Supplementary Data

Protoporphyrinogen oxidase inhibitors: from plant to human

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Content:

Compound **2**

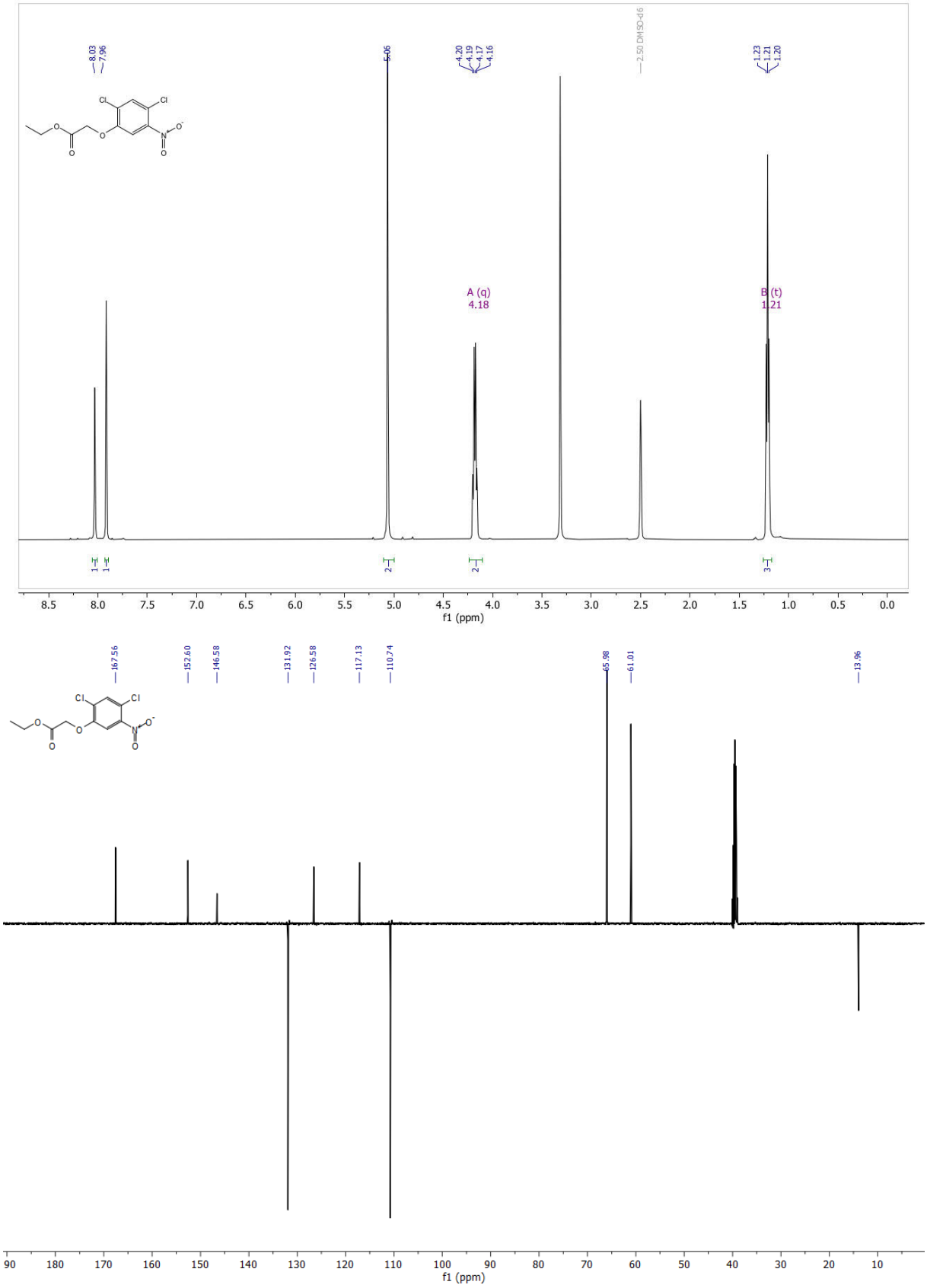

Figure S1. ^{1}H and ^{13}C NMR-spectra of the compound **2**

Compound **3**

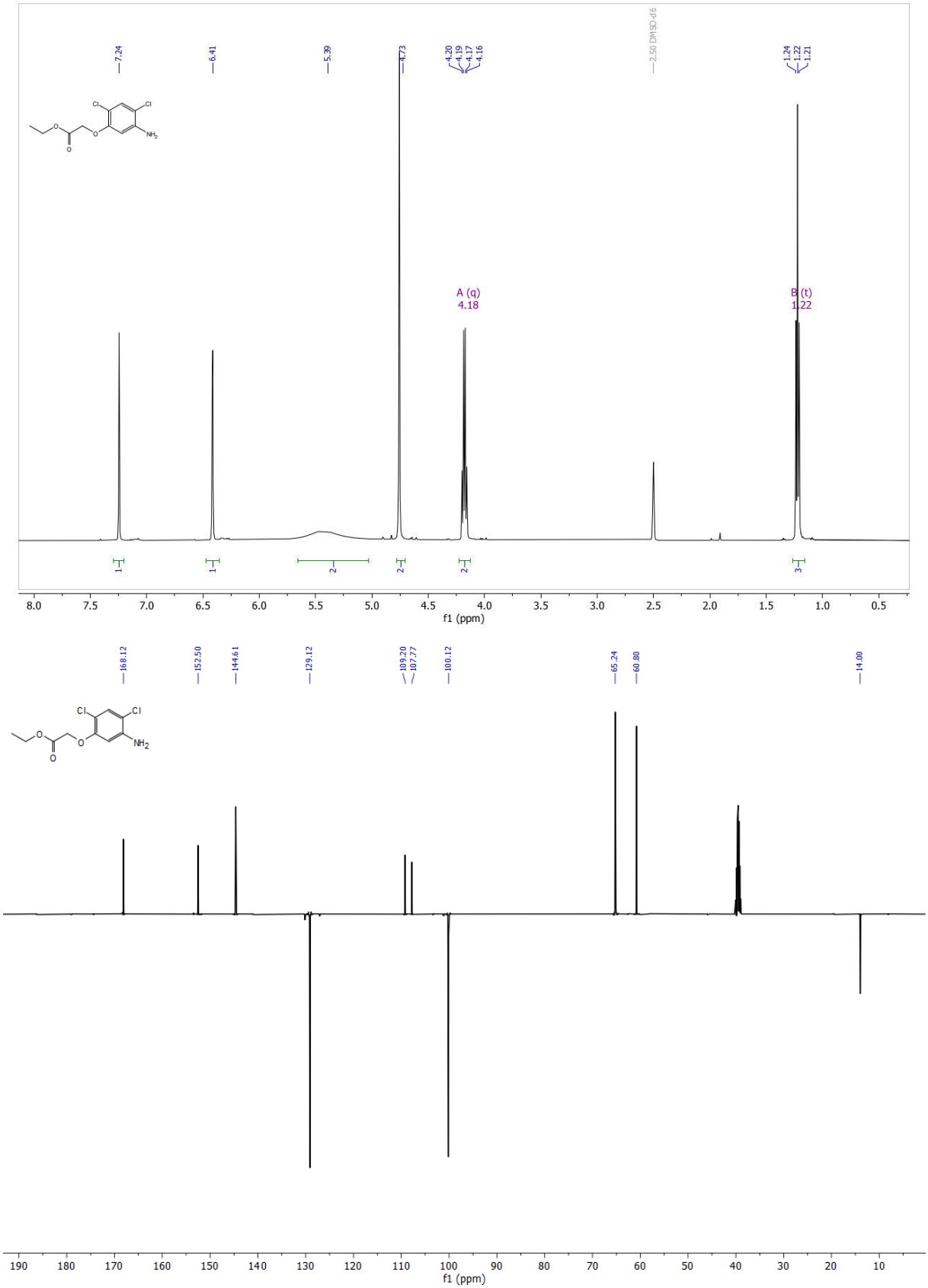

Figure S2. ^{1}H and ^{13}C NMR-spectra of the compound **3**

Schiff base **9**

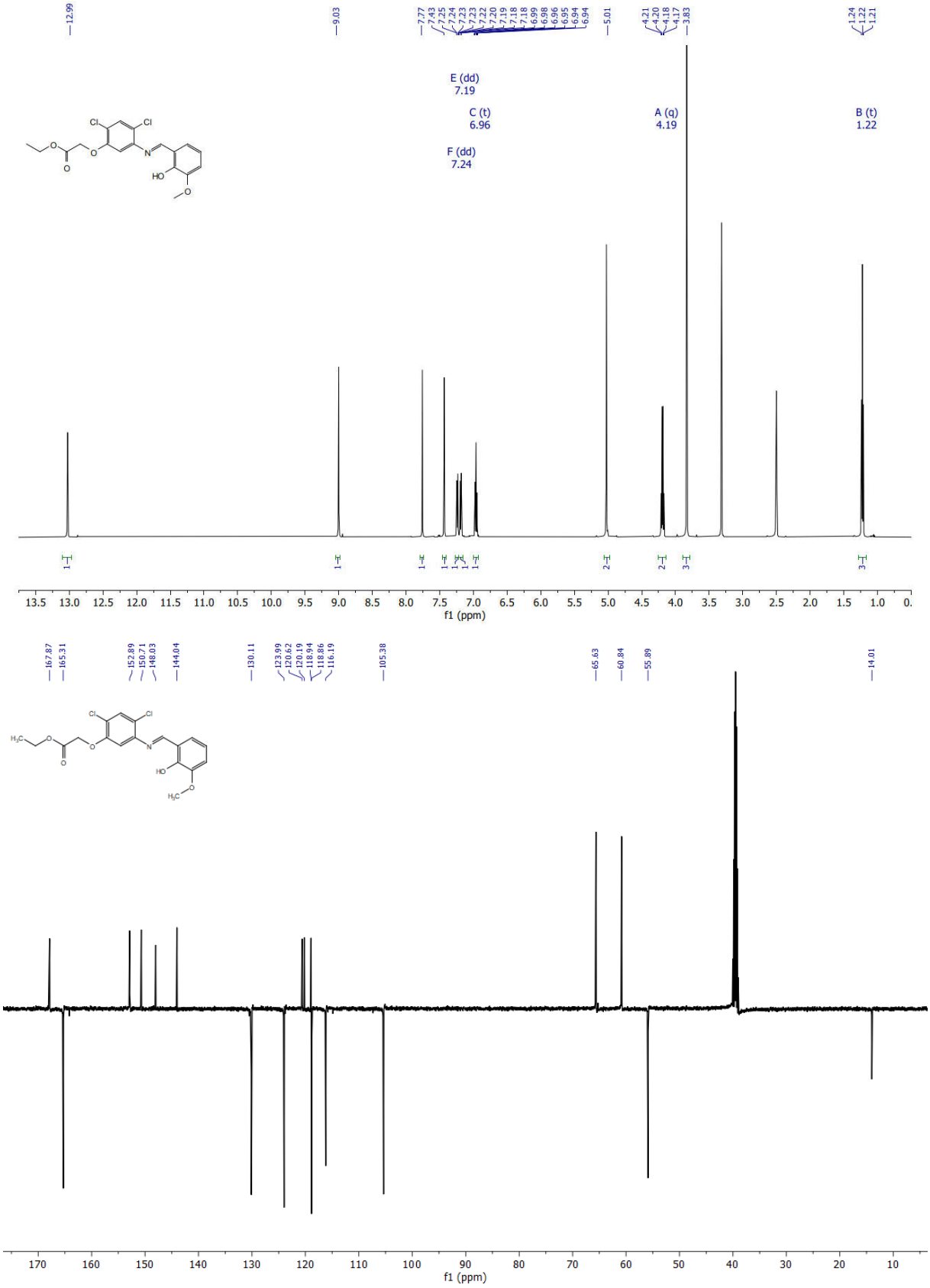

Figure S3. ^{1}H and ^{13}C NMR-spectra of the Schiff base **9**

Schiff base **10**

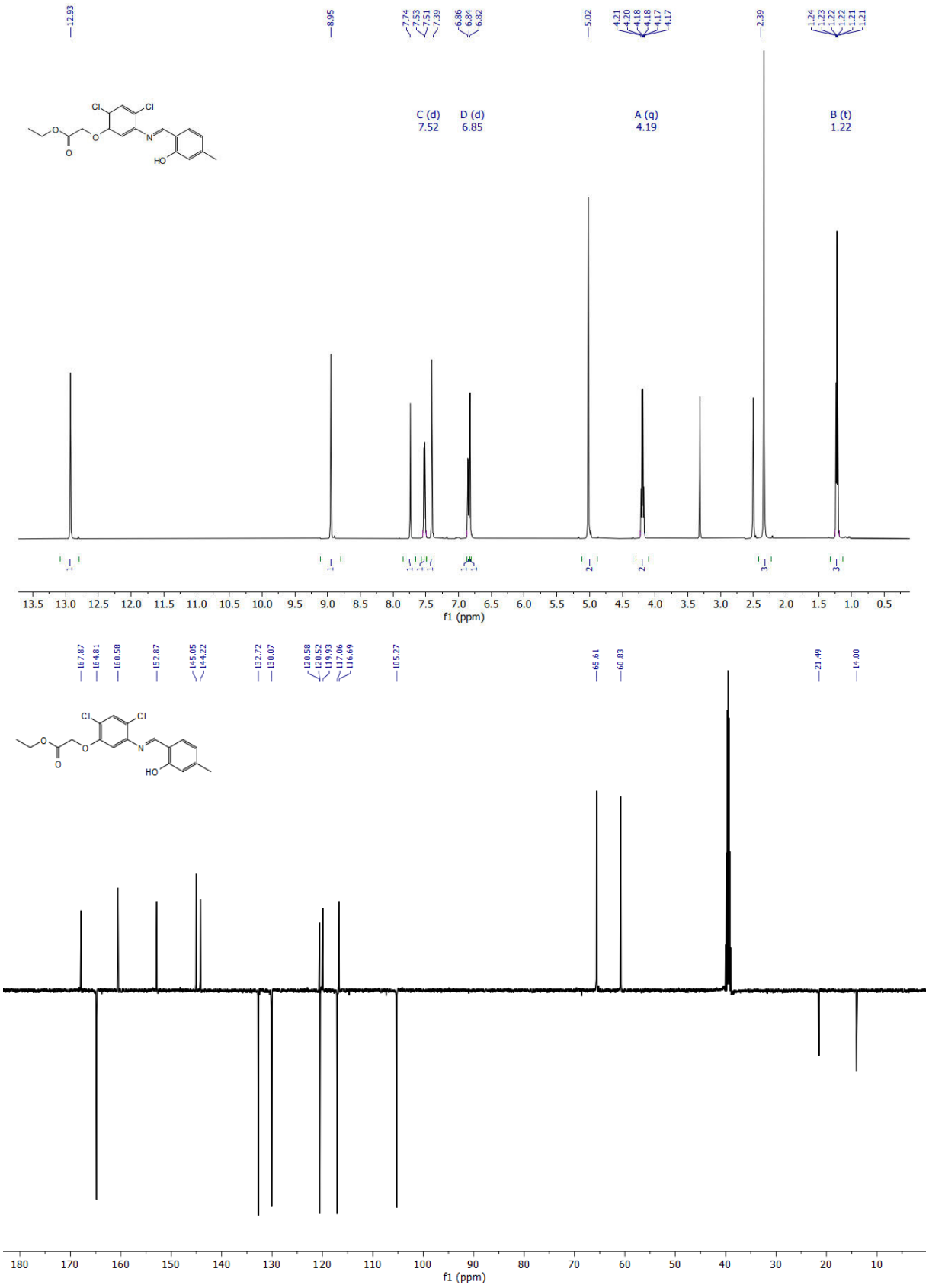

Figure S4. ^{1}H and ^{13}C NMR-spectra of the Schiff base **10**

Schiff base **11**

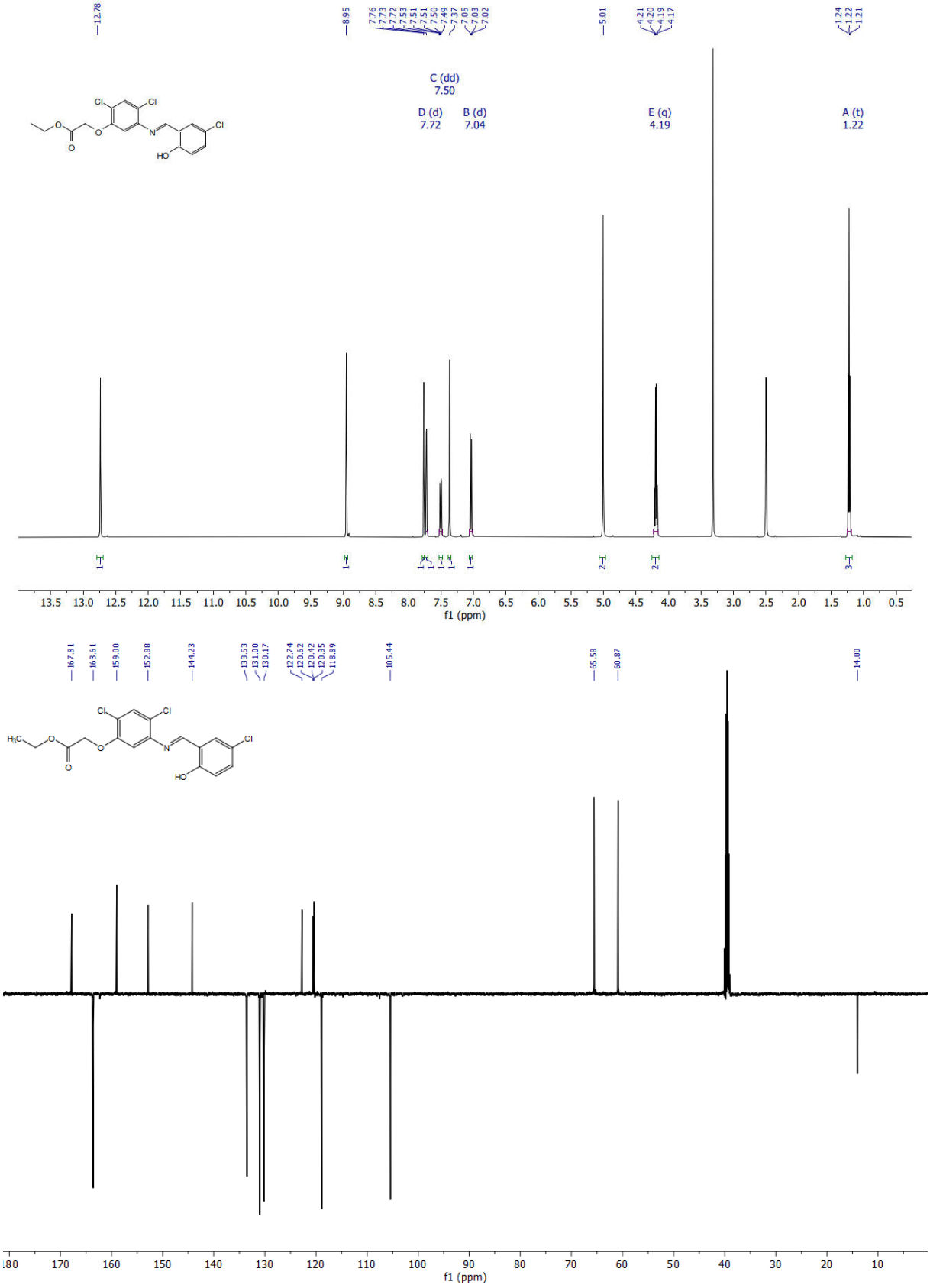

Figure S5. ^{1}H and ^{13}C NMR-spectra of the Schiff base **11**

Schiff base **12**

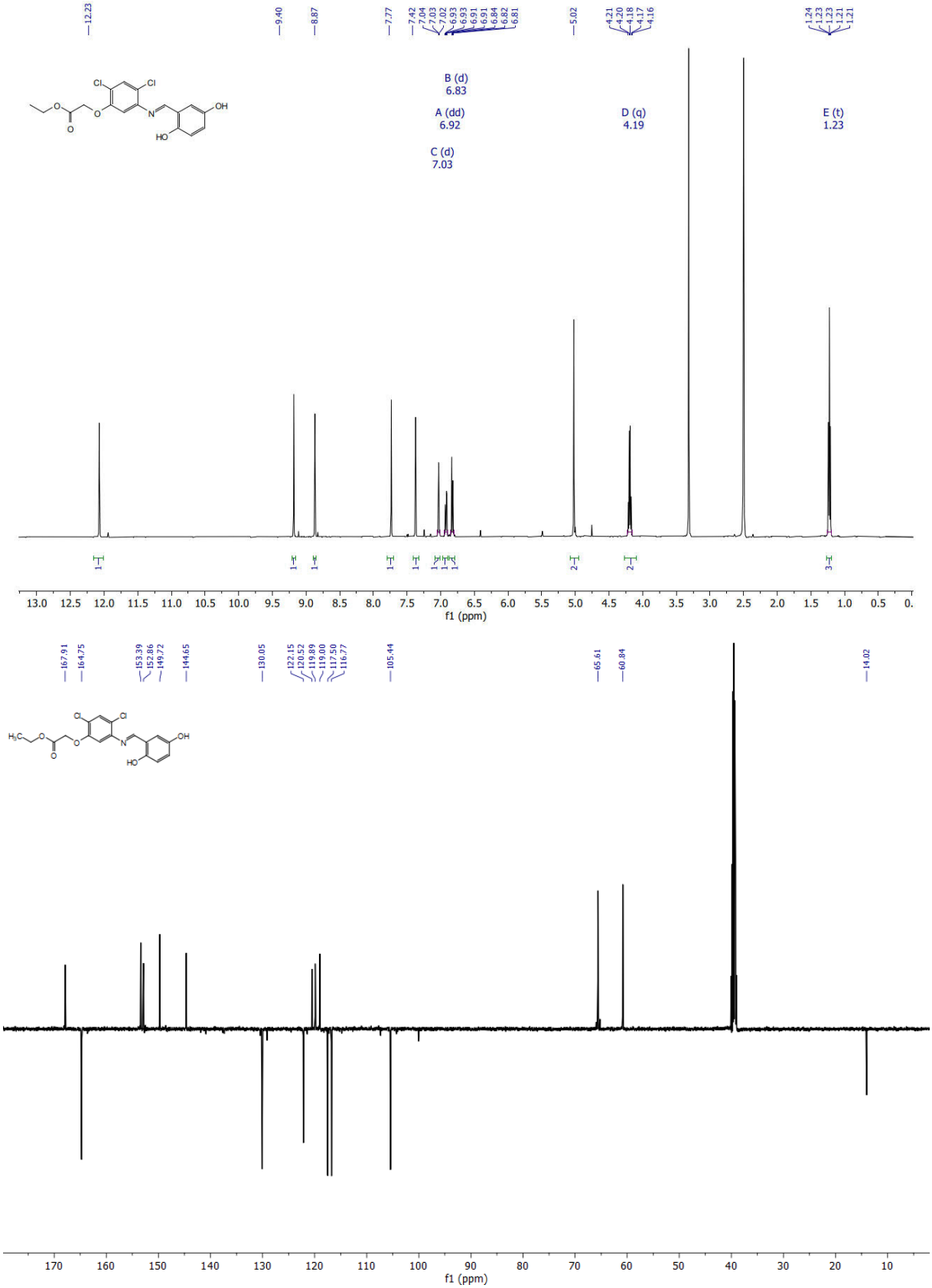

Figure S6. ^{1}H and ^{13}C NMR-spectra of the Schiff base **12**

Schiff base **13**

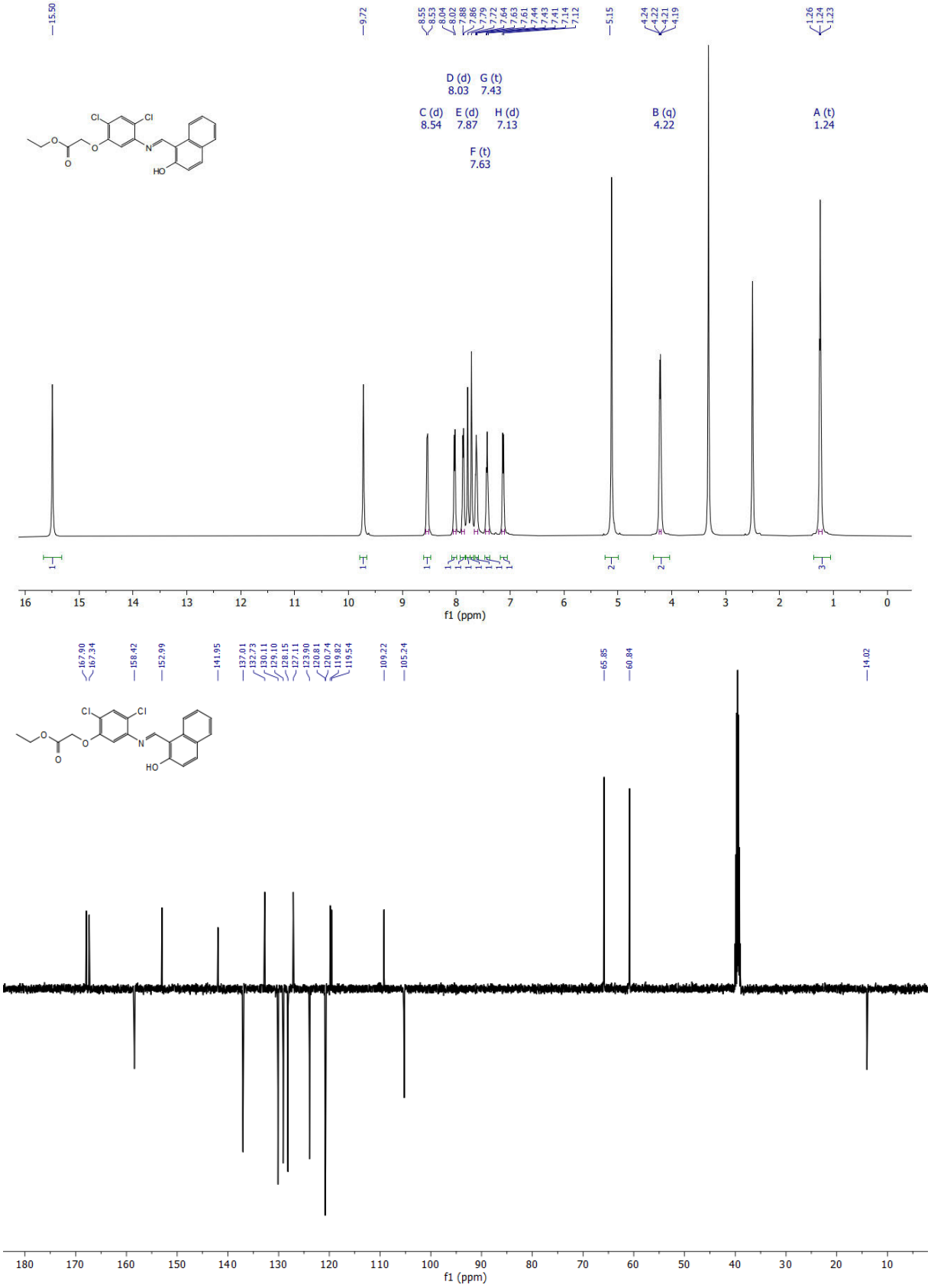

Figure S7. ^{1}H and ^{13}C NMR-spectra of the Schiff base **13**

Chromone **17**

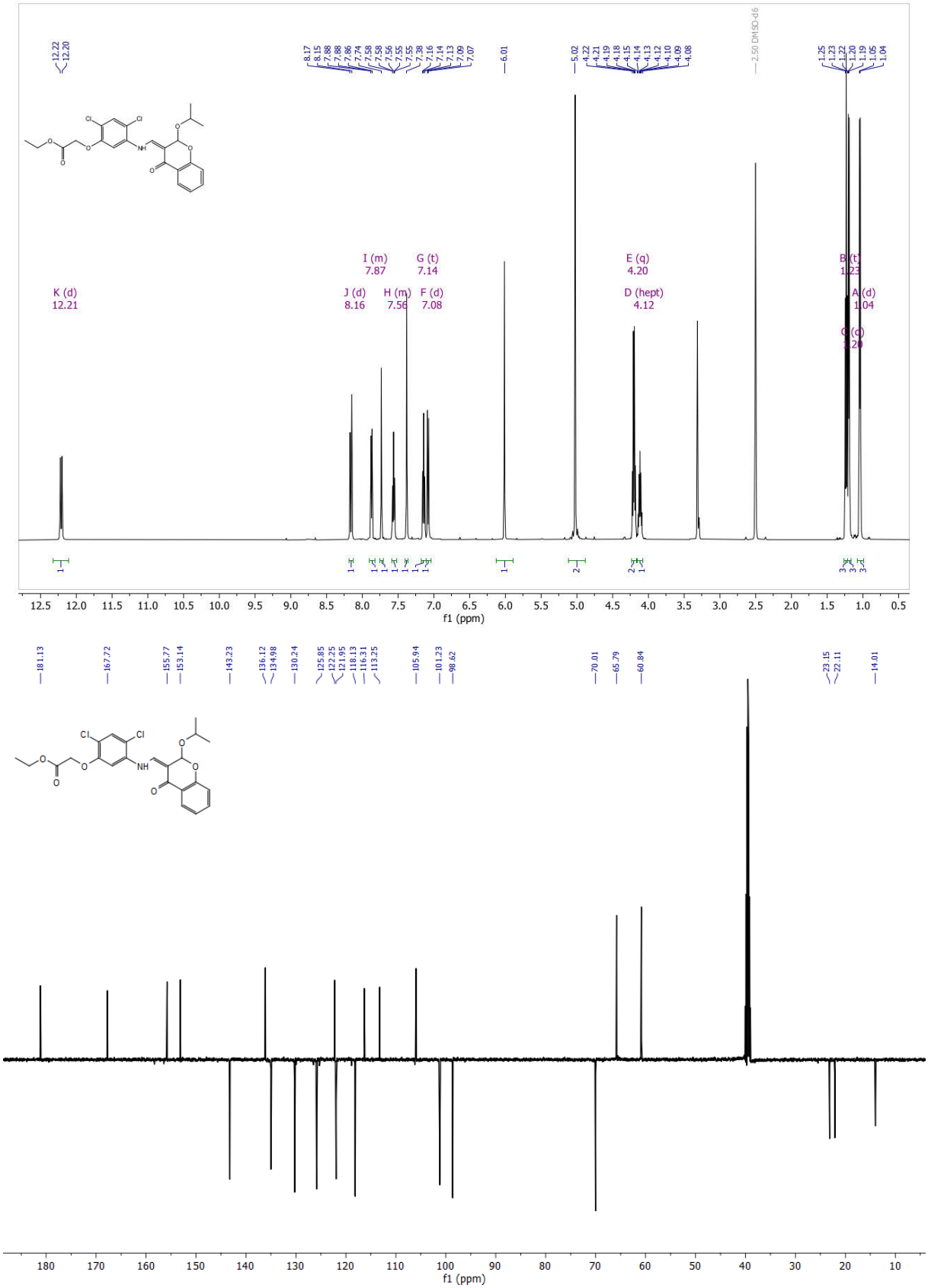

Figure S8. ^{1}H and ^{13}C NMR-spectra of the Chromone **17**

Chromone **18**

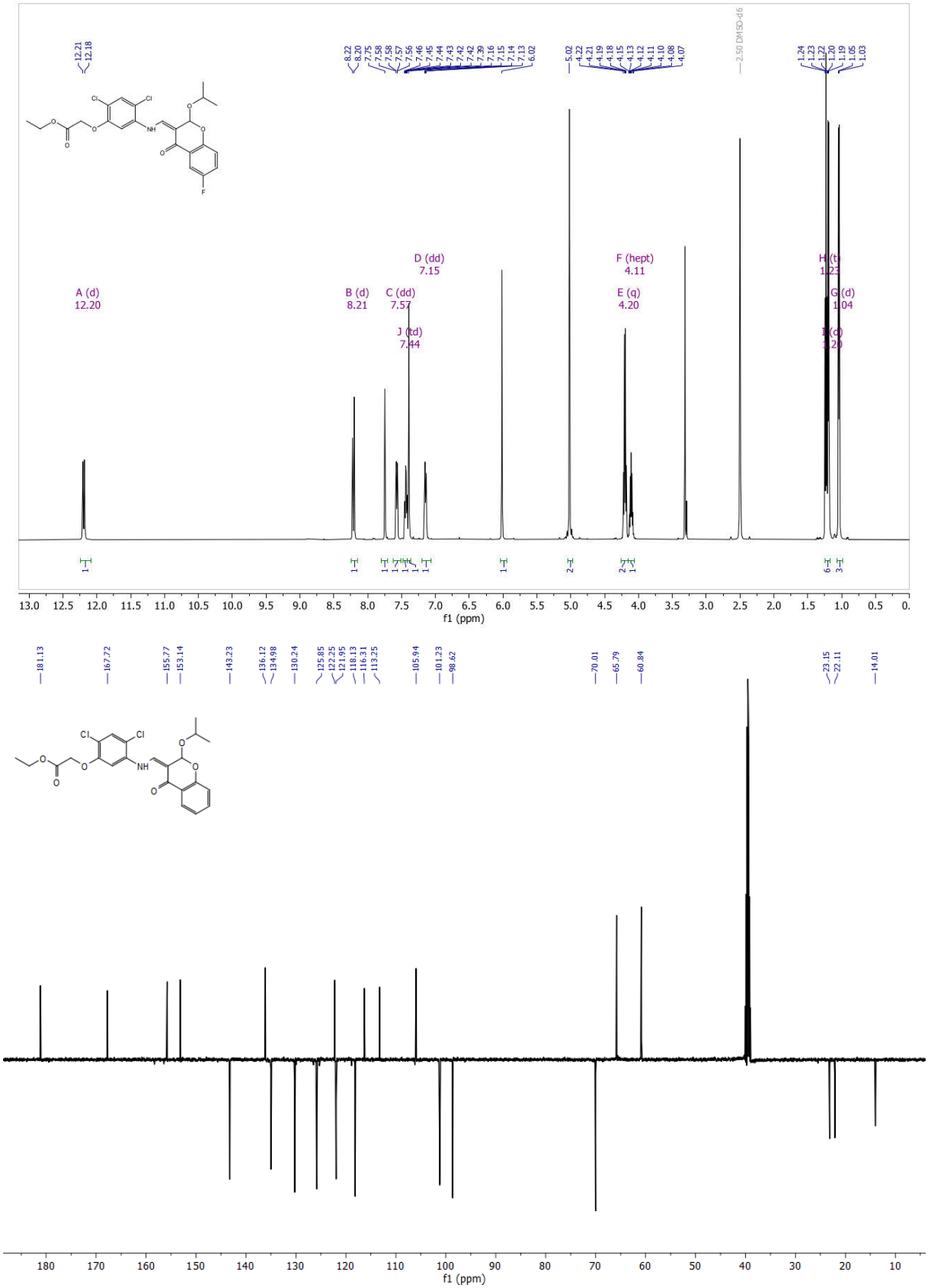

Figure S9. ^{1}H and ^{13}C NMR-spectra of the Chromone **18**

Chromone **19**

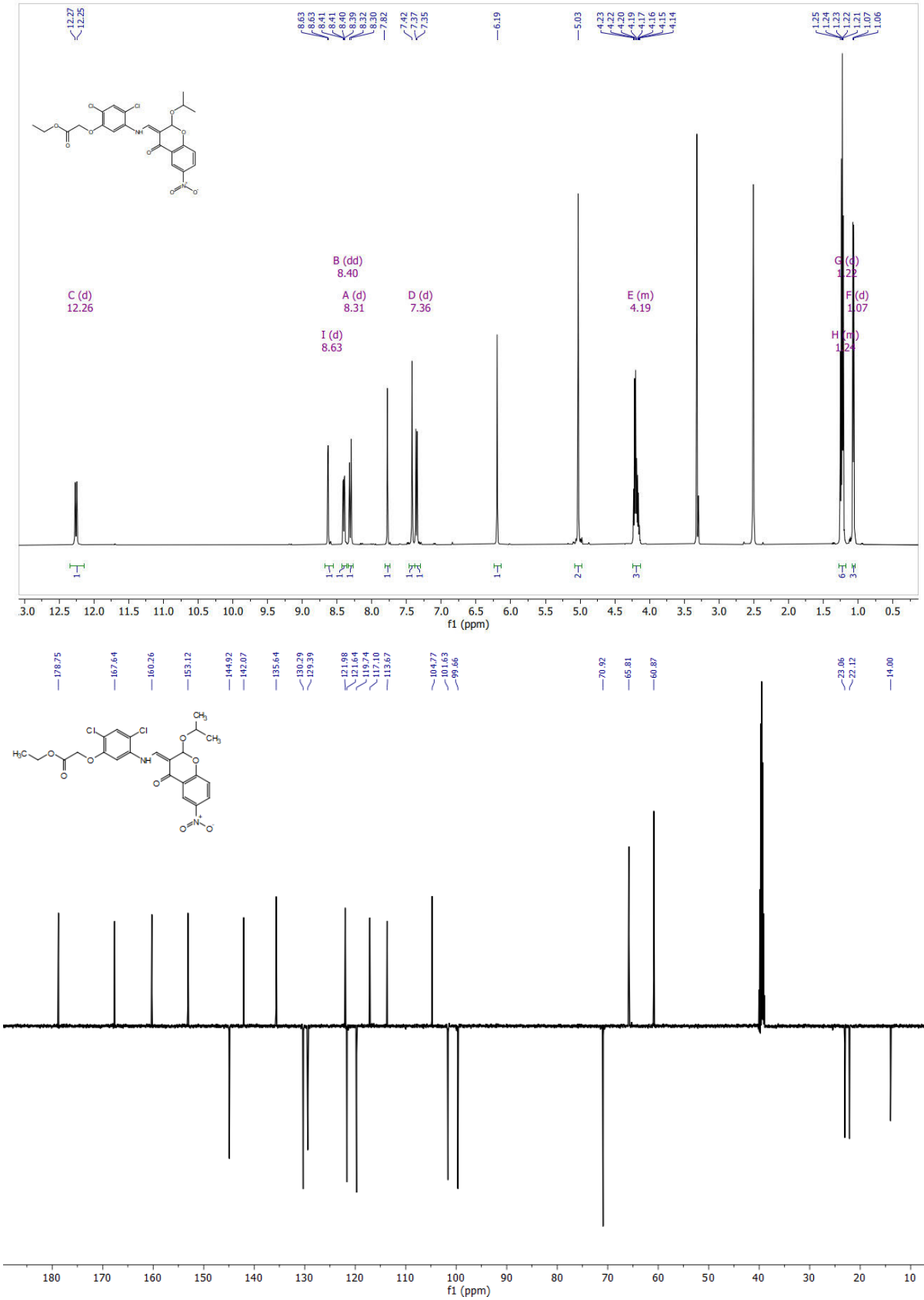

Figure S10. ^{1}H and ^{13}C NMR-spectra of the Chromone **19**

Table S1. Calculated interaction energy for the human a tobacco PPO.

Compounds	**Interaction energy (kcal/mol)**	
	hPPO[1]	**TnPPO[2]**
Schiff base **9**	-7.6	-7.3
Schiff base **10**	-8.6	-8.6
Schiff base **11**	-8.0	-9.1
Schiff base **12**	-7.6	-8.8
Schiff base **13**	-8.6	-9.9
Chromone **17**	-8.9	-8.4
Chromone **18**	-8.8	-8.6
Chromone **19**	-8.7	-8.5

[1]hPPO = human PPO, [2]TnPPO = PPO from *Nicotiana tabacum*.

Table S2. Influence of PPO herbicide on activity of the plant PPOs.

Name	**Source of PPO**	**IC_{50} (mmol/l)**	**Ref.**
Oxyfluorten	Amaranth	0.2	[1]
	Arabidopsis	0.238	
	Soybean	0.135	
	Rapeseed	0.157	
Oxadiazon	E. indica PPO1 (0.0247)	0.00247	[2]
Lactofen	Amaranthus tuberculatus	0.06	[3]
Butafenacil	*Amaranth	0.029	[1]
	*Arabidopsis	0.029	
	*Soybean	0.026	
	*Rapeseed	0.04	
	Corn	0.0005	[4]
	Black nightshade	0.0013	
	Tall morningglory	0.002	
	Velvetleaf	0.0002	
Saflufenacil	Corn	0.0006	
	Black nightshade	0.0002	
	Tall morningglory	(0.002	
	Velvetleaf	0.0004	
Oxadiargyl		~1	[5]
Fomesafen	*Amaranth	0.11	[1]
	*arabidopsis	0.176	
	*Soybean	(0.93)	
	*Rapeseed	0.102	
BAR-2	Nicotiana tabacum	~ 0.01	[6]

*Recombinant

Re-docking of acifluorfen

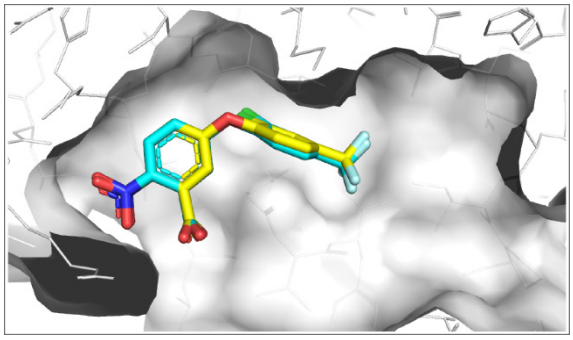

Figure S11. Re-docking of acifluorfen to the binding pocket of hPPO (PDB: 3NKS). The result of the docking experiment is shown in yellow, co-crystallized orientation in turquoise, the receptor binding-pocket in light gray.

References

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