

Supplementary information

Exploring Structure–Activity Relationships of Niclosamide-Based Colistin Potentiators in Colistin-Resistant Gram-Negative Bacteria

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NMR Spectra of compounds used for biological testing

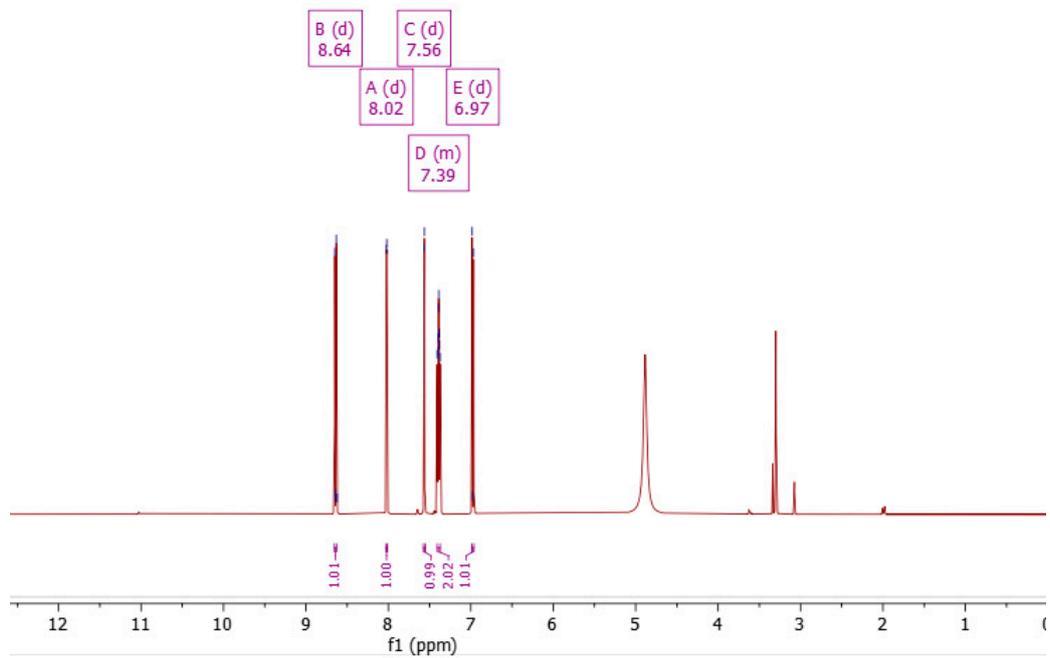


Figure S1 ¹H NMR spectrum of compound 1

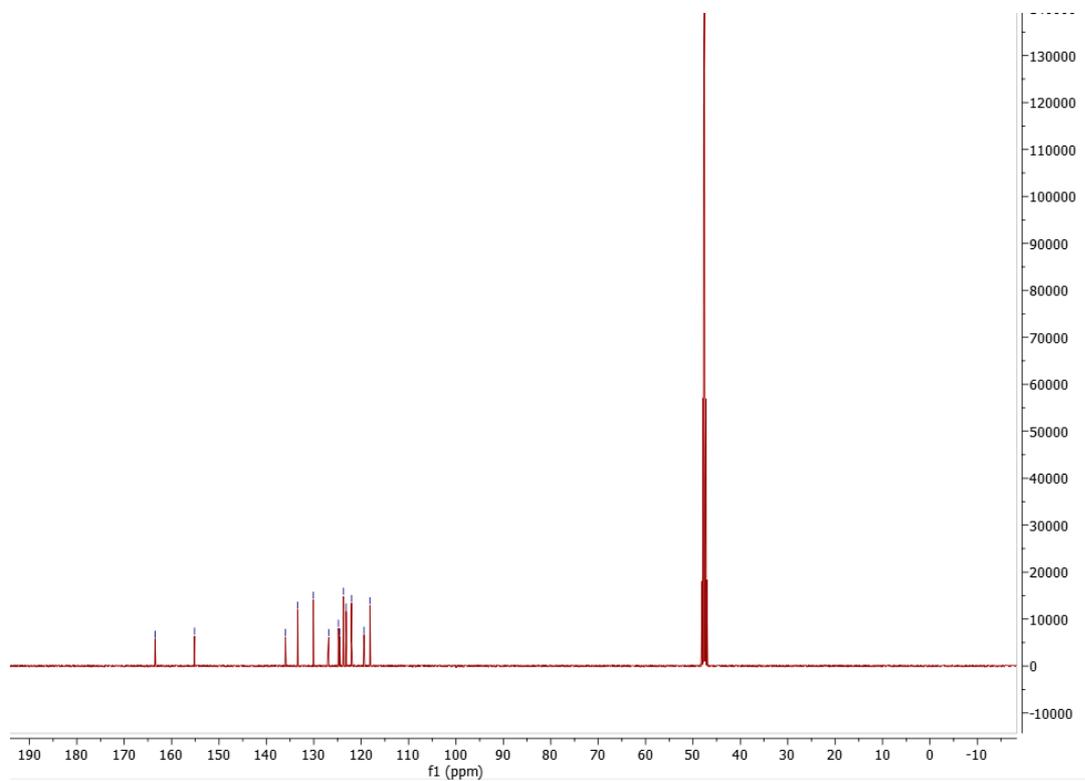


Figure S2 ^{13}C NMR spectrum of compound **1**

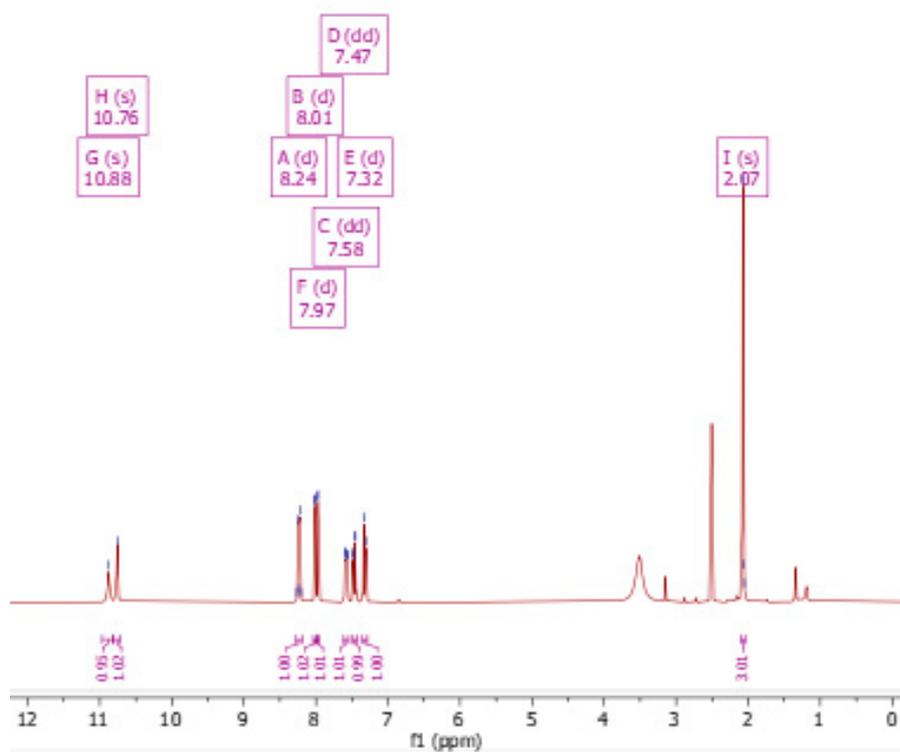


Figure S3 ^1H NMR spectrum of compound **2**

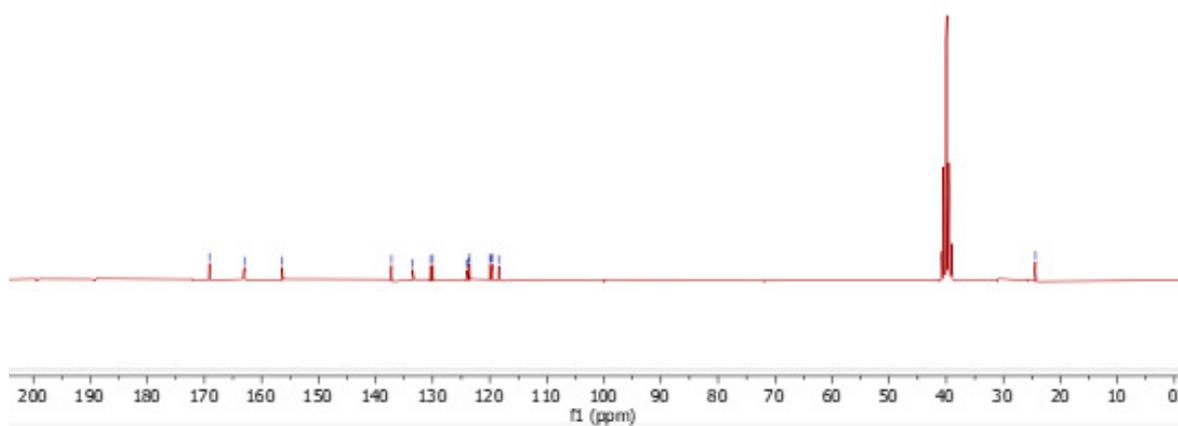


Figure S4 ^{13}C NMR spectrum of compound **2**

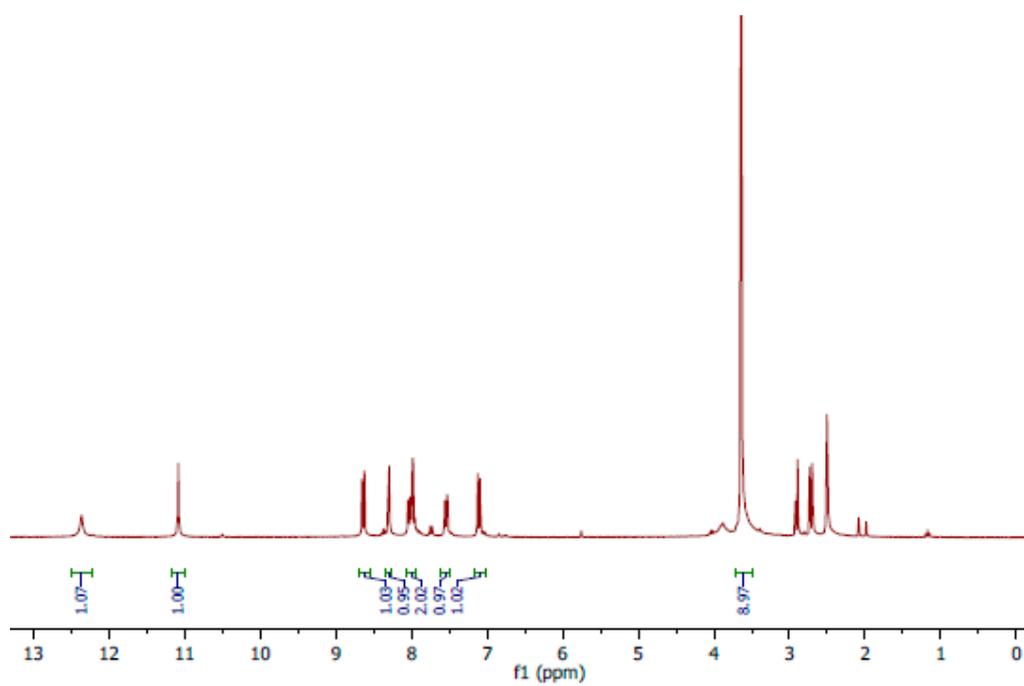


Figure S5 ^1H NMR spectrum of compound 3

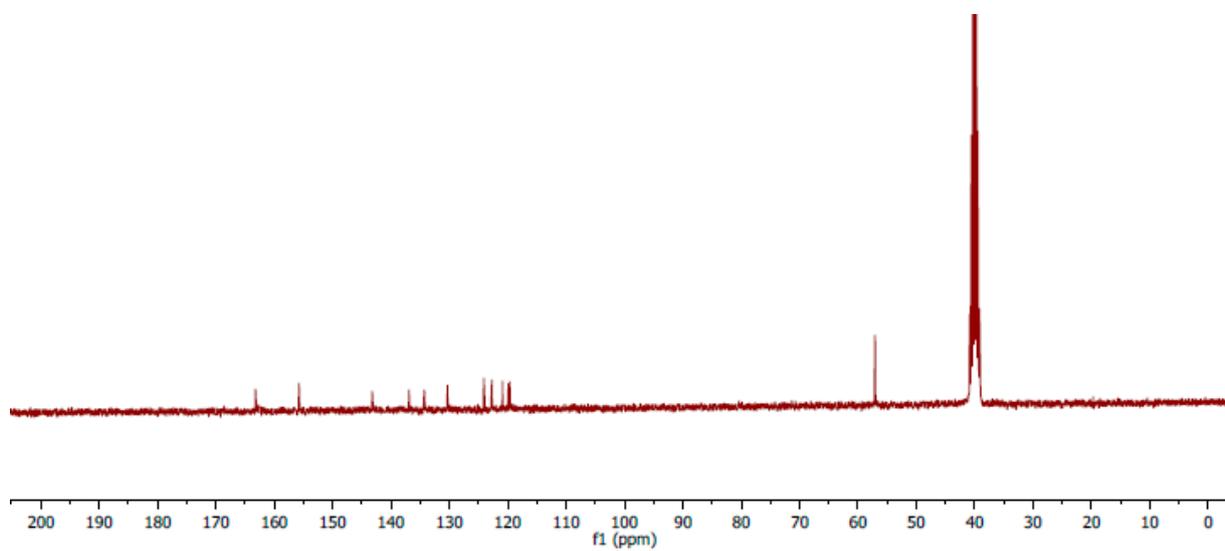


Figure S6 ^{13}C NMR spectrum of compound 3

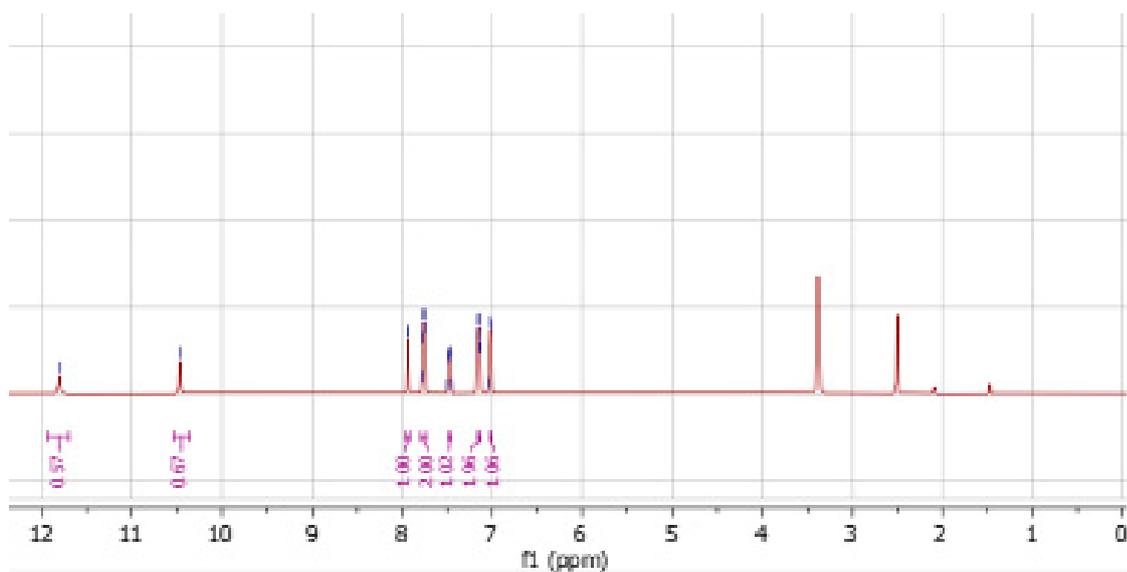


Figure S7 ^1H NMR spectrum of compound 4

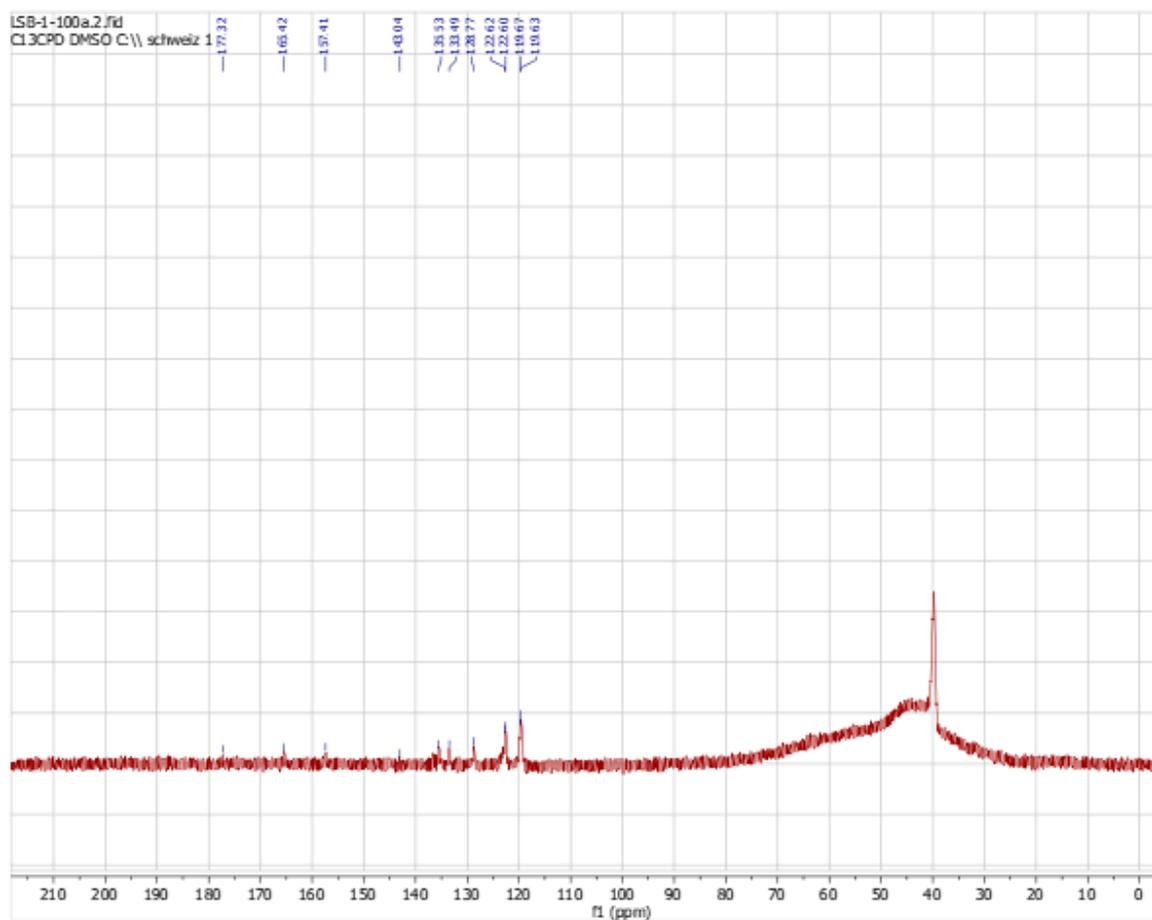


Figure S8 ^{13}C NMR spectrum of compound 4

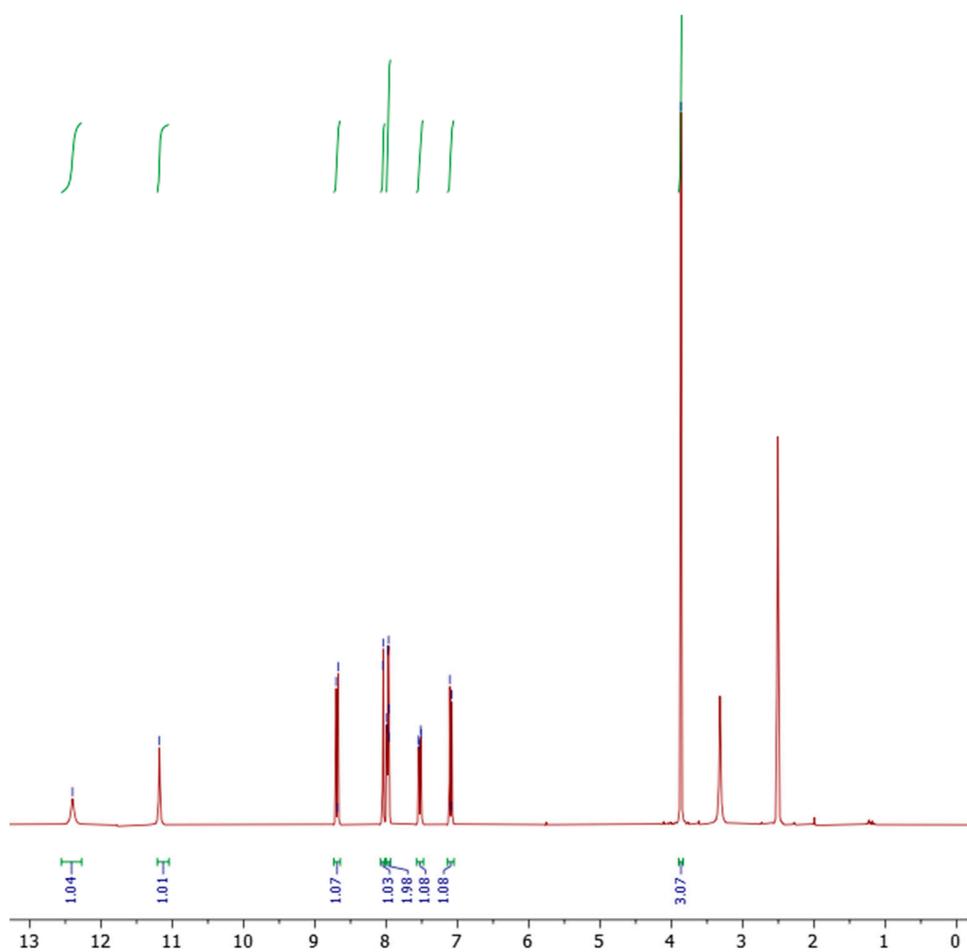


Figure S9 ¹H NMR spectrum of compound 5a

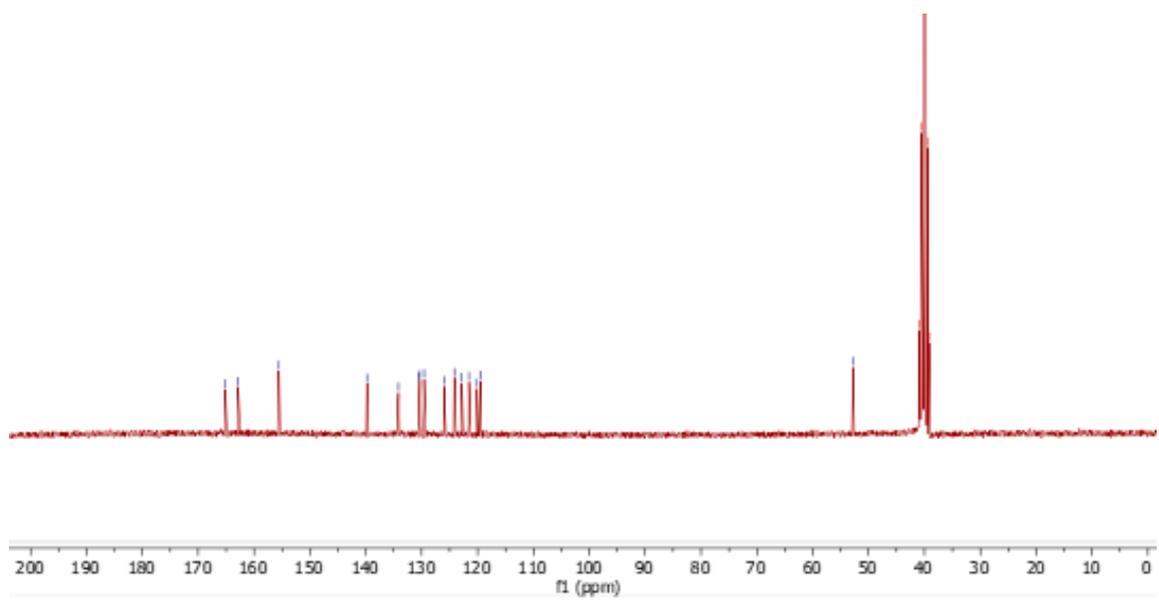


Figure S10 ¹³C NMR spectrum of compound 5a

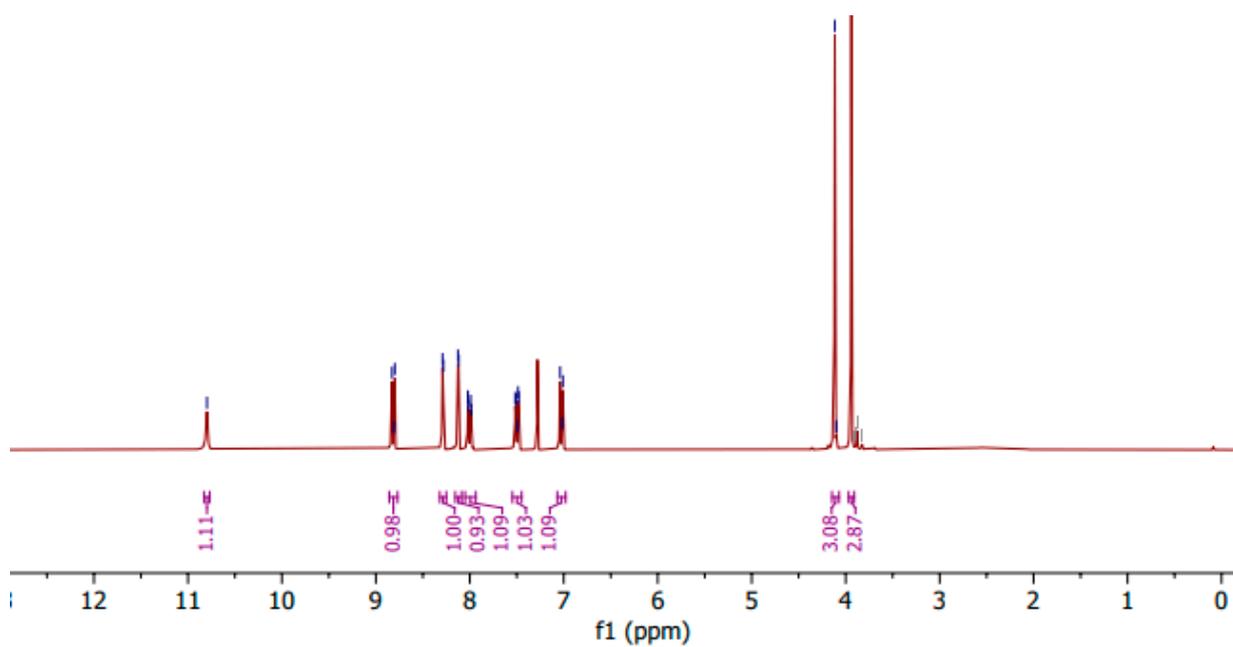


Figure S11 ¹H NMR spectrum of compound 5b

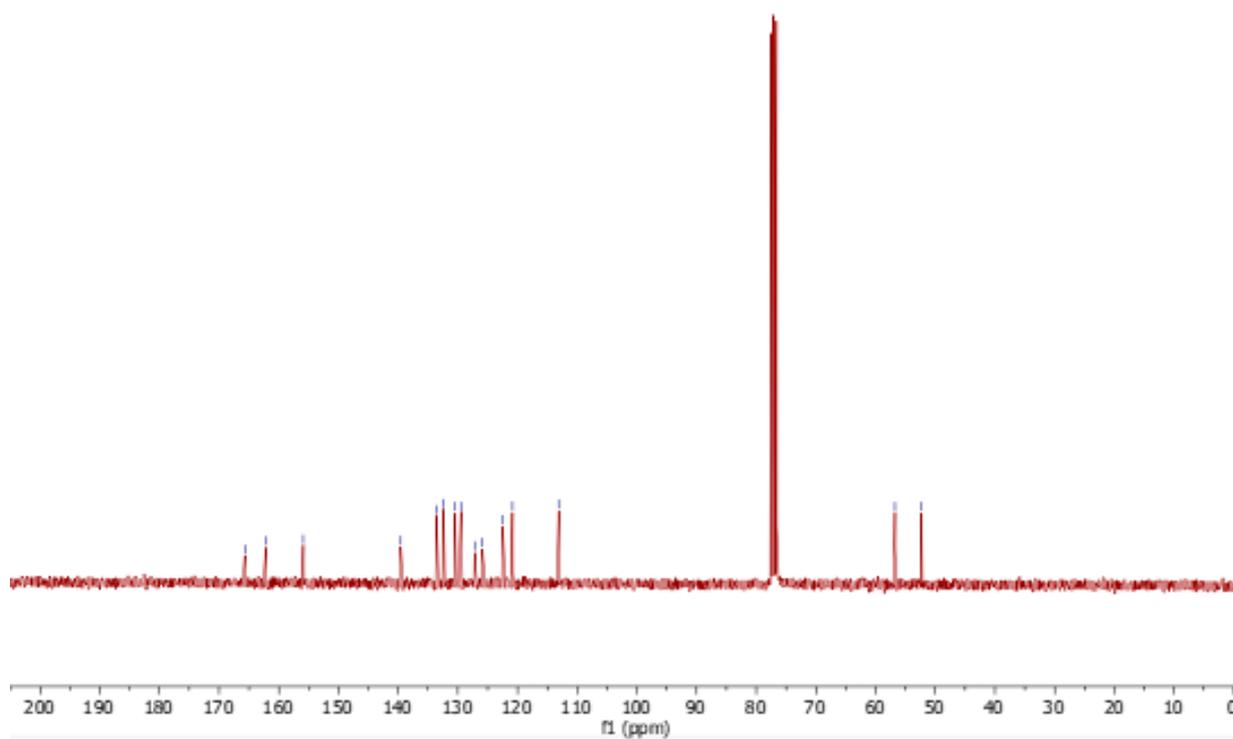


Figure S12 ¹³C NMR spectrum of compound 5b

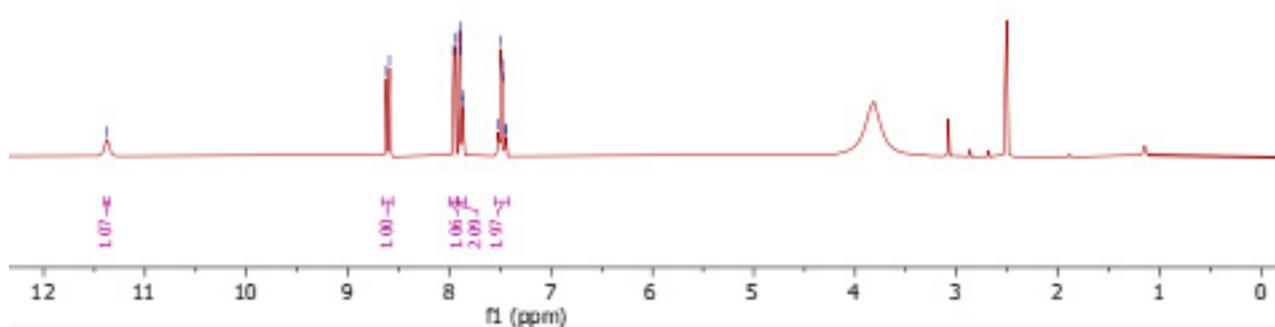


Figure S13 ^1H NMR spectrum of compound **6**

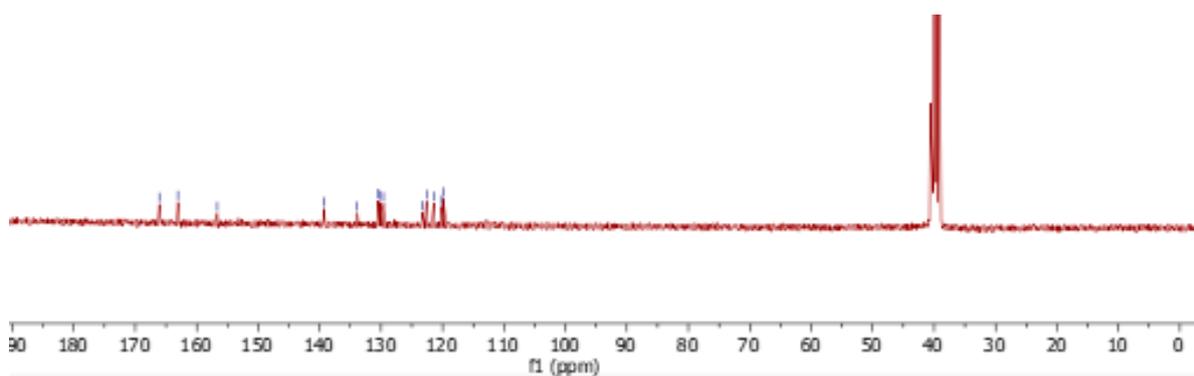


Figure S14 ^{13}C NMR spectrum of compound **6**

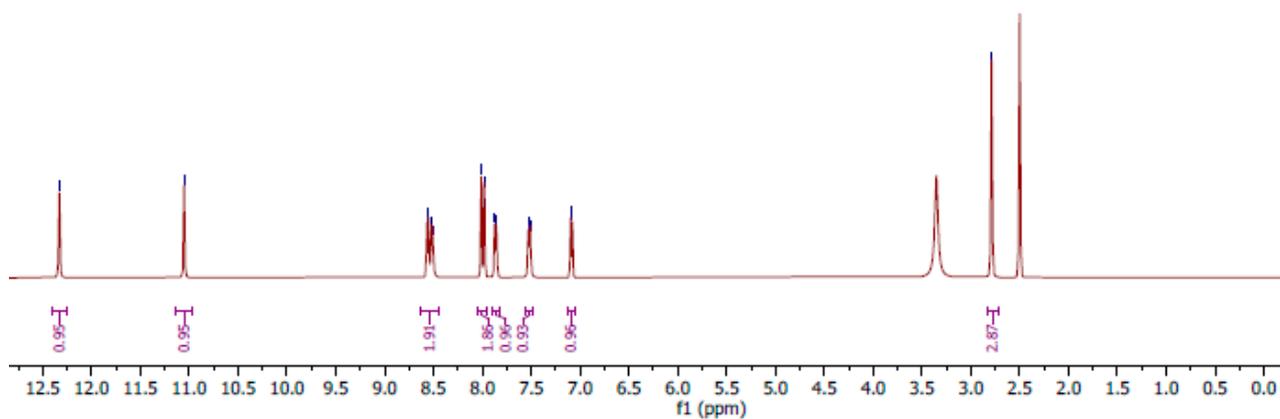


Figure S15 ^1H NMR spectrum of compound **7**

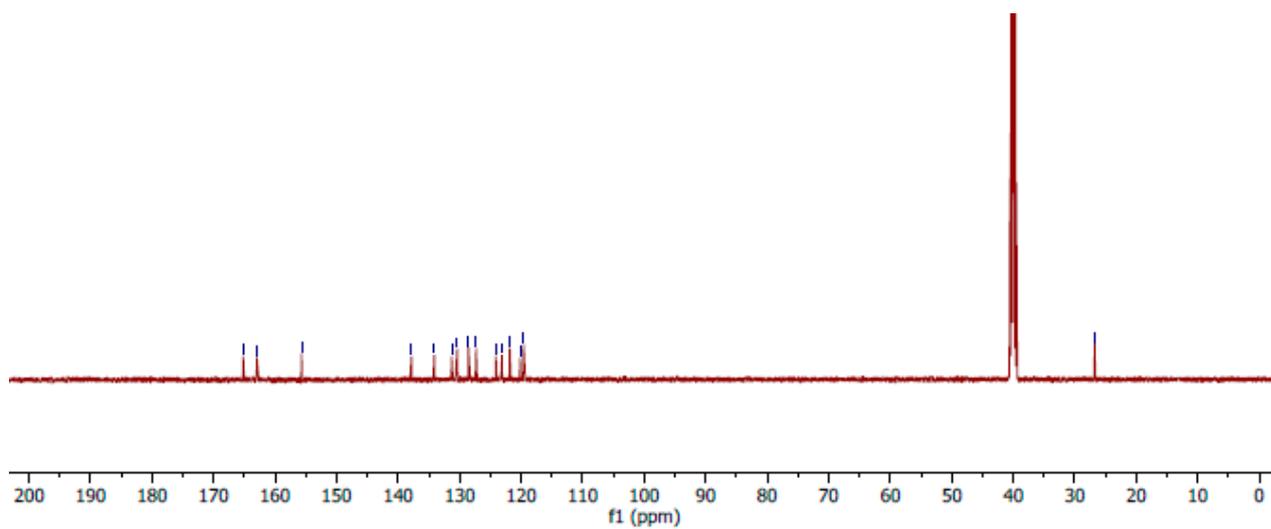


Figure S16 ¹H NMR spectrum of compound **7**

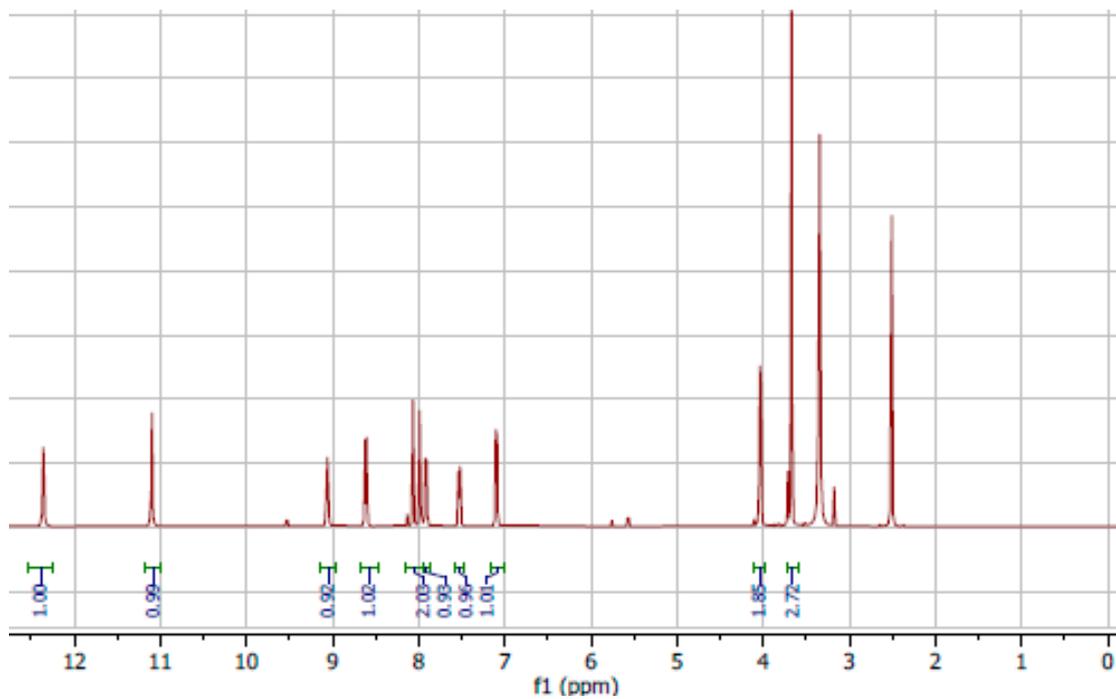


Figure S17 ¹H NMR spectrum of compound **8**

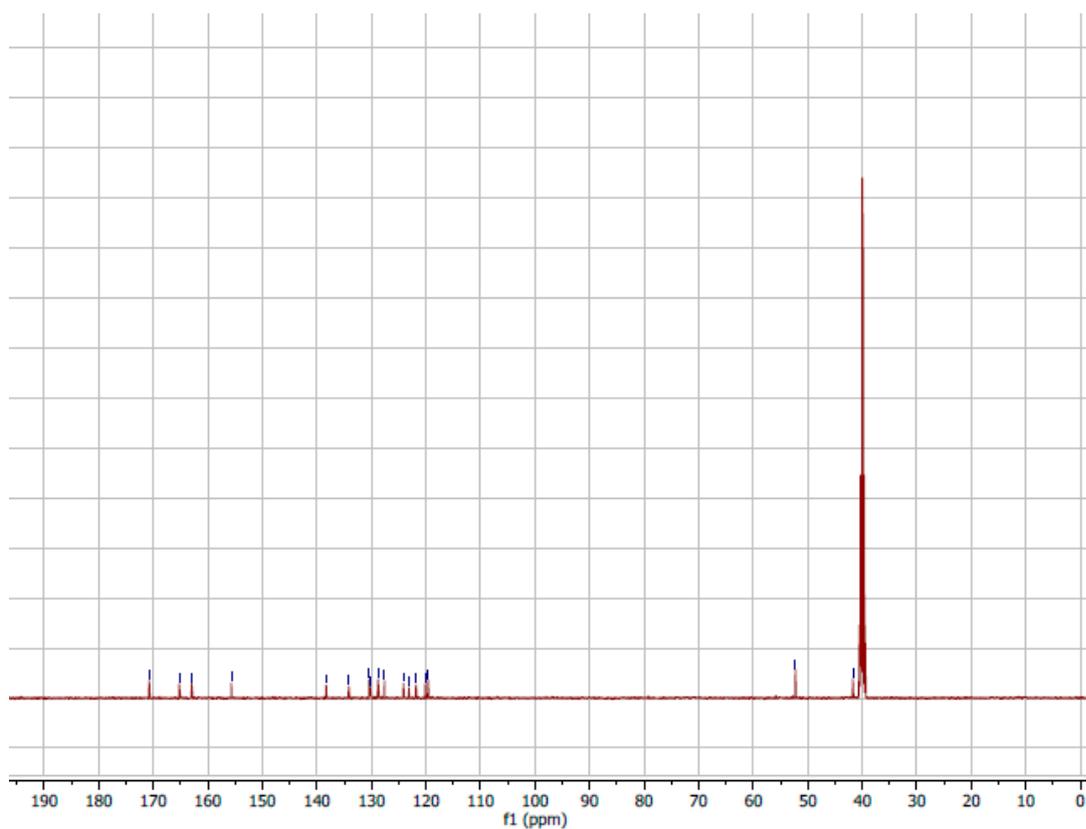


Figure S18 ^{13}C NMR spectrum of compound 8

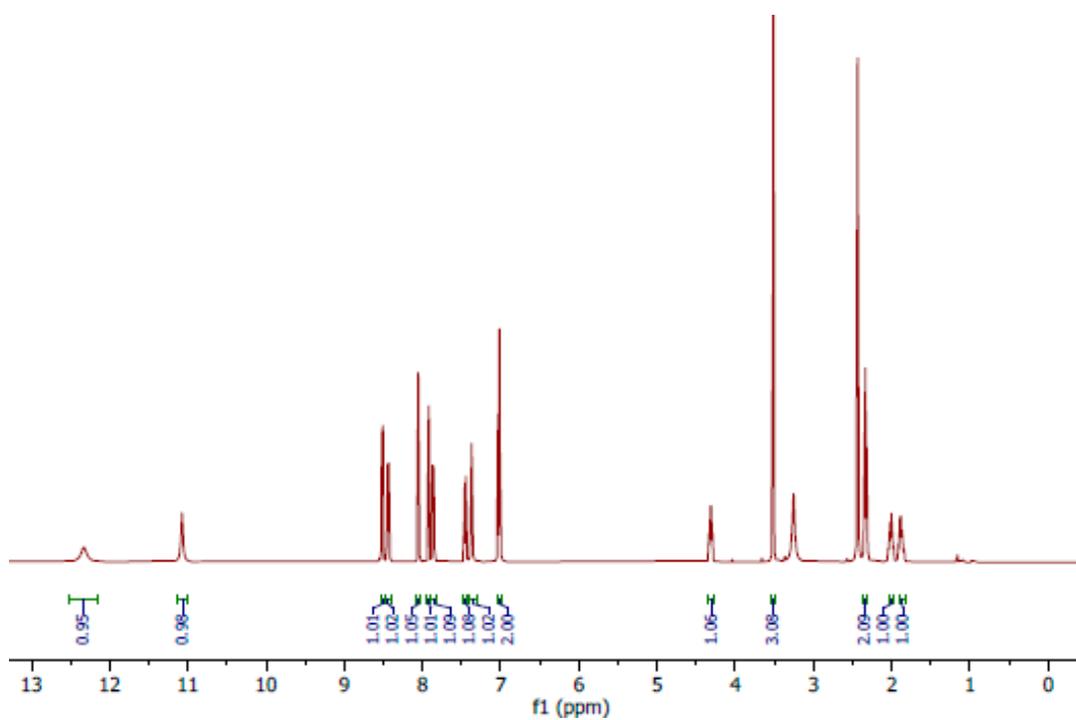


Figure S19 ^1H NMR spectrum of compound 9

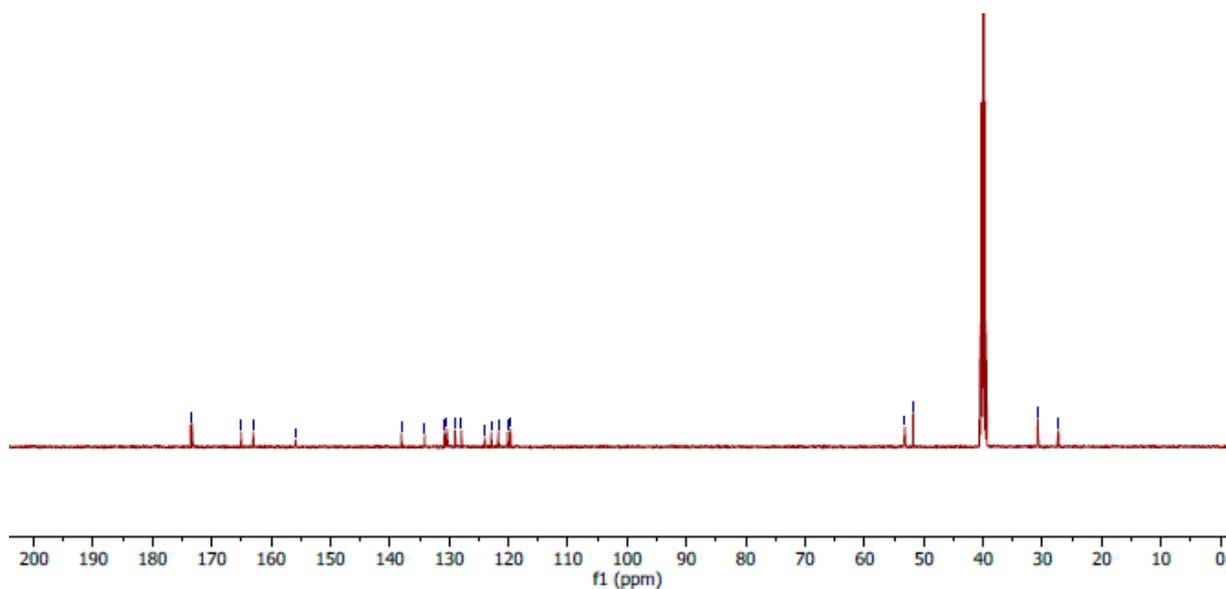


Figure S20 ^{13}C NMR spectrum of compound 9

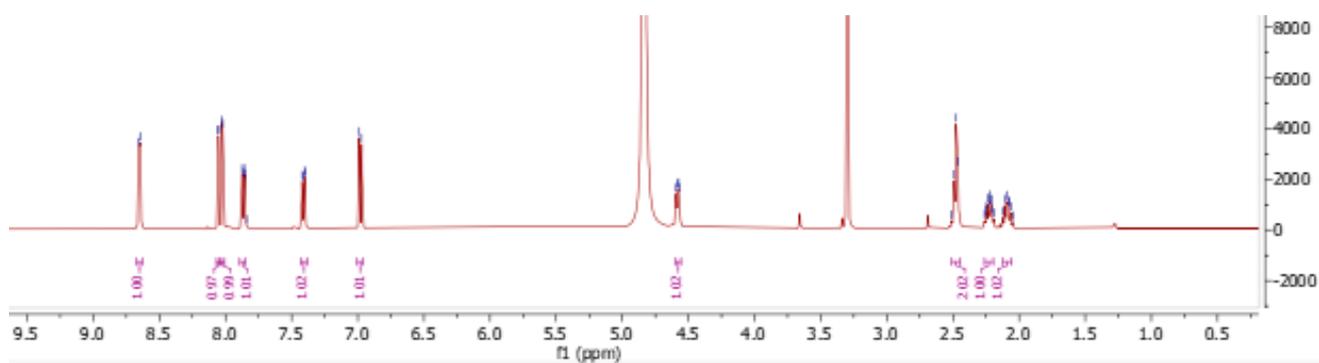


Figure S21 ^1H NMR spectrum of compound 10

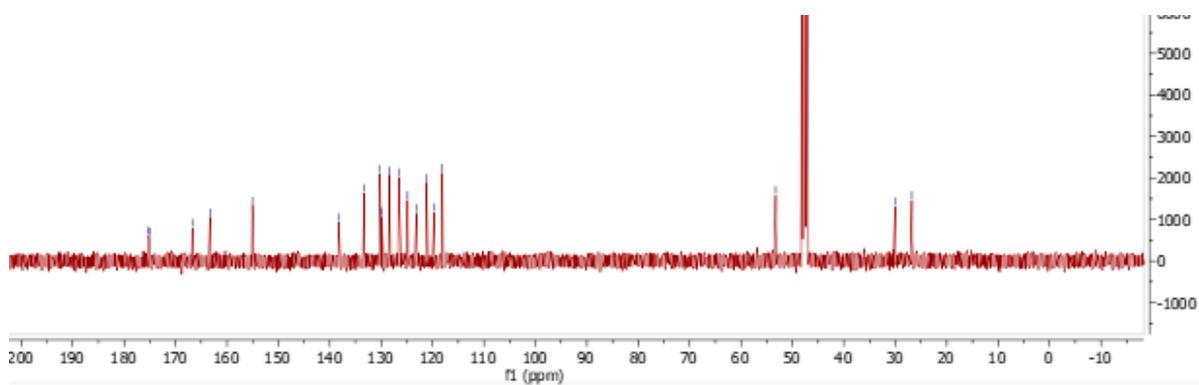


Figure S22 ^{13}C NMR spectrum of compound 10

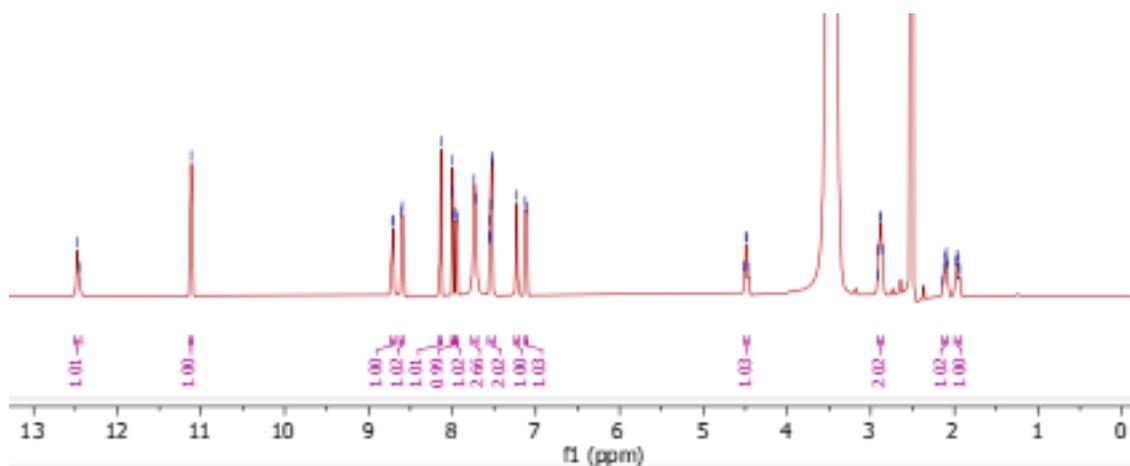


Figure S23 ¹H NMR spectrum of compound 11

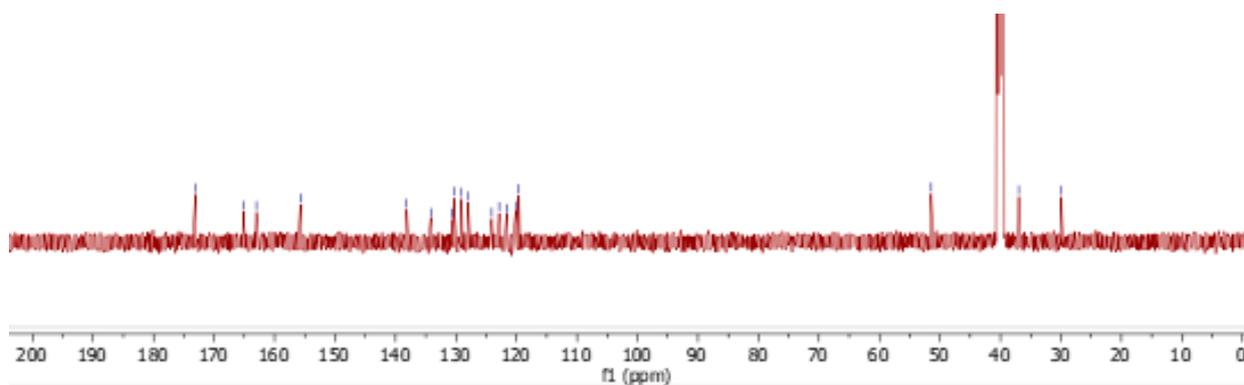


Figure S24 ¹³C NMR spectrum of compound 11

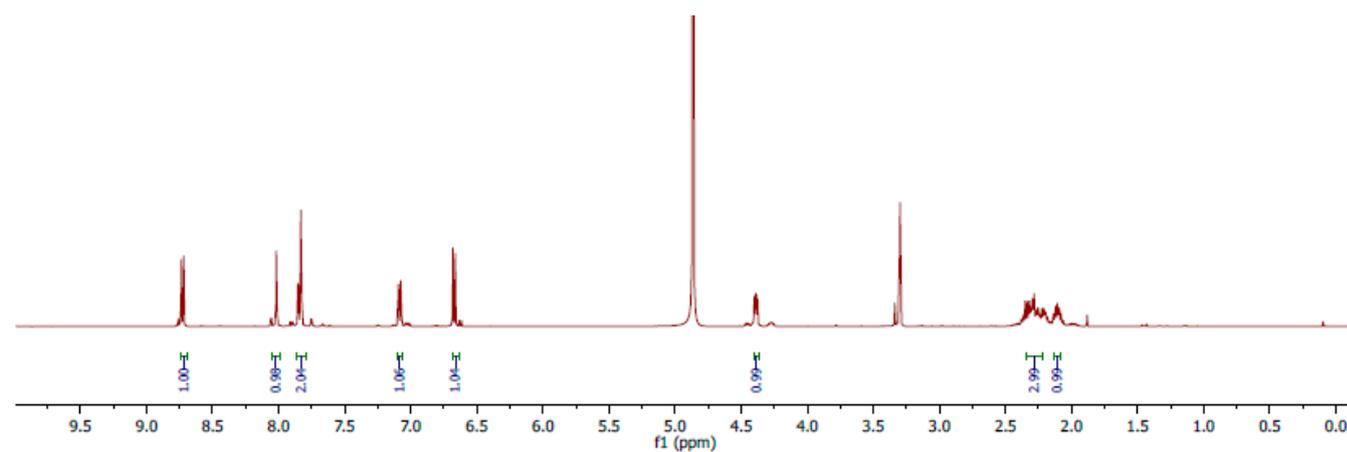


Figure S25 ¹H NMR spectrum of compound 12

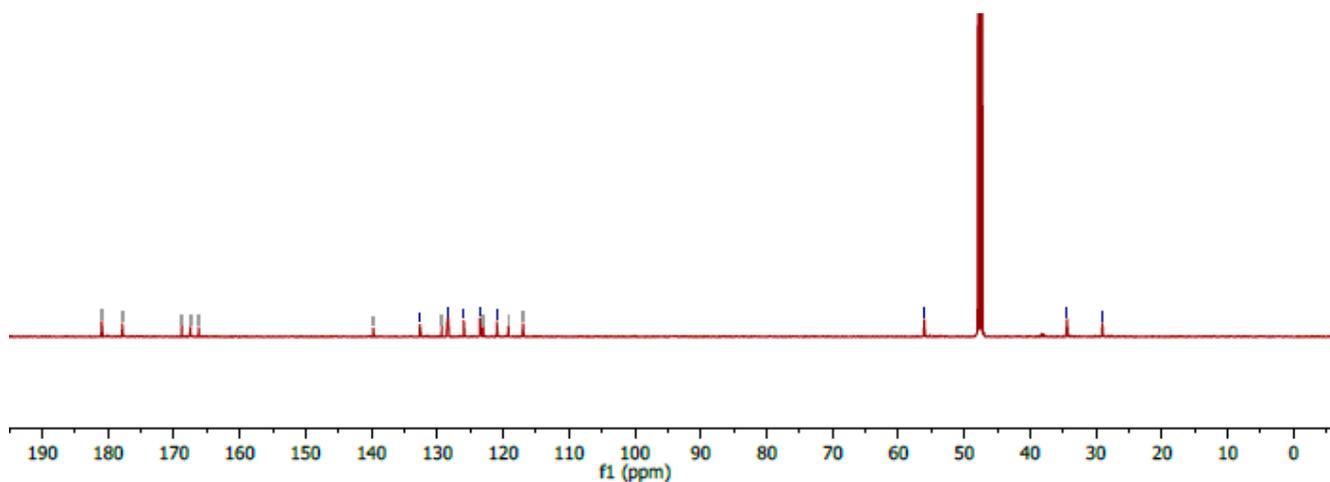


Figure S26 ^{13}C NMR spectrum of compound 12

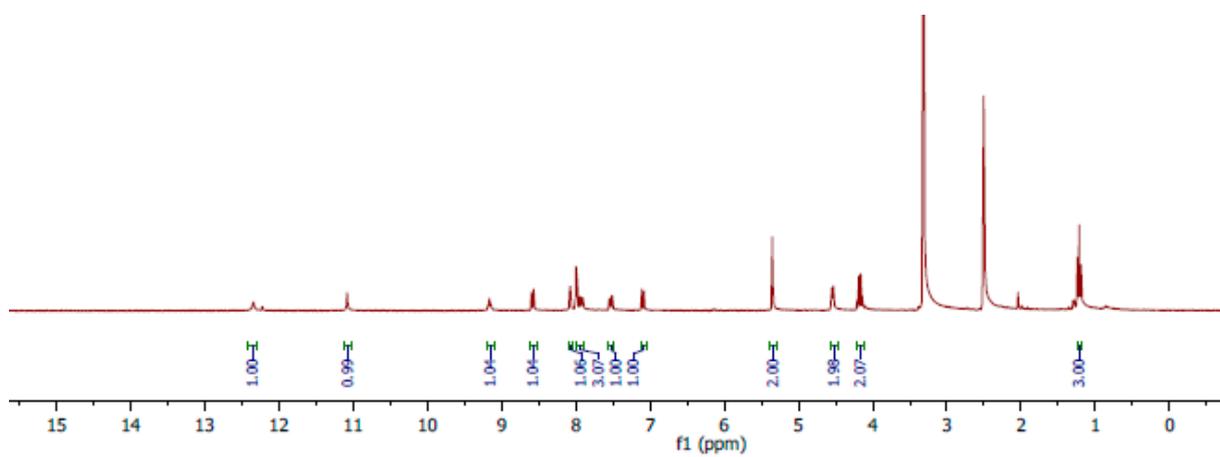


Figure S27 ^1H NMR spectrum of compound 13

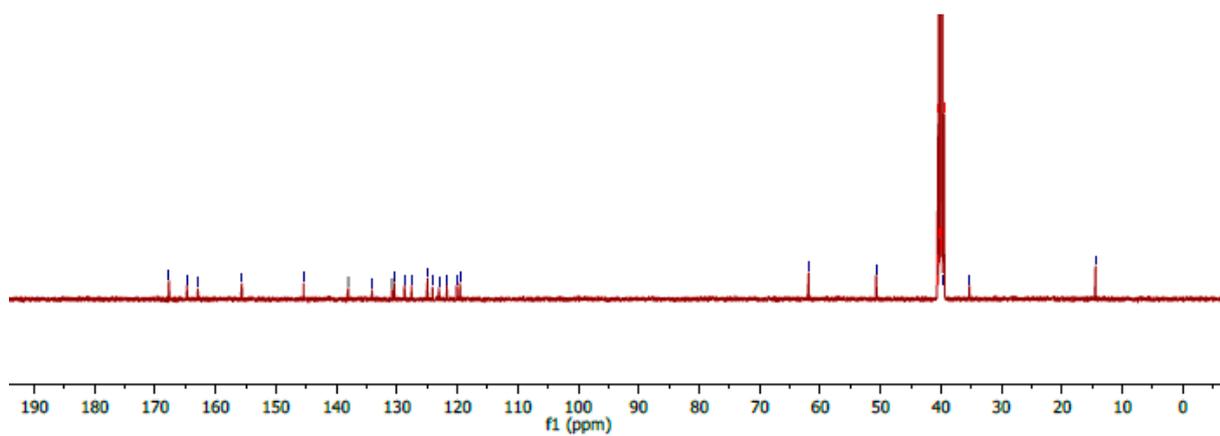


Figure S28 ^{13}C NMR spectrum of compound 13

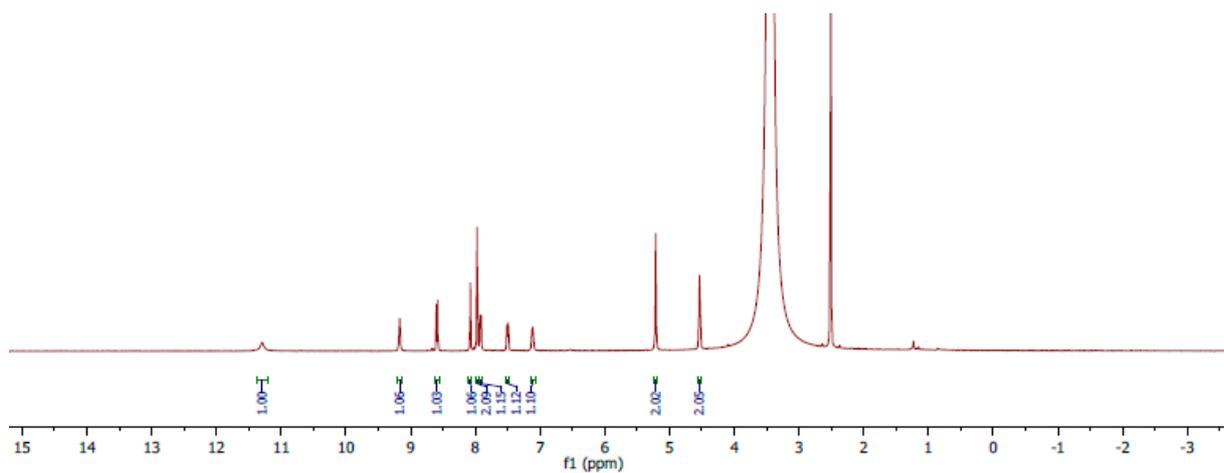


Figure S29 ^1H NMR spectrum of compound 14

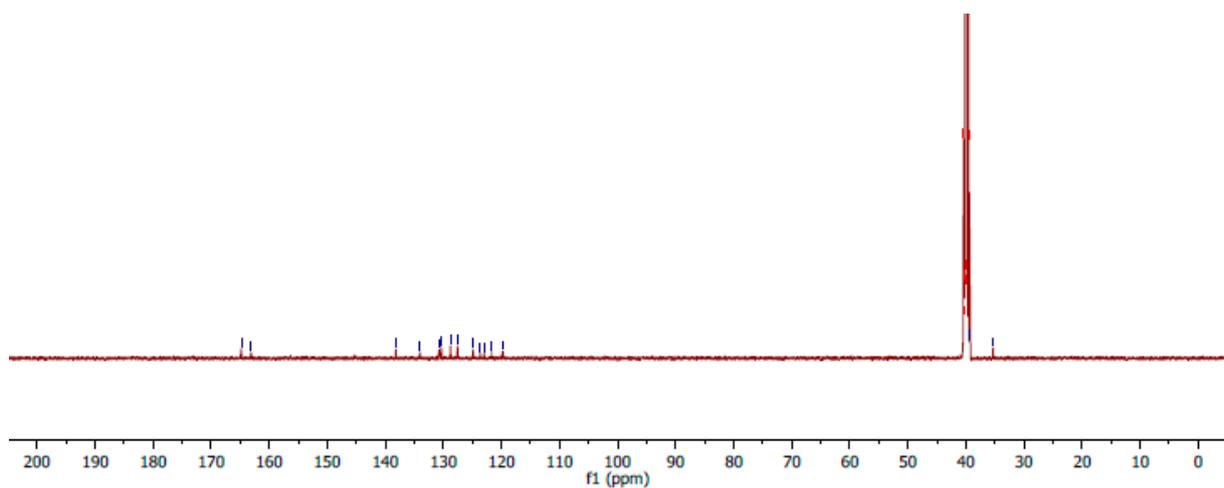


Figure S30 ^{13}C NMR spectrum of compound 14

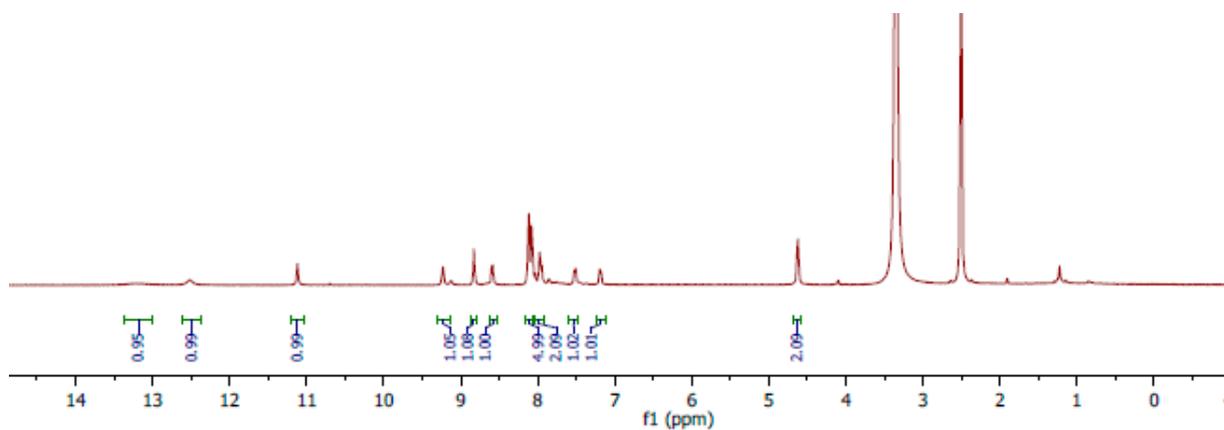


Figure S31 ^1H NMR spectrum of compound 15

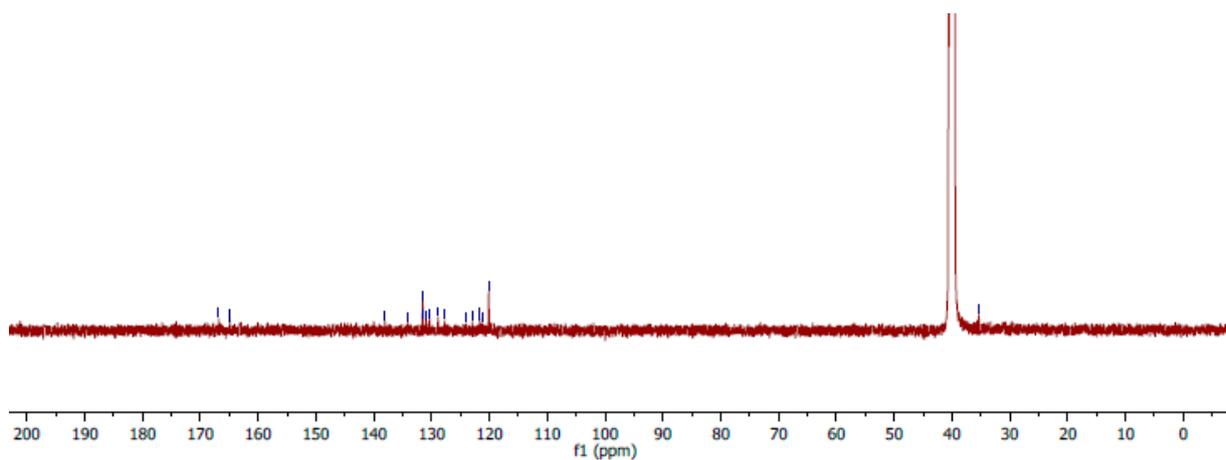


Figure S32 ¹³C NMR spectrum of compound 15

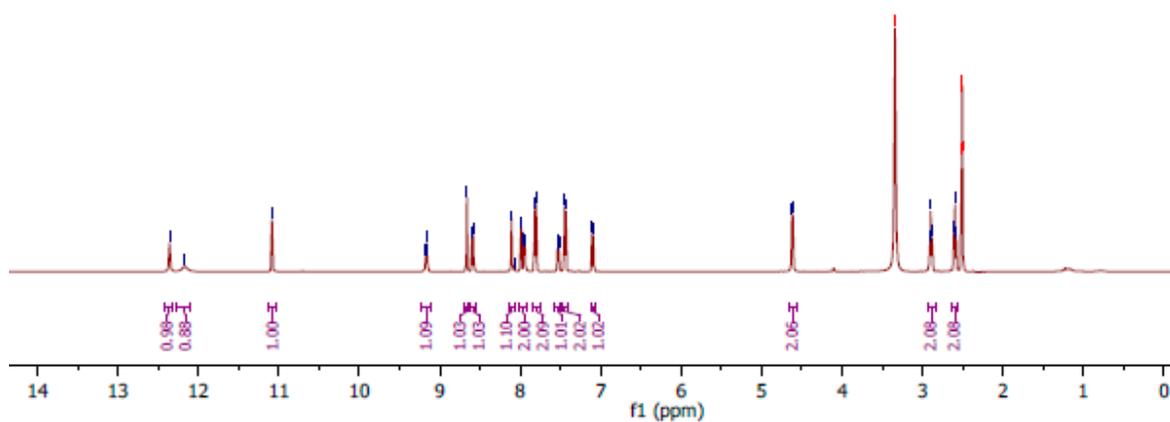


Figure S33 ¹H NMR spectrum of compound 17

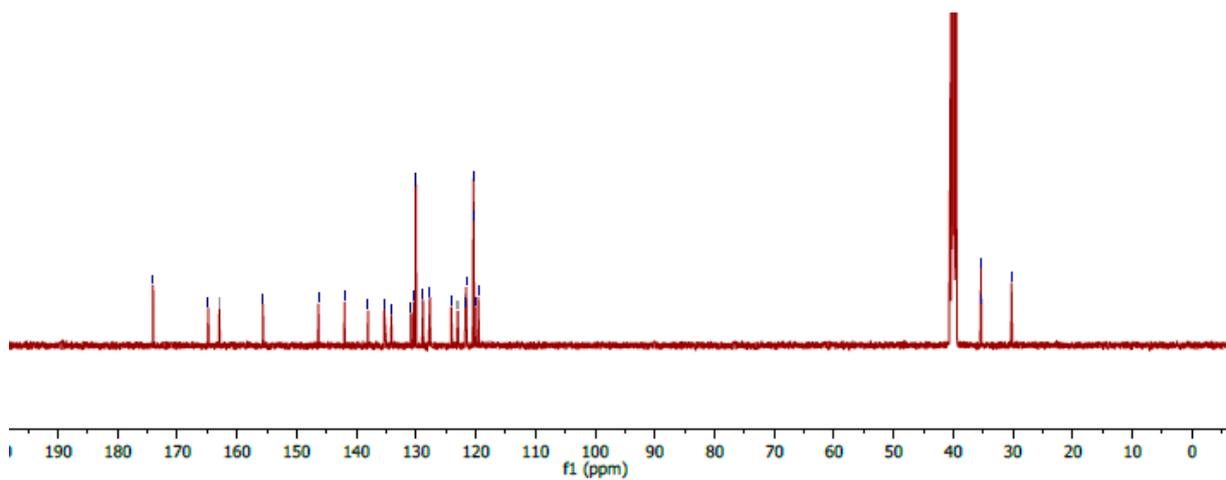


Figure S34 ¹³C NMR spectrum of compound 17

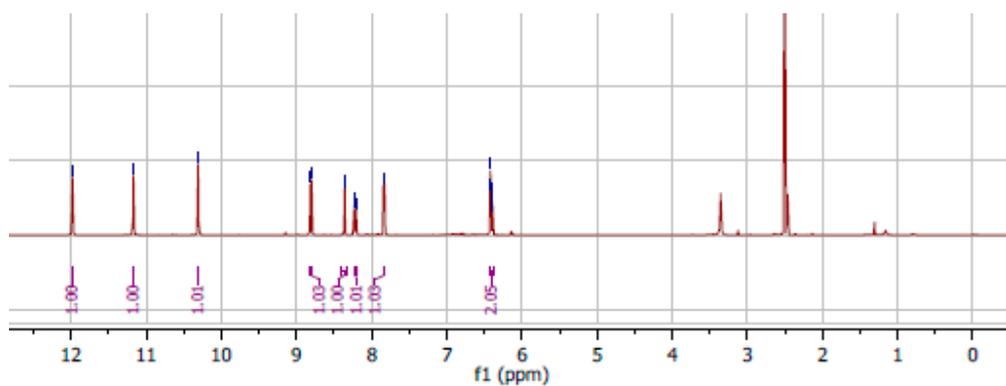


Figure S35 ^1H NMR spectrum of compound **18**

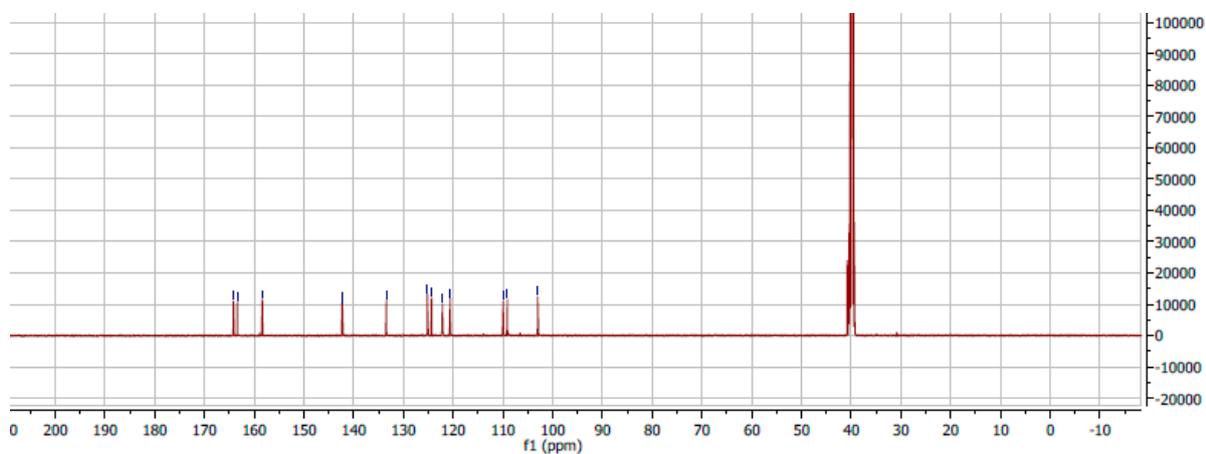


Figure S36 ^{13}C NMR spectrum of compound **18**

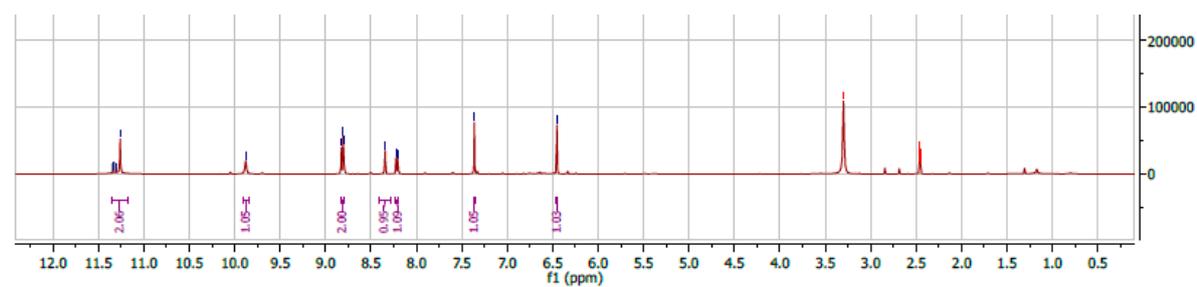


Figure S37 ^1H NMR spectrum of compound **19**

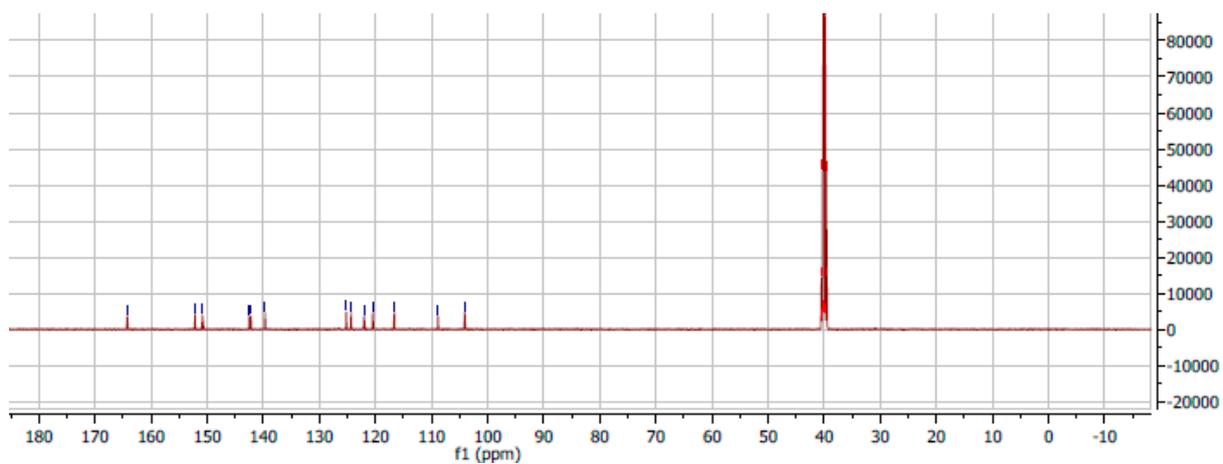


Figure S38 ^{13}C NMR spectrum of compound 19

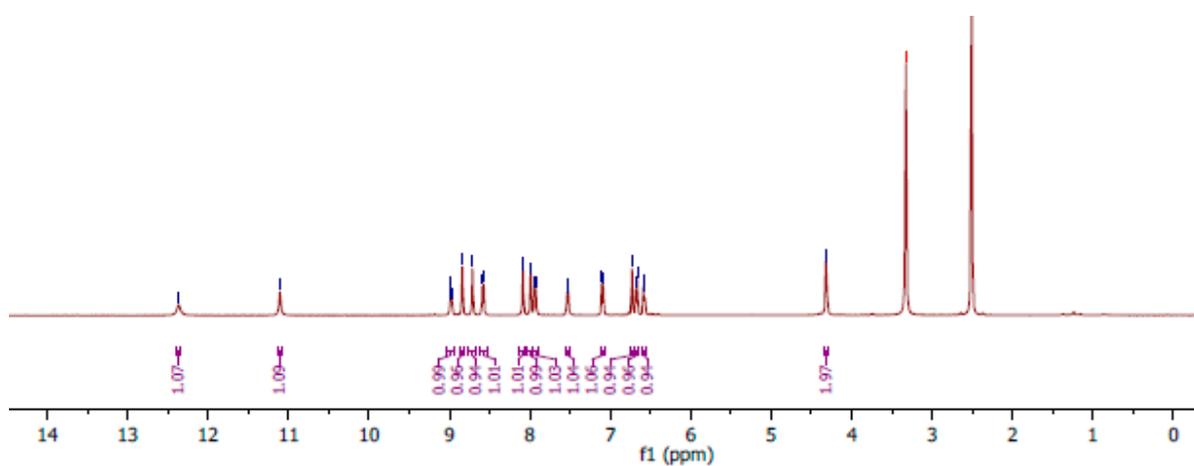


Figure S39 ^1H NMR spectrum of compound 20

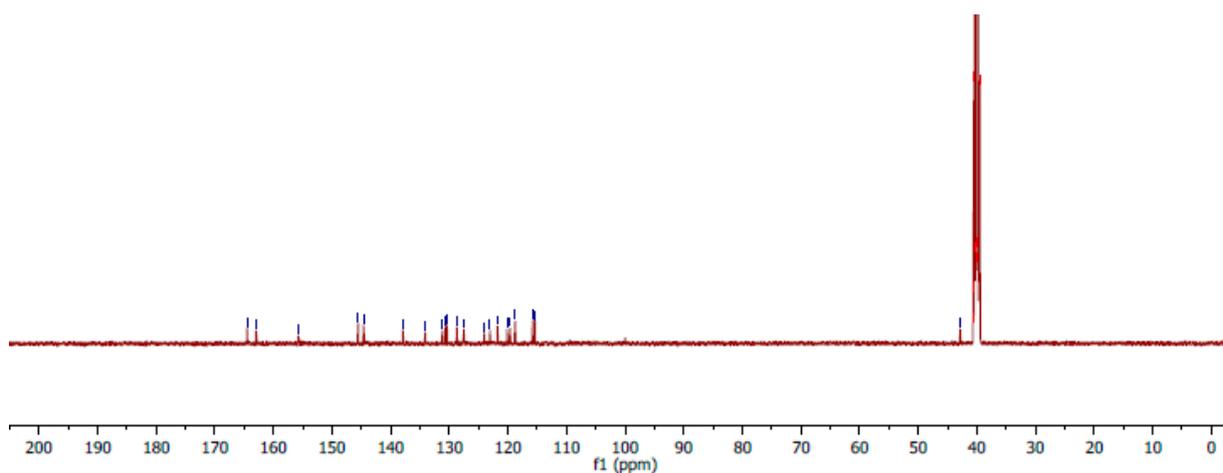


Figure S40 ^{13}C NMR spectrum of compound 20

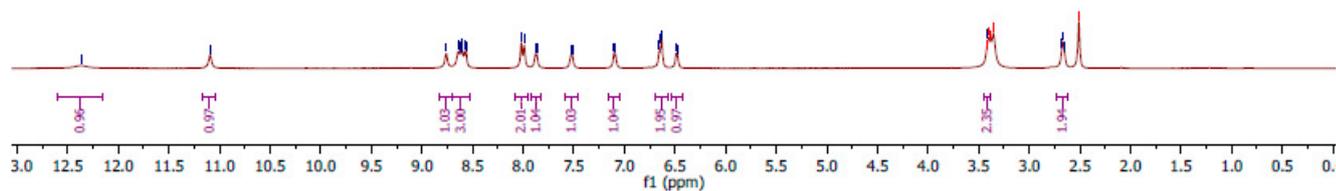


Figure S41 ¹H NMR spectrum of compound 21

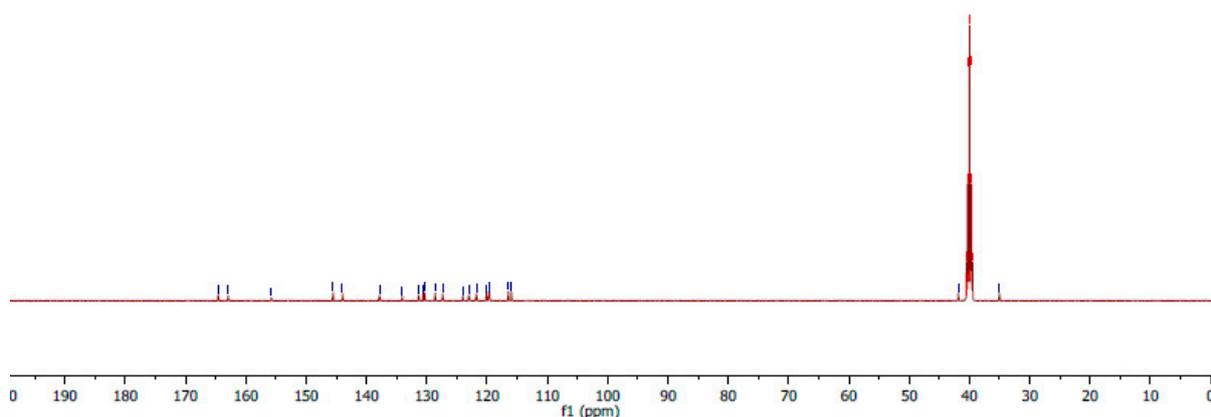


Figure S42 ¹³C NMR spectrum of compound 21

Extended Biological Data

Table S1 Minimum inhibitory concentration (MIC) in µg/mL of compounds 1-21 against 4 colistin-resistant strains of GNB. KP = *Klebsiella pneumoniae*, EC = *Escherichia coli*.

Compound	KP113250	KP113254	EC94393	EC94474
1	>128	>128	>128	>128
2	>128	>128	>128	>128
3	>128	>128	>128	>128
4	>128	>128	>128	>128
5a	>128	>128	>128	>128
5b	>128	>128	>128	>128
6	>128	>128	>128	>128
7	>128	>128	>128	>128

8	>128	>128	>128	>128
9	>128	>128	>128	>128
10	>128	>128	>128	>128
11	>128	>128	>128	>128
12	>128	>128	>128	>128
14	>128	>128	>128	>128
15	>128	>128	>128	>128
16	>128	>128	>128	>128
17	>128	>128	>128	>128
18	>128	>128	>128	>128
19	>128	>128	>128	>128
20	>128	>128	>128	>128
21	>128	>128	>128	>128

Table S2. Colistin minimum inhibitory concentration (MIC) in combination with 4 μ M of compound **5b** and niclosamide against 4 colistin-resistant strains of GNB. KP = *Klebsiella pneumoniae*, EC = *Escherichia coli*.

Compound	Colistin MIC with 4 μ M compound (μ g/mL)			
	KP113250	KP113254	EC94393	EC94474
Niclosamide	0.25	0.5	0.25	0.5
5b	256	256	8	16
Colistin alone	256	256	8	16