Synthesis, anti-bacterial and anti-protozoal activities of amidinobenzimidazole derivatives and their interactions with DNA and RNA

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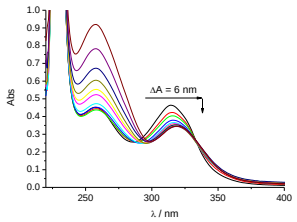
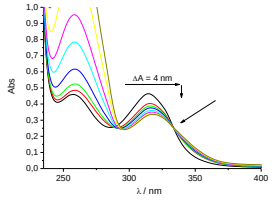
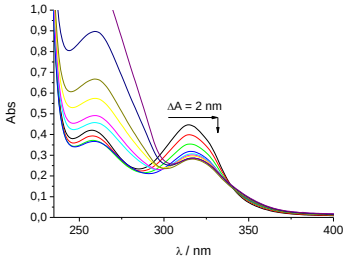
1. Spectroscopic characterization of compounds

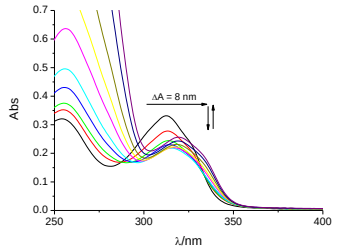
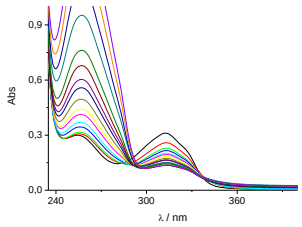
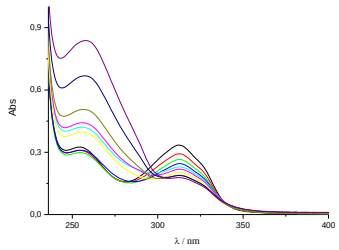
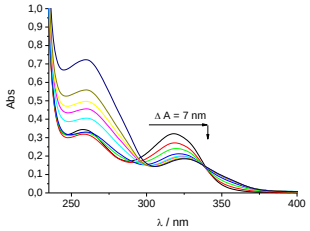
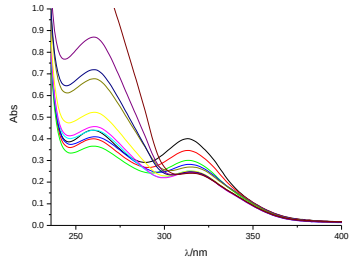
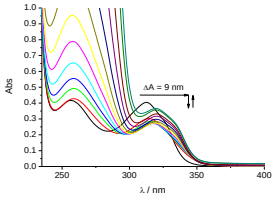
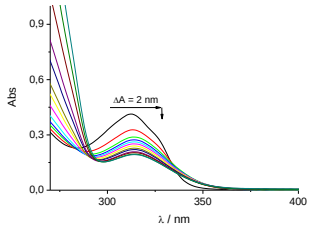
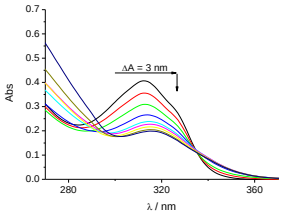
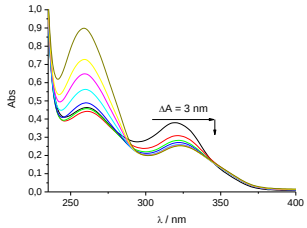
Due to the low solubility of investigate compounds in pure water, a stock solutions were prepared in DMSO, $c = 1 \times 10^{-3}$ mol dm^{-3}. Stock solutions have been characterized by UV-Vis spectroscopy. DMSO solutions of all studied compounds were shown to be stable over longer period at 4−8 °C. Table 1 gives values for the molar absorption coefficients of compounds in water-DMSO (≥ 1 %) mixture.

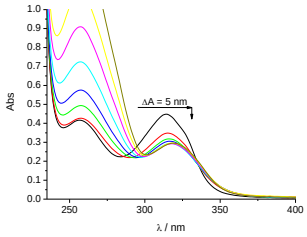
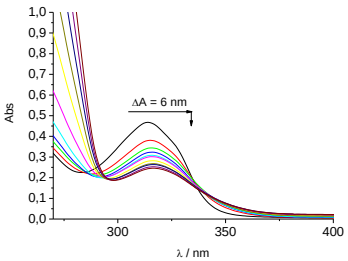
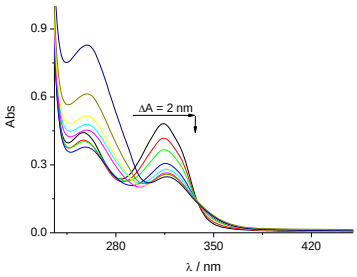
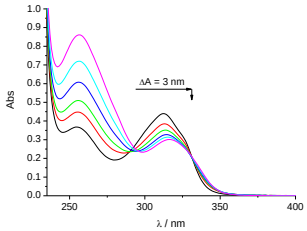
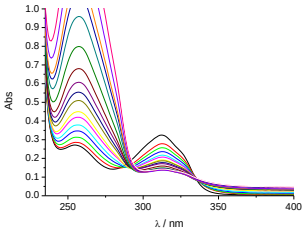
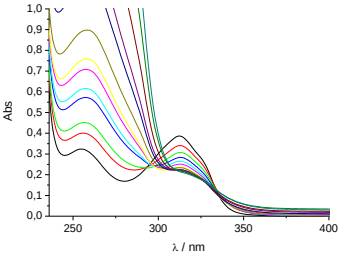
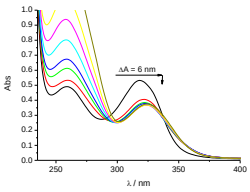
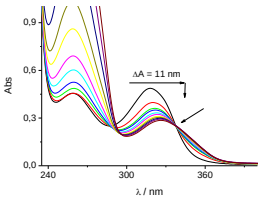
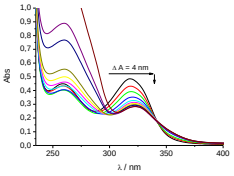
Table S1. Molar absorption coefficients of investigated compounds

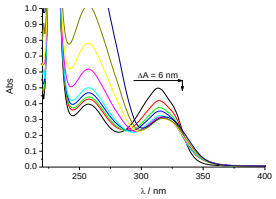
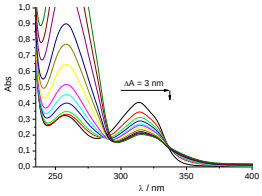
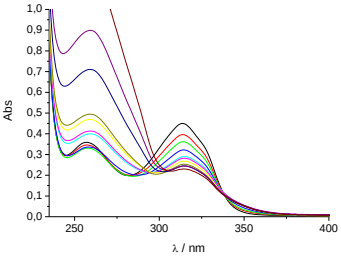
	λ_{max} / nm	$\varepsilon \cdot 10^3$ / dm^{3}mol^{-1}cm^{-1}		λ_{max} / nm	$\varepsilon \cdot 10^3$ / dm^{3}mol^{-1}cm^{-1}		λ_{max} / nm	$\varepsilon \cdot 10^3$ / dm^{3}mol^{-1}cm^{-1}
7a	257 315	30.7 31.4	**8a**	255 313	22.4 23.1	**9a**	259 313	24.9 22.4
7b	259 313	29.6 27.0	**8b**	256 312	28.1 27.5	**9b**	261 321	30.5 25.2
7c	256 313	26.9 28.7	**8c**	255 313	24.3 30.0	**9c**	258 317	32.5 35.9
7d	257 313	27.5 35.1	**8d**	255 313	22.1 26.9	**9d**	259 317	23.3 26.9
7e	257 314	31.6 37.7	**8e**	254 312	20.6 24.3	**9e**	259 319	34.5 35.3

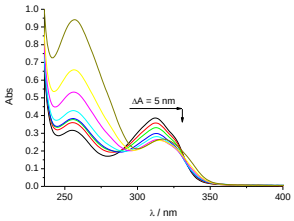
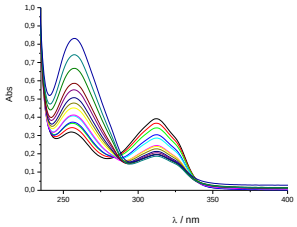
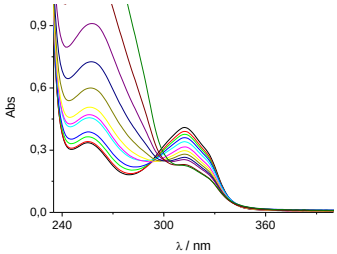
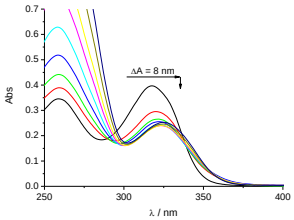
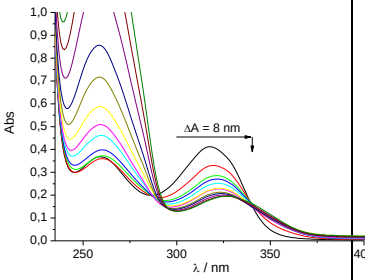
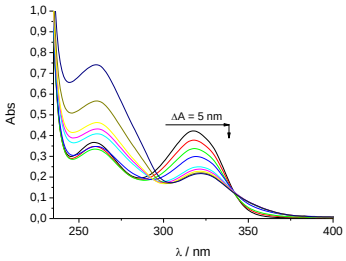
Fig. S1. UV/VIS spectra

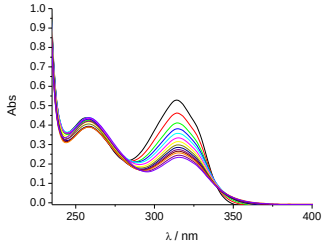
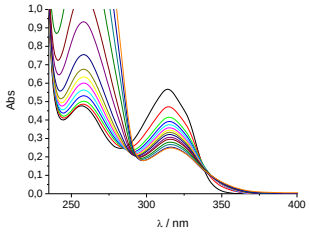
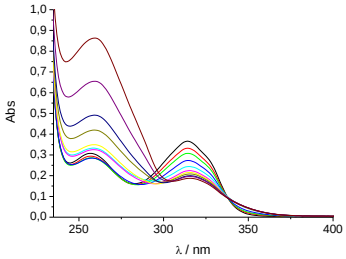
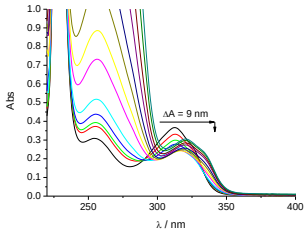
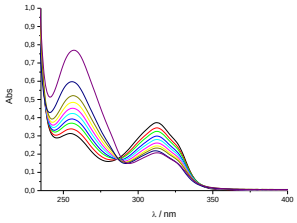
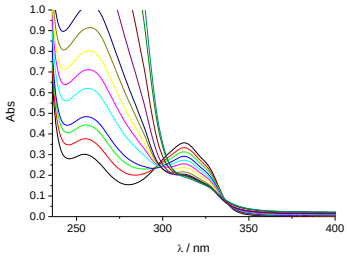
	***ct*DNA**	**polyA-polyU**	**polyC-polyG**
7a			

8a	 ΔA = 8 nm Abs λ/nm	 Abs λ / nm	 Abs λ / nm
9a			 Δ A = 7 nm Abs λ / nm
7b			 Abs λ/nm
8b	 ΔA = 9 nm Abs λ / nm	 ΔA = 2 nm Abs λ / nm	 ΔA = 3 nm Abs λ / nm
9b		 ΔA = 3 nm Abs λ / nm	

	*ct*DNA	polyA-polyU	polyC-polyG
7c			
8c			
9c			

	*ct*DNA	polyA-polyU	polyC-polyG
7d			

8d			
9d			

	***ct*DNA**	**polyA-polyU**	**polyC-polyG**
7e			
8e			

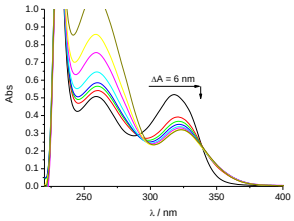
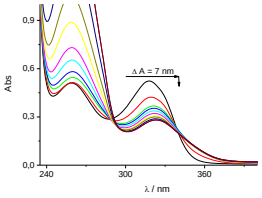
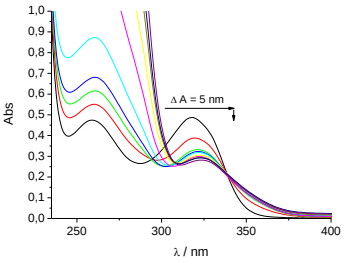
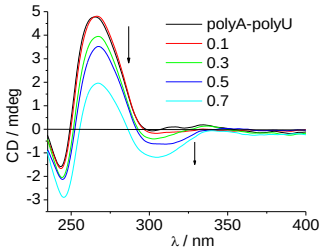
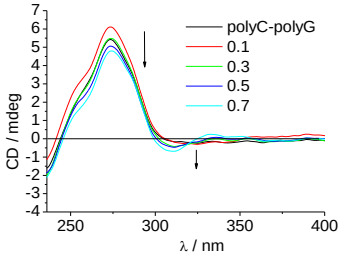
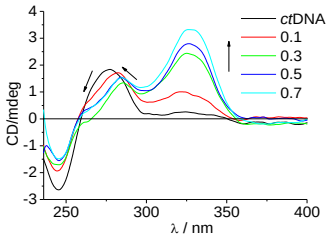
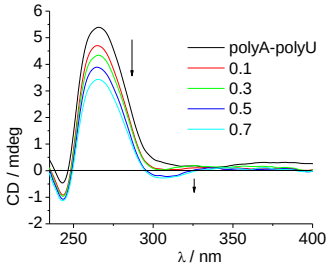
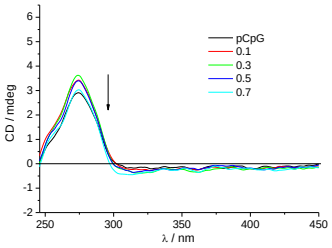
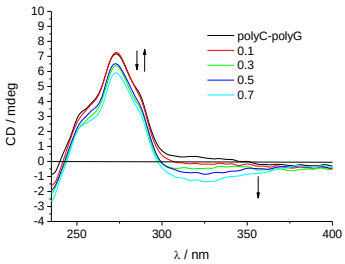
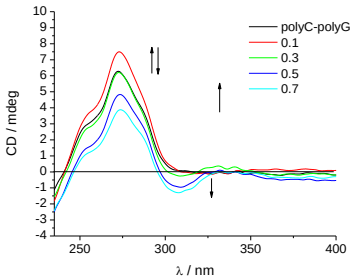
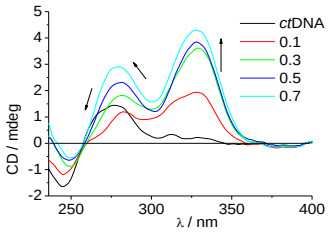
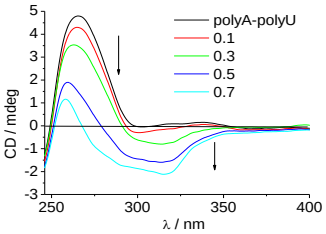
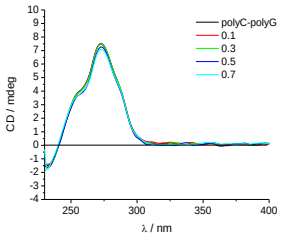
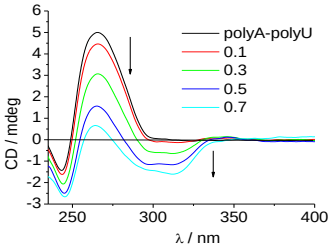
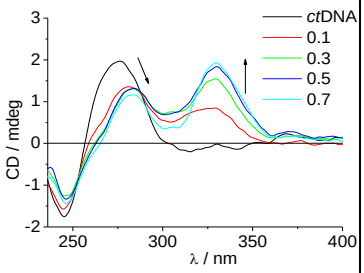
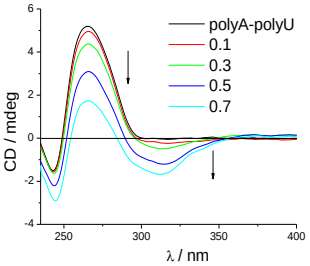
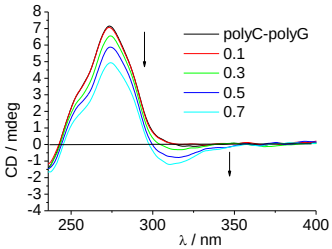
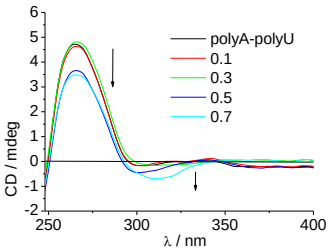
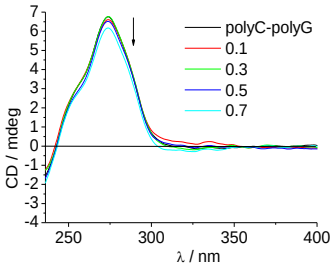
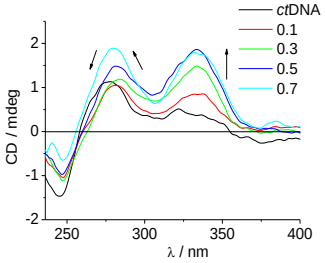
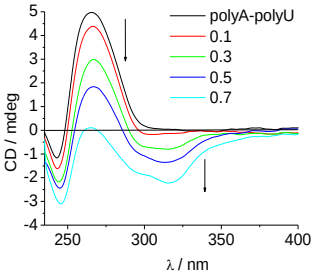
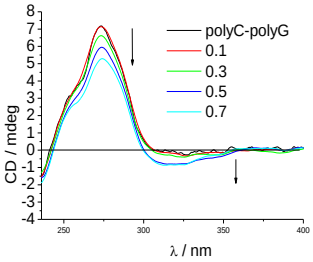
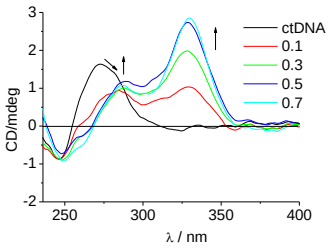
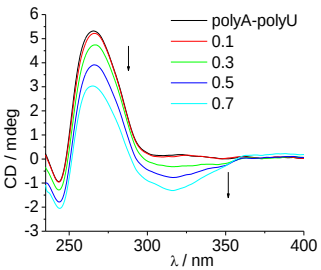
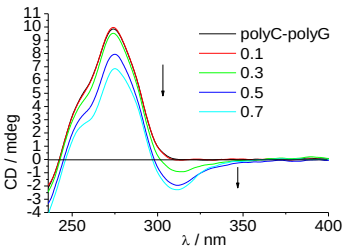
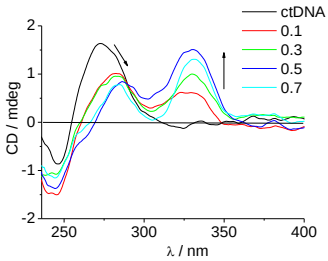
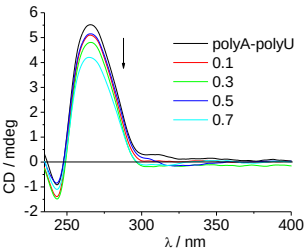
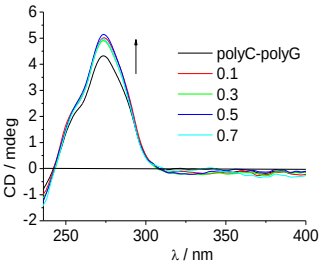
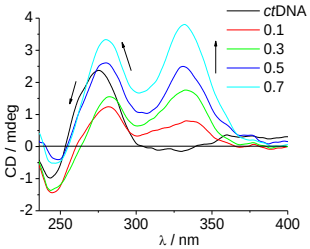
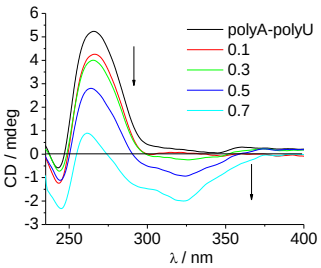
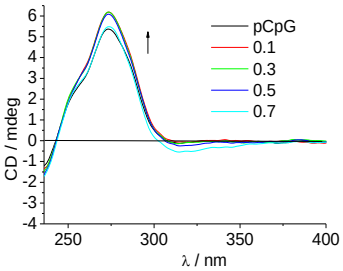
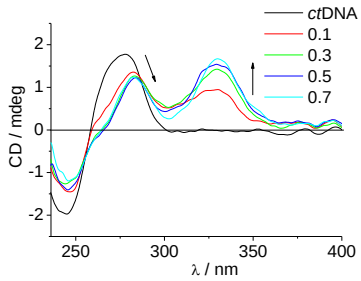
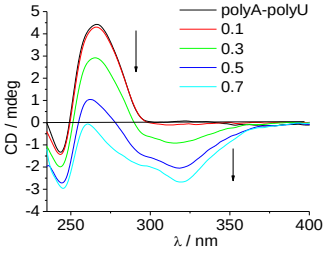
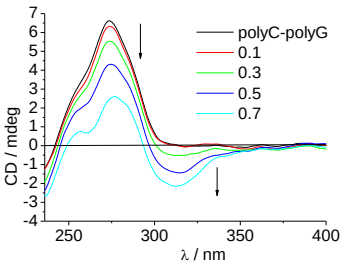
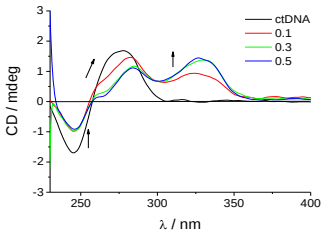
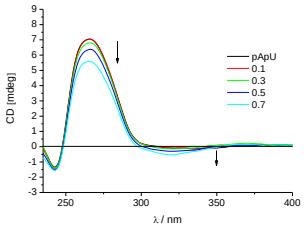
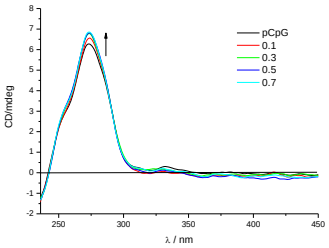
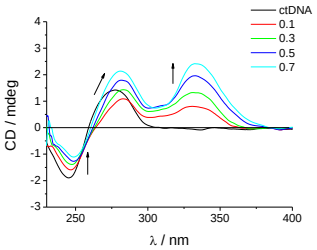
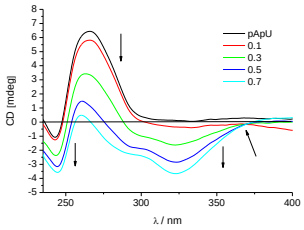
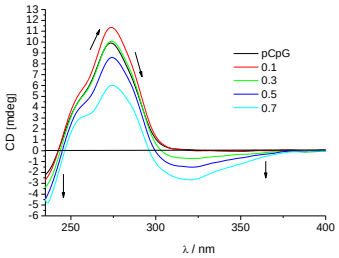
9e			

Fig. S2. CD titrations

	*ct*DNA	polyA-polyU	polyC-polyG
7a			
8a			
9a			
7b			

8b	 ctDNA 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyA-polyU 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyC-polyG 0.1 0.3 0.5 0.7 CD / mdeg λ / nm
9b		 polyA-polyU 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	
7c	 ctDNA 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyA-polyU 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyC-polyG 0.1 0.3 0.5 0.7 CD / mdeg λ / nm
8c		 polyA-polyU 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyC-polyG 0.1 0.3 0.5 0.7 CD / mdeg λ / nm
9c	 ctDNA 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyA-polyU 0.1 0.3 0.5 0.7 CD / mdeg λ / nm	 polyC-polyG 0.1 0.3 0.5 0.7 CD / mdeg λ / nm

7d	 CD/mdeg λ / nm ctDNA 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyA-polyU 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyC-polyG 0.1 0.3 0.5 0.7
8d	 CD / mdeg λ / nm ctDNA 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyA-polyU 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyC-polyG 0.1 0.3 0.5 0.7
9d	 CD / mdeg λ / nm ctDNA 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyA-polyU 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm pCpG 0.1 0.3 0.5 0.7
7e	 CD / mdeg λ / nm ctDNA 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyA-polyU 0.1 0.3 0.5 0.7	 CD / mdeg λ / nm polyC-polyG 0.1 0.3 0.5 0.7

8e	 CD / mdeg λ / nm ctDNA 0.1 0.3 0.5	 CD [mdeg] λ / nm pApU 0.1 0.3 0.5 0.7	 CD/mdeg λ / nm pCpG 0.1 0.3 0.5 0.7
9e	 CD / mdeg λ / nm ctDNA 0.1 0.3 0.5 0.7	 CD [mdeg] λ / nm pApU 0.1 0.3 0.5 0.7	 CD [mdeg] λ / nm pCpG 0.1 0.3 0.5 0.7

3. Antimicrobial activities

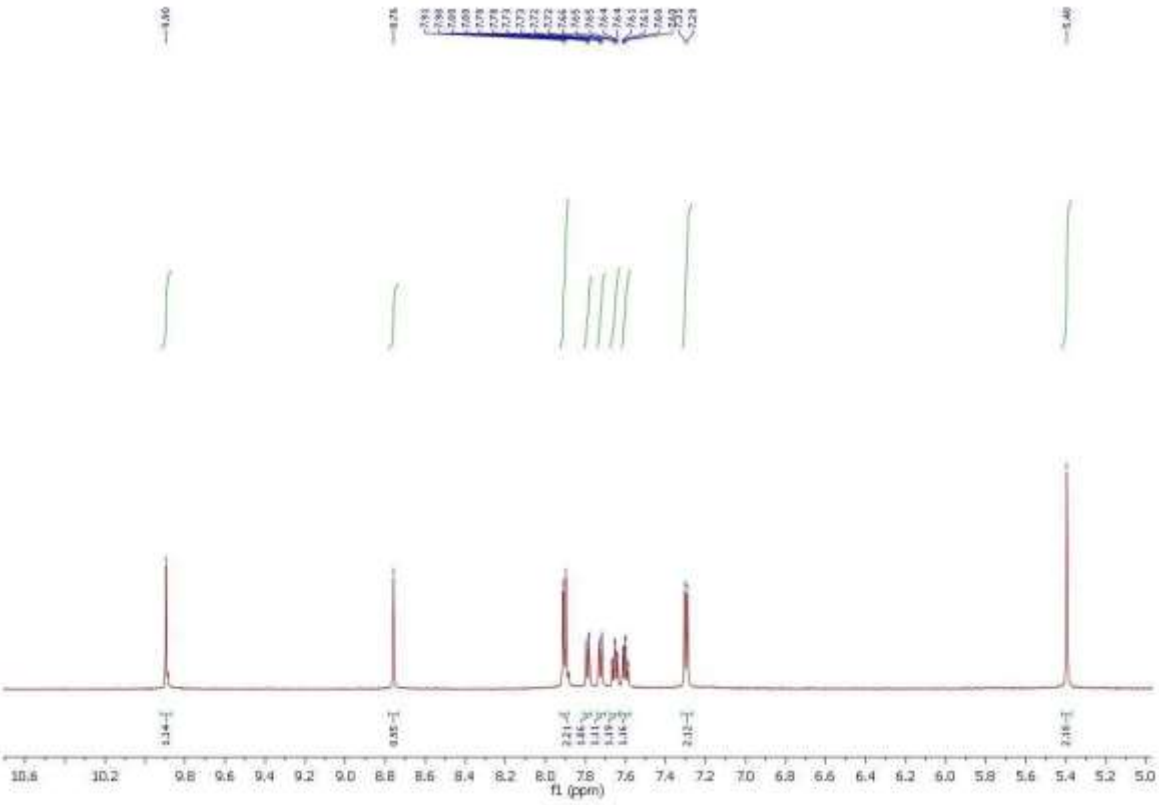
Table S2

Antimicrobial activities of compounds **7a**–**7e**, **8a**–**8e** and **9a**–**9e** against Gram-positive and Gram-negative bacteria.

Compd	MIC (μg/mL)					
	S. aureus ATCC 25923	*E. faecalis* ATCC 29212	*E. coli* ATCC 25925	*K. pneumonia* ATCC 700803	*P. aeruginosa* ATCC 27853	*A. baumannii* ATCC 19606
7a	32	64	32	128	128	>256
7b	>256	128	>256	>256	>256	>256
7c	64	64	256	>256	>256	>256
7d	32	64	32	64	32	>256
7e	32	128	32	128	64	>256
8a	128	256	256	>256	>256	>256
8b	128	64	256	>256	>256	>256
8c	32	64	256	>256	>256	>256
8d	64	128	>256	>256	>256	>256
8e	64	256	256	>256	>256	>256
9a	128	128	256	>256	>256	>256
9b	128	256	256	>256	>256	>256
9c	128	32	256	>256	>256	>256
9d	64	128	128	>256	128	>256
9e	32	128	64	>256	128	>256
Ceftazidime	-	-	0.5	-	4	-
Ciprofloxacin	-	-	0.004	0.06	0.5	0.06
Ampicilin	1	2	-	-	-	-
Gentamicin	0.125	8	-	-	-	-

Fig. S3 a) ^{1}H NMR and b) ^{13}C NMR of compd. **3c**

a)



b)

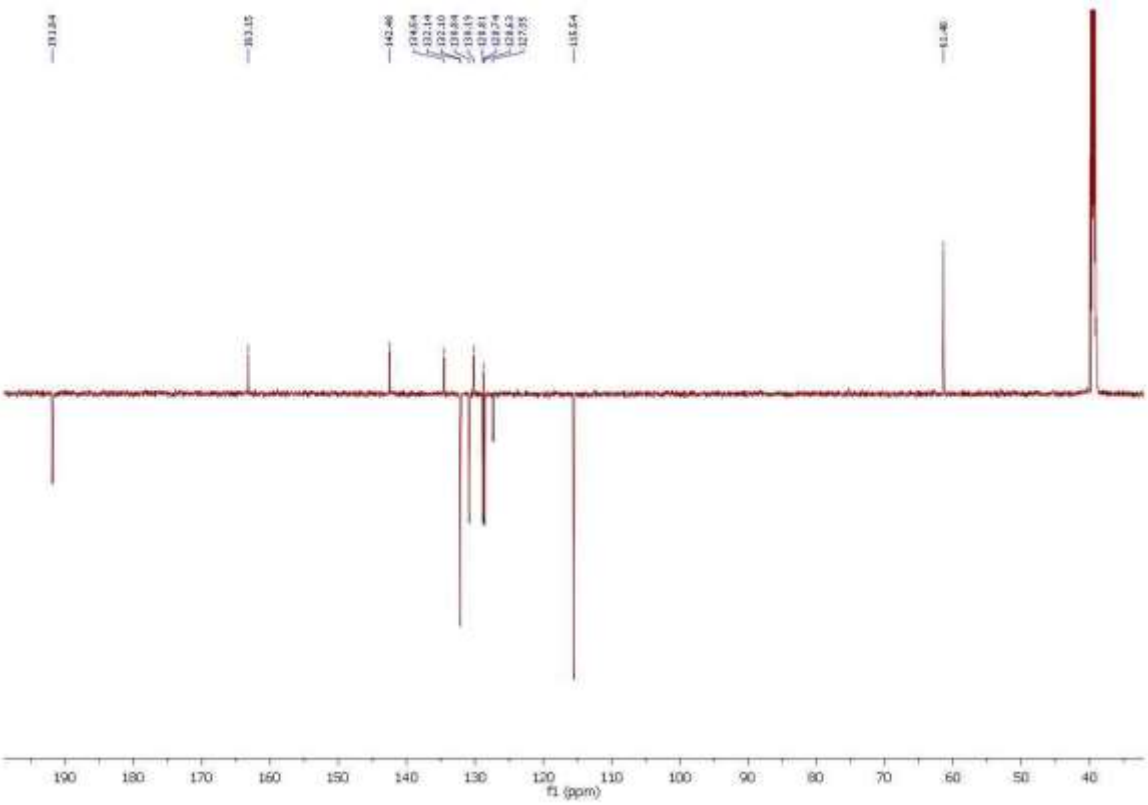
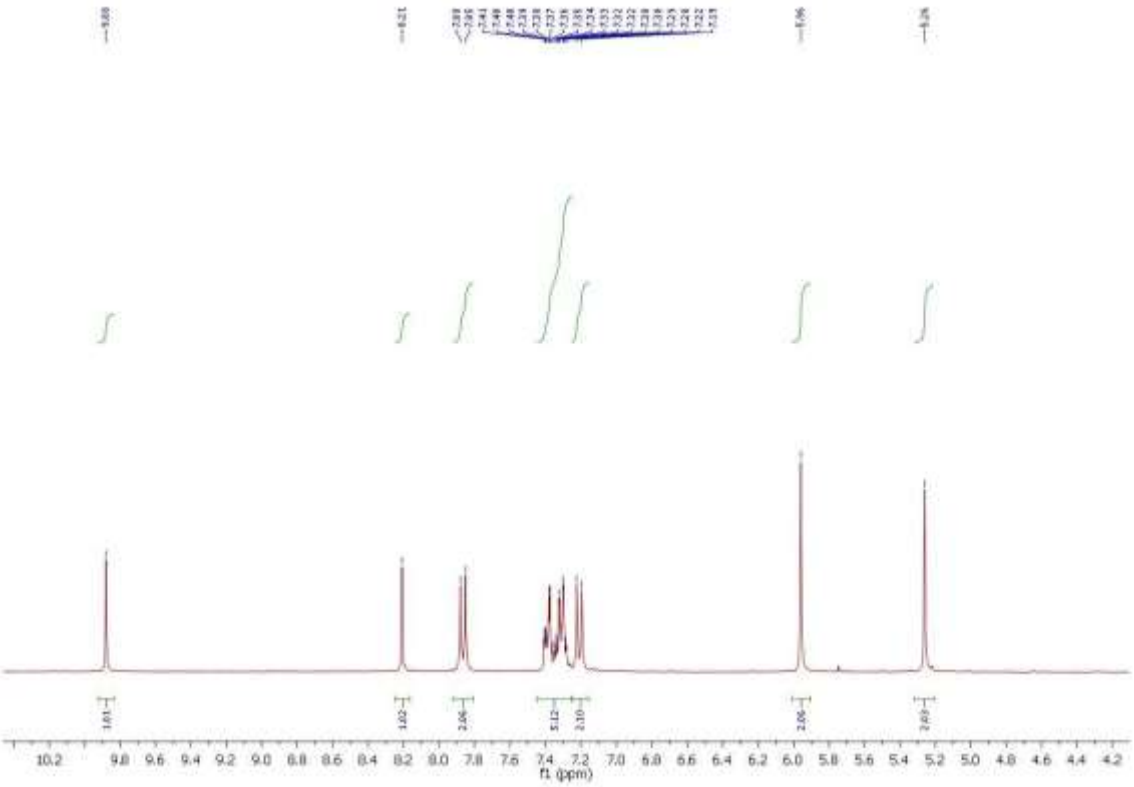


Fig. S4 a) ^{1}H NMR and b) ^{13}C NMR of compd. **3e**

a)



b)

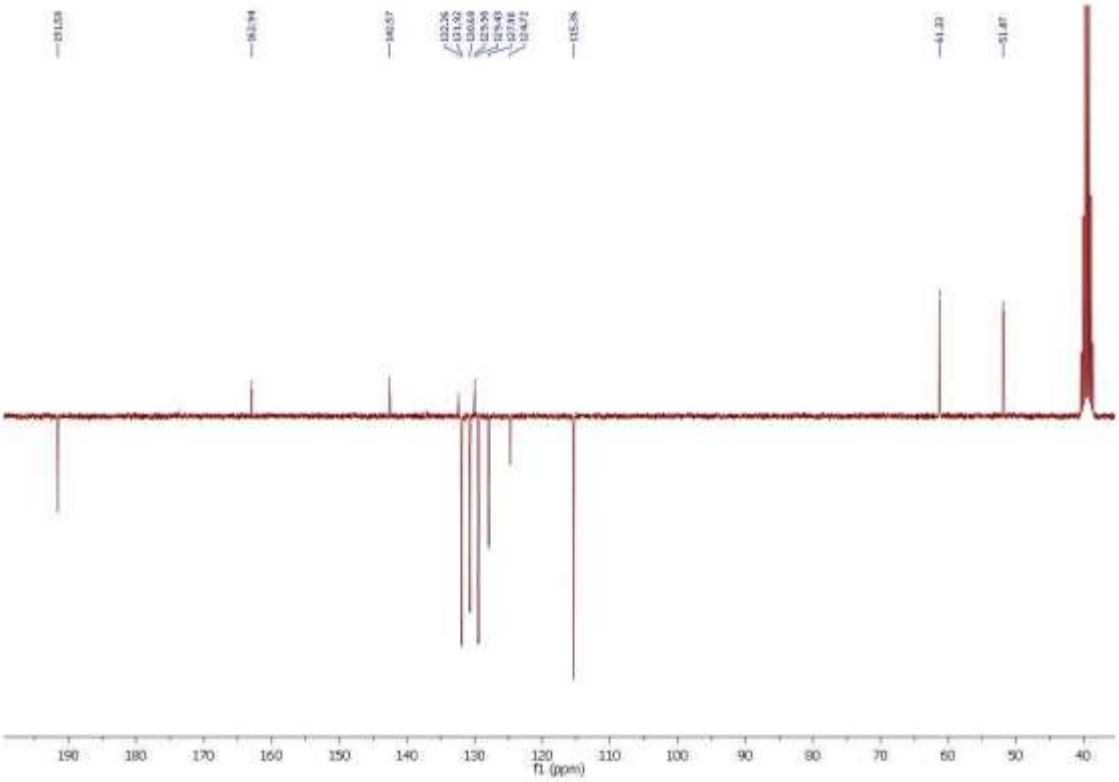
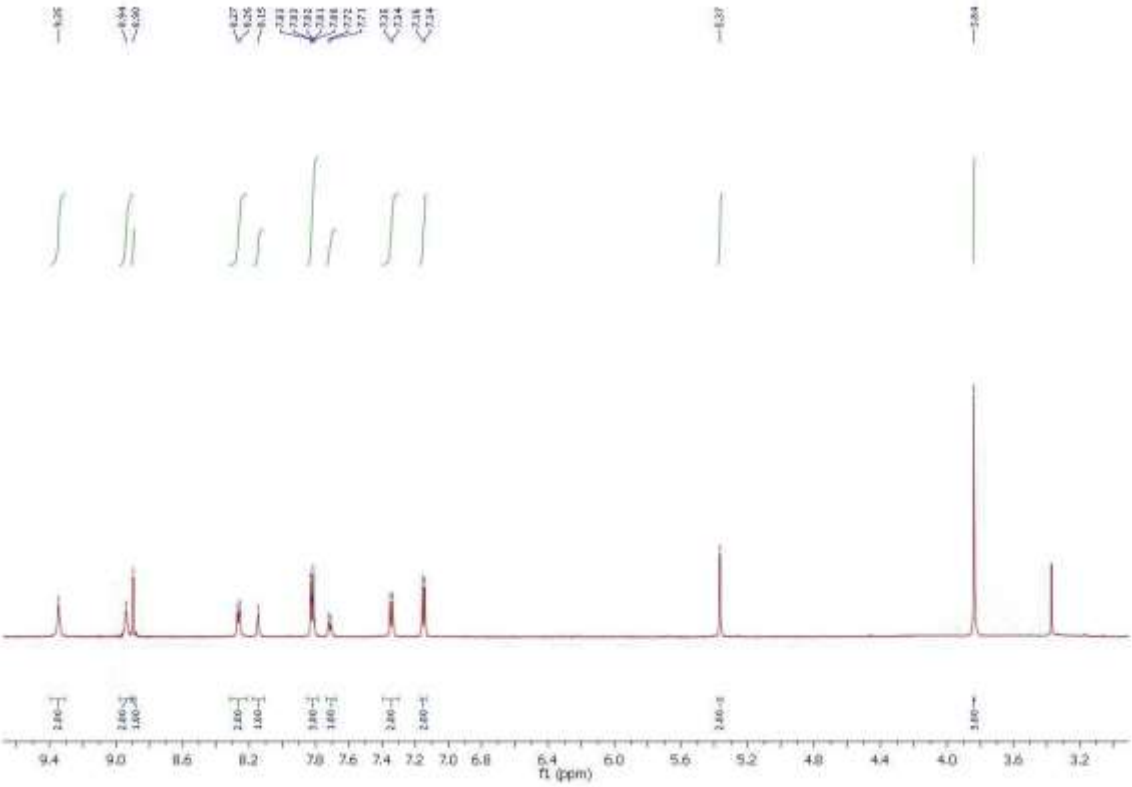


Fig. S5 a) ^{1}H NMR and b) ^{13}C NMR of compd. **7b**

a)



b)

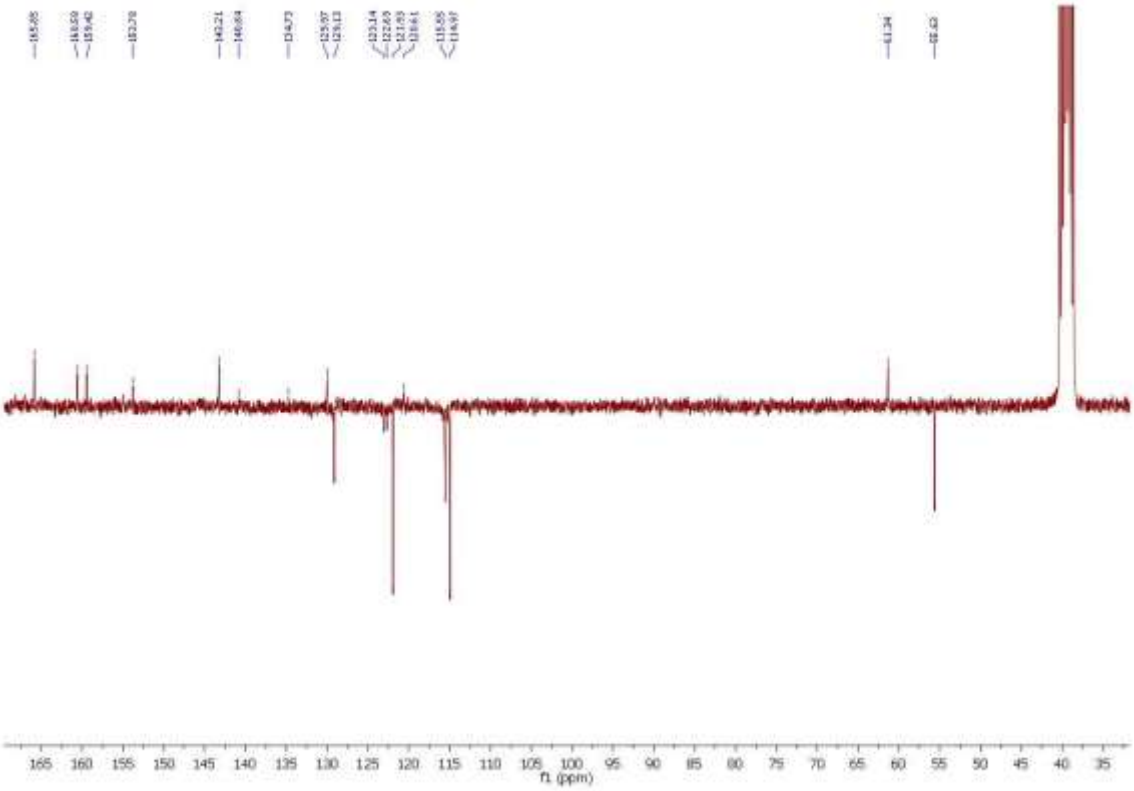
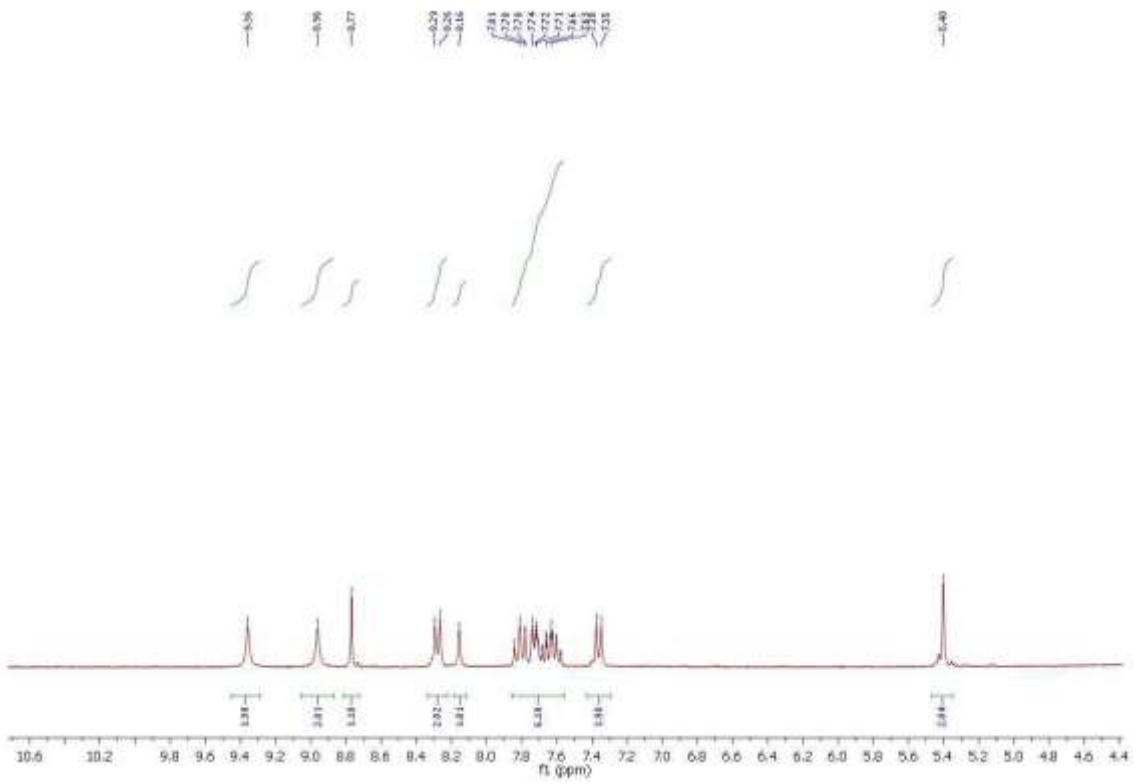


Fig. S6 a) ^{1}H NMR and b) ^{13}C NMR of compd. **7c**

a)



b)

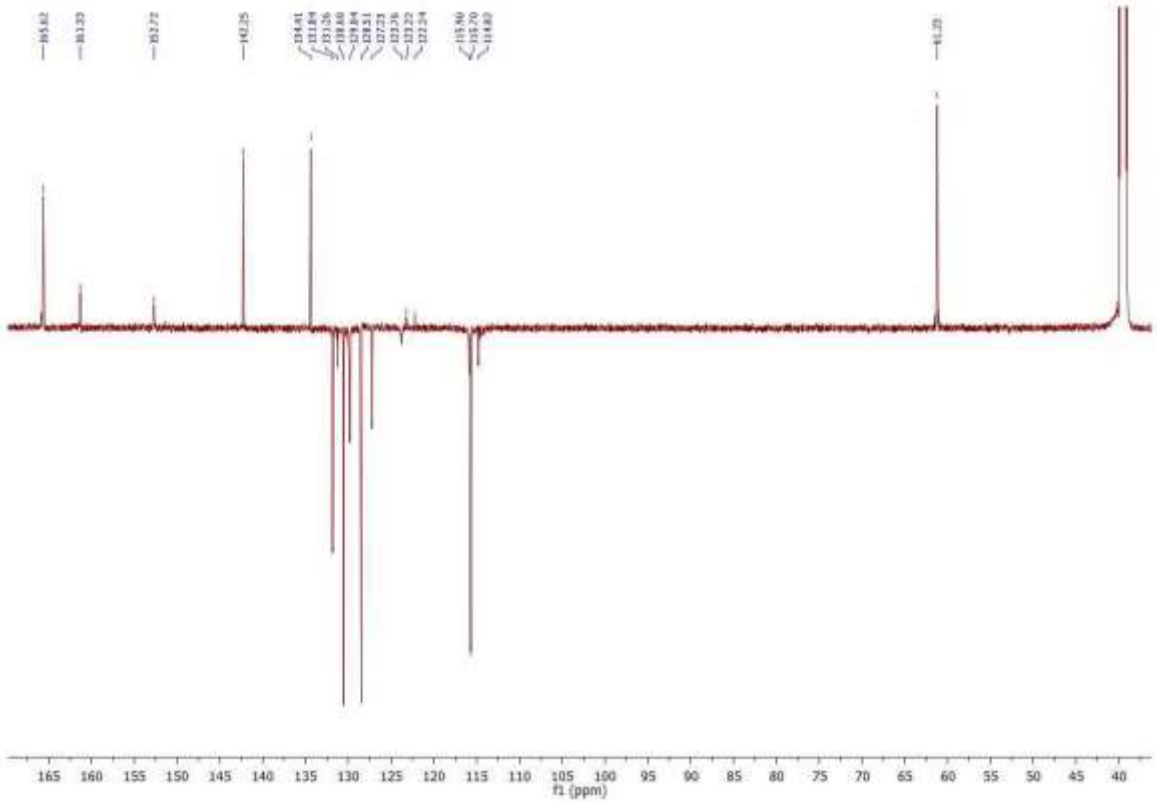
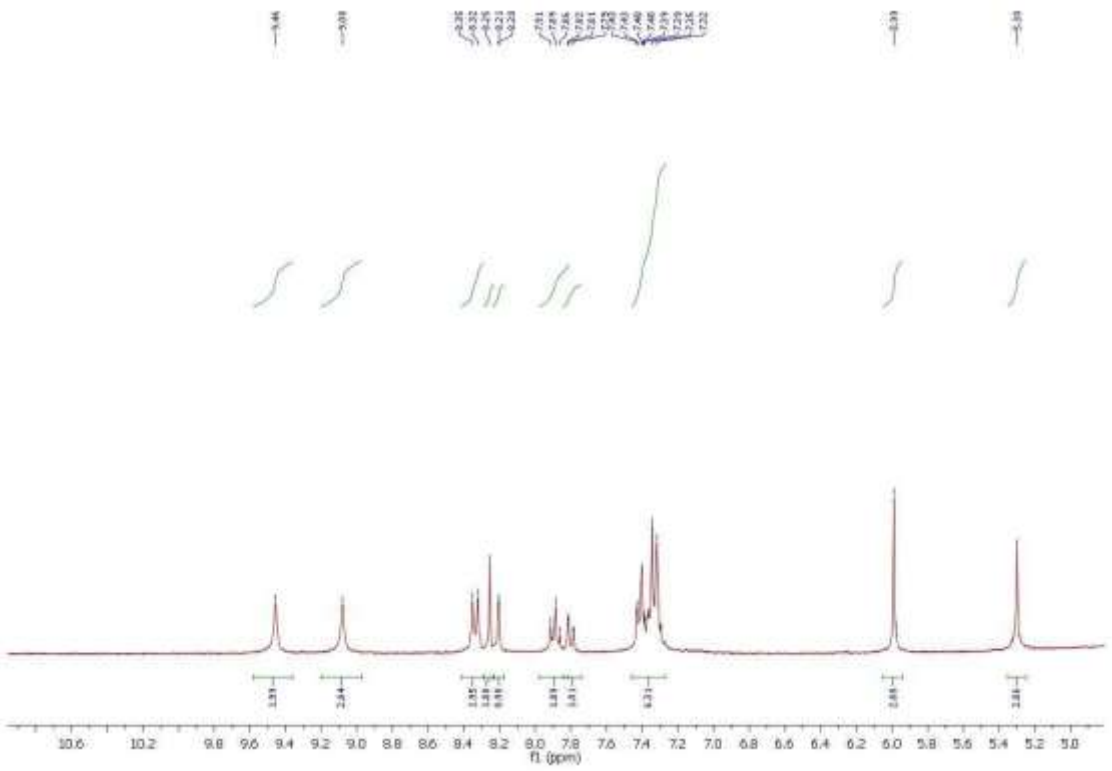


Fig. S7 a) ^{1}H NMR and b) ^{13}C NMR of compd. **7e**

a)



b)

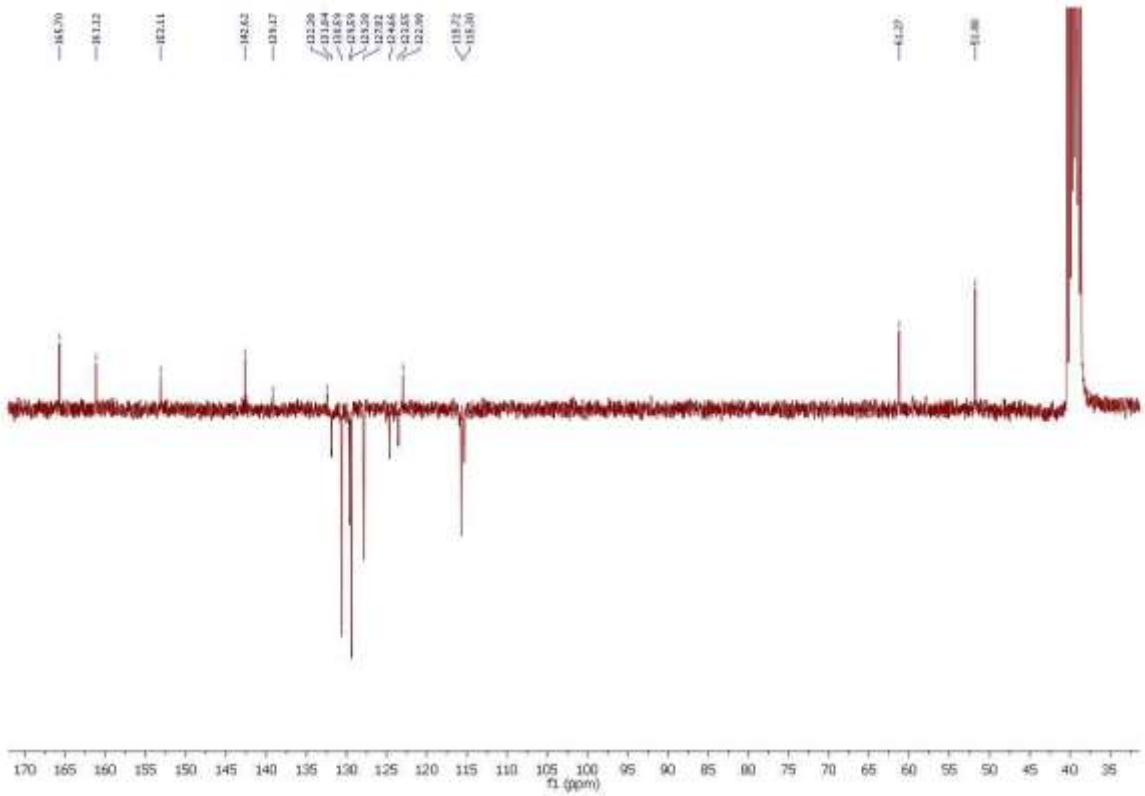
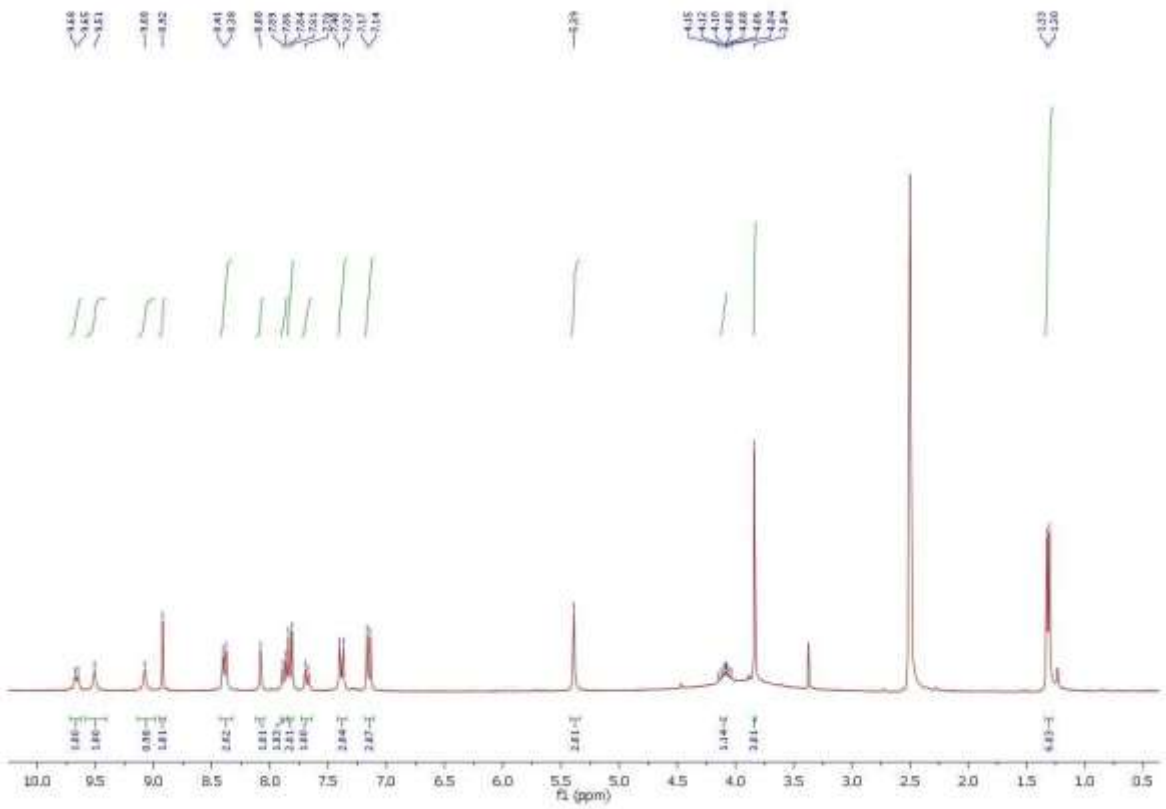


Fig. S8 a) ^{1}H NMR and b) ^{13}C NMR of compd. **8b**

a)



b)

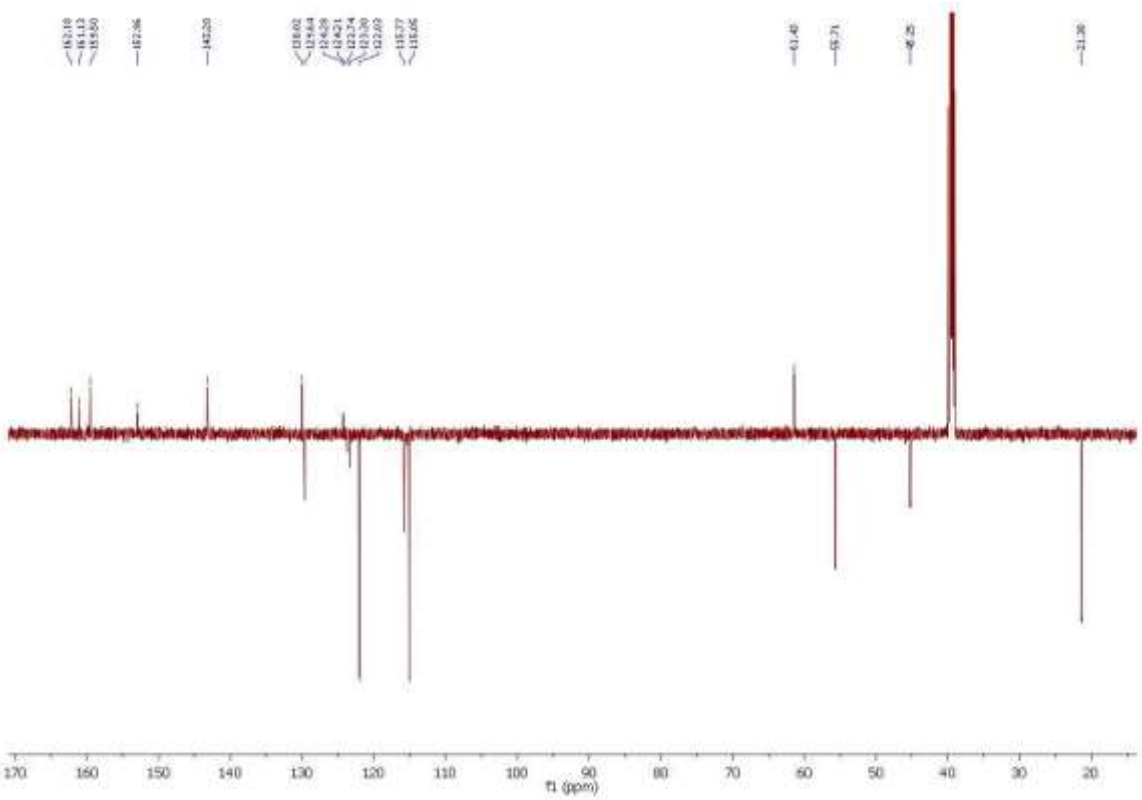
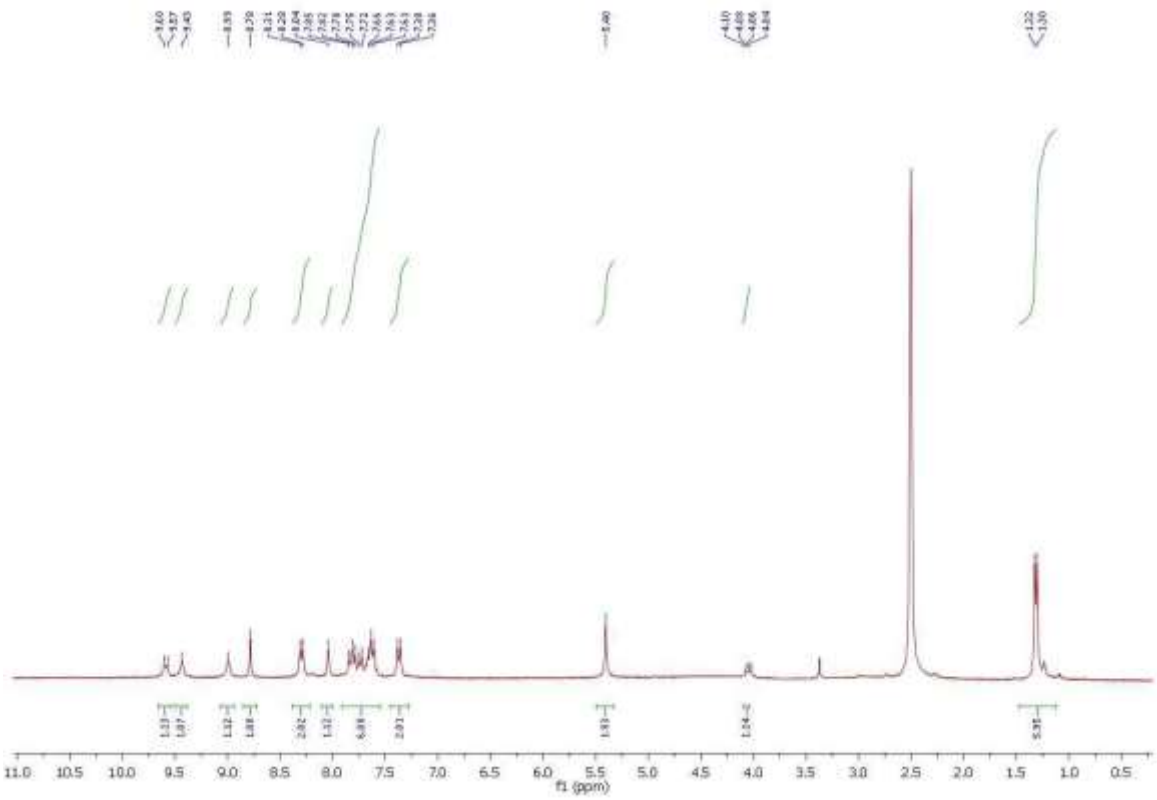


Fig. S9 a) ^{1}H NMR and b) ^{13}C NMR of compd. **8c**

a)



b)

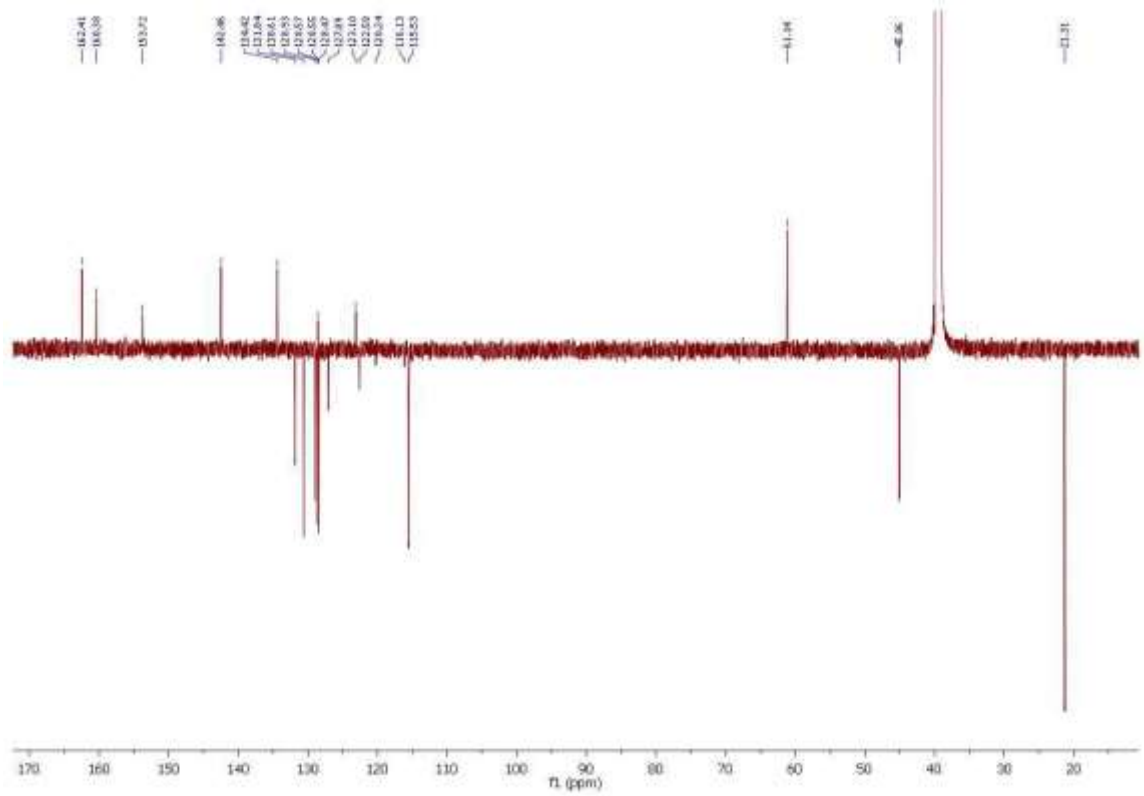
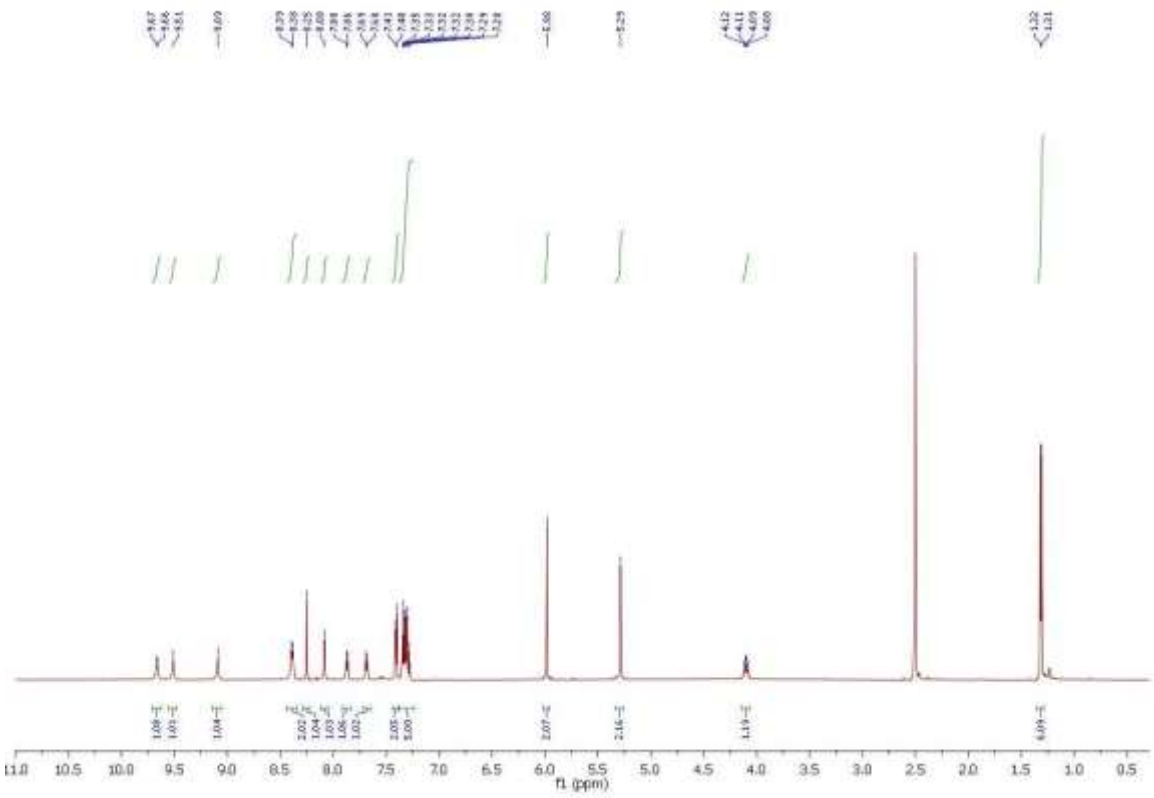


Fig. S10 a) ^{1}H NMR and b) ^{13}C NMR of compd. **8e**

a)



b)

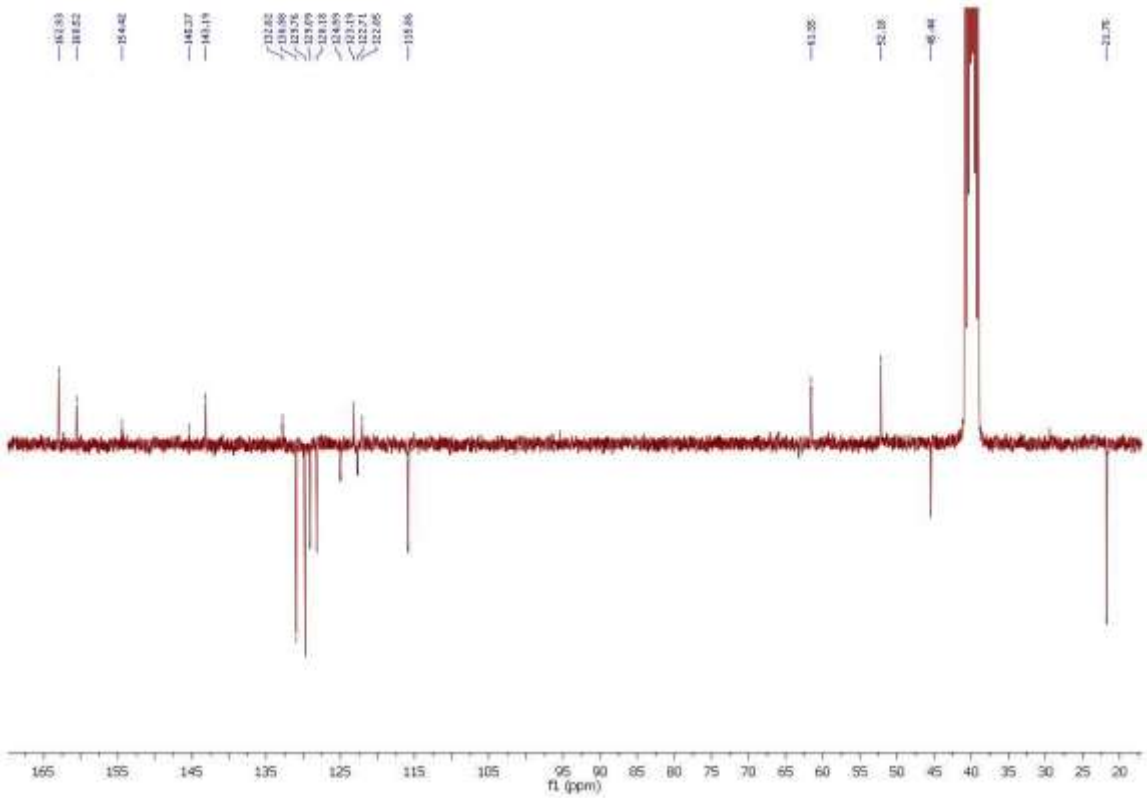
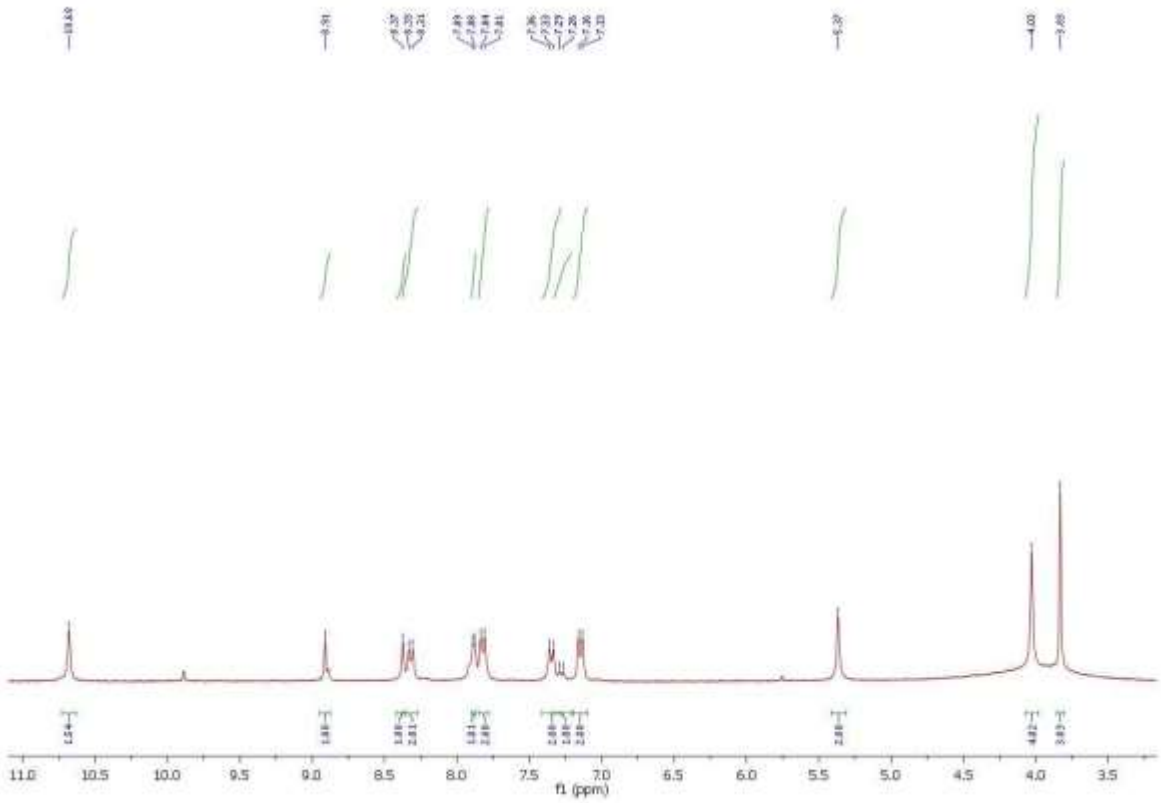


Fig. S11 a) ^{1}H NMR and b) ^{13}C NMR of compd. **9b**

a)



b)

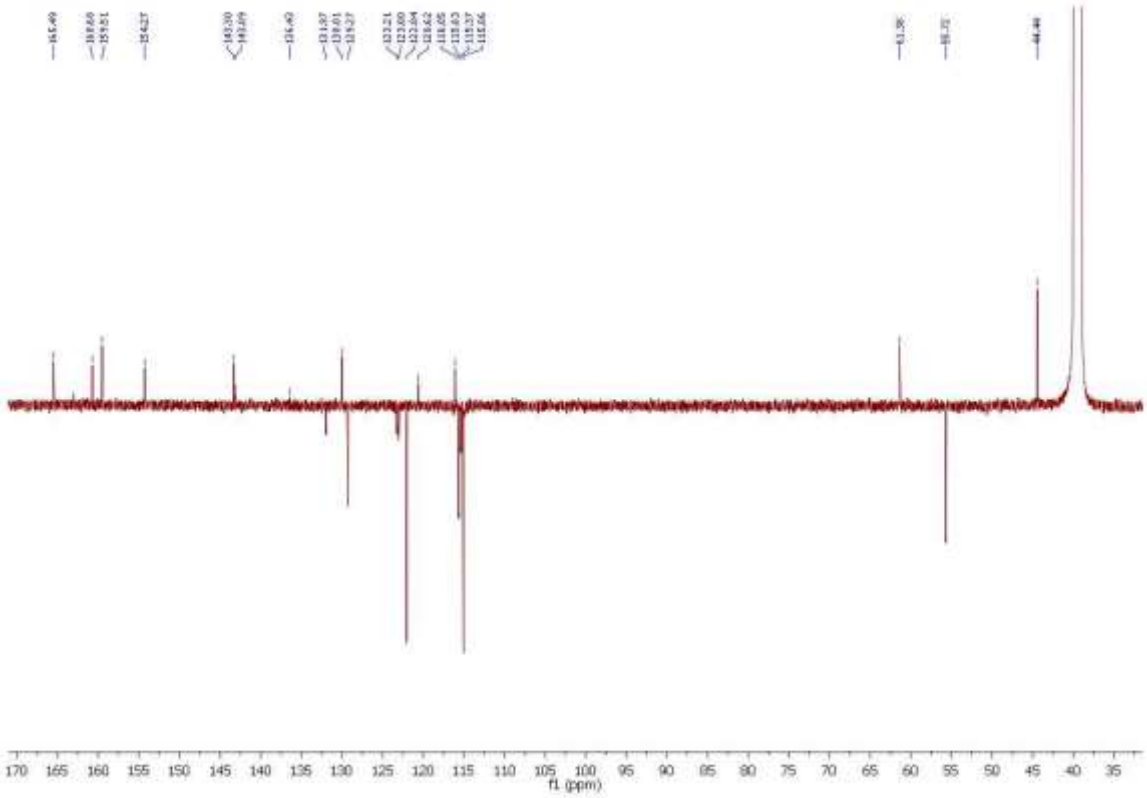
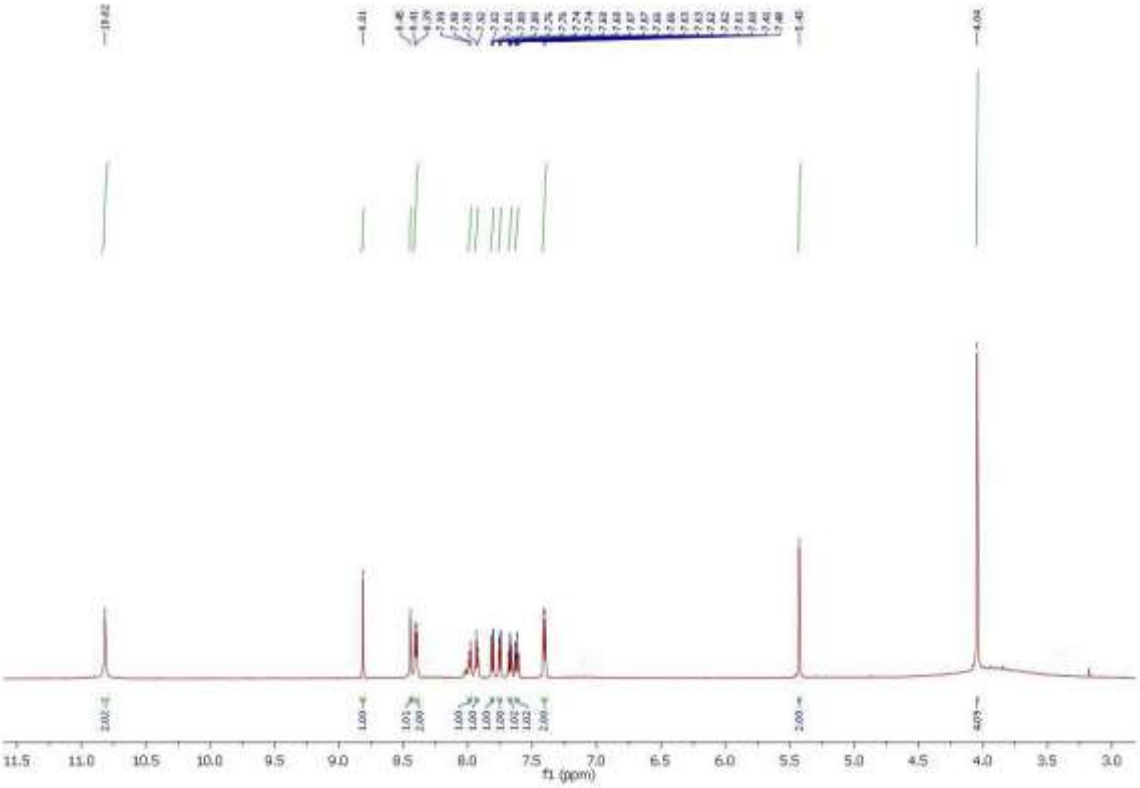


Fig. S12 a) ^{1}H NMR and b) ^{13}C NMR of compd. **9c**

a)



b)

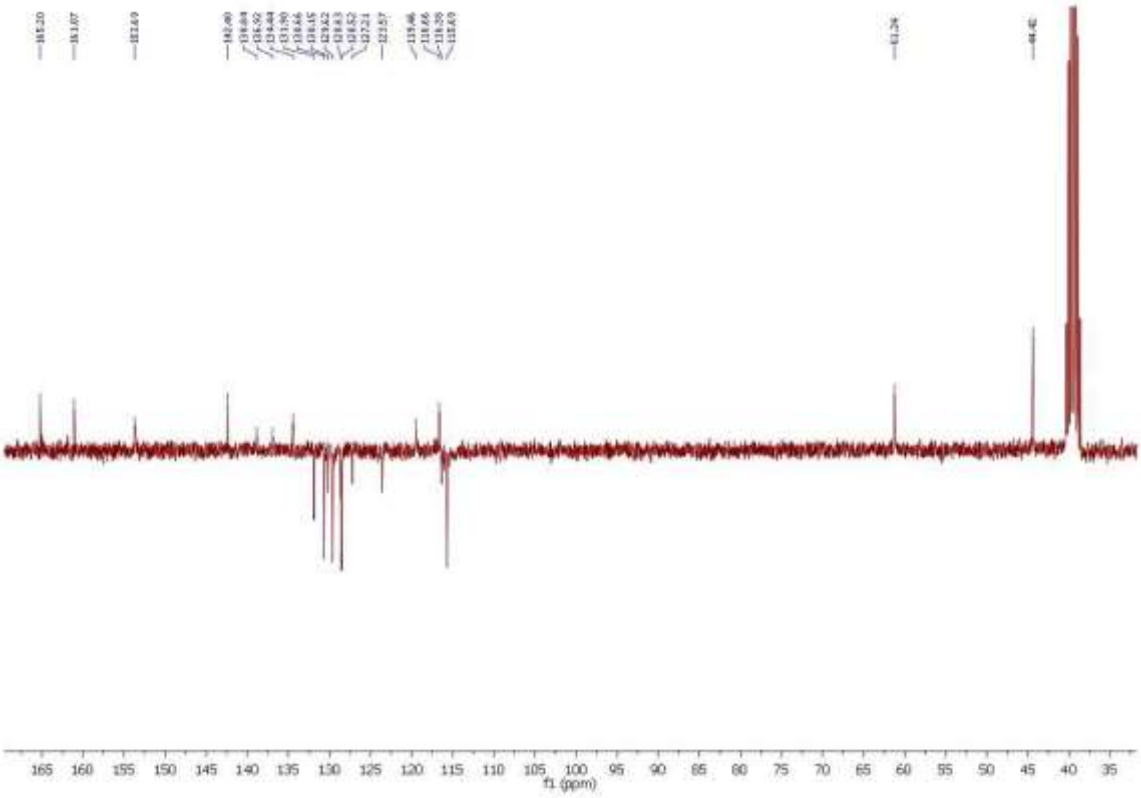
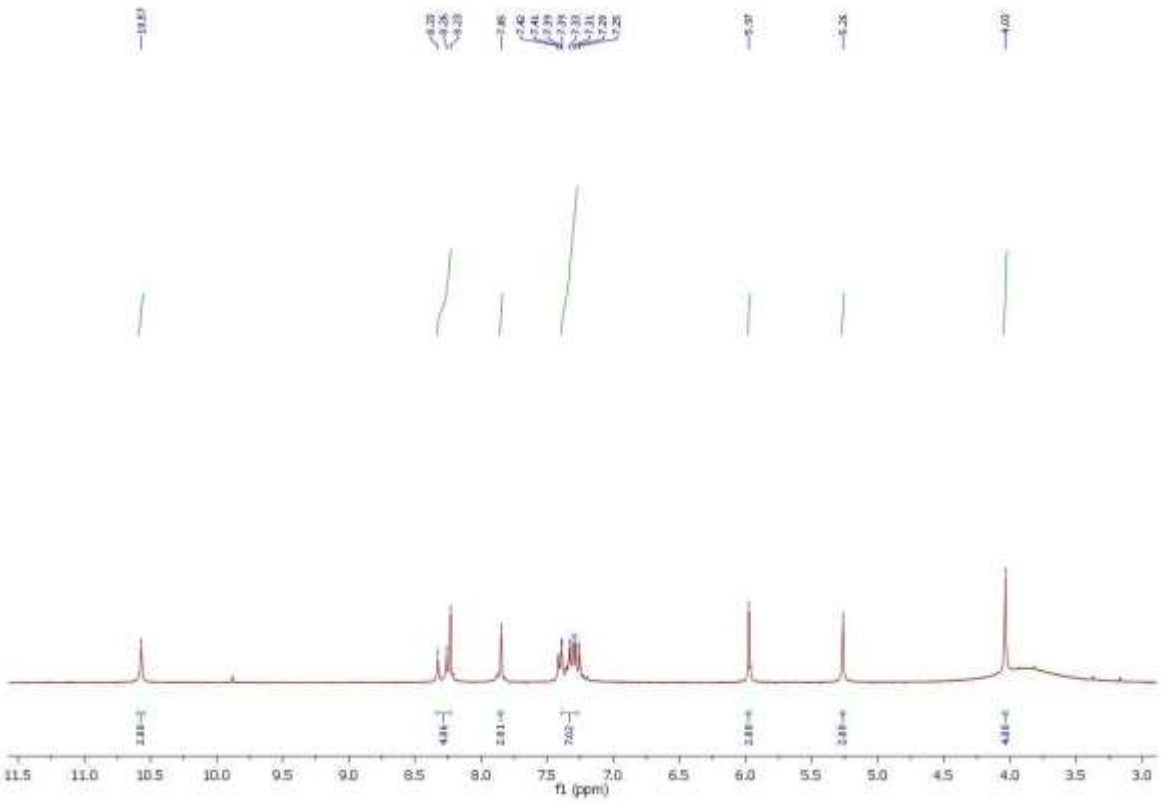


Fig. S13 a) ^{1}H NMR and b) ^{13}C NMR of compd. **9e**

a)



b)