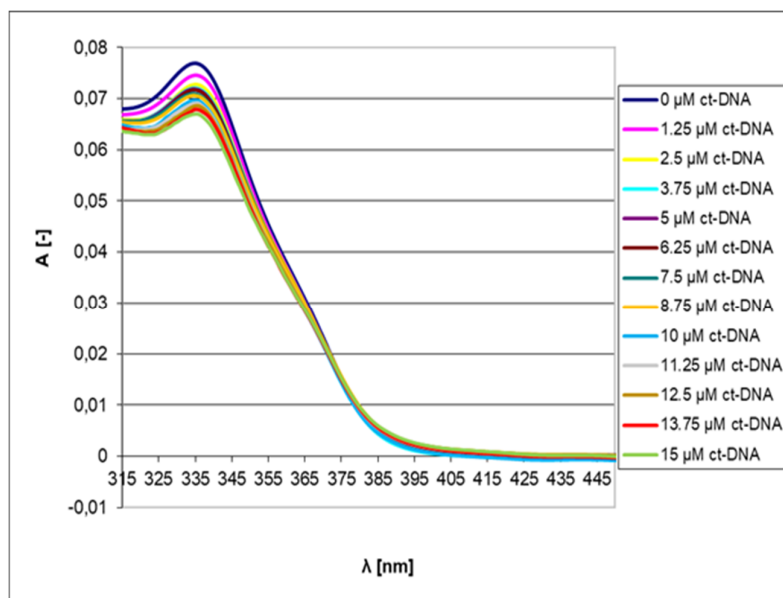


Figure S202. UV-vis absorption spectra of mitonafide (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[DNA]$ yielded the binding constant (right).

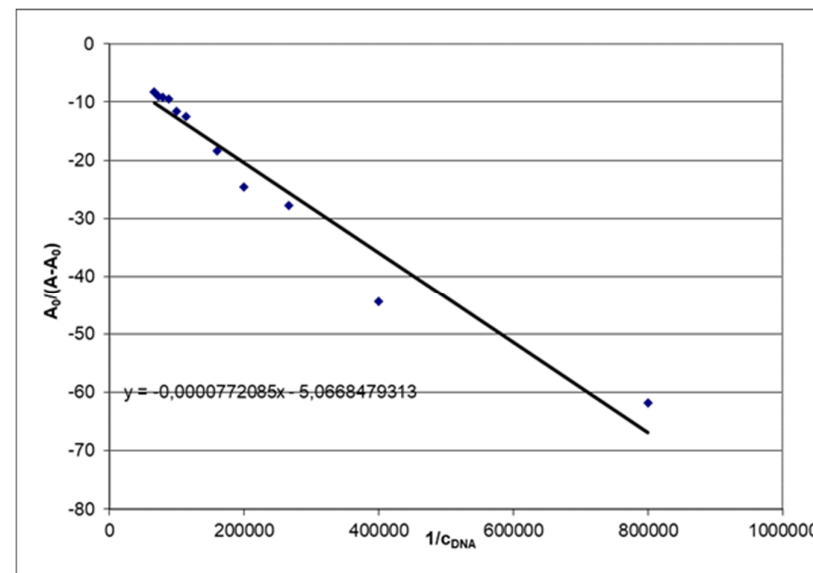
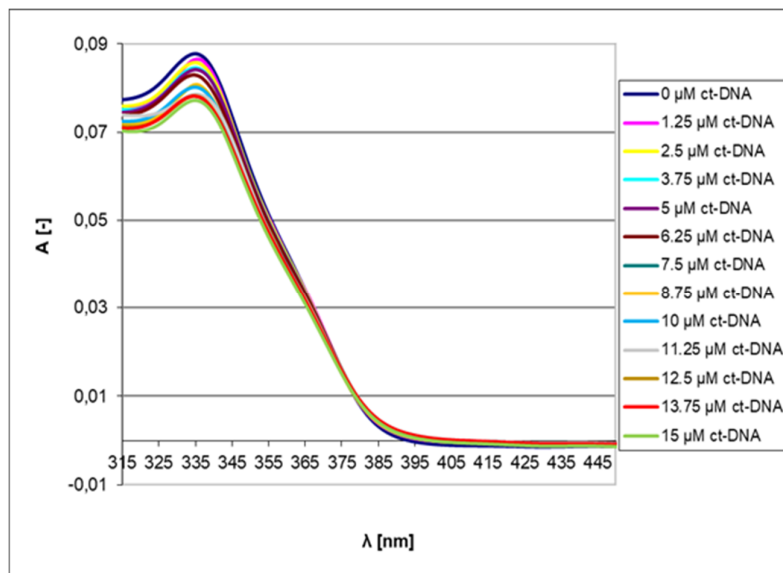


Figure S203. UV-vis absorption spectra of pinafide (20 μM) in the presence of increasing amount of ct-DNA (0-15 μM) (left). The plot of $A_0/(A-A_0)$ versus $1/[DNA]$ yielded the binding constant (right).

Table 2S. Crystallographic data.

Compound	39	41
Wavelength [Å]	0.7749	1.54178
Temperature [K]	100	130
Space group	P-1	P-1
Z	2	2
<i>a</i> [Å]	6.923(2)	7.0385(8)
<i>b</i> [Å]	13.239(8)	9.5223(8)
<i>c</i> [Å]	15.571(3)	21.4413(17)
α [°]	105.721(0)	79.497(7)
β [°]	102.188(3)	81.569(8)
γ [°]	95.815(0)	87.093(8)
R _{int}	0.0550	0.0892
Resolution [Å]	0.79	0.79
% completeness	74.3	94.8
Independent reflections	4262	5628
R/R(for F _o >4 σ)	0.0840/0.1106	0.1012/0.1755
CSD code	2059432	2059431