Supporting Information for:

Perylene Bisimide Dyes with Up to Five Independently Introduced Substituents: Controlling the Functionalization Pattern and Photo-physical Properties Using Regiospecific Bay-Substitution

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The supporting information contains following items:

Section 1. Cyclic voltammograms

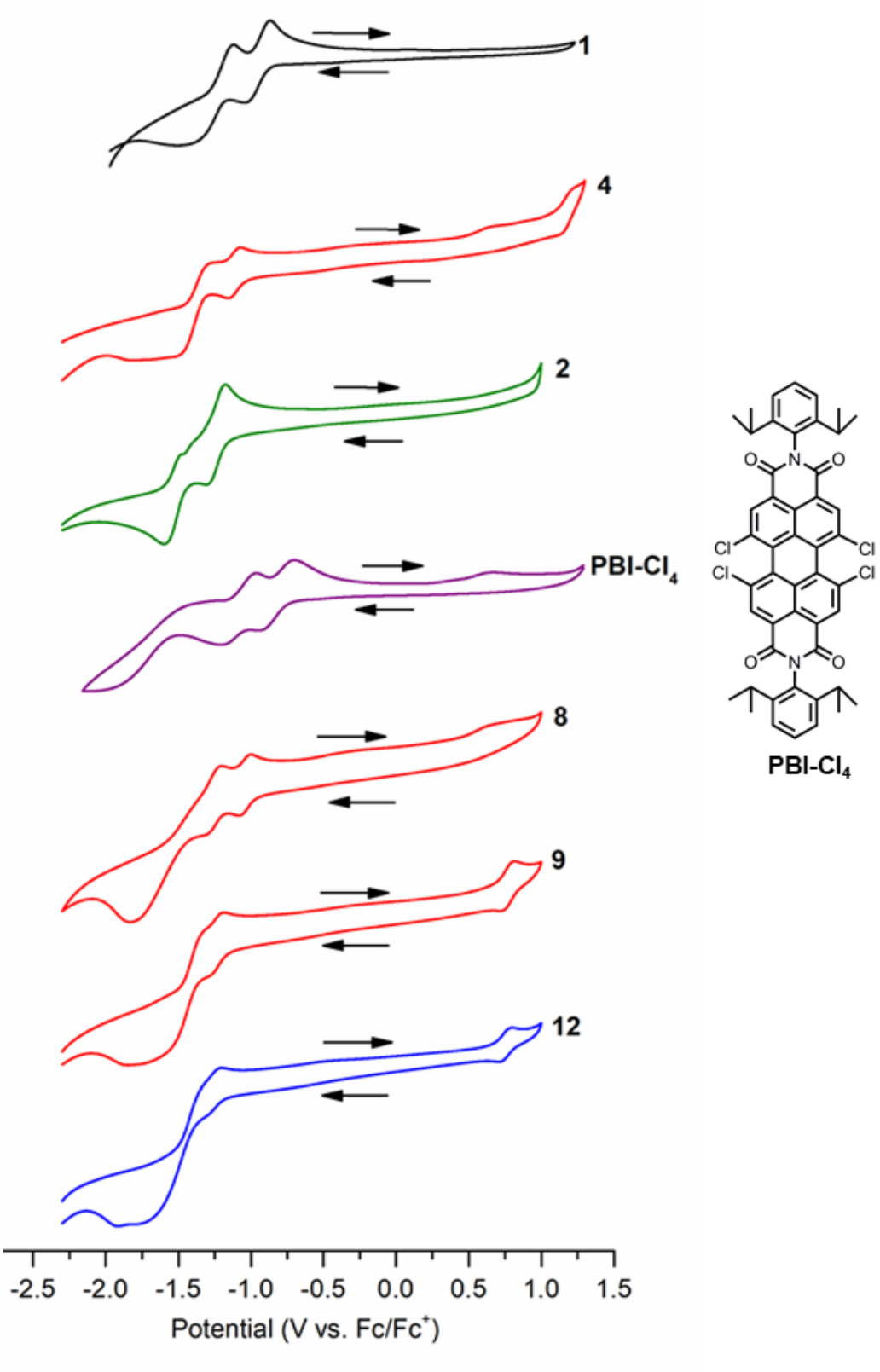


Figure S-1.1: Cyclic voltammograms of compounds **1**, **4**, **2**, **PBI-Cl$_4$**, **8**, **9**, and **12**.

Section 2. Spectroscopy related data

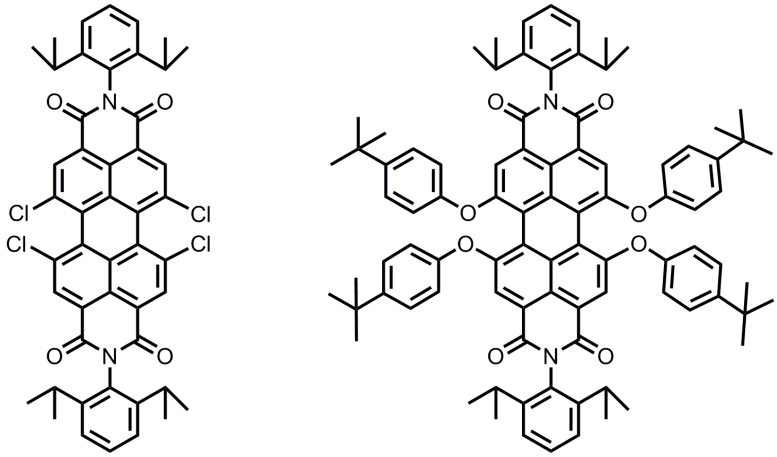


Figure S-2.1: Structures of compound **PBI-Cl$_4$** (left) and **PBI-(OPh)$_4$** (right).

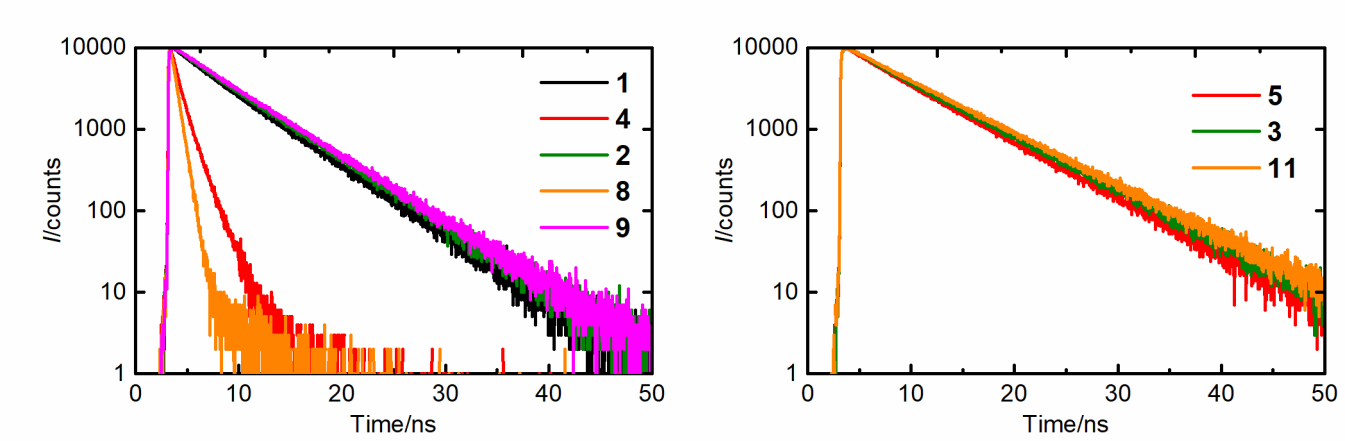


Figure S-2.2: Fluorescence decay-curves of compounds **1**, **4**, **2**, **8**, **9** and relevant model compounds (**5**, **3**, and **11**) in toluene after excitation at 400 nm.

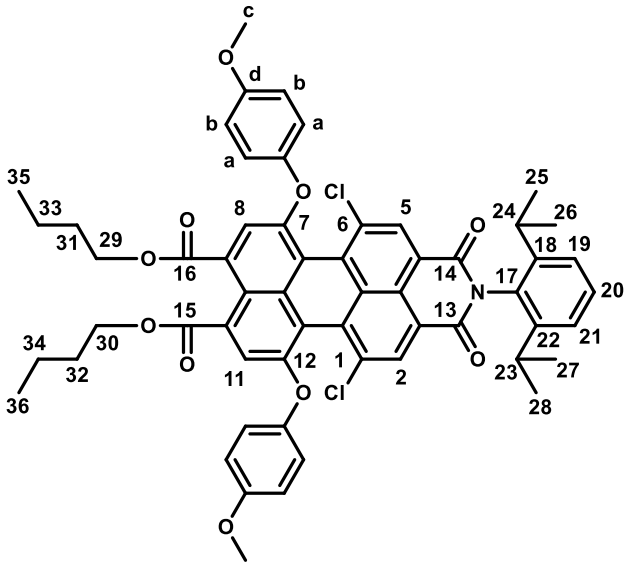
Table S-1: Optical properties of the model compounds **5**, **3**, **PBI-Cl$_4$**, **11**, and **PBI-(OPh)$_4$** in toluene.

Compound	λ_{abs}(nm)	ε ($M^{-1}cm^{-1}$)	λ_{em}(nm)	Φ_f[a]	τ_f (ns)[b]
5	507	28700	560	0.92	6.09
3	529	25100	589	0.79	6.42
PBI-Cl$_4$	523	45000	552	0.95	5.11
11	560	43200	606	0.72	6.73
PBI-(OPh)$_4$	581	61700	611	0.76	5.79

[a] Fluorescence quantum yield. [b] Fluorescence life-time.

Section 3. Structure elucidation of compounds 2, 3, 4, 6, 9, 12, and 15 by 1D and 2D NMR Spectroscopy

3.1 Compound 2:



The structure of compound **2** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.1. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.2). The evidences of the regiospecific substitution at 7- and 12-positions were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.3), which clearly showed the cross couplings of ester carbonyl carbons (C^{15} and C^{16}) with perylene core protons (H^{8} and H^{11}) and butyl-chain protons (H^{29} and H^{30}). Furthermore, the imide carbonyl carbon atoms C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments (Figure S-3.4) in which through-space cross couplings between H^{c}–H^{b}, H^{a}–$H^{8,11}$, and $H^{2,5}$–$H^{23,24}$ were clearly observed. The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.5).

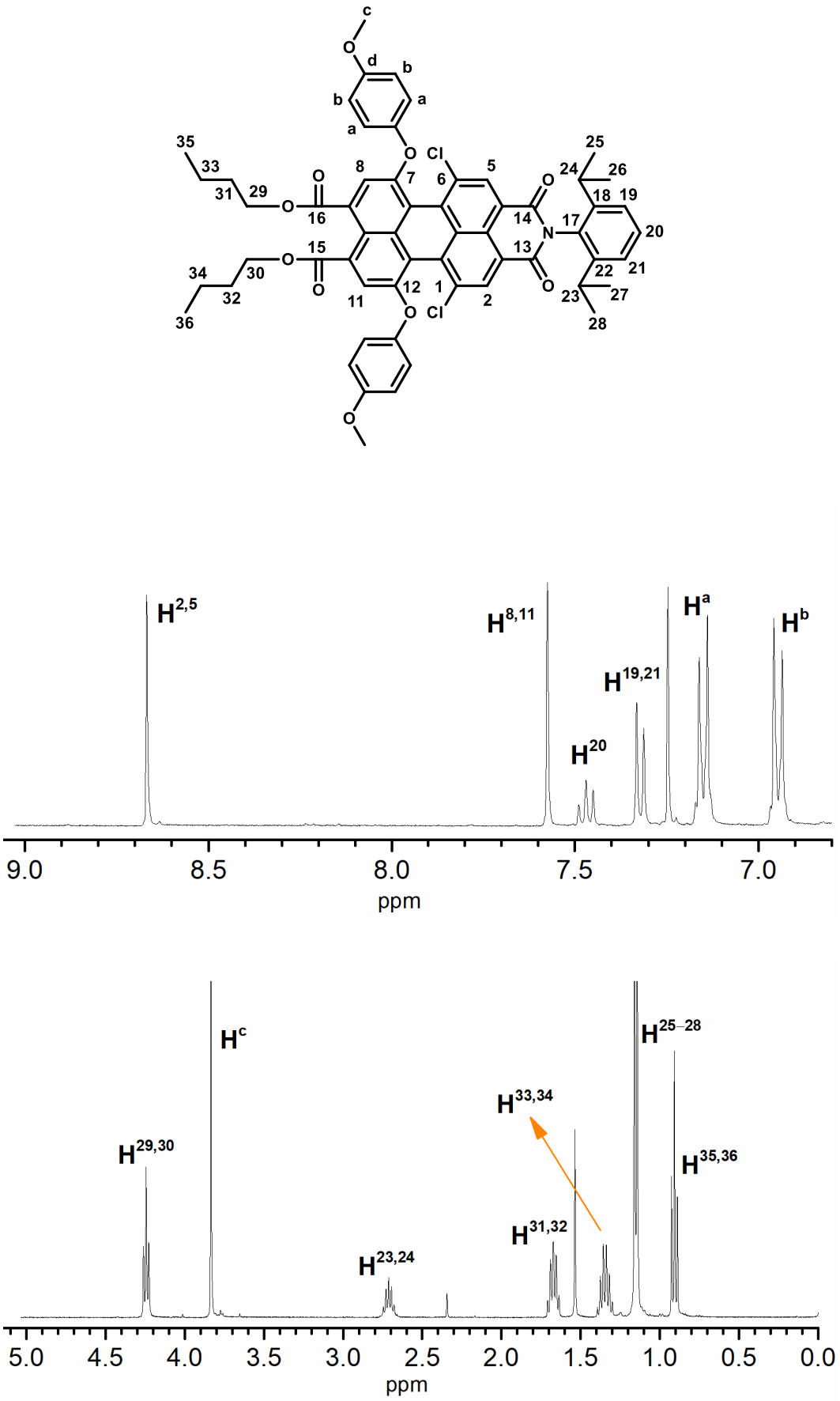


Figure S-3.1: ^{1}H NMR spectrum (CDCl3, 400 MHz) of compound **2** with complete assignments of proton signals (aromatic region at the top and aliphatic region at the bottom).

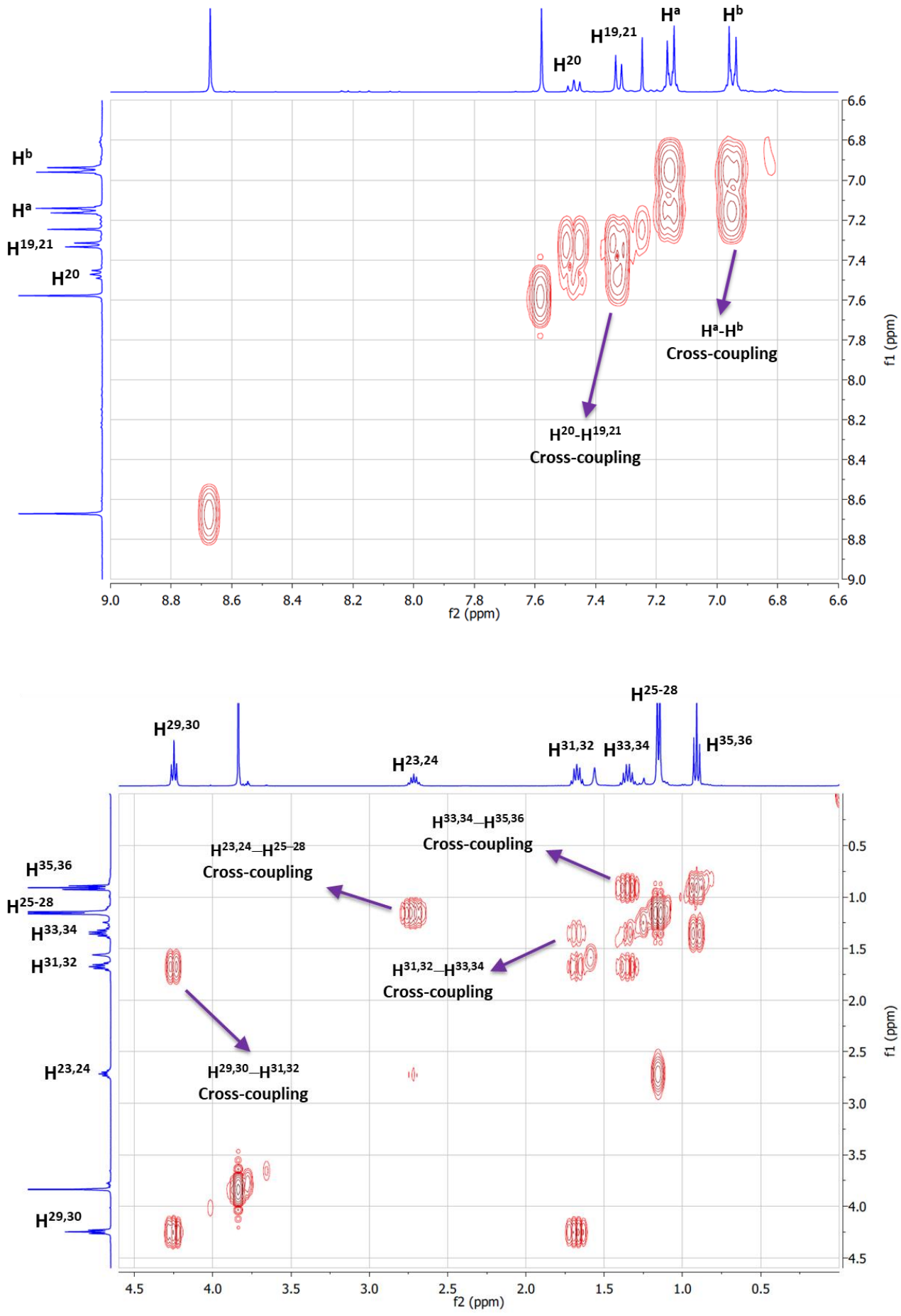


Figure S-3.2: $^{1}H–^{1}H$ gCOSY NMR spectrum (CDCl3, 400 MHz) of compound **2** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

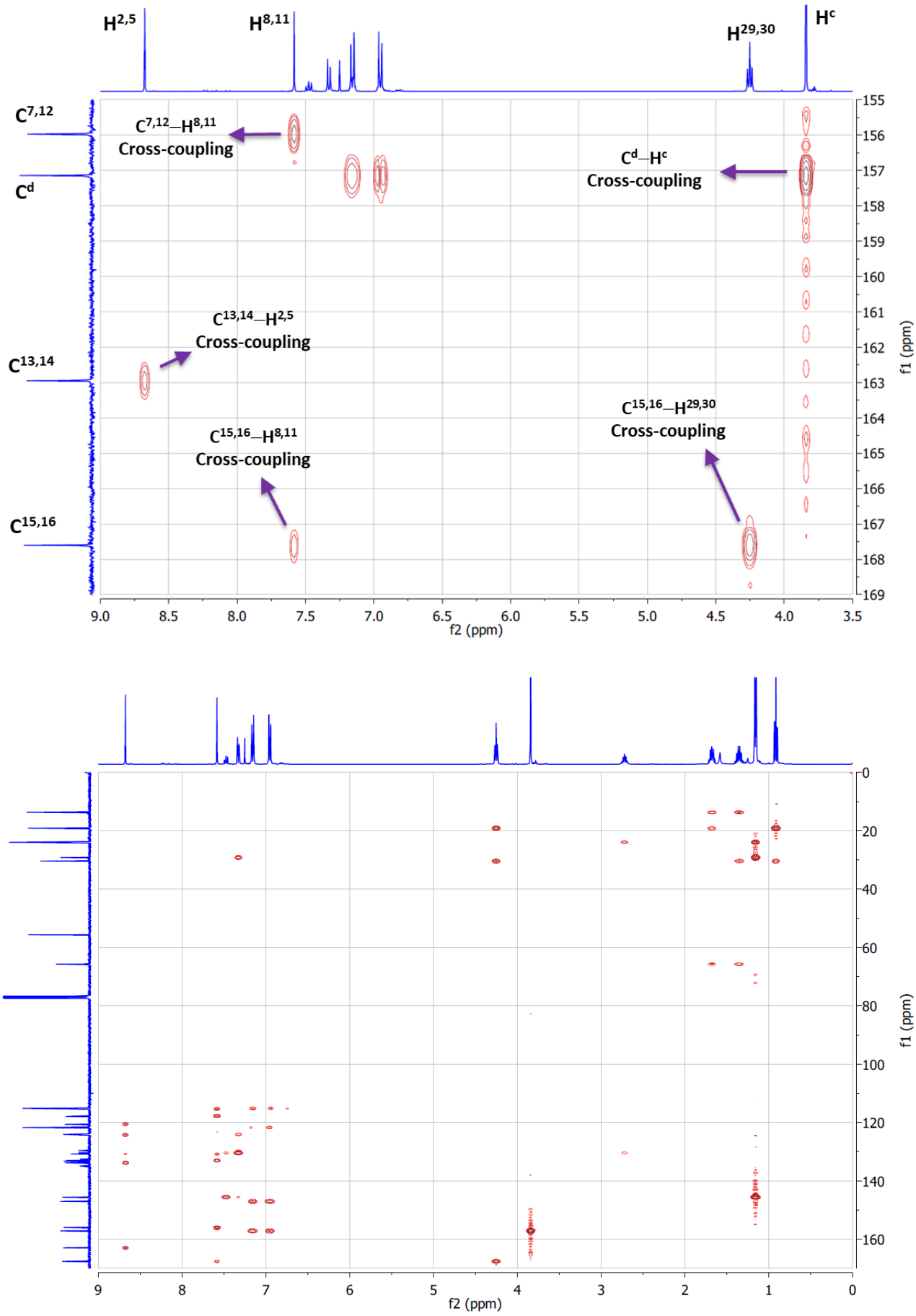


Figure S-3.3: $^{1}H–^{13}C$ gHMBC NMR spectrum (CDCl3, 400 MHz) of compound **2** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

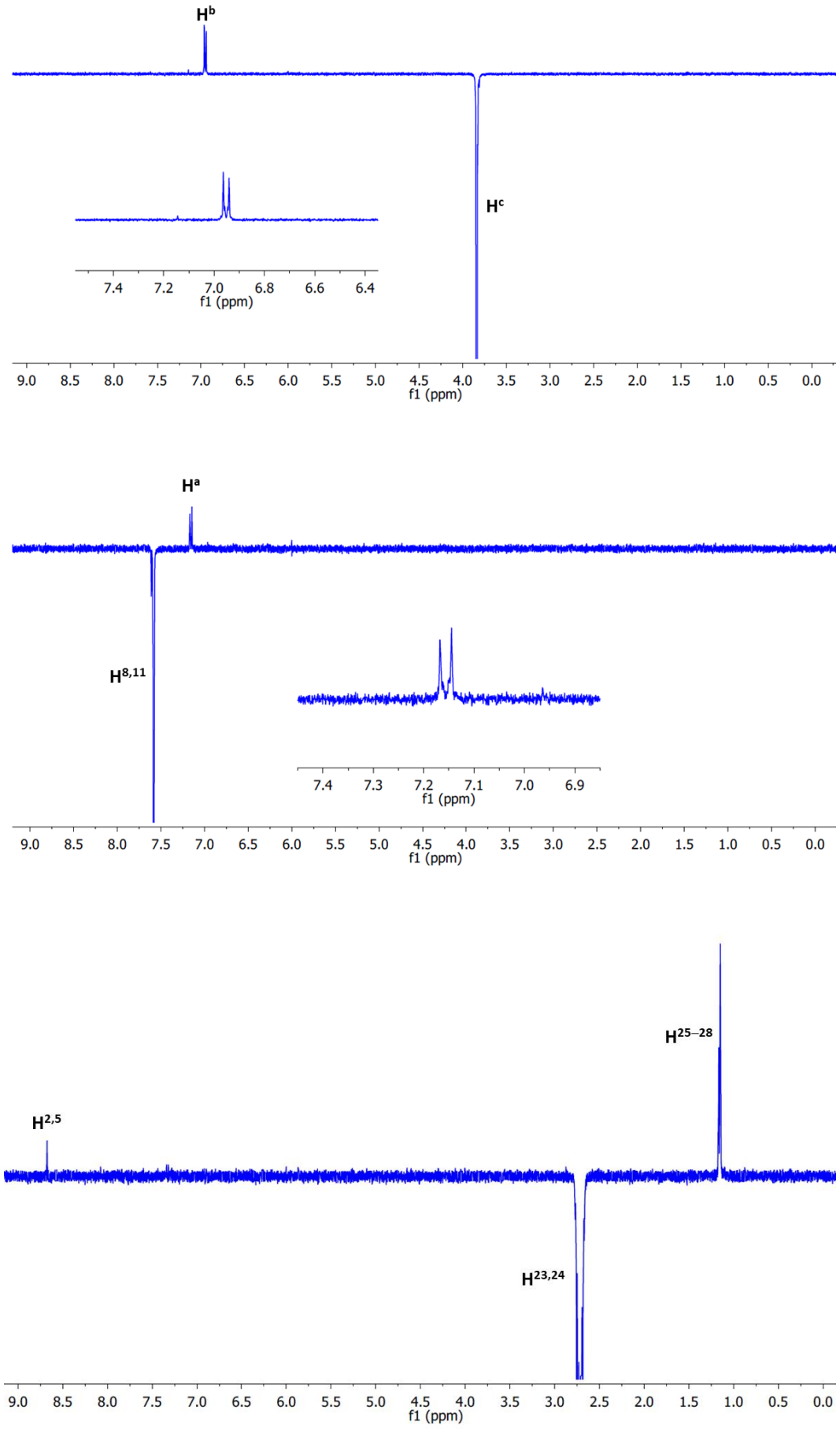


Figure S-3.4: ^{1}H–^{1}H 1D NOESY NMR spectra (CDCl3, 400 MHz) of compound **2** with the indication of through-space cross-couplings between crucial protons (H^{c}–H^{b} coupling at the top, H^{a}–$H^{8,11}$ coupling at the middle, and $H^{2,5}$–$H^{23,24}$ coupling at the bottom).

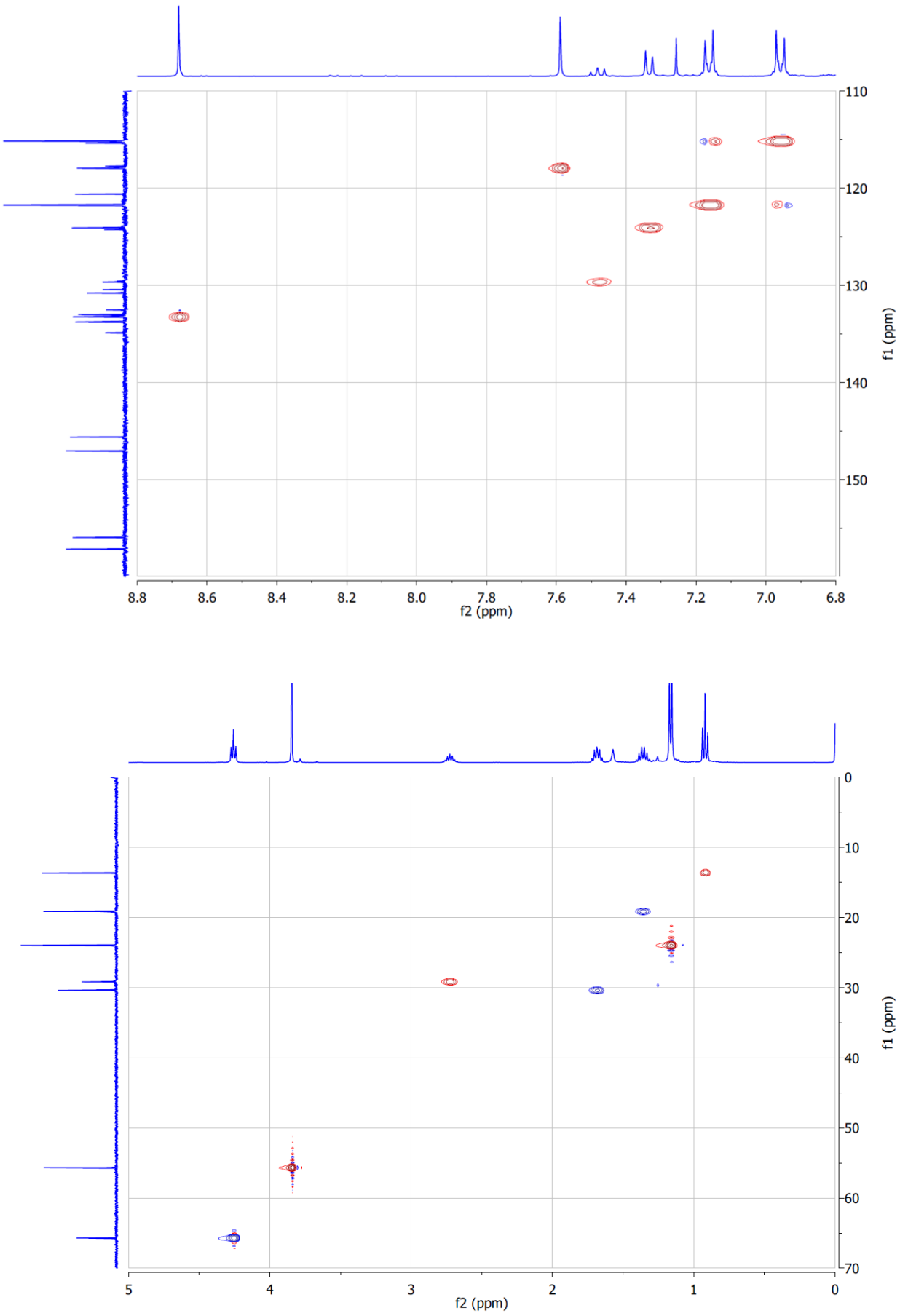
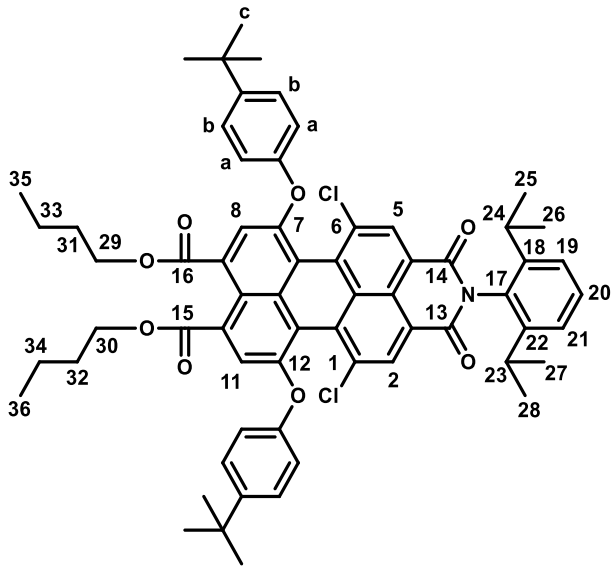


Figure S-3.5: $^{1}H–^{13}C$ gHSQC NMR spectrum (CDCl3, 400 MHz) of compound **2** (Aromatic part at the top and aliphatic part at the bottom).

3.2 Compound 3:



The structure of compound **3** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.6. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.7). The evidences of the regiospecific substitution at 7- and 12-positions were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.8), which clearly showed the cross couplings of ester carbonyl carbons (C^{15} and C^{16}) with perylene core protons (H^{8} and H^{11}) and butyl-chain protons (H^{29} and H^{30}). Furthermore, the imide carbonyl carbon atoms C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments (Figure S-3.9) in which through-space cross couplings between H^{a}–$H^{8,11}$, and $H^{2,5}$–$H^{23,24}$ were clearly observed. The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.10).

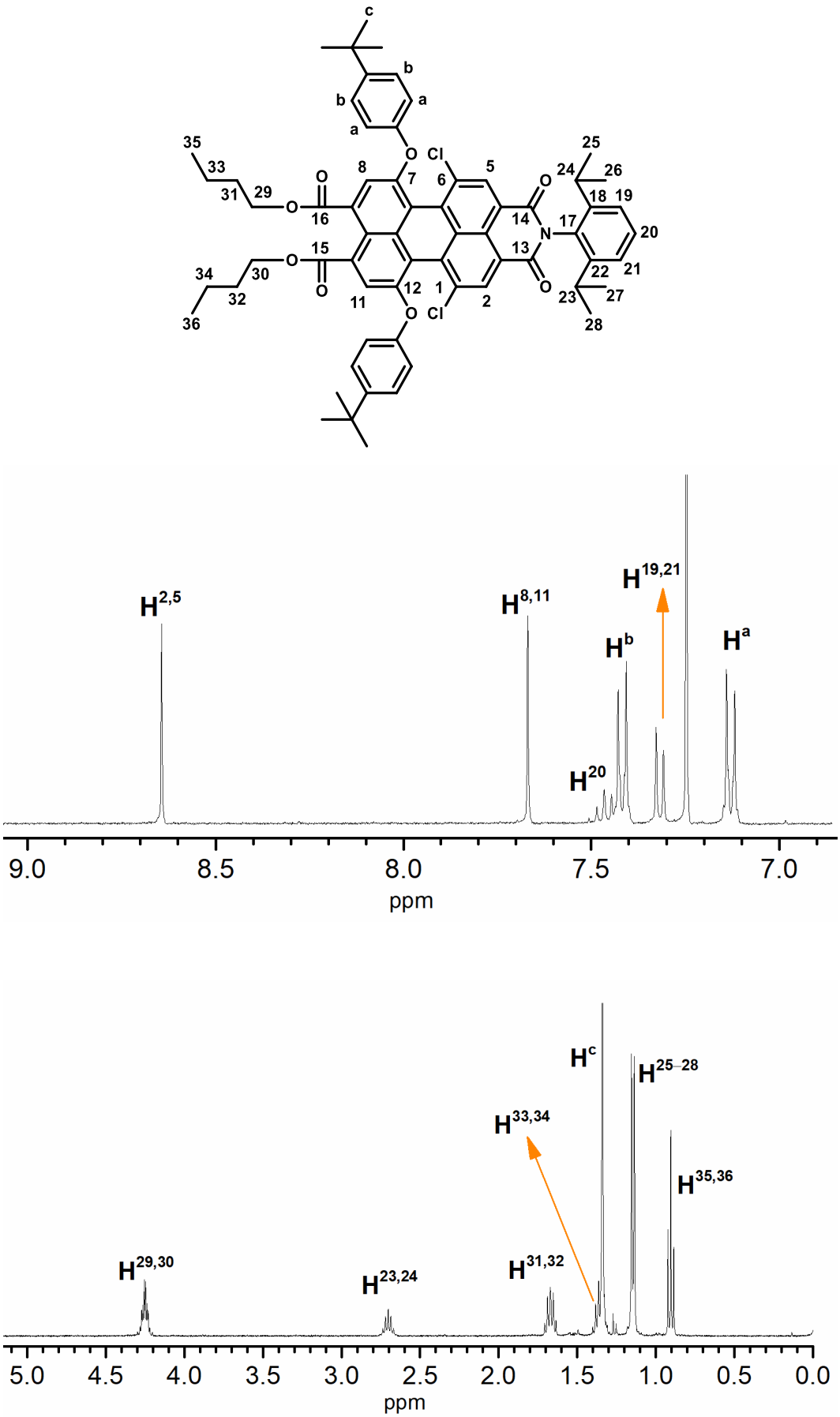


Figure S-3.6: ^{1}H NMR spectrum (CDCl3, 400 MHz) of compound **3** with complete assignments of proton signals (aromatic region at the top and aliphatic region at the bottom).

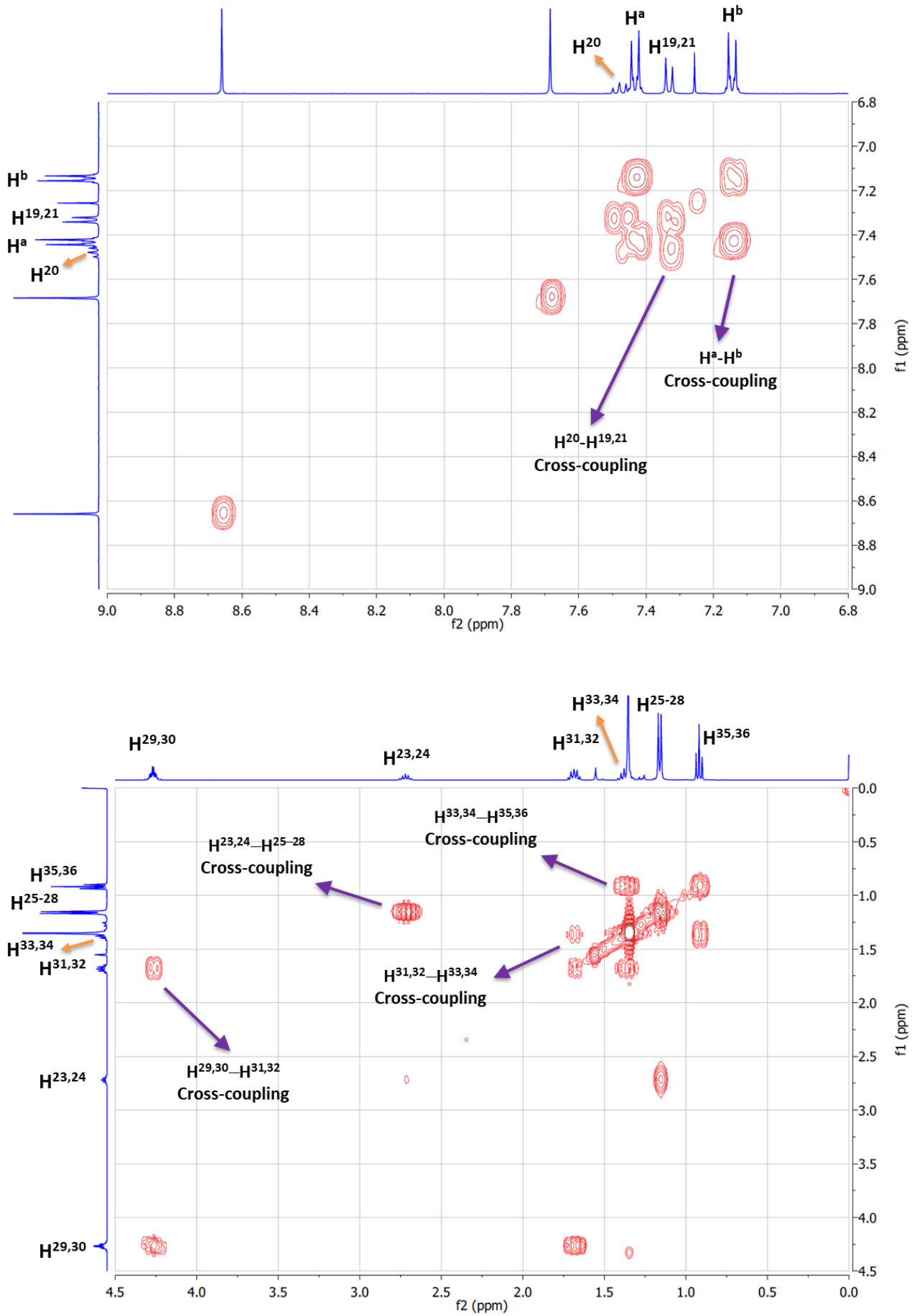


Figure S-3.7: $^{1}H–^{1}H$ gCOSY NMR spectrum (CDCl3, 400 MHz) of compound **3** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

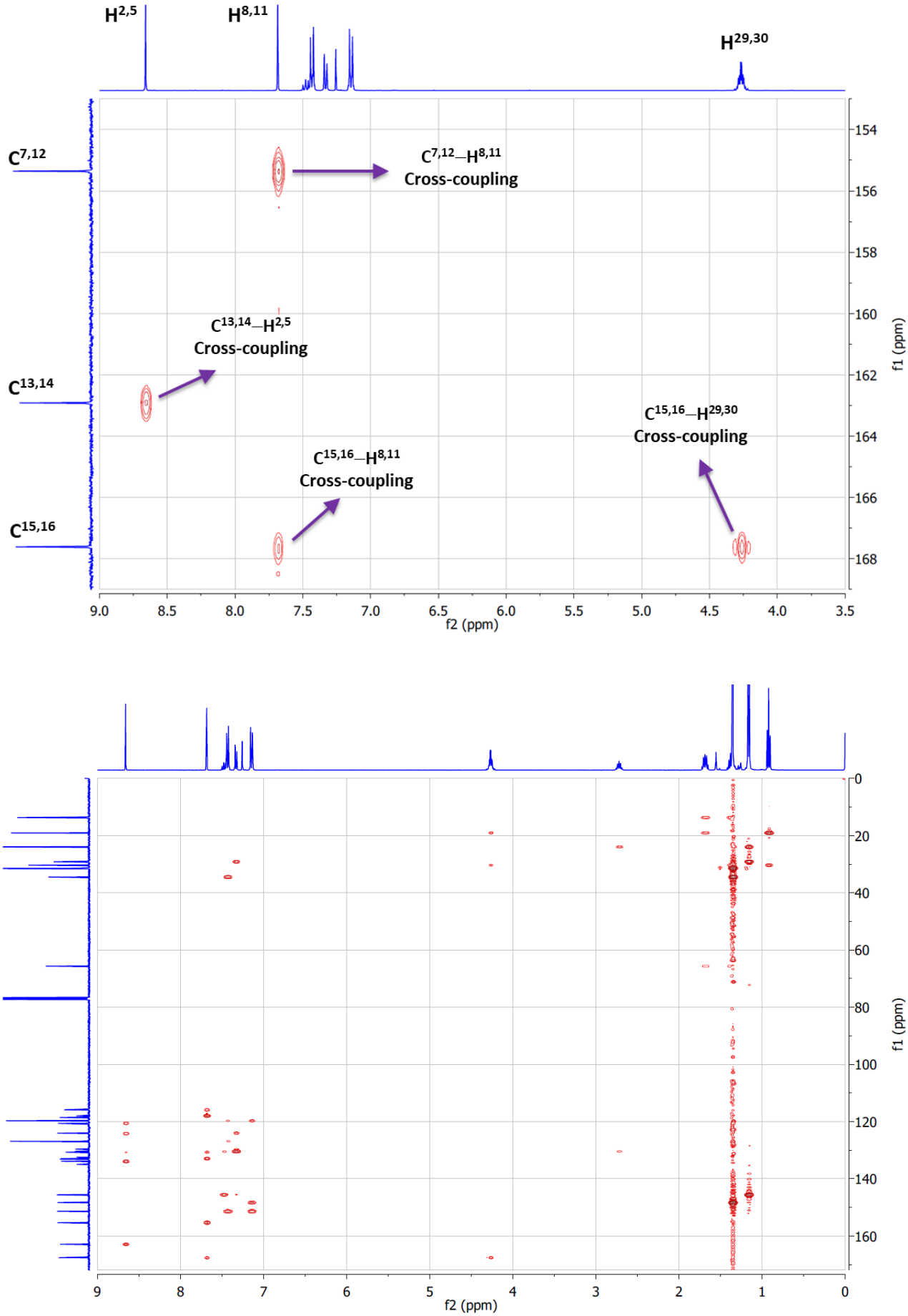


Figure S-3.8: $^{1}H–^{13}C$ gHMBC NMR spectrum (CDCl3, 400 MHz) of compound **3** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

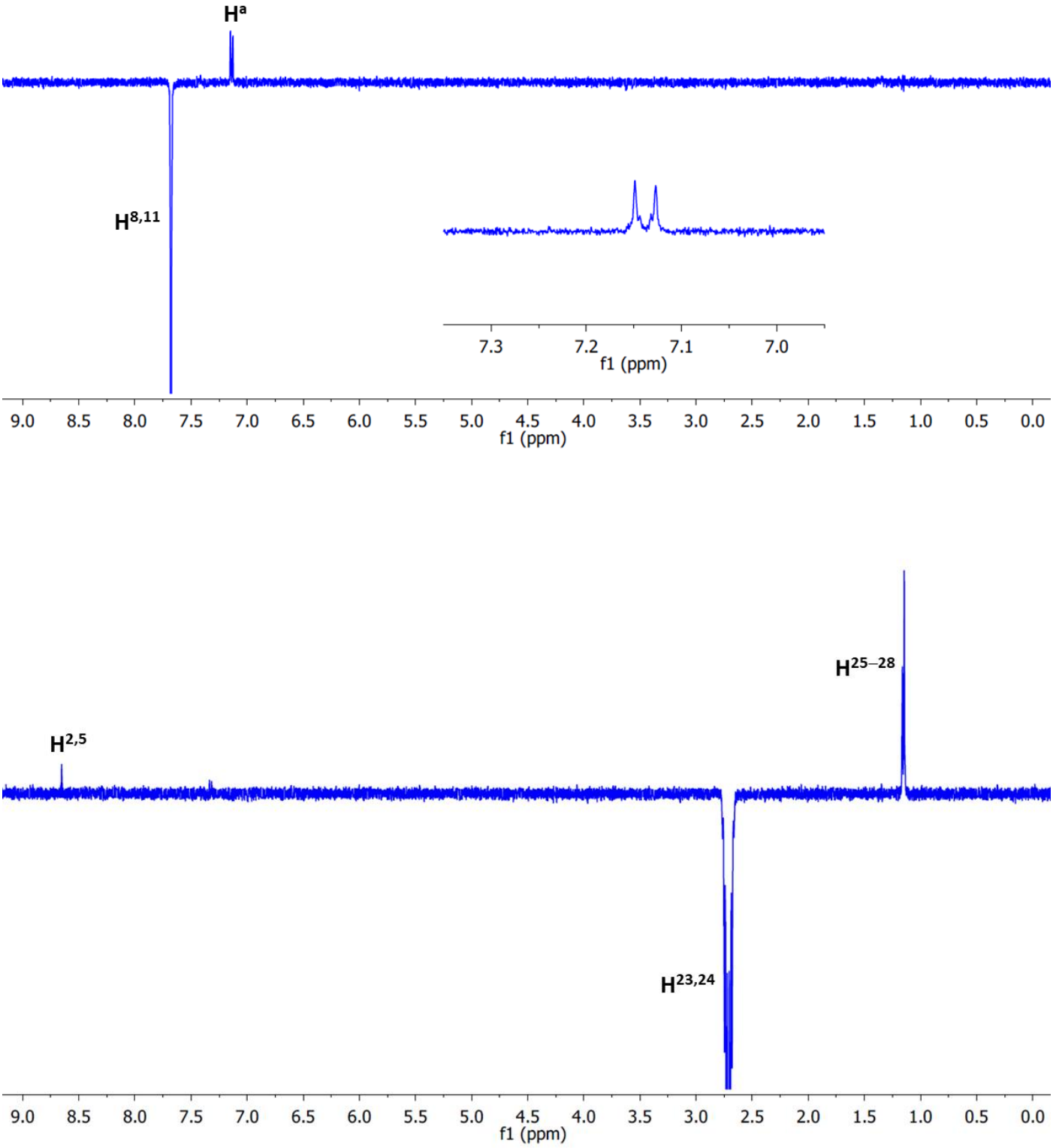


Figure S-3.9: ^{1}H–^{1}H 1D NOESY NMR spectra (CDCl3, 400 MHz) of compound **3** with the indication of through-space cross-couplings between crucial protons (H^{a}–$H^{8,11}$ coupling at the top and $H^{2,5}$–$H^{23,24}$ coupling at the bottom).

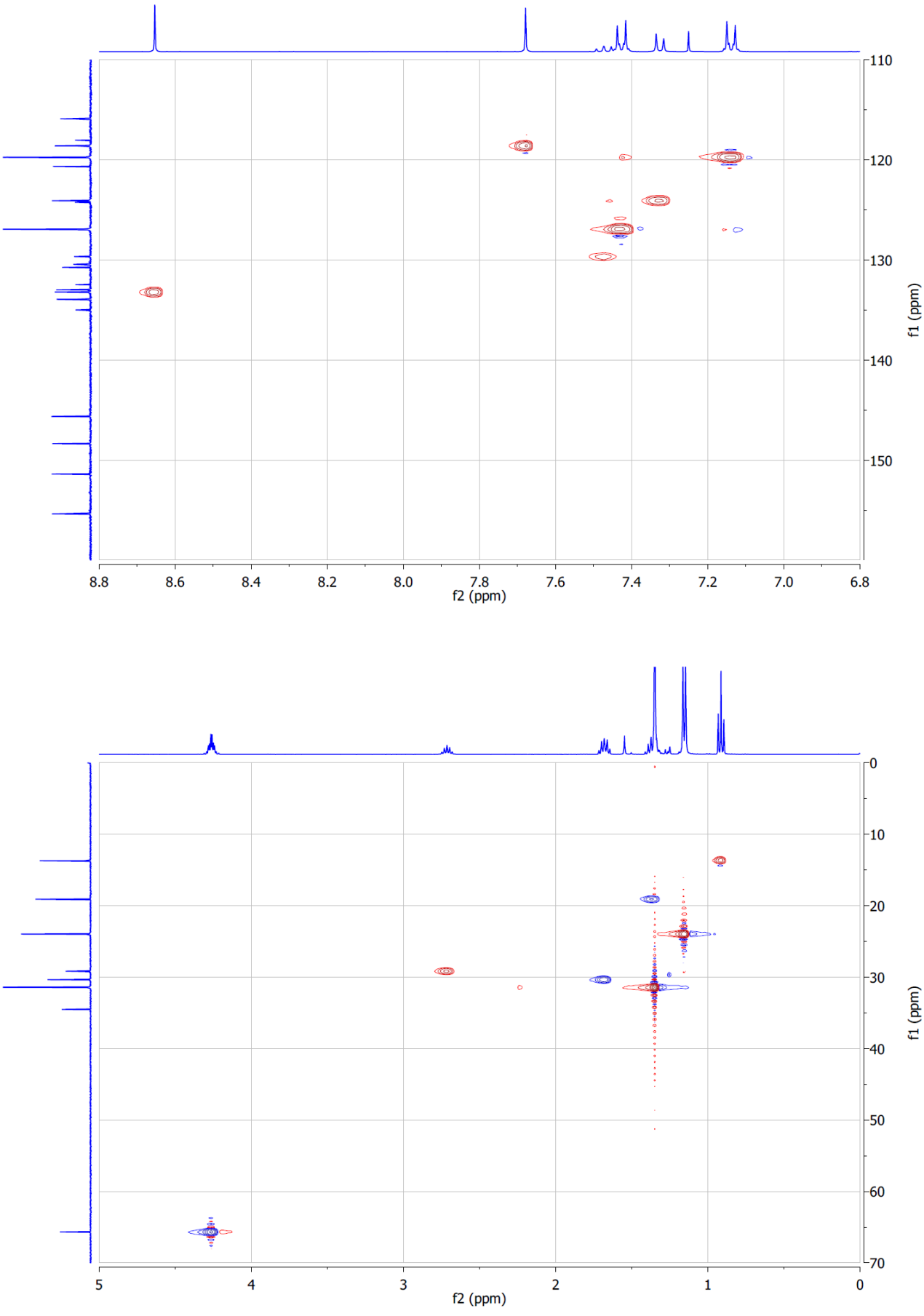
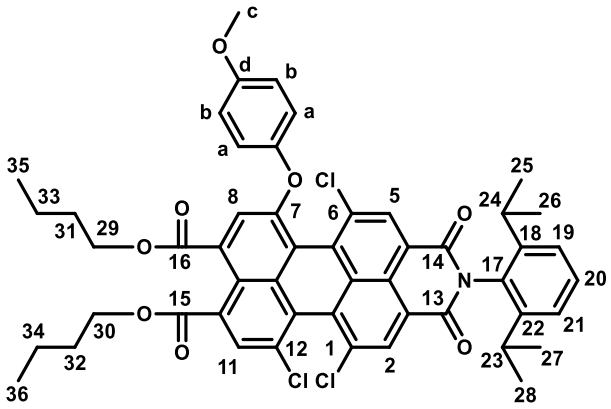


Figure S-3.10: $^{1}H–^{13}C$ gHSQC NMR spectrum (CDCl3, 400 MHz) of compound **3** (Aromatic part at the top and aliphatic part at the bottom).

3.3 Compound 4:



The structure of compound **4** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H-, ^{13}C-, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.11. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.12). The evidences of the regiospecific substitution at 7-position were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.13), which clearly showed the cross couplings of ester carbonyl carbon C^{16} with perylene core protons H^{8} and butyl chain protons H^{29}. Furthermore, the imide carbonyl carbon atoms C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments (Figure S-3.14) in which through-space cross couplings between H^{c}–H^{b} and H^{a}–H^{8} were clearly observed. The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.15).

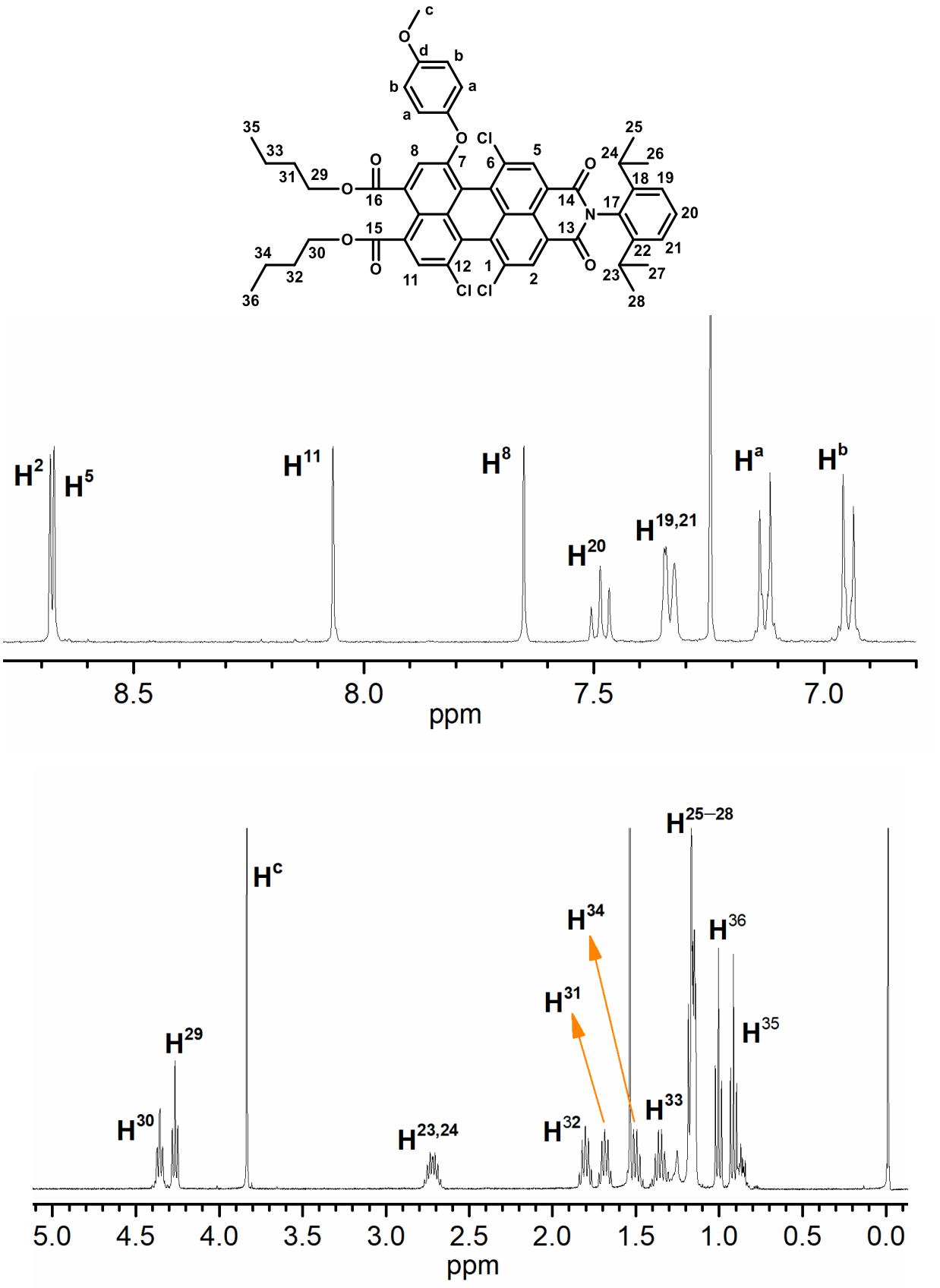


Figure S-3.11: ^{1}H NMR spectrum (CDCl3, 400 MHz) of compound **4** with complete assignments of proton signals (aromatic region at the top and aliphatic region at the bottom).

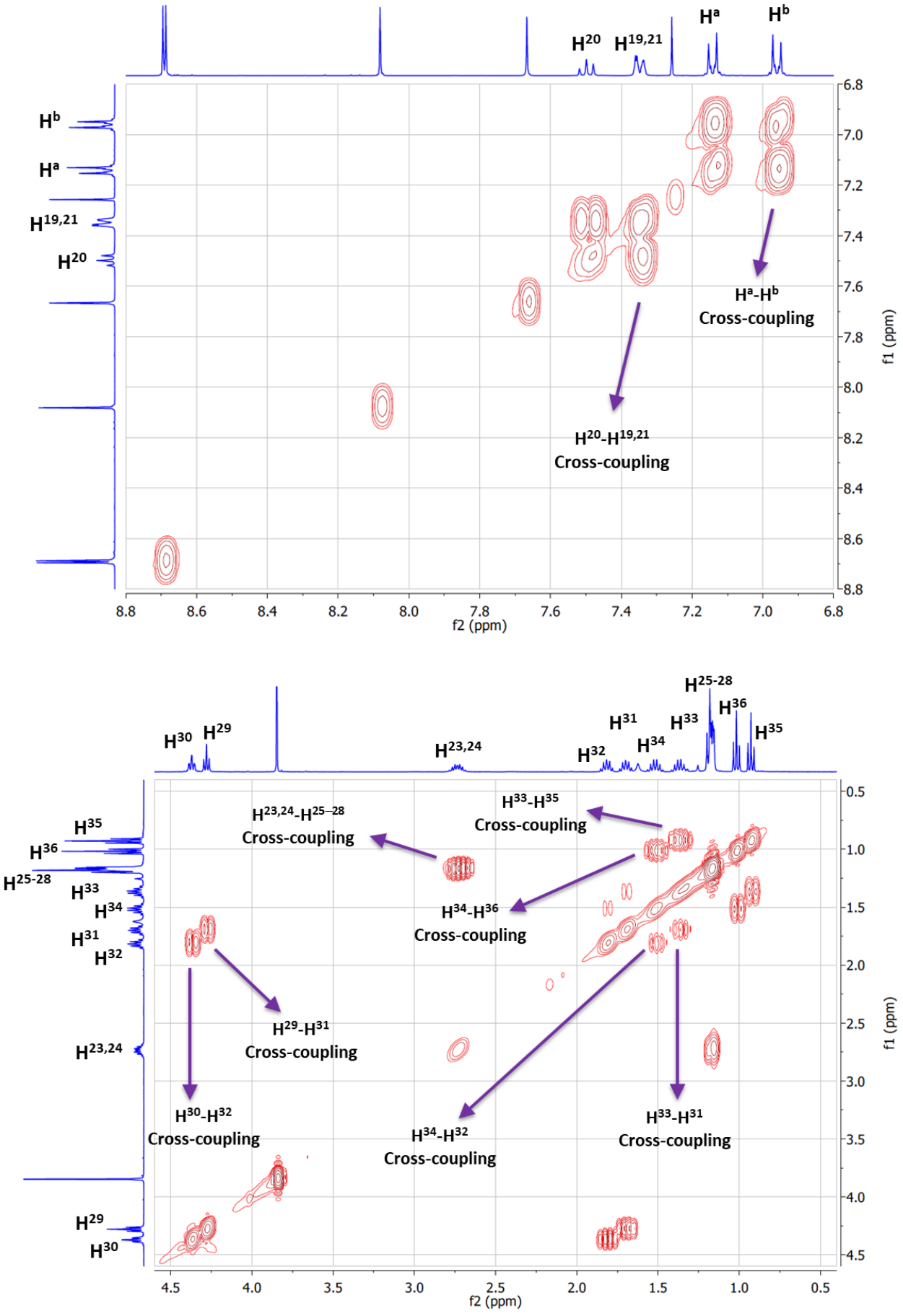


Figure S-3.12: ^{1}H–^{1}H gCOSY NMR spectrum (CDCl3, 400 MHz) of compound **4** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

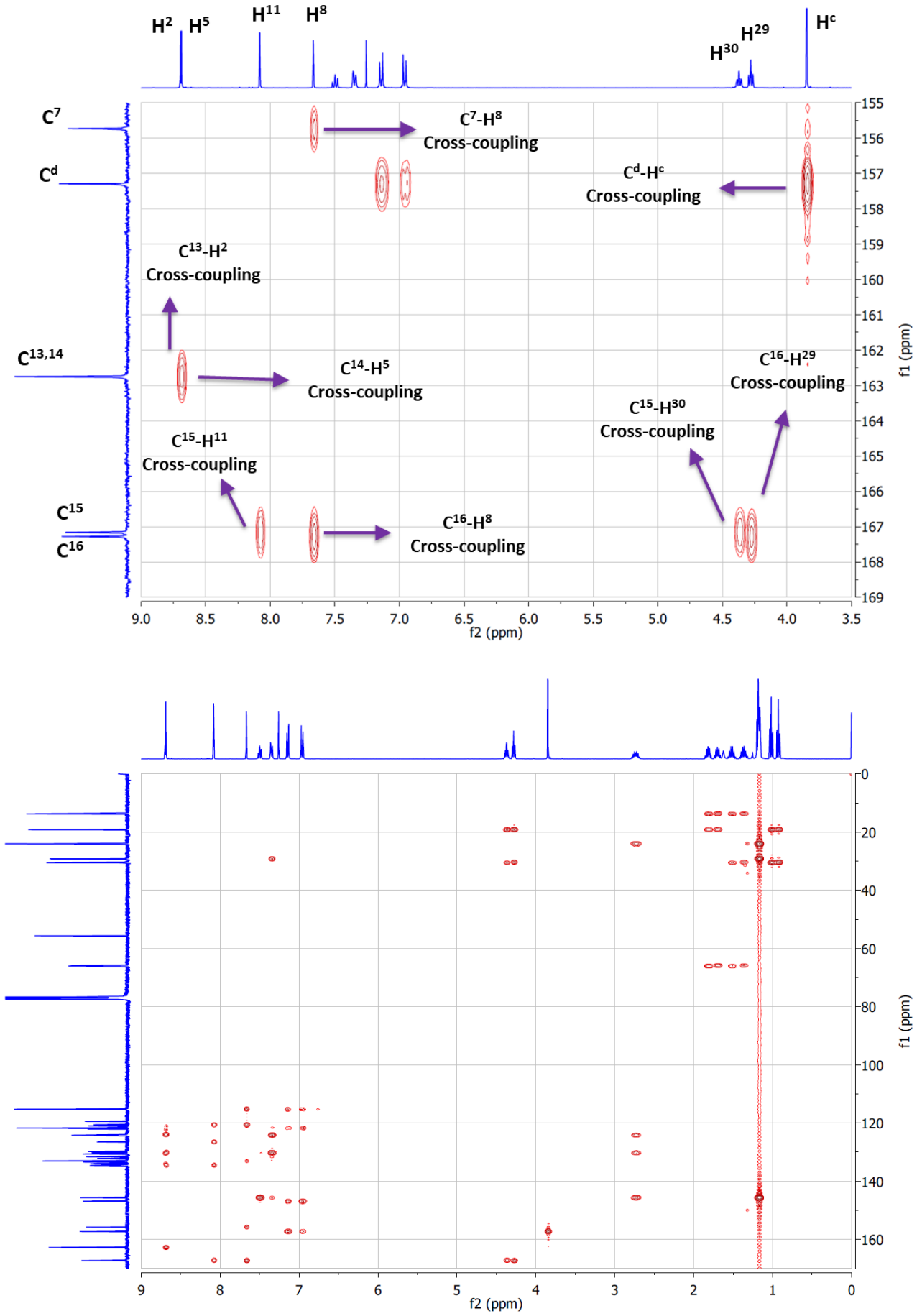


Figure S-3.13: ^{1}H–^{13}C gHMBC NMR spectrum (CDCl3, 400 MHz) of compound **4** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

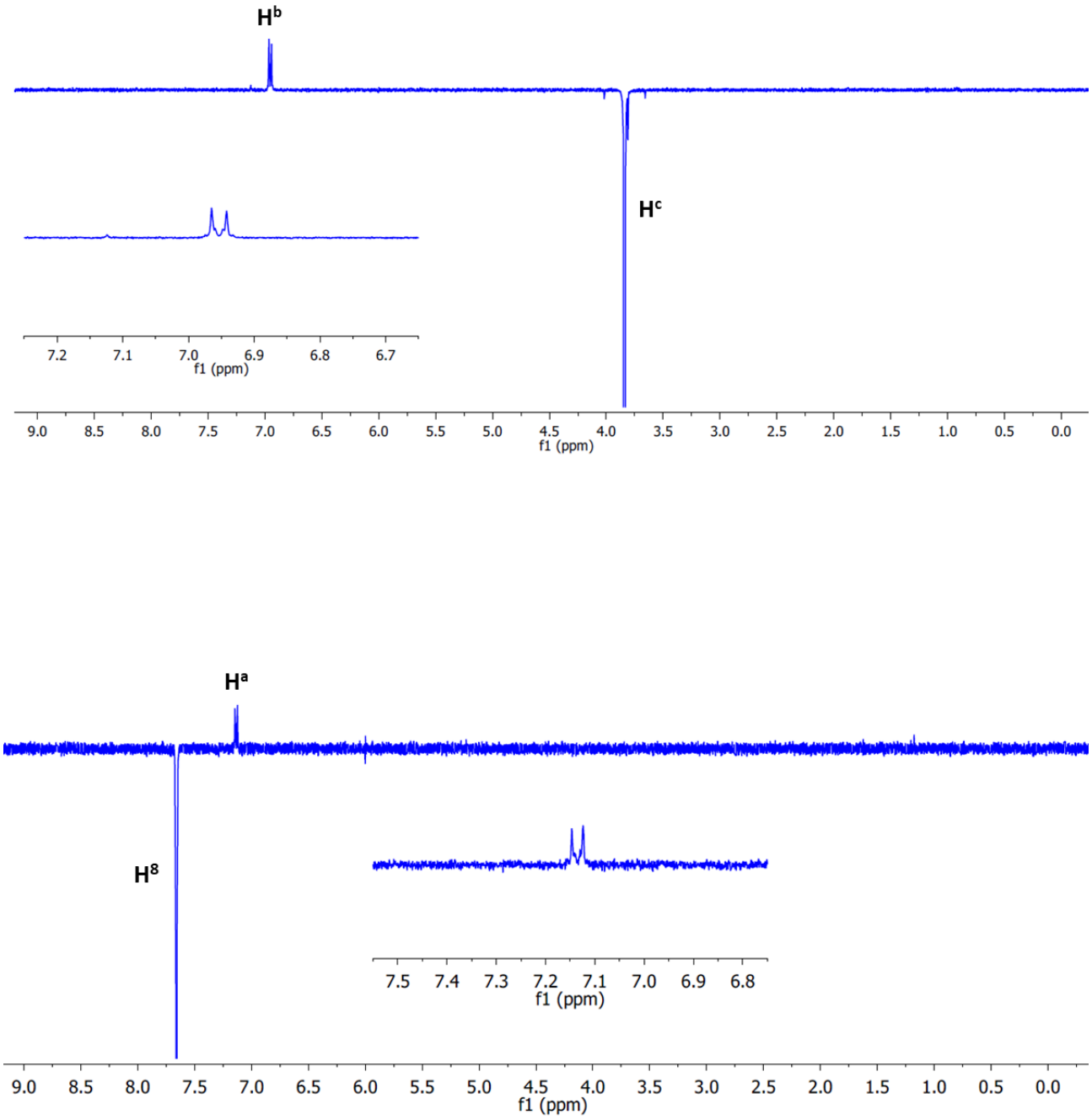


Figure S-3.14: ^{1}H–^{1}H 1D NOESY NMR spectra (CDCl3, 400 MHz) of compound **4** with the indication of through-space cross-couplings between crucial protons (H^{c}–H^{b} coupling at the top and H^{a}–H^{8} coupling at the bottom).

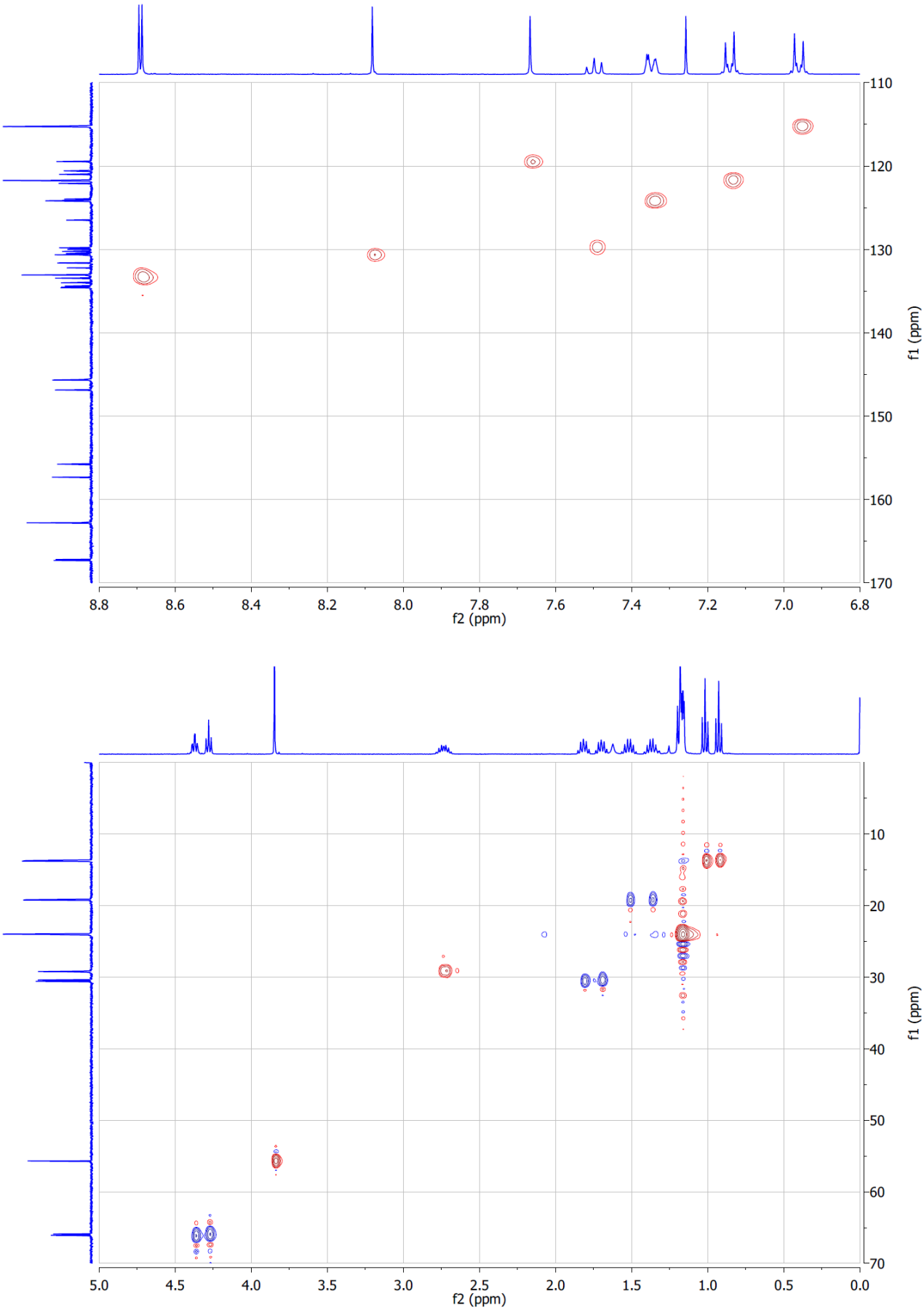
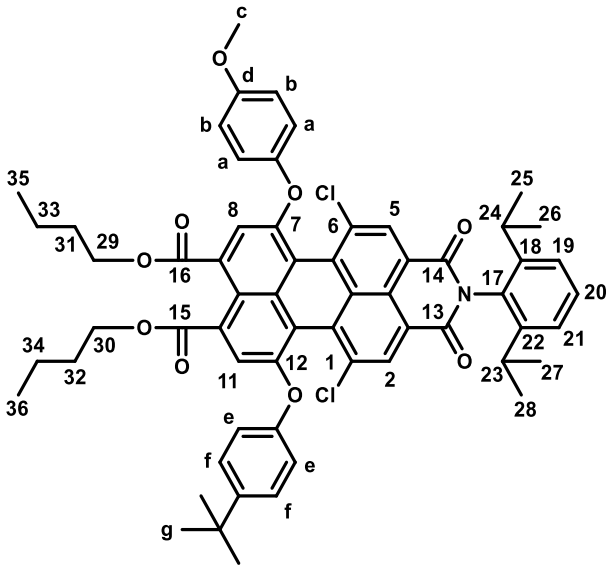


Figure S-3.15: $^{1}H–^{13}C$ HSQC NMR spectrum (CDCl3, 400 MHz) of compound **4** (Aromatic part at the top and aliphatic part at the bottom).

3.4 Compound 6:



The structure of compound **6** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, HOMO 2DJ, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.16. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.17). The first evidences of regiospecific substitution of 4-methoxyphenoxy- and 4-*tert*-butylphenoxy at 7- and 12-positions, respectively, were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.18). This clearly showed the cross couplings of ester carbonyl carbons (C^{15} and C^{16}) with perylene core protons (H^{11} and H^{8}) and butyl-chain protons (H^{29} and H^{30}). Furthermore, the imide carbonyl carbon atoms C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments (Figure S-3.19) in which through-space cross couplings between H^{c}–H^{b}, H^{a}–H^{8}, and H^{e}–H^{11} were clearly observed. The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.20).

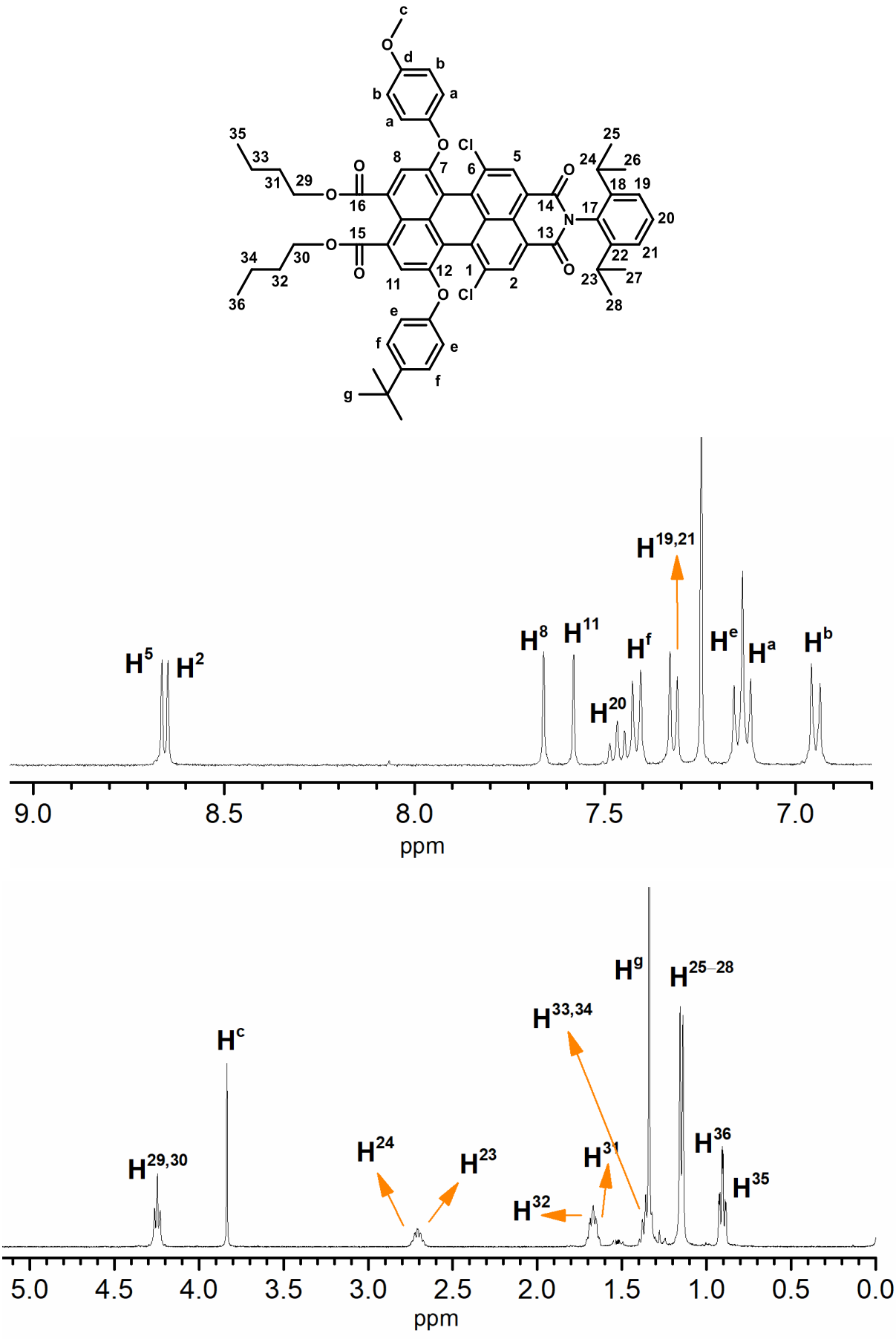


Figure S-3.16: ^{1}H NMR spectrum (CDCl3, 400 MHz) of compound **6** with complete assignments of proton signals (aromatic region at the top and aliphatic region at the bottom). *Note: The signals of following protons are overlapping, but resolved in Homonuclear J-resolved (HOMO 2DJ) spectrum: H23 & H24; H31 & H32; H35 & H36.*

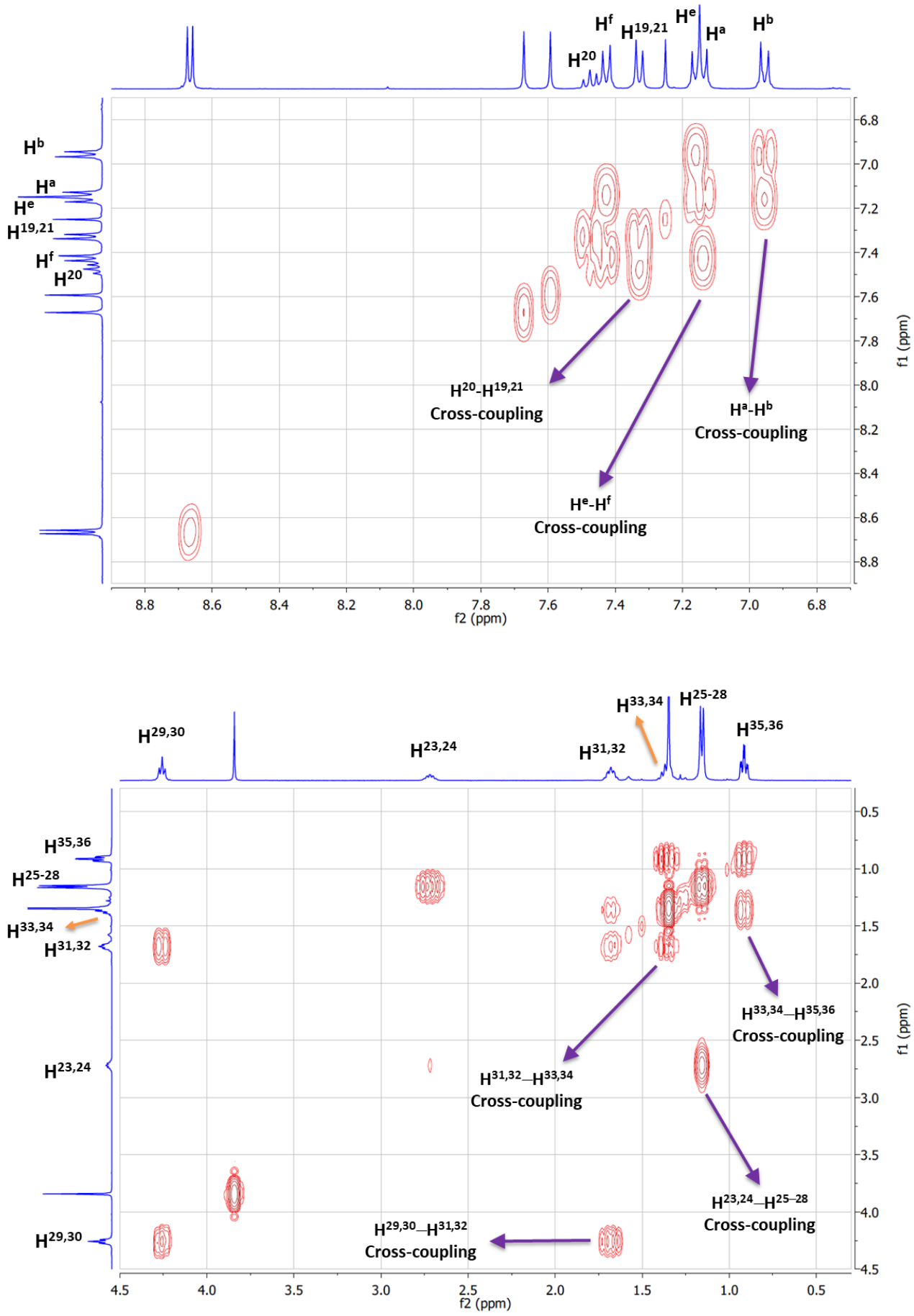


Figure S-3.17: ^{1}H–^{1}H gCOSY NMR spectrum (CDCl3, 400 MHz) of compound **6** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

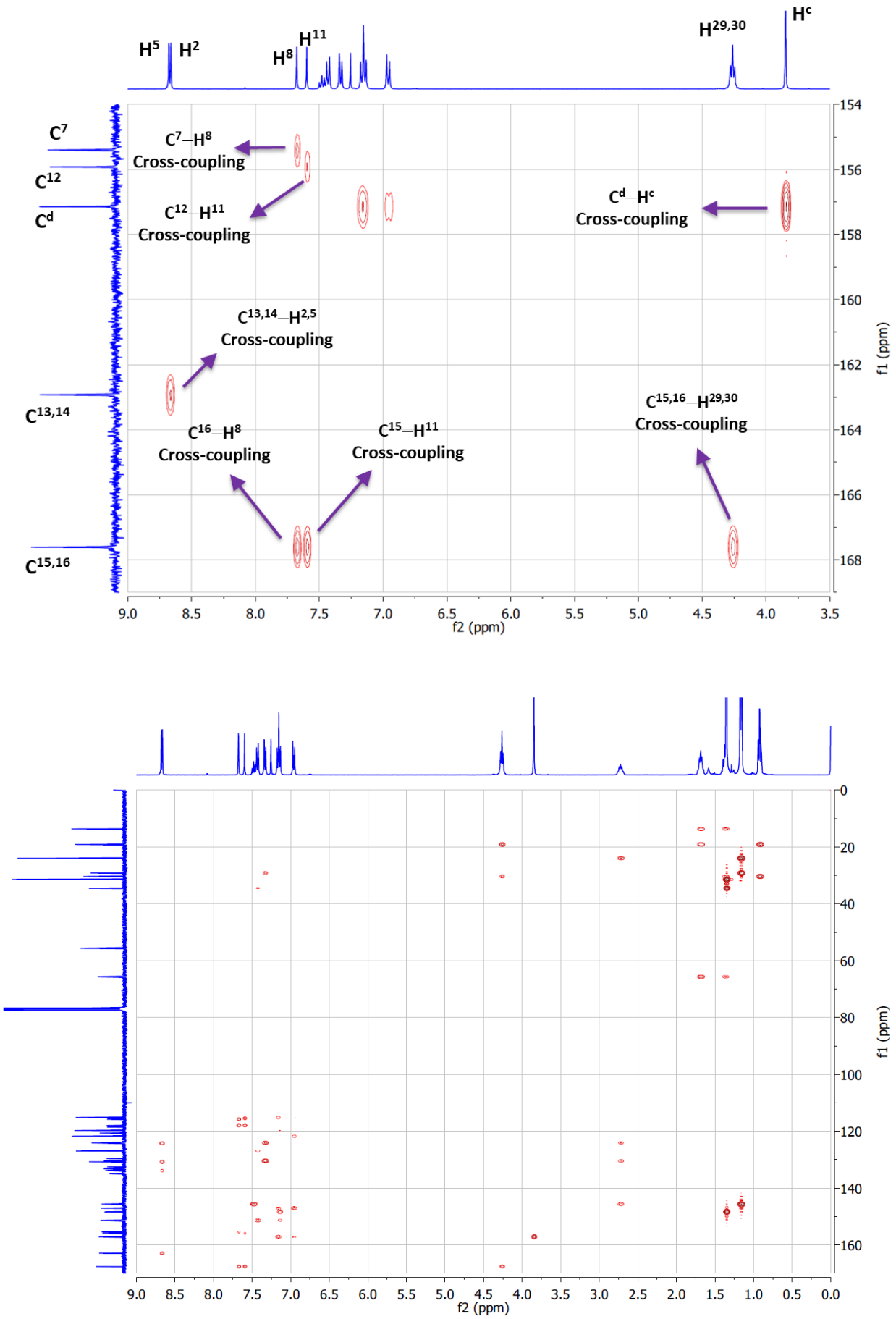


Figure S-3.18: $^{1}H–^{13}C$ gHMBC NMR spectrum (CDCl3, 400 MHz) of compound **6** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

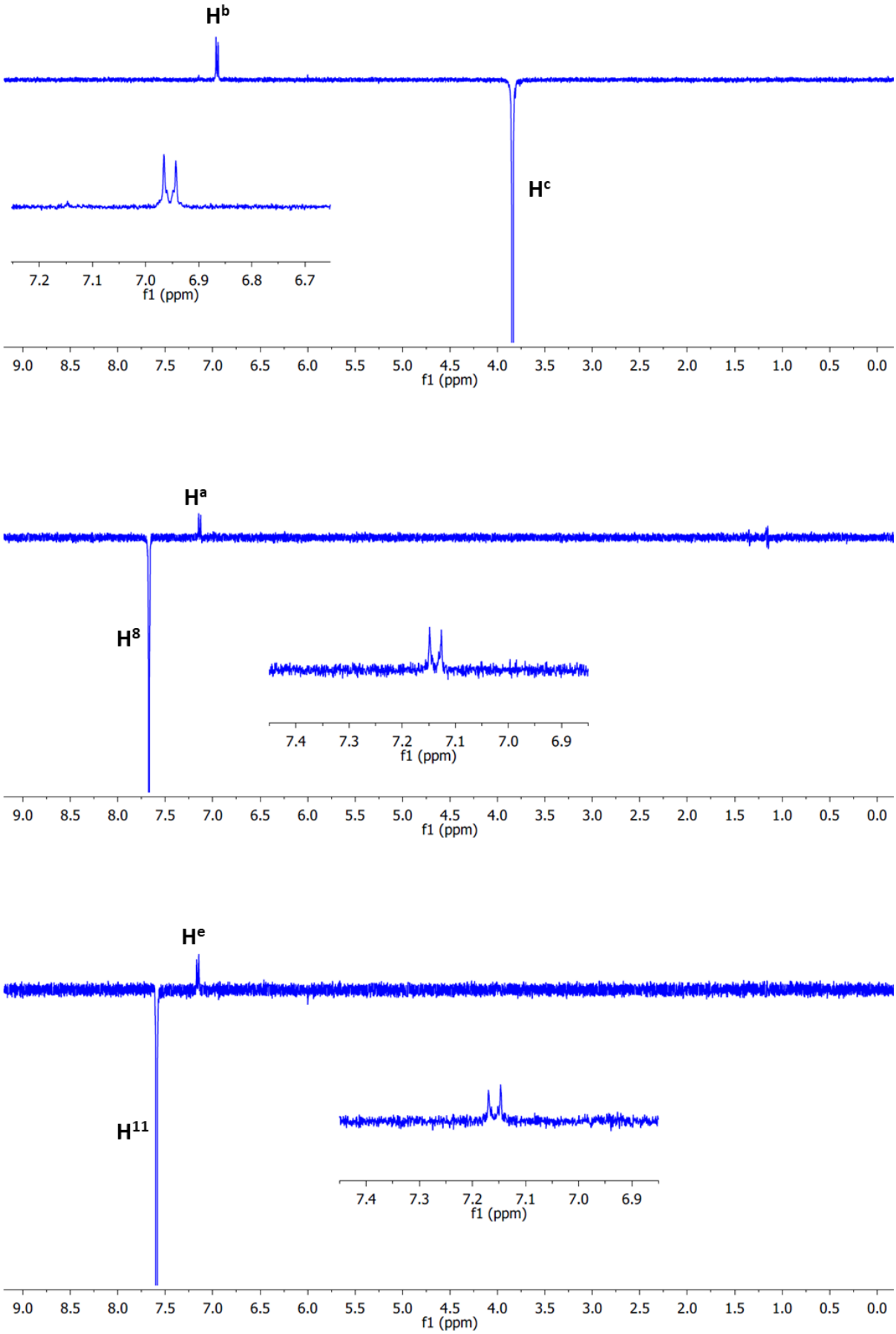


Figure S-3.19: ^{1}H–^{1}H 1D NOESY NMR spectra (CDCl3, 400 MHz) of compound **6** with the indication of through-space cross-couplings between crucial protons (H^{c}–H^{b} coupling at the top, H^{a}–H^{8} coupling at the middle, and H^{e}–H^{11} coupling at the bottom).

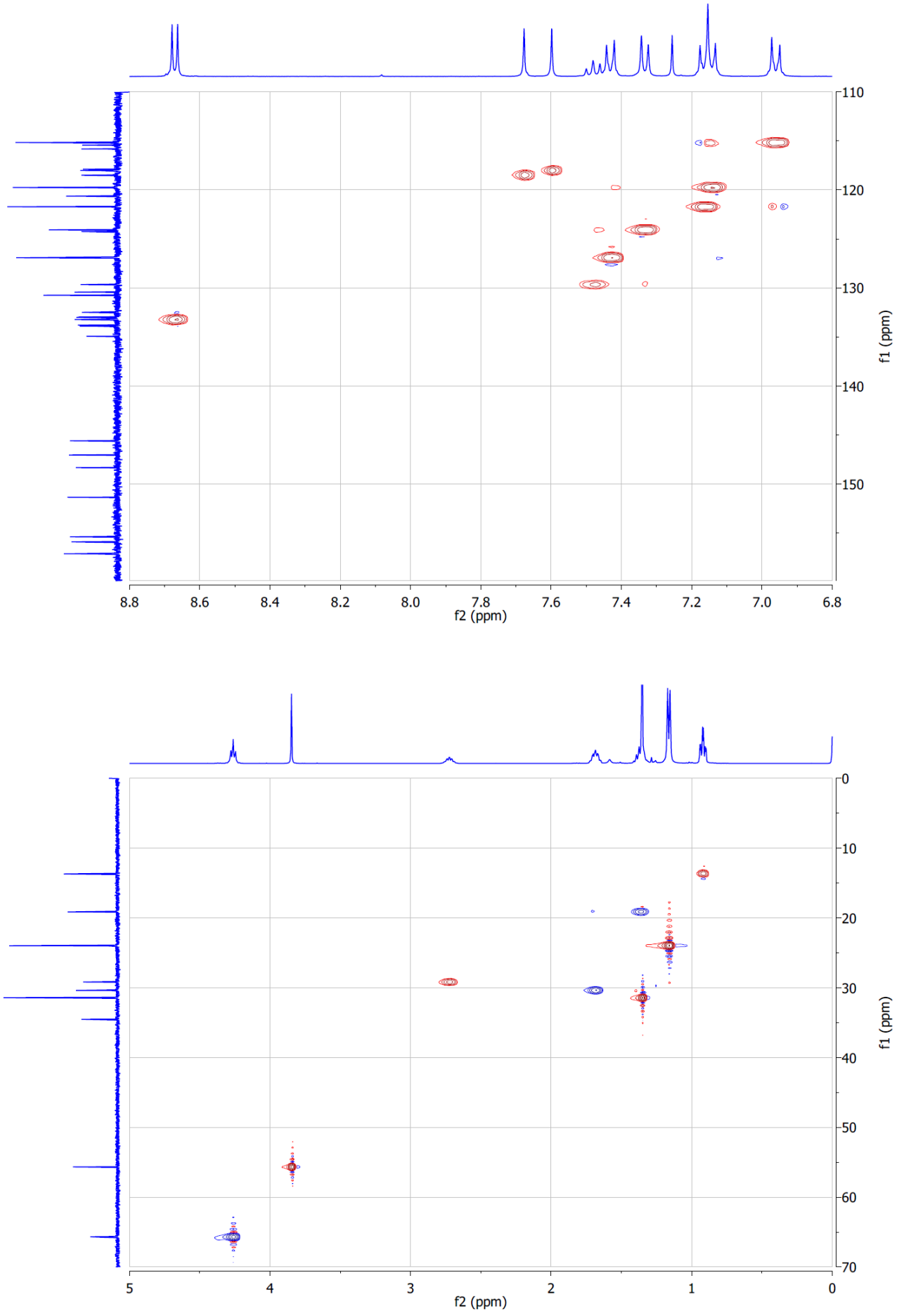
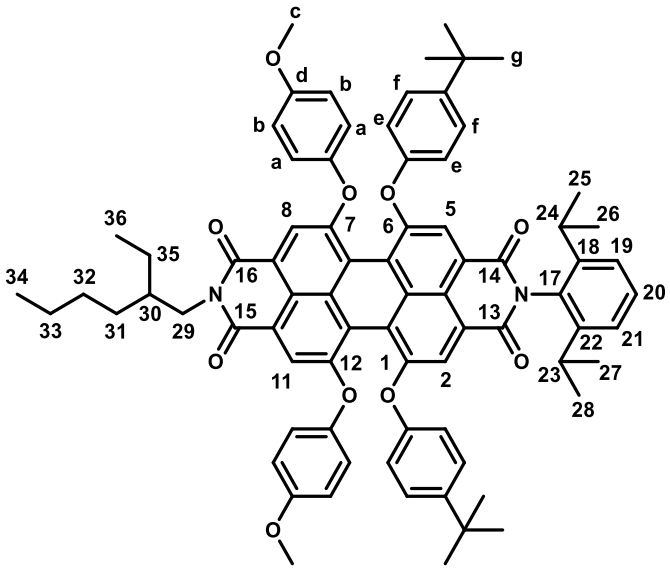


Figure S-3.20: $^{1}H–^{13}C$ HSQC NMR spectrum (CDCl3, 400 MHz) of compound **6** (Aromatic part at the top and aliphatic part at the bottom).

3.5 Compound 9:



The structure of compound **9** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.21. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.22). The first evidences of presence of 4-methoxyphenoxy-groups at 7, 12-positions and 4-*tert*-butylphenoxy-groups at 1, 6-positions were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.23). This clearly showed the cross couplings of carbonyl carbons (C^{15} and C^{16}) with perylene core protons (H^{8} and H^{11}) and 2-ethylhexyl-chain protons H^{29}. Furthermore, the other set of carbonyl carbons C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments in which through-space cross couplings between important protons were investigated. These experiments further confirmed the presence of 4-*tert*-butylphenoxy-gropus at 1, 6-positions by clearly showing through-space cross couplings between H^{g}–H^{f}, H^{e}–$H^{2,5}$, and $H^{23,24}$–$H^{2,5}$ protons (Figure S-3.24). Similarly, the presence of 4-methoxyphenoxy-gropus at 7, 12-positions was proved by through-space cross couplings between H^{c}–H^{b} and H^{a}–$H^{8,11}$ protons (Figure S-3.25). The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.26).

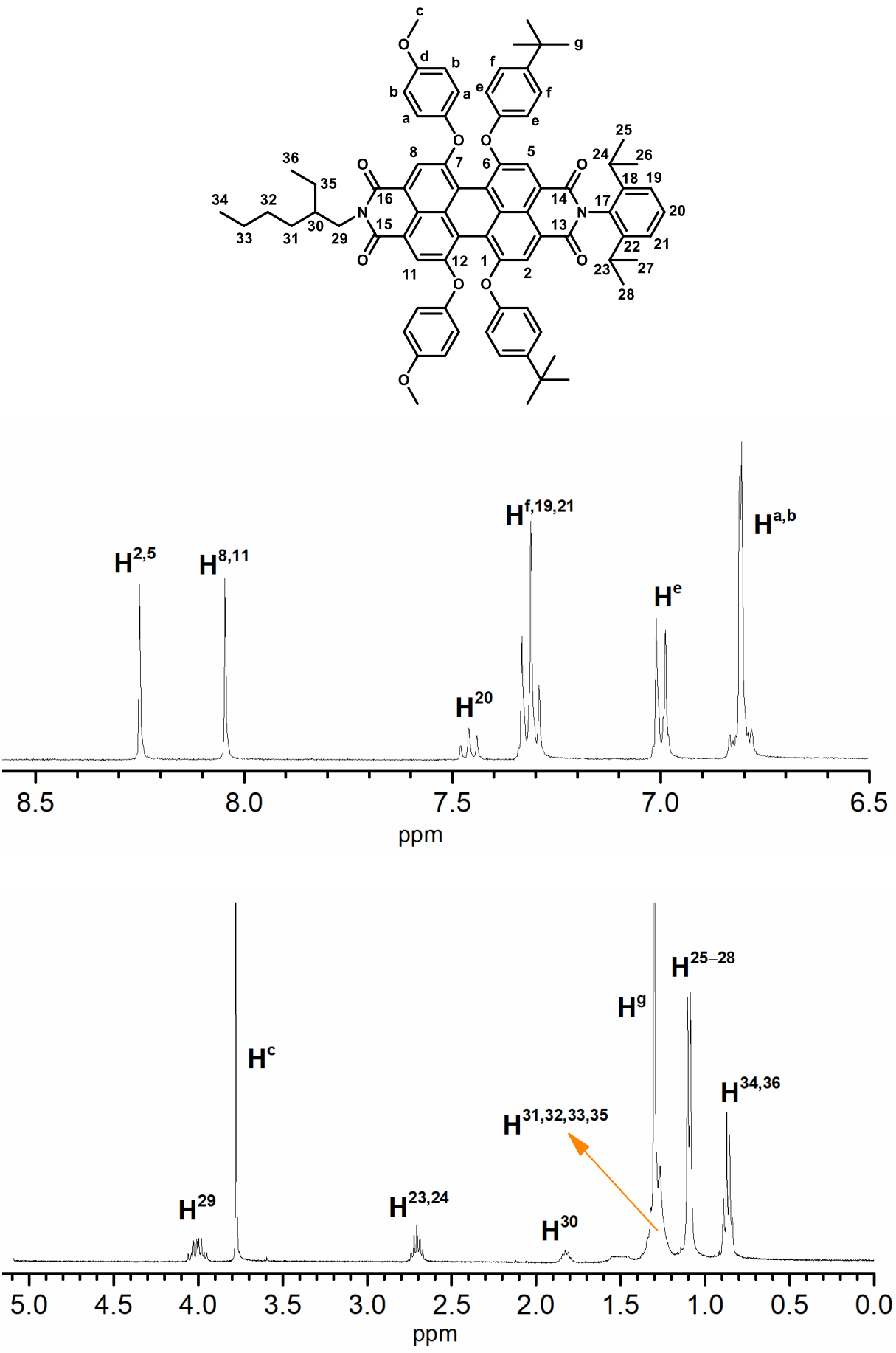


Figure S-3.21: ^{1}H NMR spectrum (CD_2Cl_2, 400 MHz) of compound **9** with complete assignments of proton signals.

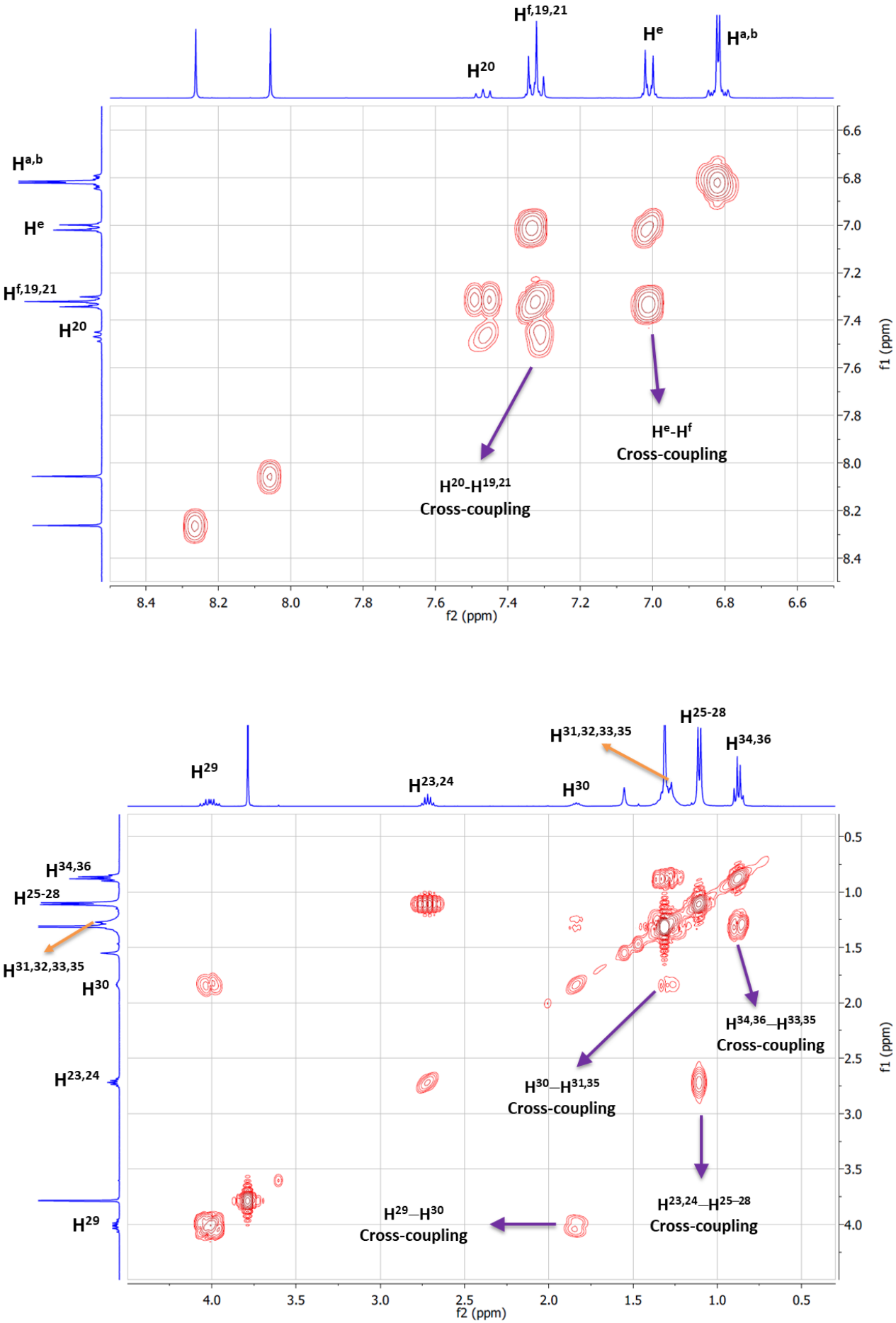


Figure S-3.22: ^{1}H–^{1}H gCOSY NMR spectrum (CD_2Cl_2, 400 MHz) of compound **9** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

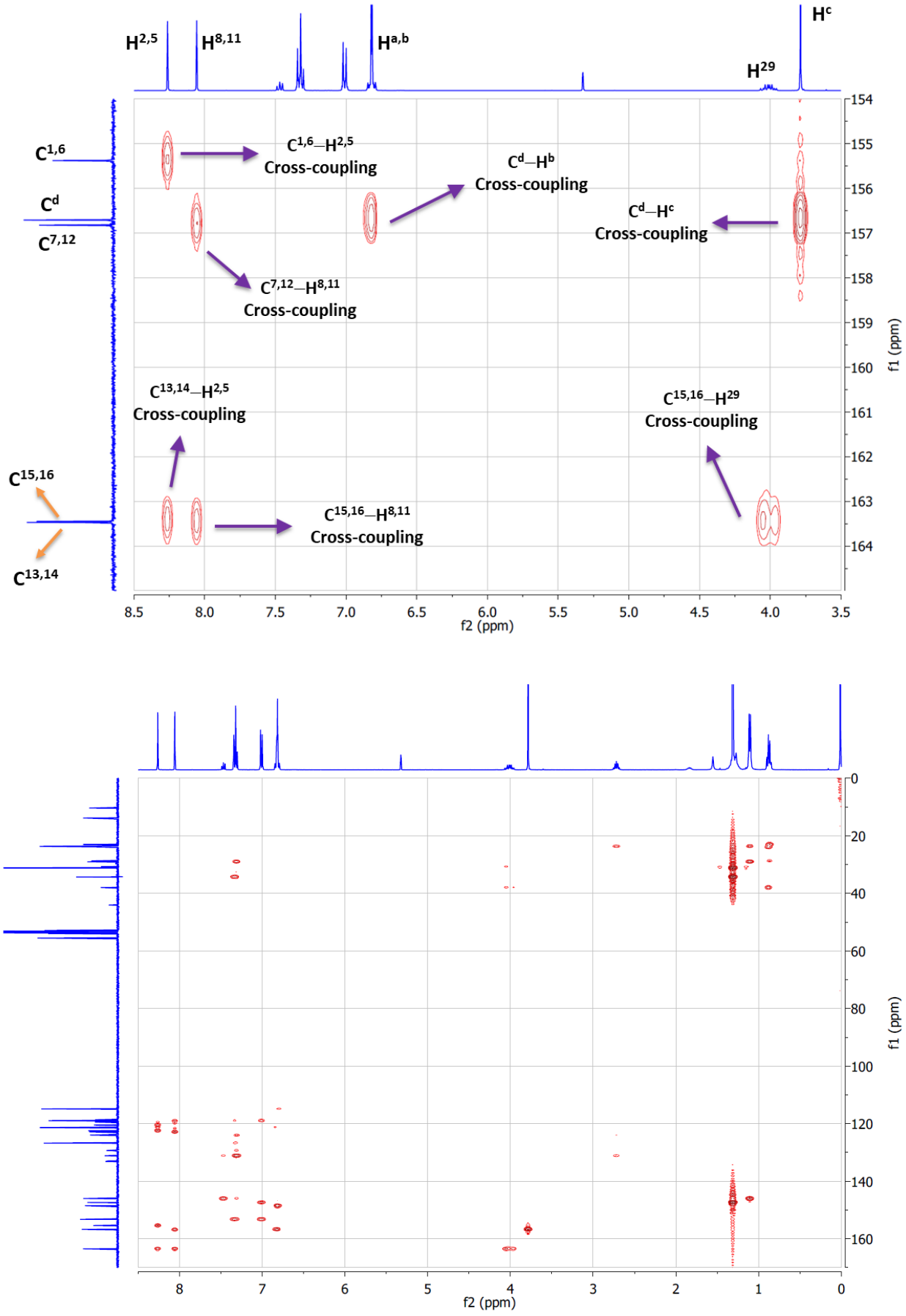


Figure S-3.23: $^{1}H–^{13}C$ gHMBC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **9** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

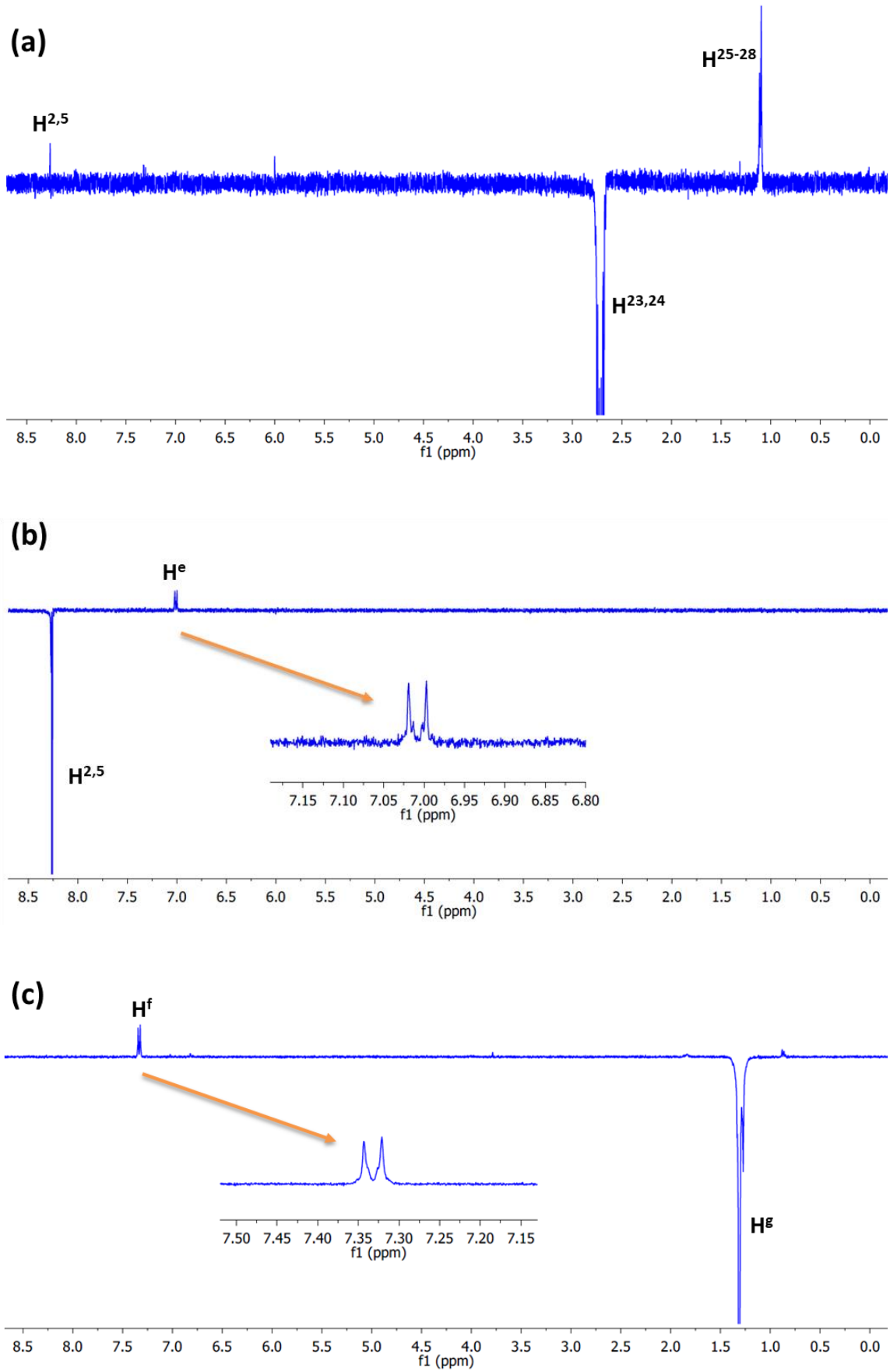


Figure S-3.24: ^{1}H–^{1}H 1D NOESY NMR spectra (CD_2Cl_2, 400 MHz) of compound **9** with the indication of through-space cross-couplings between crucial protons: (a) $H^{23,24}$–$H^{2,5}$ coupling; (b) $H^{2,5}$–H^{e} coupling; (c) H^{g}–H^{f} coupling.

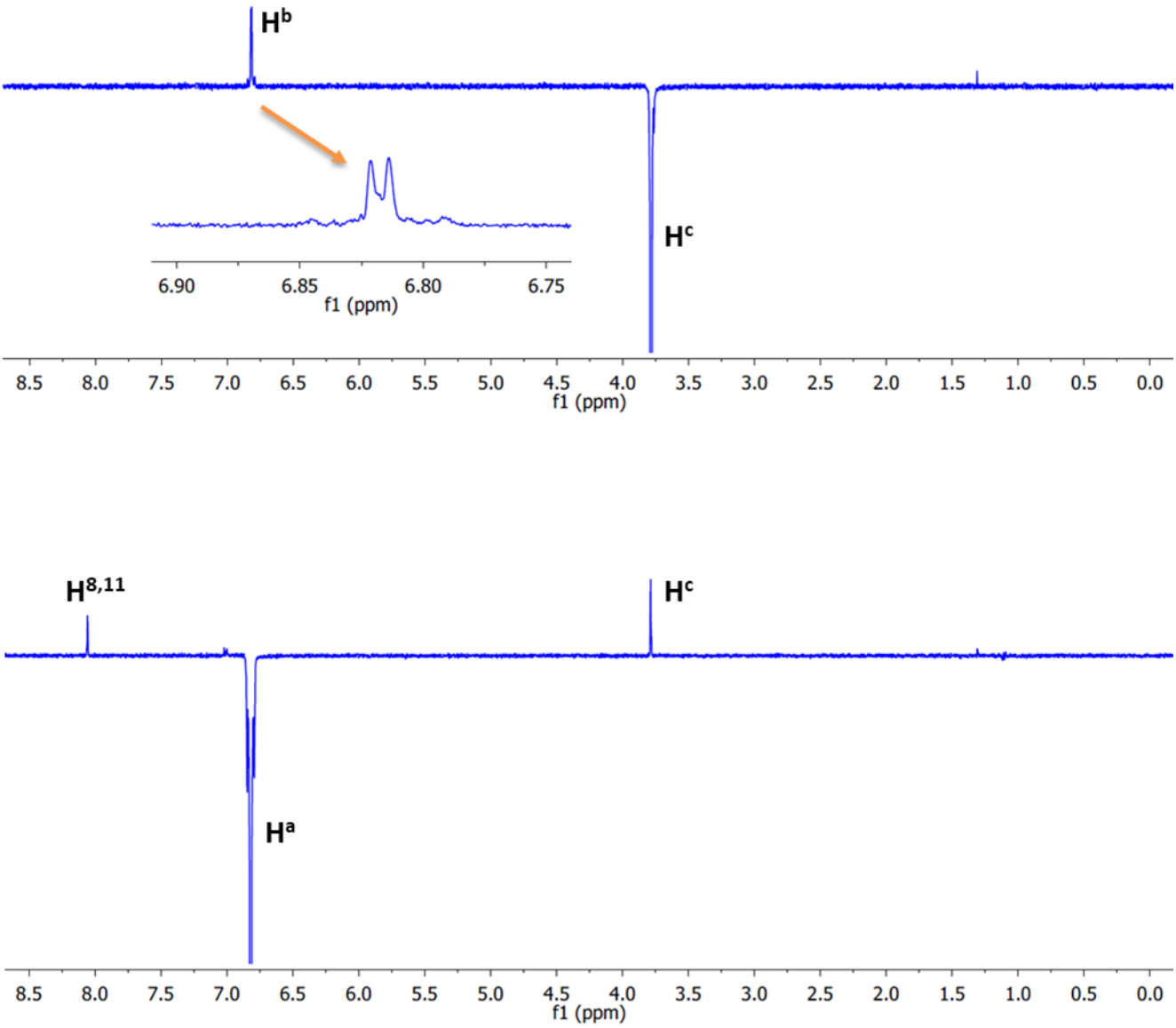


Figure S-3.25: $^{1}H–^{1}H$ 1D NOESY NMR spectra (CD_2Cl_2, 400 MHz) of compound **9** with the indication of through-space cross-couplings between crucial protons ($H^{c}–H^{b}$ coupling at the top and $H^{a}–H^{8,11}$ coupling at the bottom).

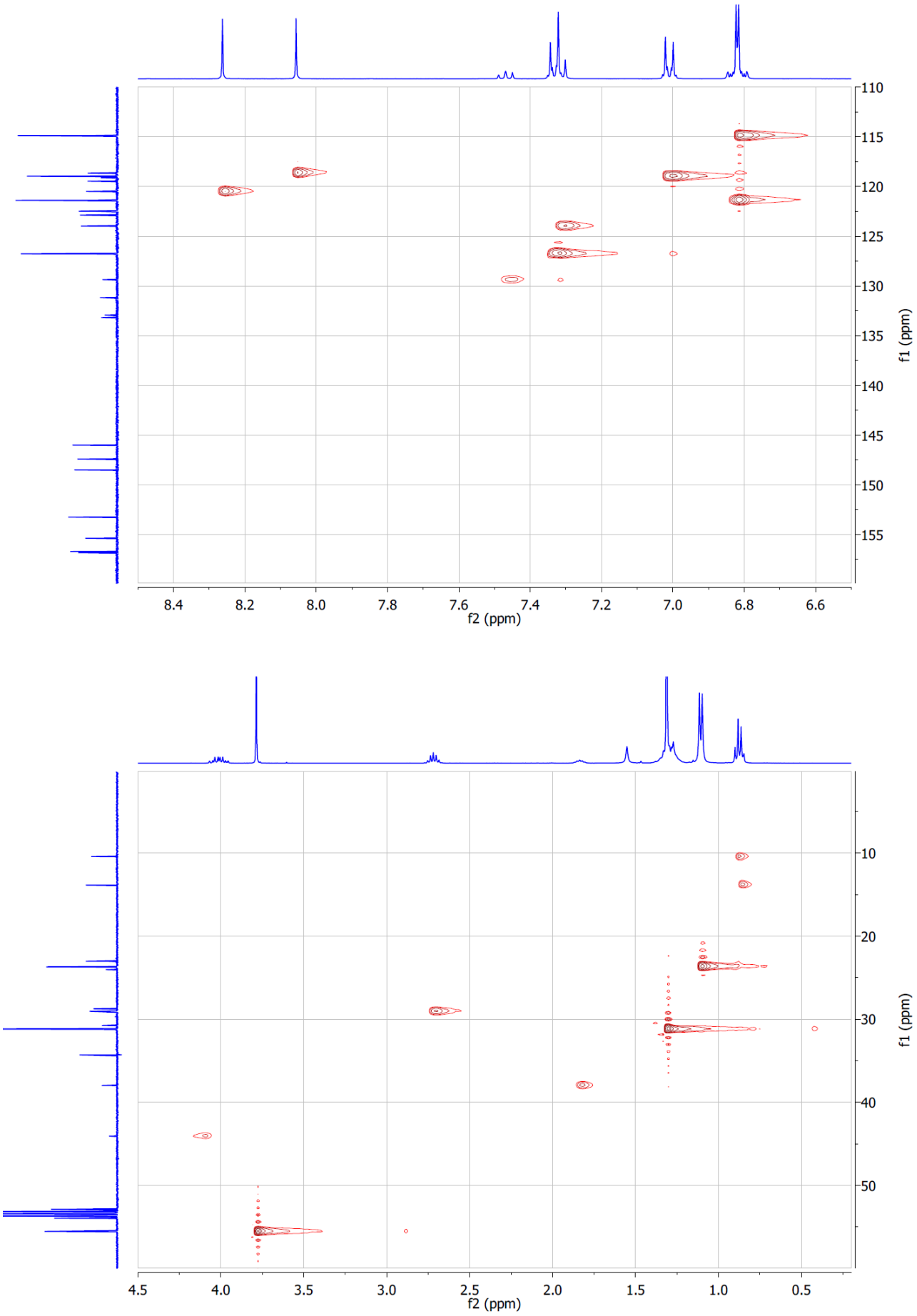
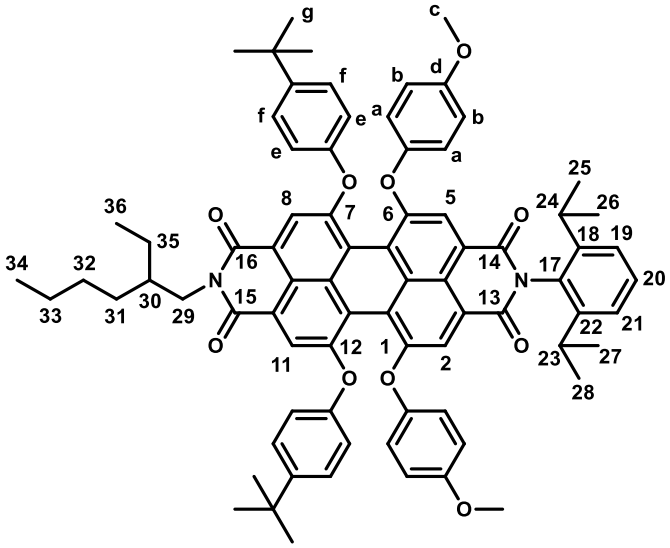


Figure S-3.26: $^{1}H–^{13}C$ HSQC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **9** (Aromatic part at the top and aliphatic part at the bottom).

3.6 Compound 12:



The structure of compound **12** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.27. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.28). The first evidences of presence of 4-*tert*-butylphenoxy-groups at 7, 12-positions and 4-methoxyphenoxy-groups at 1, 6-positions were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.29). This clearly showed the cross couplings of carbonyl carbons (C^{15} and C^{16}) with perylene core protons (H^{8} and H^{11}) and 2-ethylhexyl-chain protons H^{29}. Furthermore, the other set of carbonyl carbons C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments in which through-space cross couplings between important protons were investigated (Figures S-3.30 & S-3.31). These experiments further confirmed the presence of 4-*tert*-butylphenoxy-gropus at 7, 12-positions by clearly showing through-space cross couplings between H^{g}–H^{f}, and H^{e}–$H^{8,11}$ protons (Figure S-3.30). The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.32).

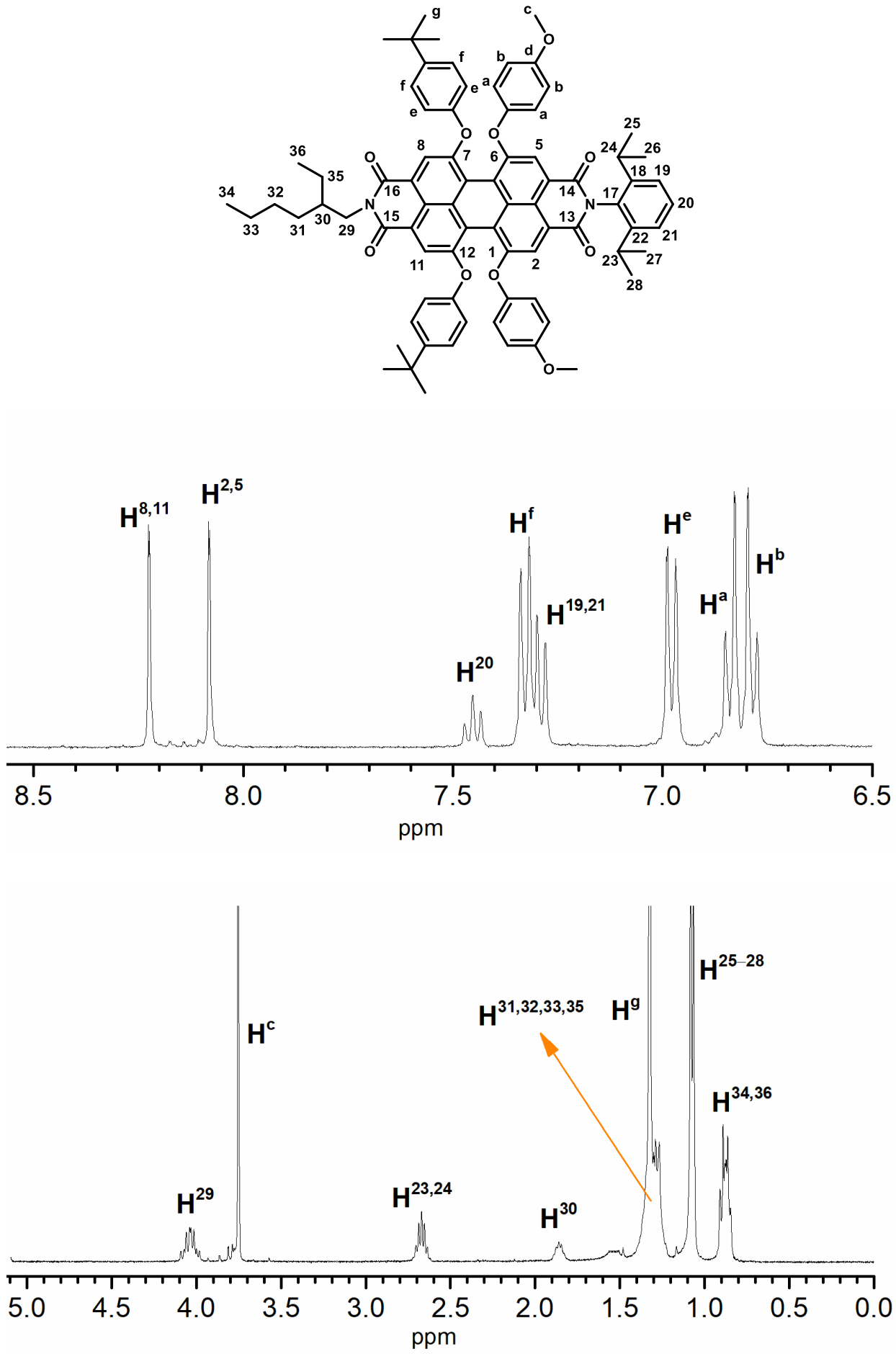


Figure S-3.27: ^{1}H NMR spectrum (CD_2Cl_2, 400 MHz) of compound **12** with complete assignments of proton signals.

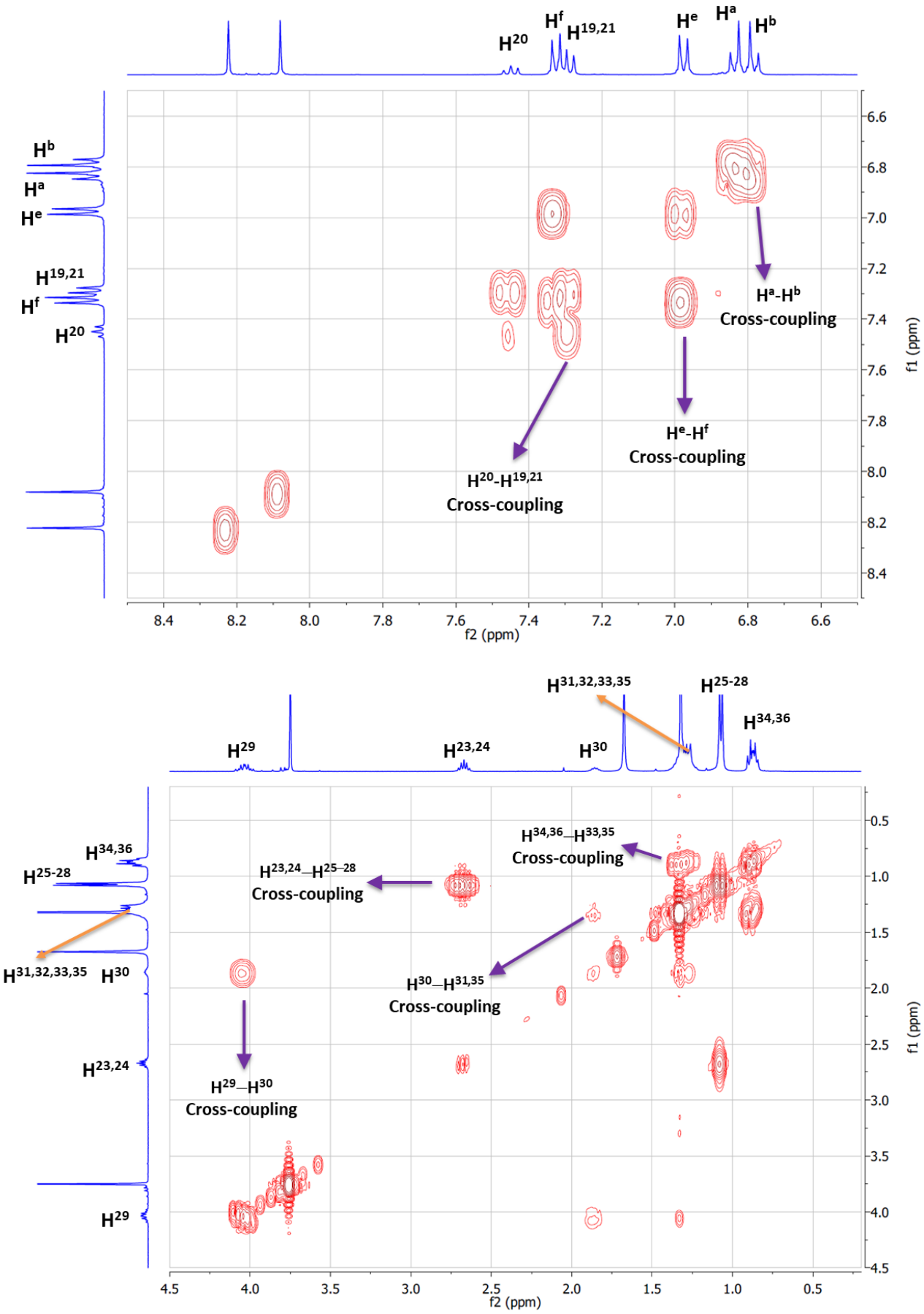


Figure S-3.28: ^{1}H–^{1}H gCOSY NMR spectrum (CD_2Cl_2, 400 MHz) of compound **12** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

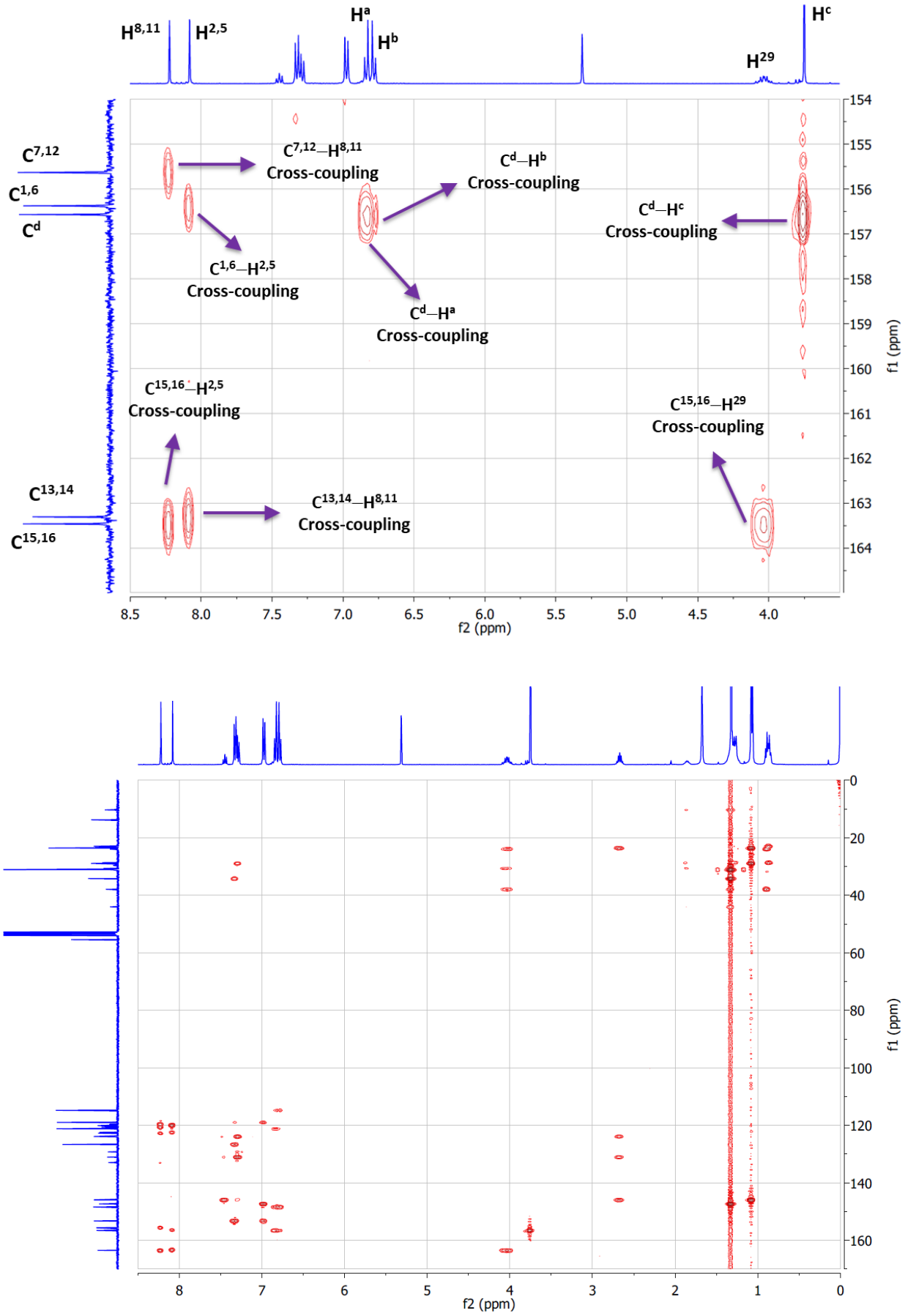


Figure S-3.29: ^{1}H–^{13}C gHMBC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **12** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

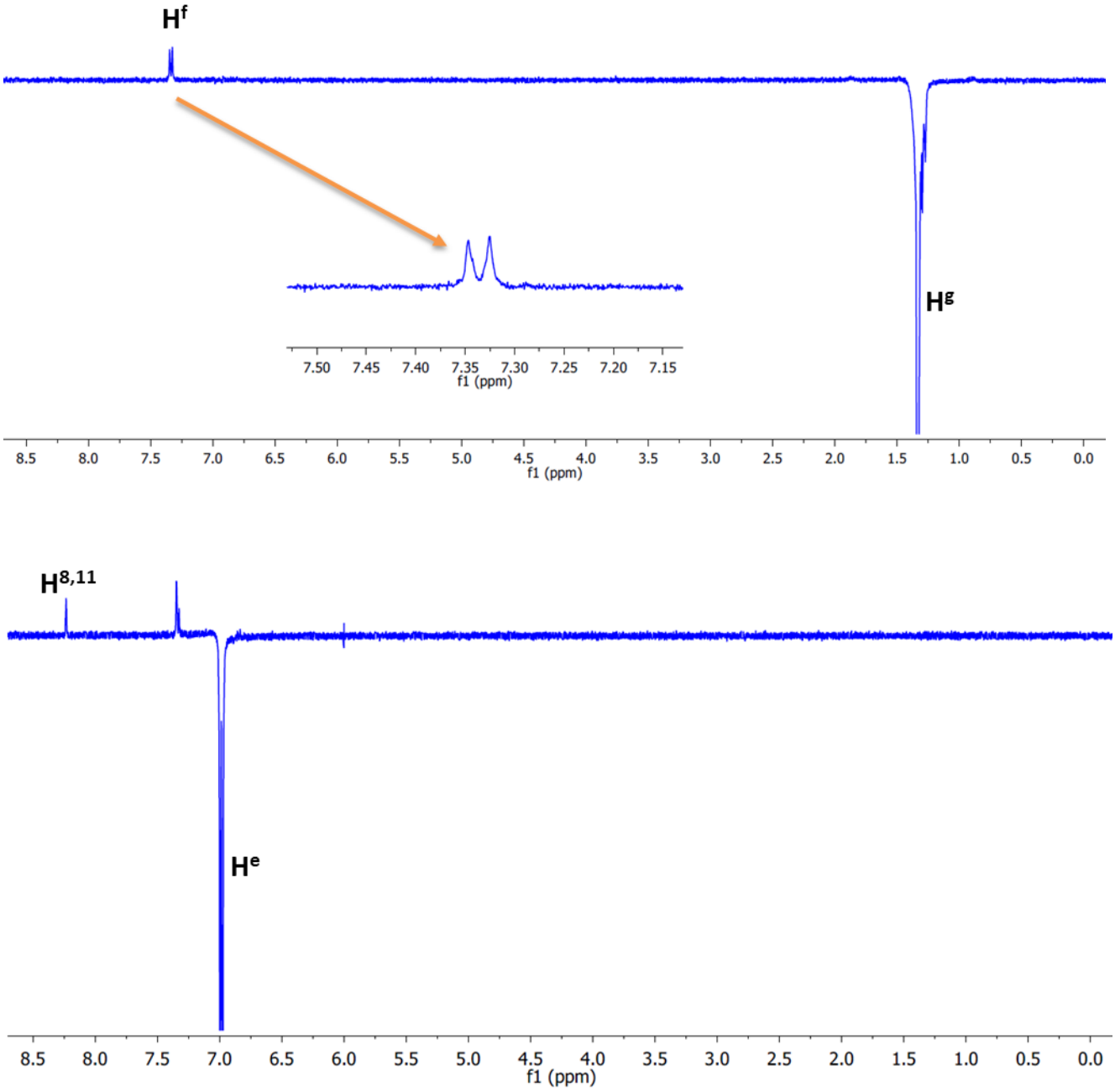


Figure S-3.30: $^{1}H–^{1}H$ 1D NOESY NMR spectra (CD_2Cl_2, 400 MHz) of compound **12** with the indication of through-space cross-couplings between crucial protons ($H^g–H^f$ coupling at the top and $H^e–H^{8,11}$ coupling at the bottom).

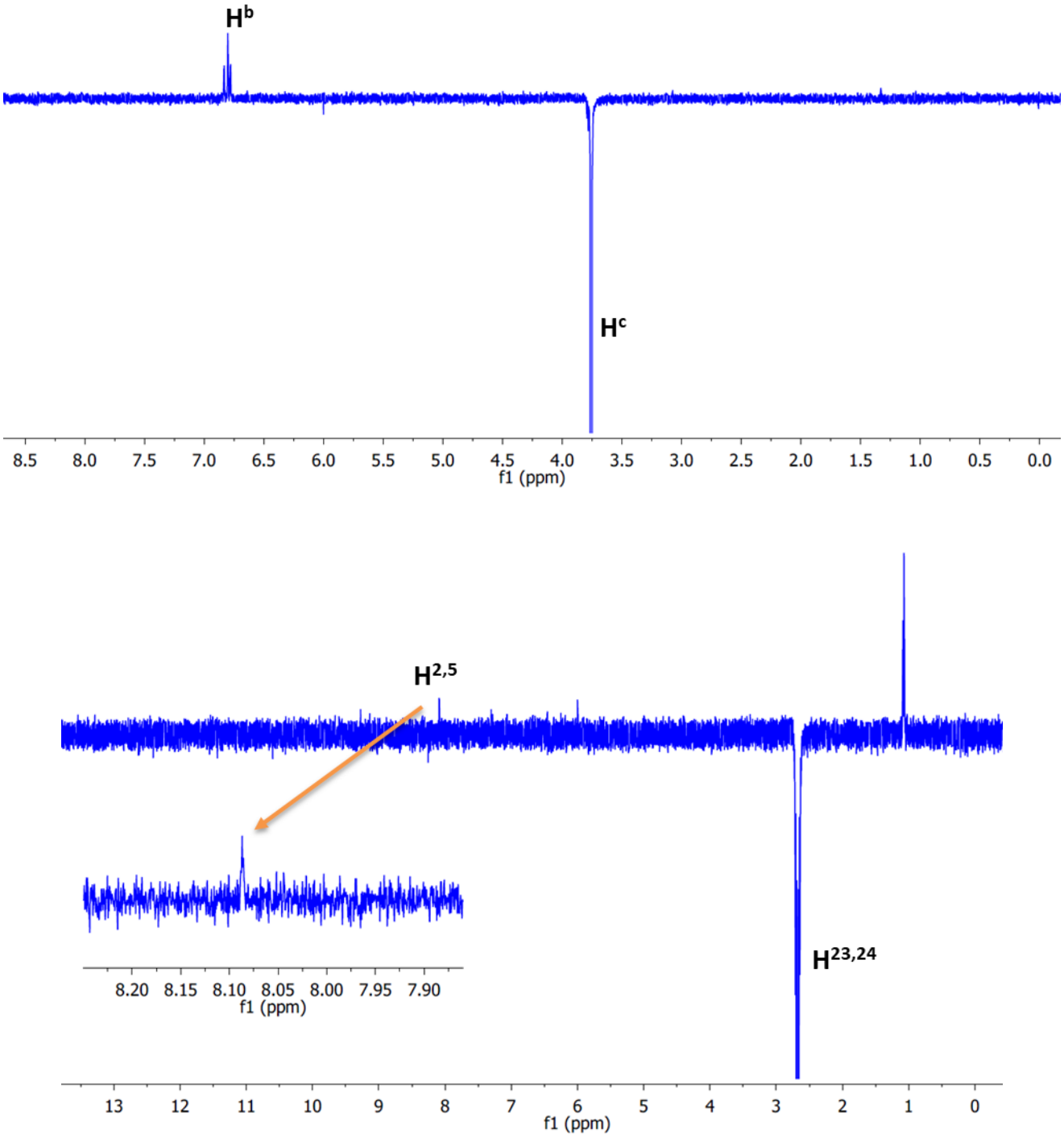


Figure S-3.31: ^{1}H–^{1}H 1D NOESY NMR spectra (CD_2Cl_2, 400 MHz) of compound **12** with the indication of through-space cross-couplings between crucial protons (H^c–H^b coupling at the top and $H^{23,24}$–$H^{2,5}$ coupling at the bottom).

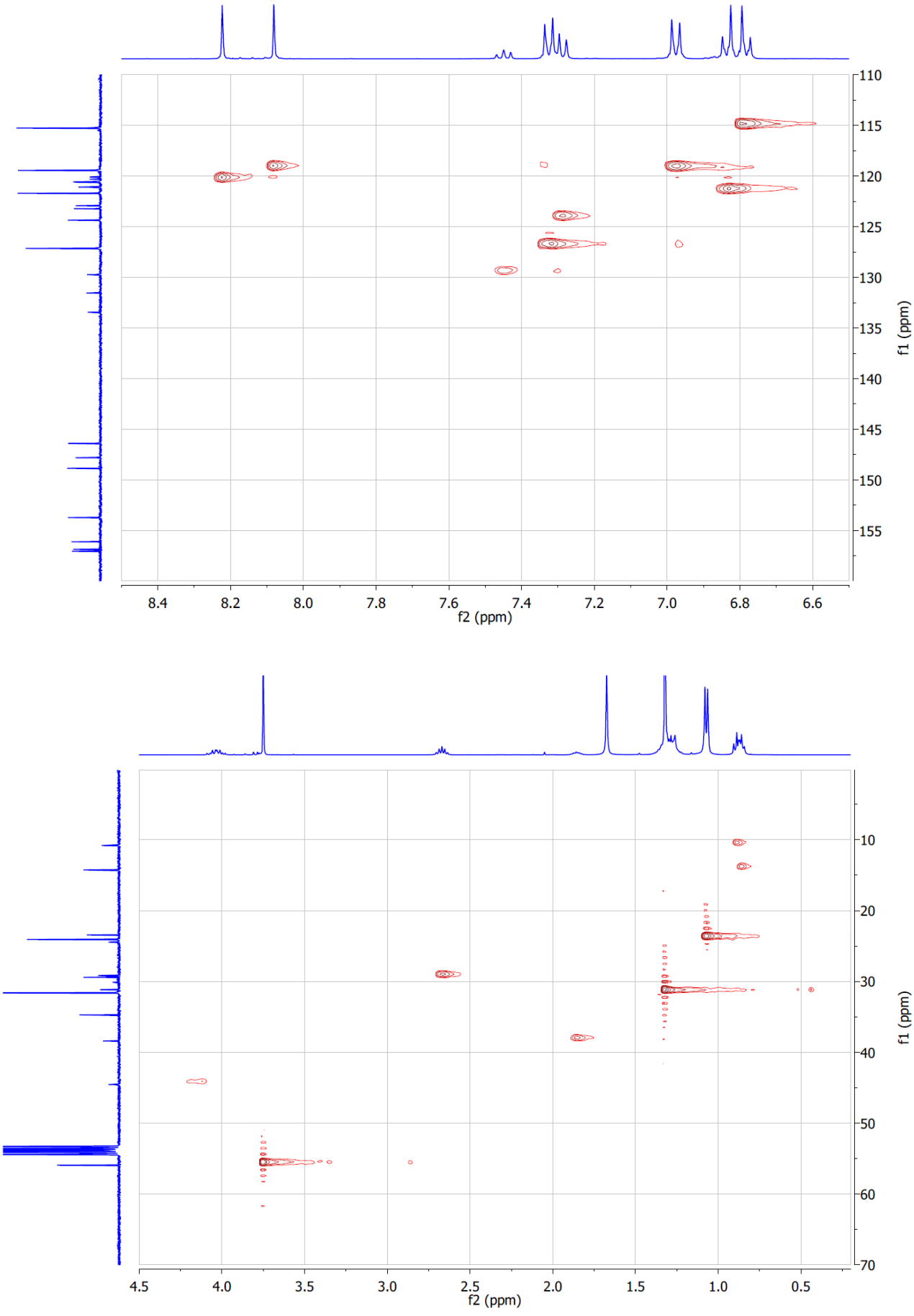
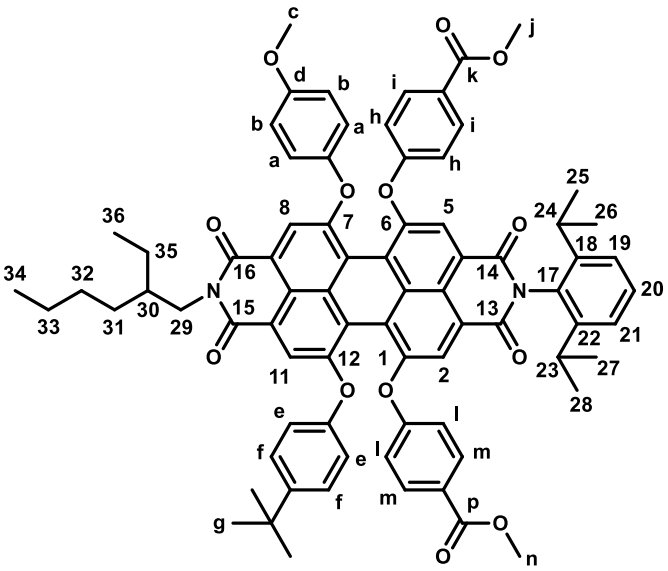


Figure S-3.32: $^{1}H–^{13}C$ gHSQC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **12** (Aromatic part at the top and aliphatic part at the bottom).

3.7 Compound 15:



The structure of compound **15** was unambiguously confirmed by a series of systematic 1D and 2D-NMR measurements, namely ^{1}H, ^{13}C, ^{13}C-APT and DEPT-135, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, and ^{1}H–^{1}H NOESY. The complete assignment of peaks in the ^{1}H-NMR spectrum is shown in Figure S-3.33. The signals of all through-bond coupled protons were identified using ^{1}H–^{1}H COSY spectrum (Figure S-3.34). The first evidences of presence of 4-methoxyphenoxy-group at 7-position, 4-*tert*-butylphenoxy-group at 12-position, and 4-methoxycarbonylphenoxy-groups at 1, 6-positions were provided by the ^{1}H–^{13}C HMBC experiment (Figure S-3.35). This clearly showed the cross couplings of carbonyl carbon C^{15} with perylene core proton H^{11} and 2-ethylhexyl-chain protons H^{29}. Similarly, cross couplings of carbonyl carbon C^{16} with perylene core proton H^{8} and 2-ethylhexyl-chain protons H^{29} were observed. Furthermore, the other set of carbonyl carbons C^{13} and C^{14} exhibited the cross couplings with perylene core protons H^{2} and H^{5}. The crucial and final confirmation to the proposed structural assignment was provided by 1D ^{1}H-^{1}H NOESY experiments in which through-space cross couplings between important protons were investigated. These experiments further confirmed the presence of 4-methoxycarbonylphenoxy-groups at 1, 6-positions by clearly showing through-space cross coupling between $H^{h,l}$–$H^{2,5}$ protons (Figure S-3.36). Similarly, the presence of 4-*tert*-butylphenoxy-group at 12-position was proved by through-space cross couplings between H^{e}–H^{11} protons (Figure S-3.36). The identification of all proton-attached carbon atoms was achieved by ^{1}H–^{13}C HSQC spectroscopy (Figure S-3.37).

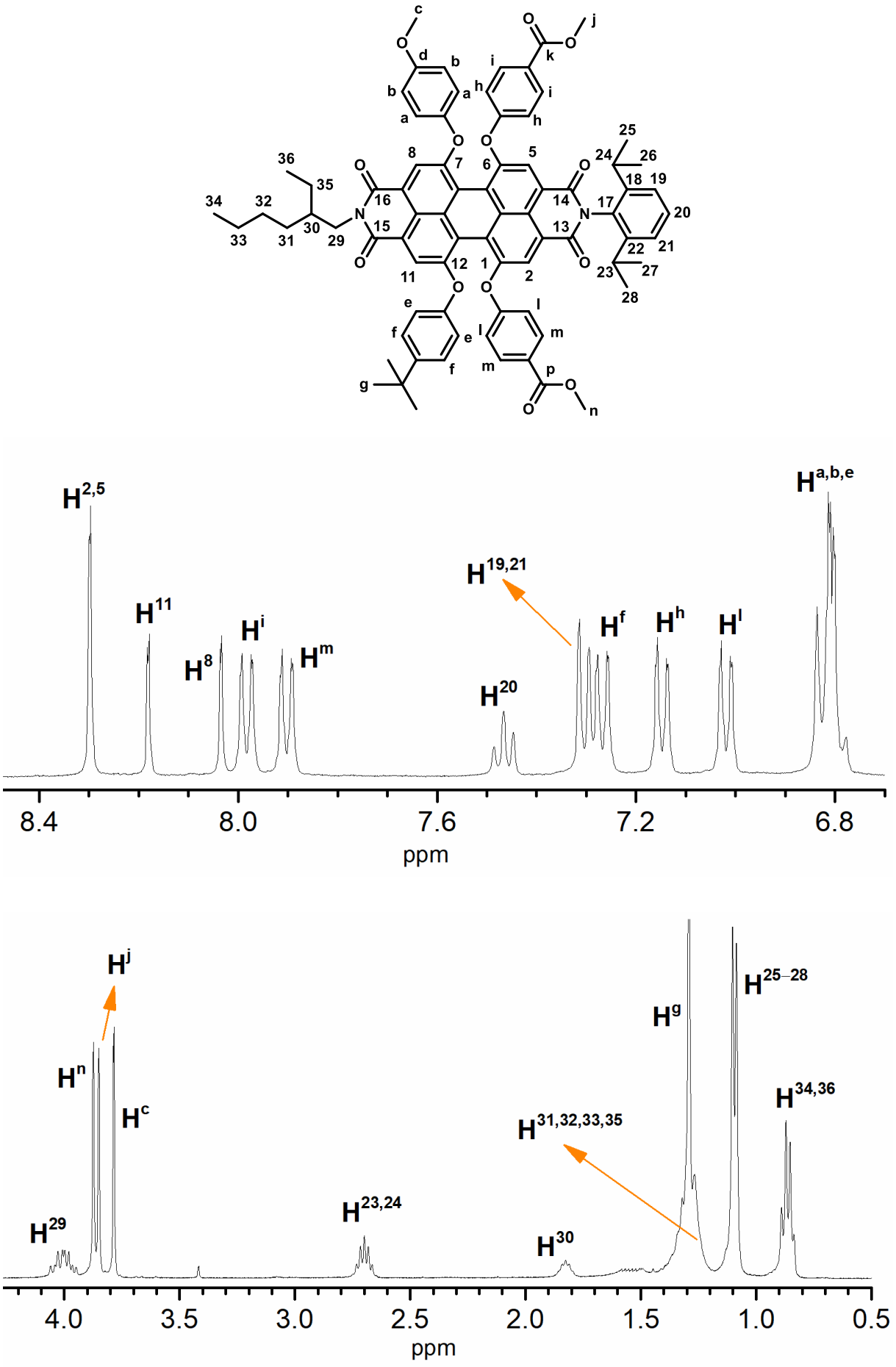


Figure S-3.33: ^{1}H NMR spectrum (CD_2Cl_2, 400 MHz) of compound **15** with complete assignments of proton signals.

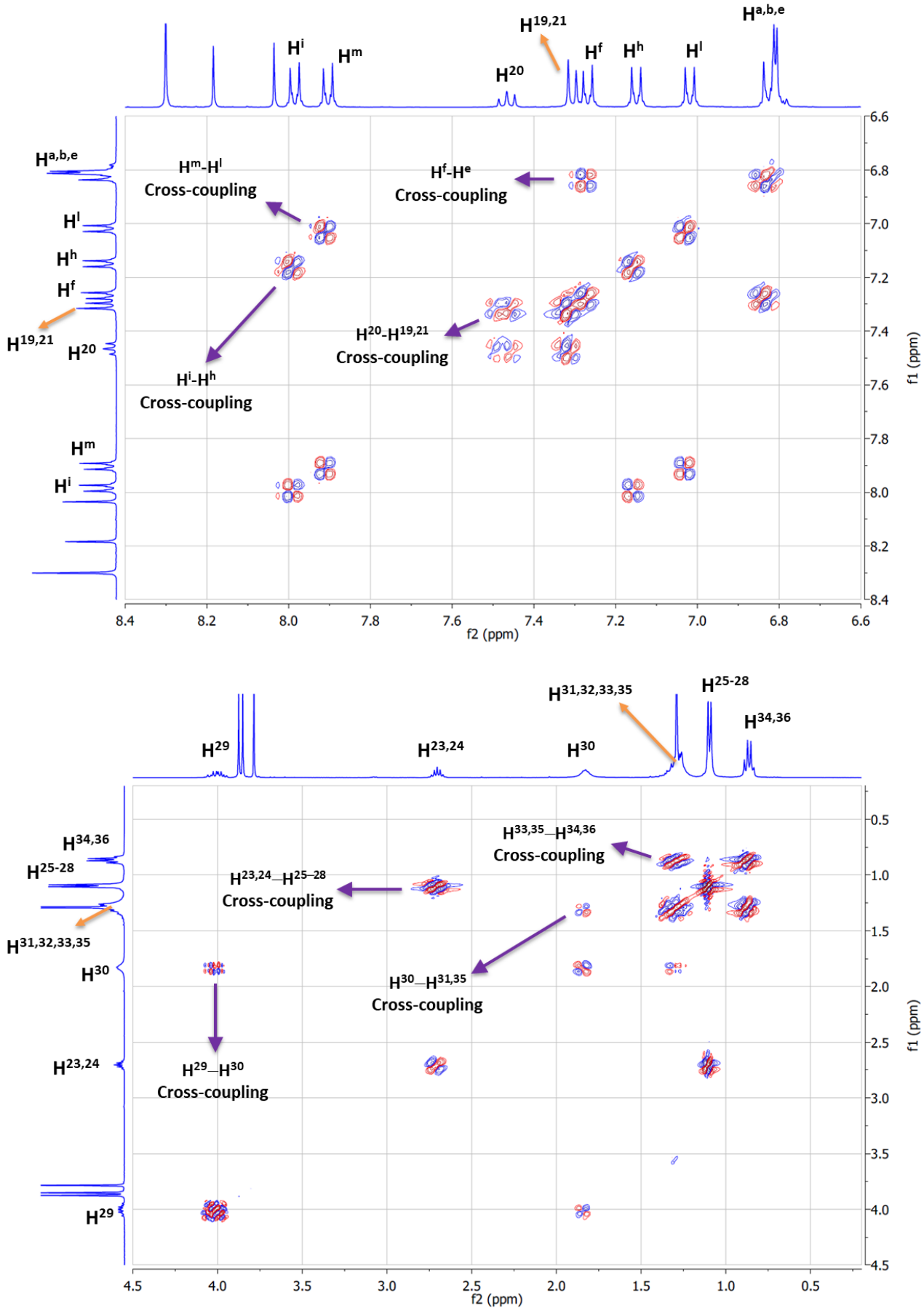


Figure S-3.34: ^{1}H–^{1}H gDQCOSY NMR spectrum (CD_2Cl_2, 400 MHz) of compound **15** with the indication of through-bond coupled protons (aromatic region at the top and aliphatic region at the bottom).

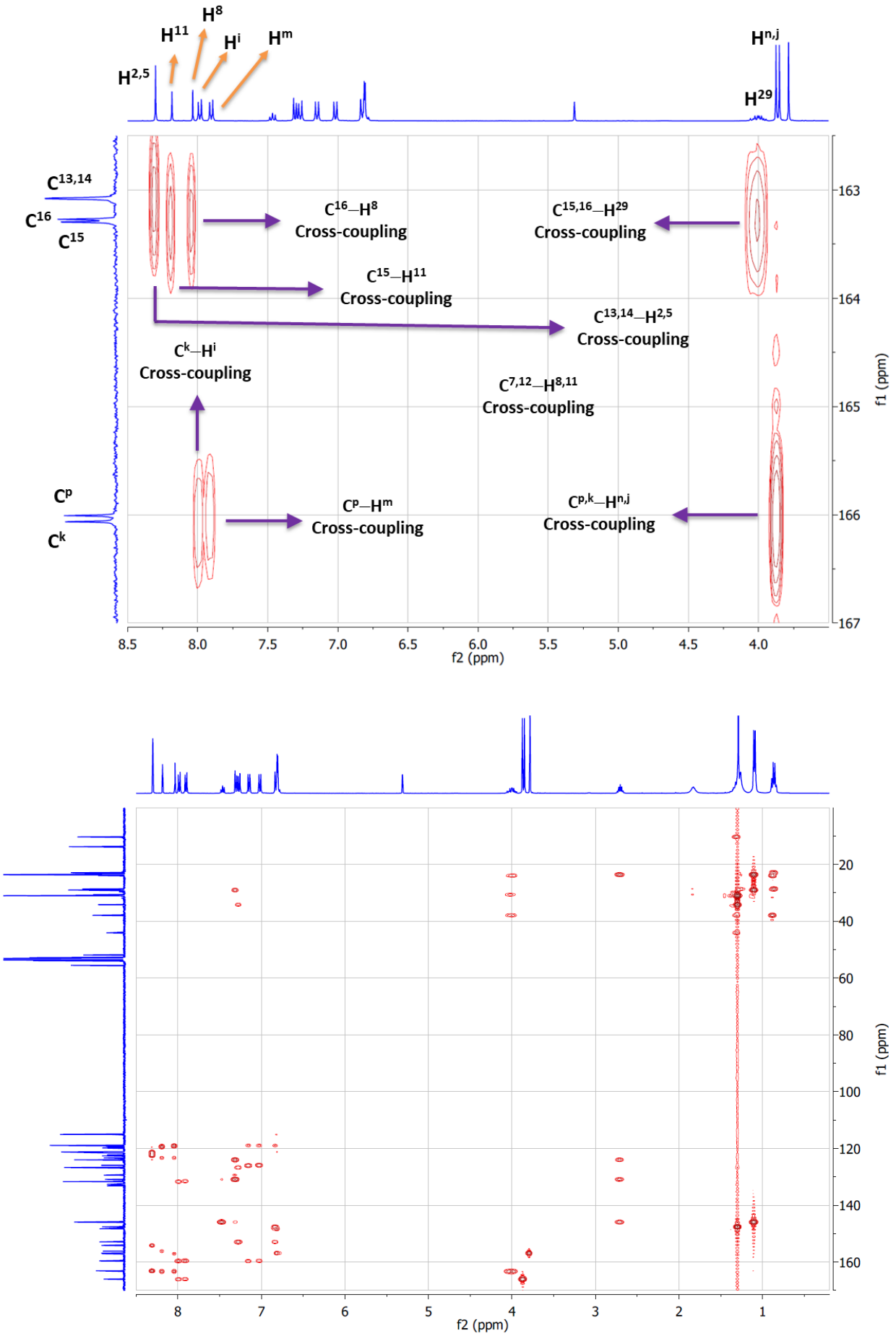


Figure S-3.35: ^{1}H–^{13}C gHMBC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **15** with the indication of important long-range cross-couplings between proton and carbon atoms (zoomed spectrum at the top and full spectrum at the bottom).

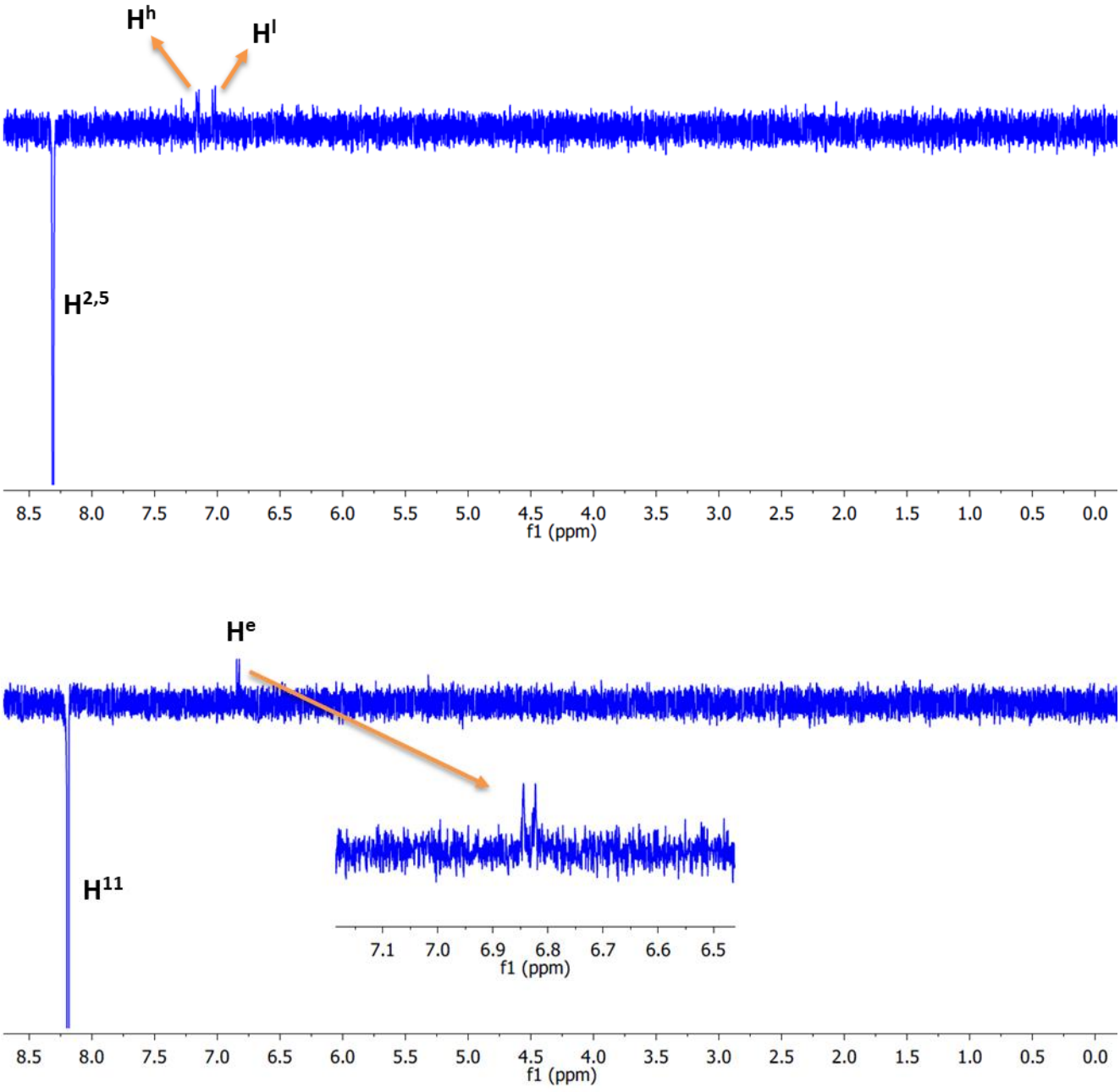


Figure S-3.36: $^{1}H–^{1}H$ 1D NOESY NMR spectra (CD_2Cl_2, 400 MHz) of compound **15** with the indication of through-space cross-couplings between crucial protons ($H^{2,5}–H^{h,l}$ coupling at the top and $H^{e}–H^{11}$ coupling at the bottom).

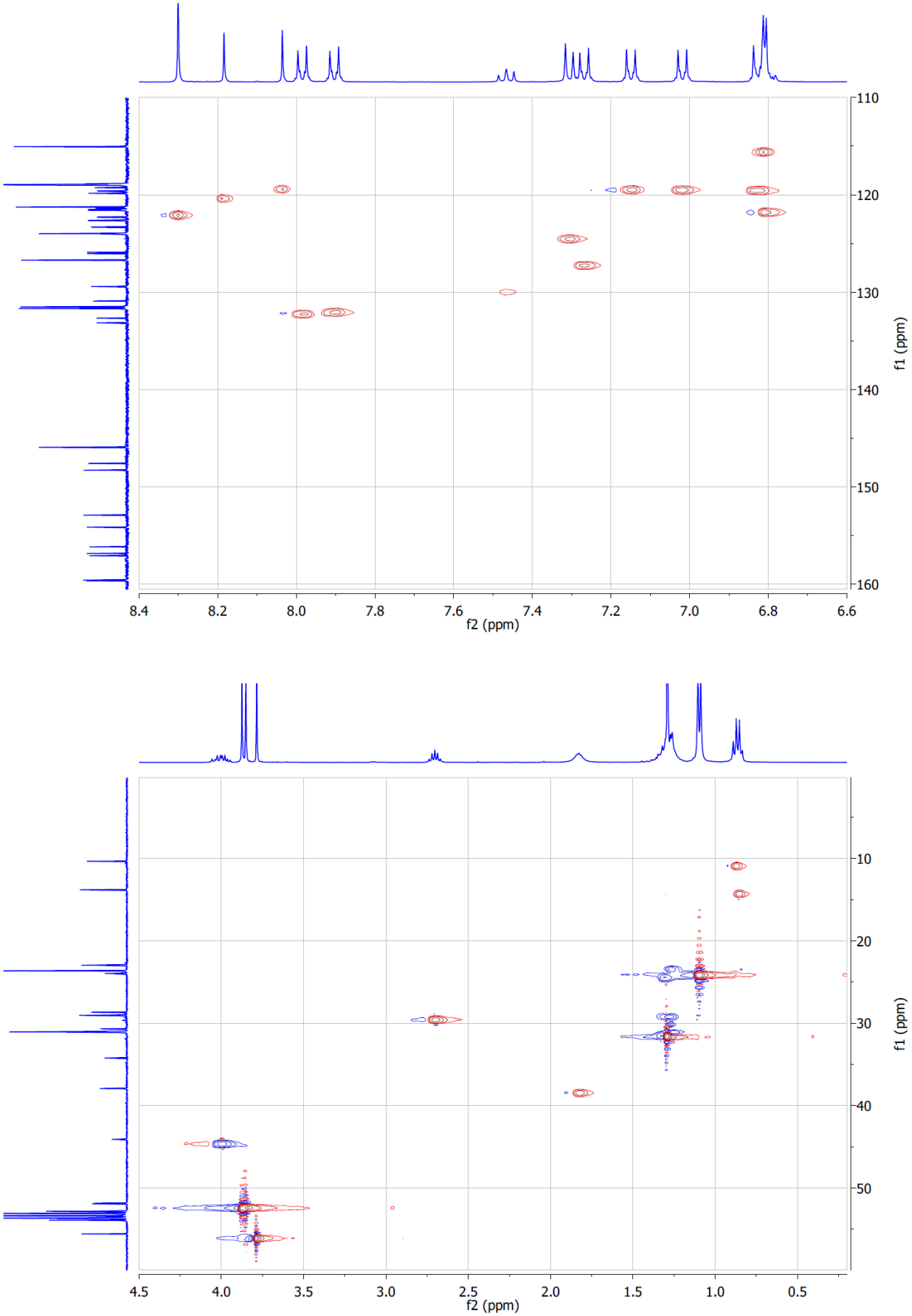


Figure S-3.37: $^{1}H–^{13}C$ gHSQC NMR spectrum (CD_2Cl_2, 400 MHz) of compound **15** (Aromatic part at the top and aliphatic part at the bottom).

Section 4. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra

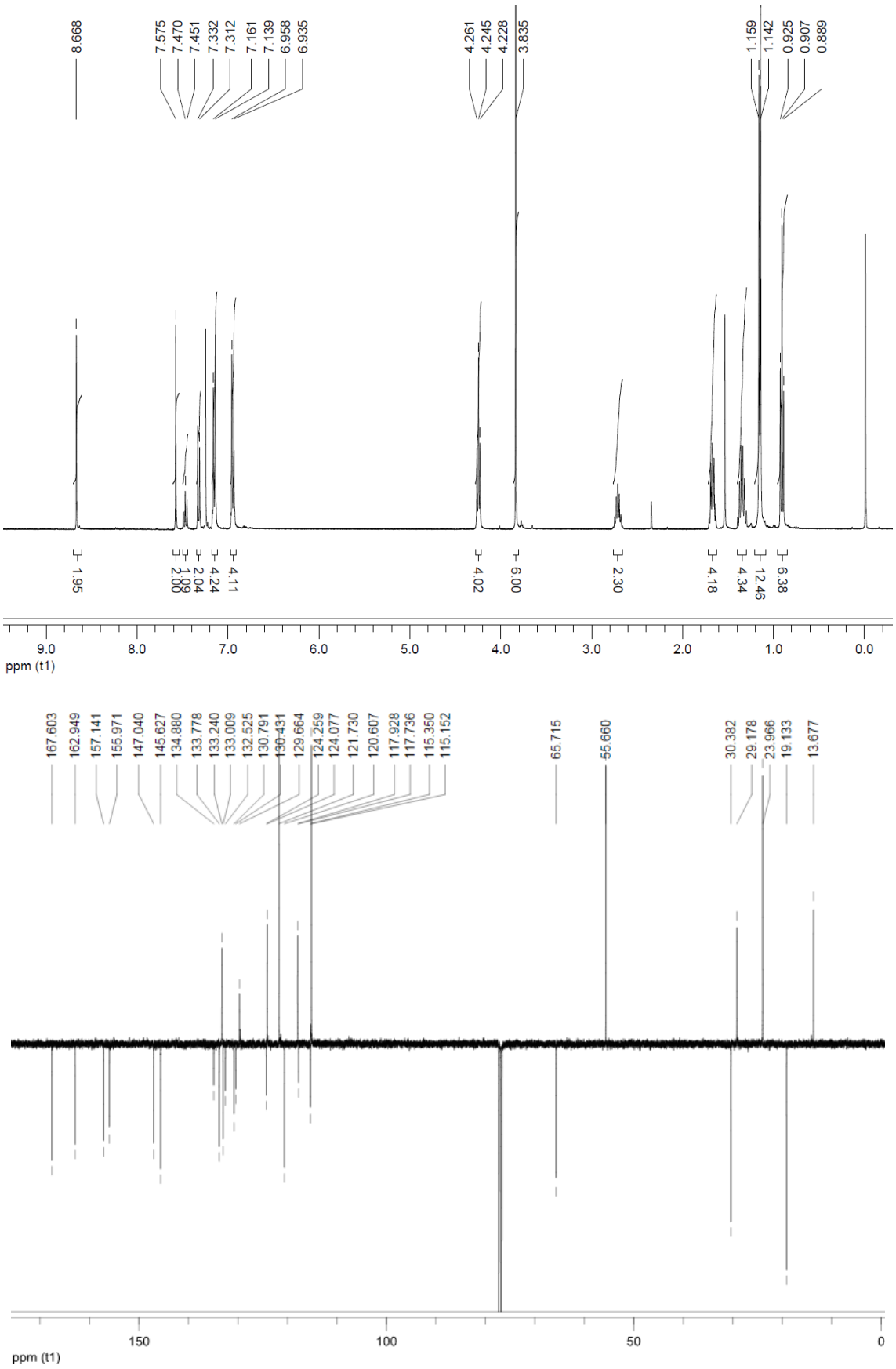


Figure S-4.1: ^{1}H and ^{13}C-APT NMR spectra of compound **2**.

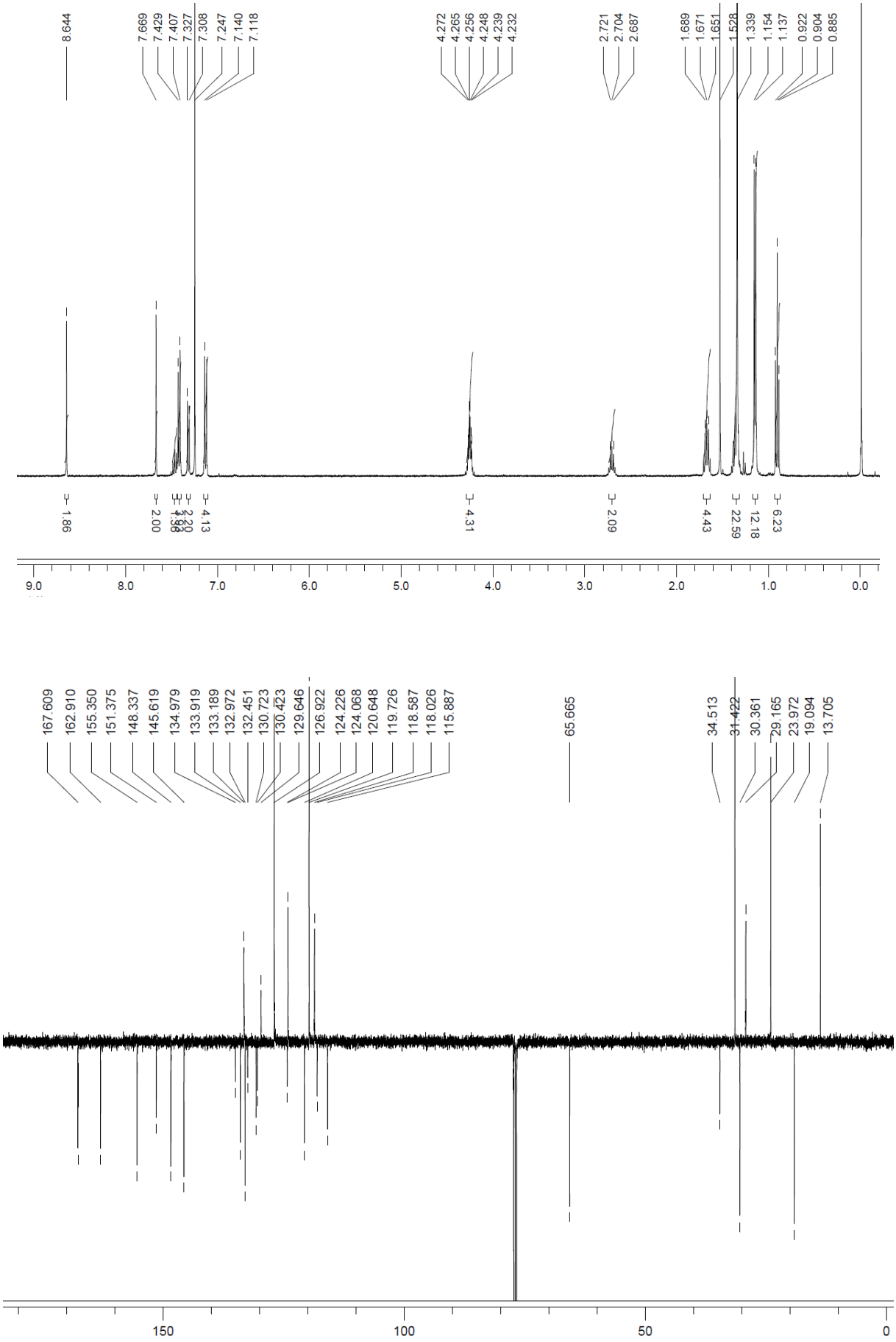


Figure S-4.2: ^{1}H and ^{13}C APT NMR spectra of compound **3**.

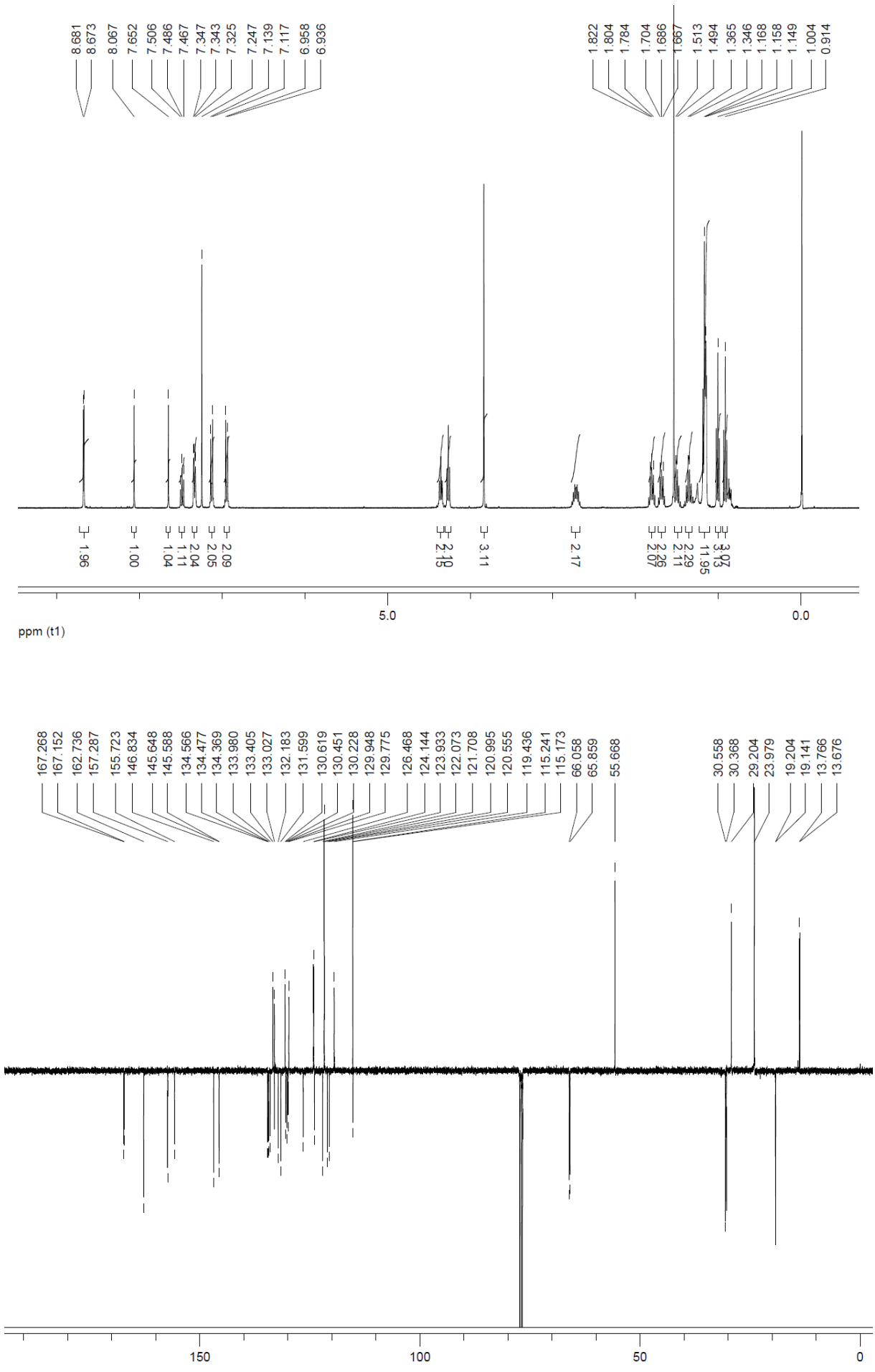


Figure S-4.3: ^{1}H and ^{13}C APT NMR spectra of compound **4**.

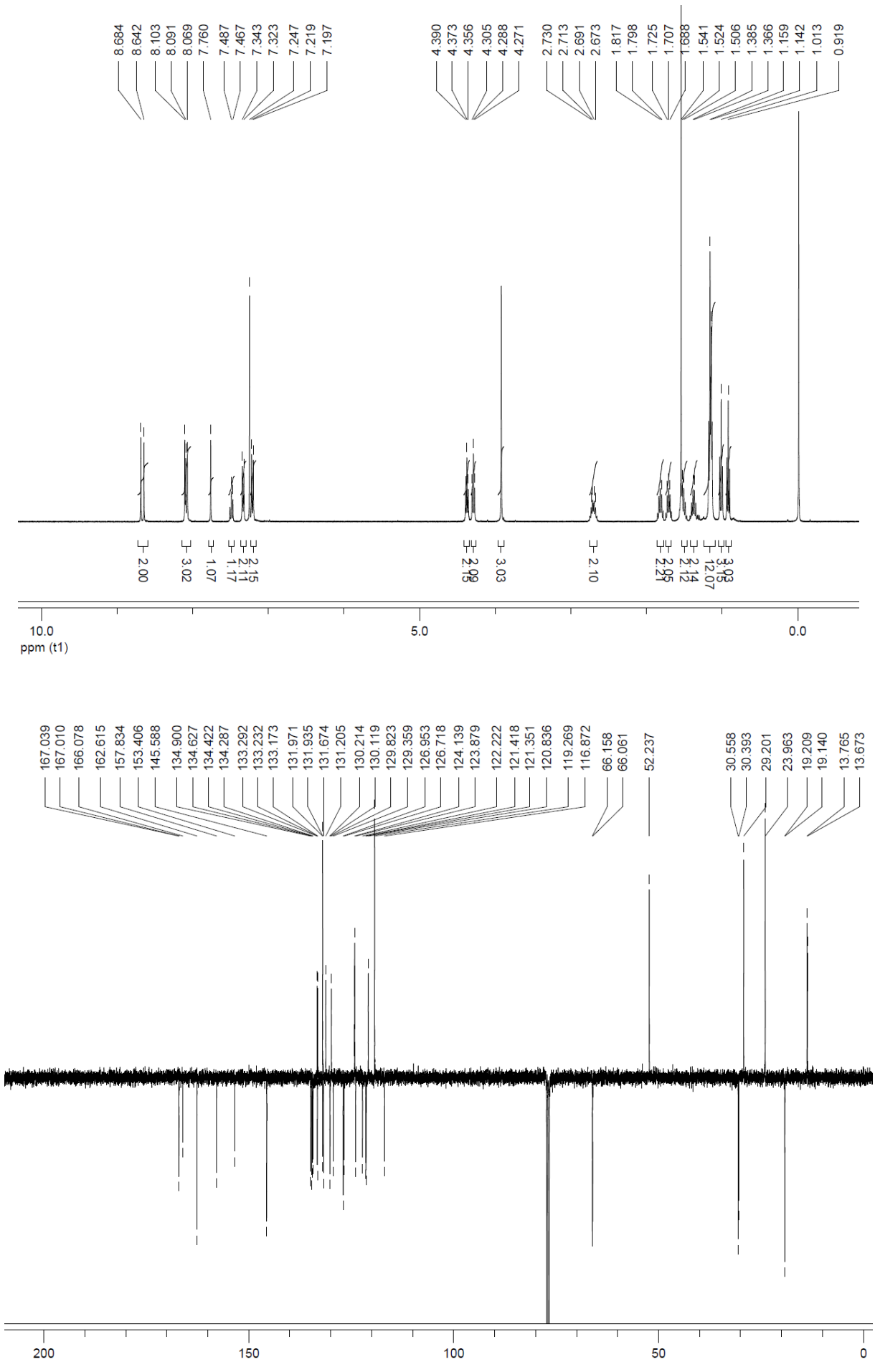


Figure S-4.4: ^{1}H and ^{13}C APT NMR spectra of compound **5**.

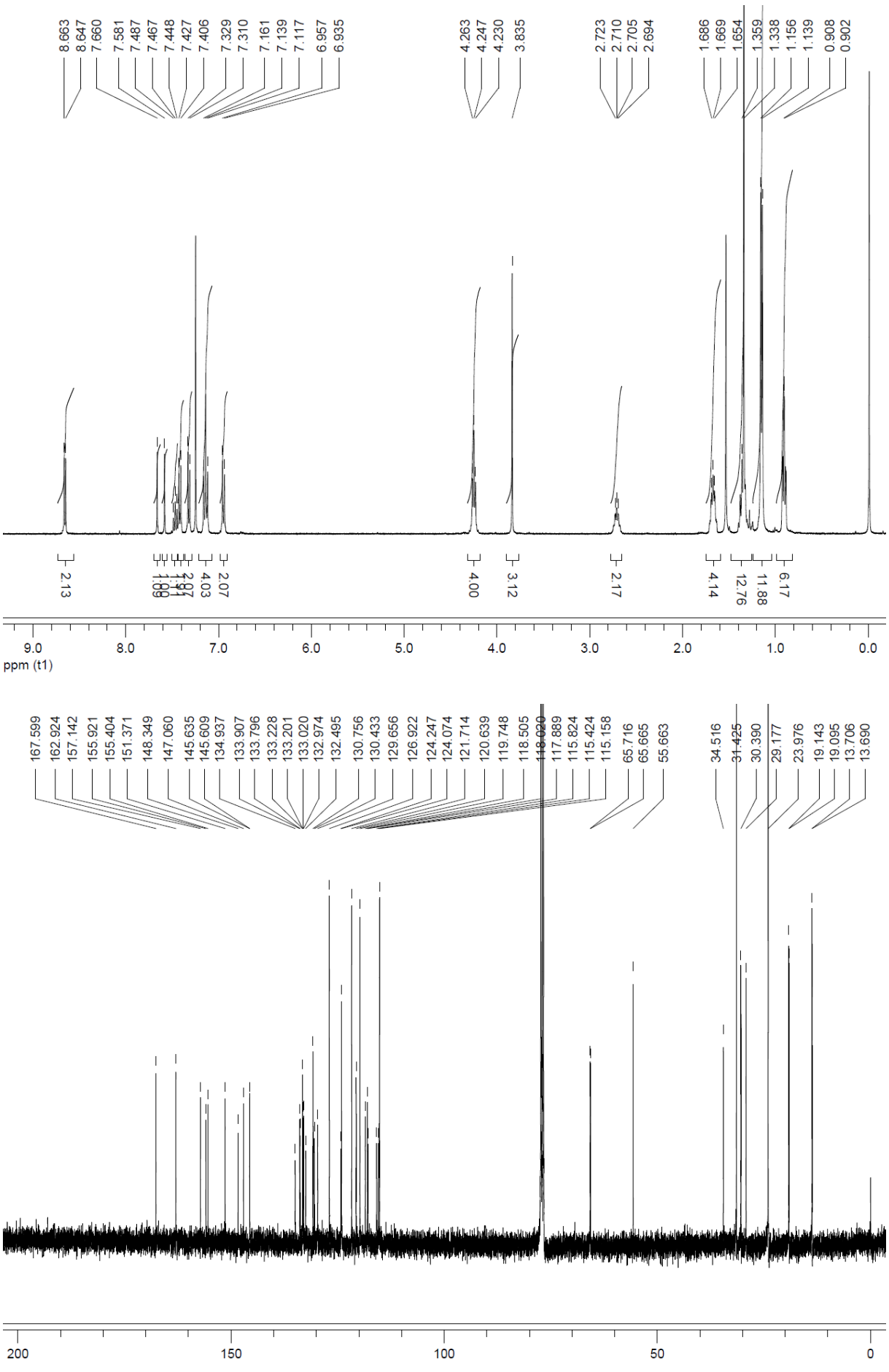


Figure S-4.5: ^{1}H and ^{13}C NMR spectra of compound **6**.

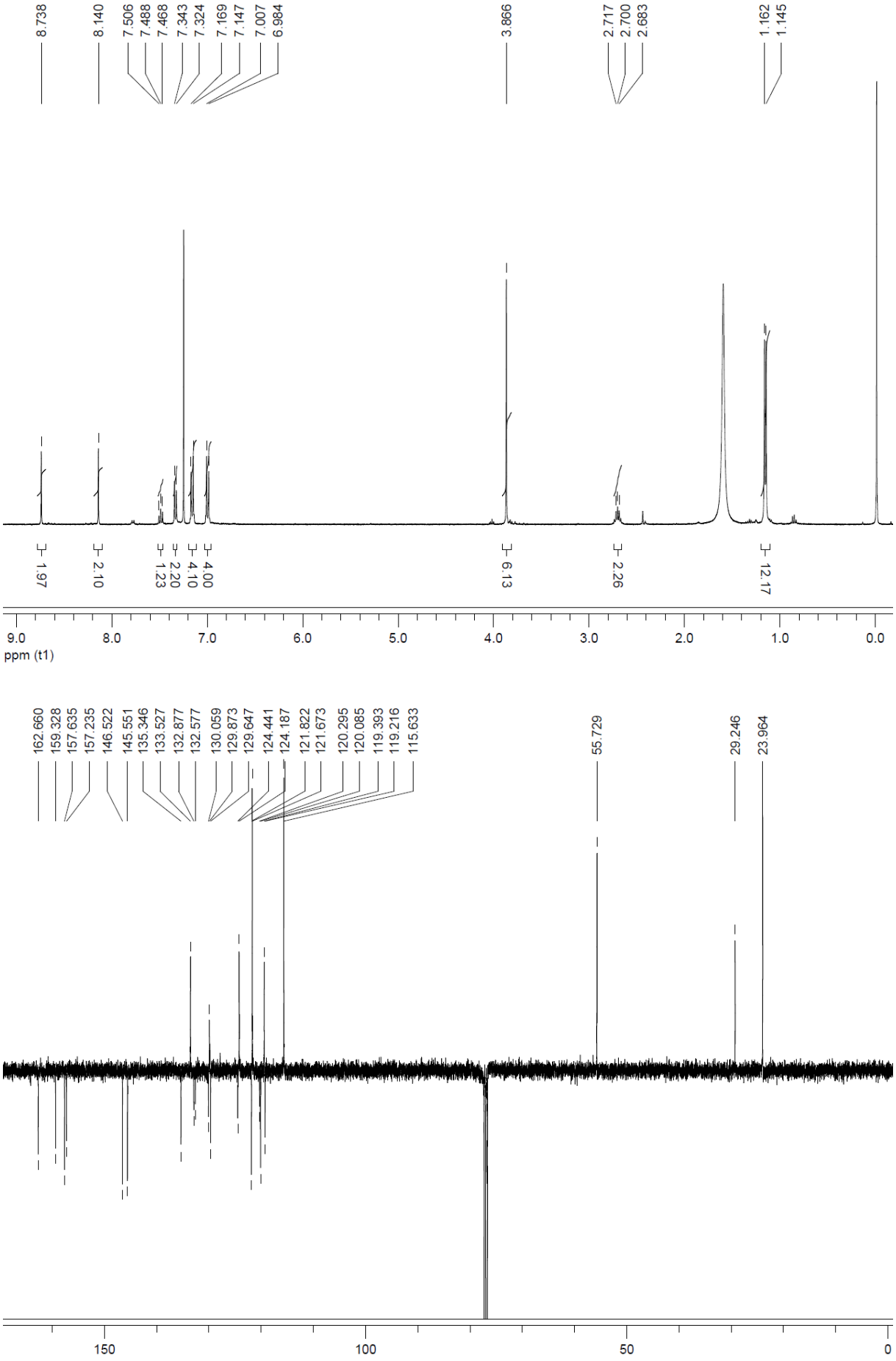


Figure S-4.6: ^{1}H and ^{13}C APT NMR spectra of compound **7**.

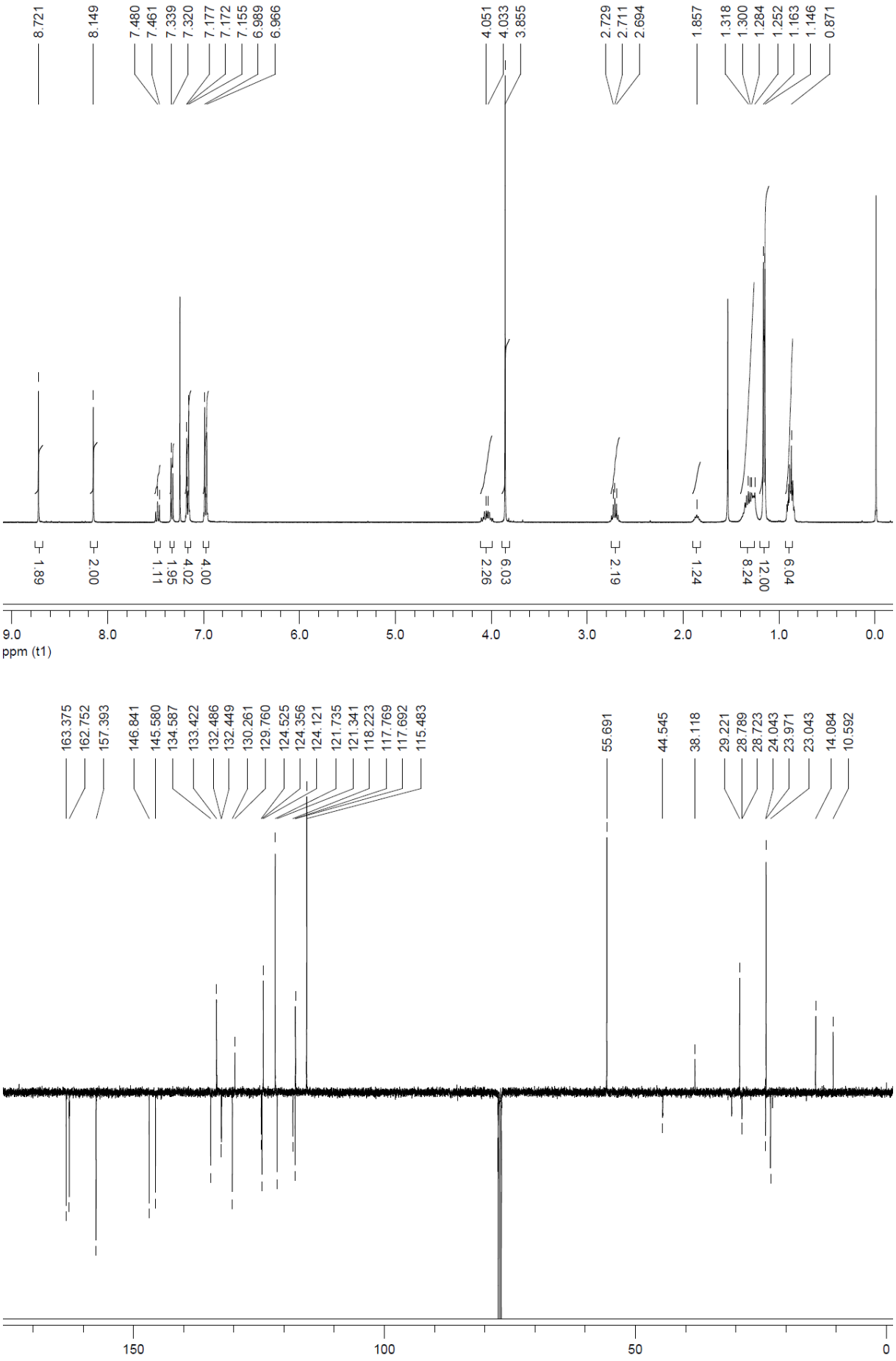


Figure S-4.7: ^{1}H and ^{13}C APT NMR spectra of compound **8**.

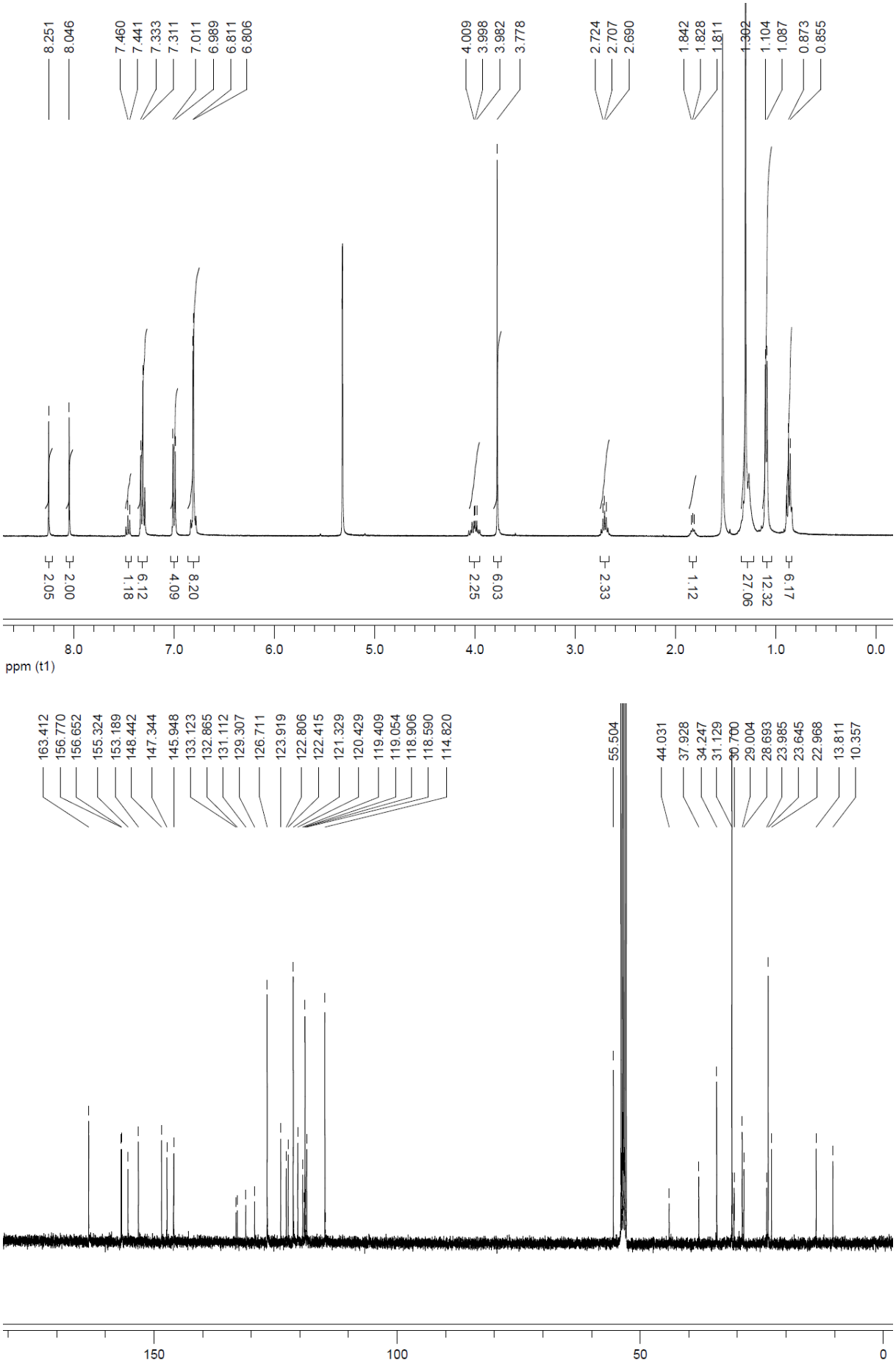
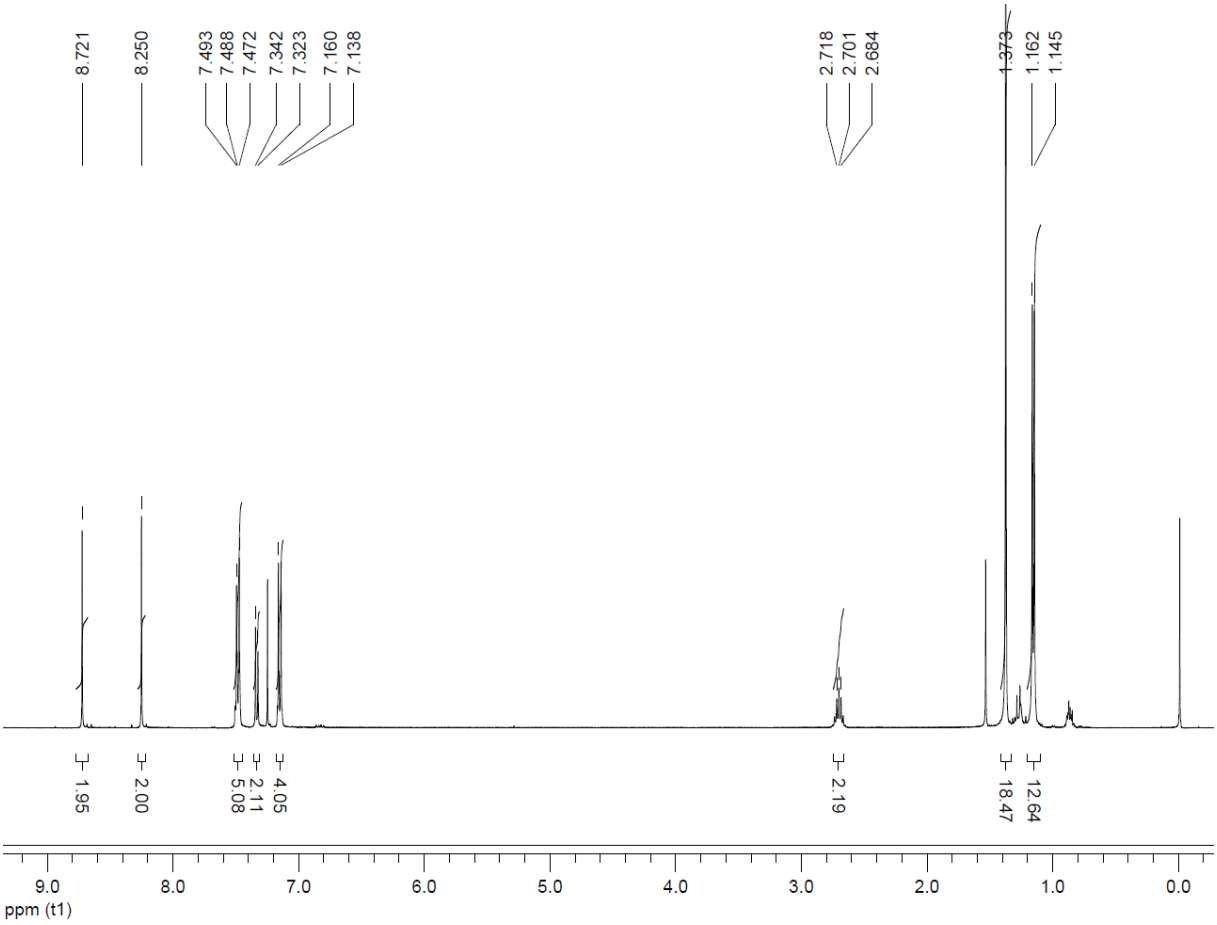


Figure S-4.8: ^{1}H and ^{13}C NMR spectra of compound **9**.



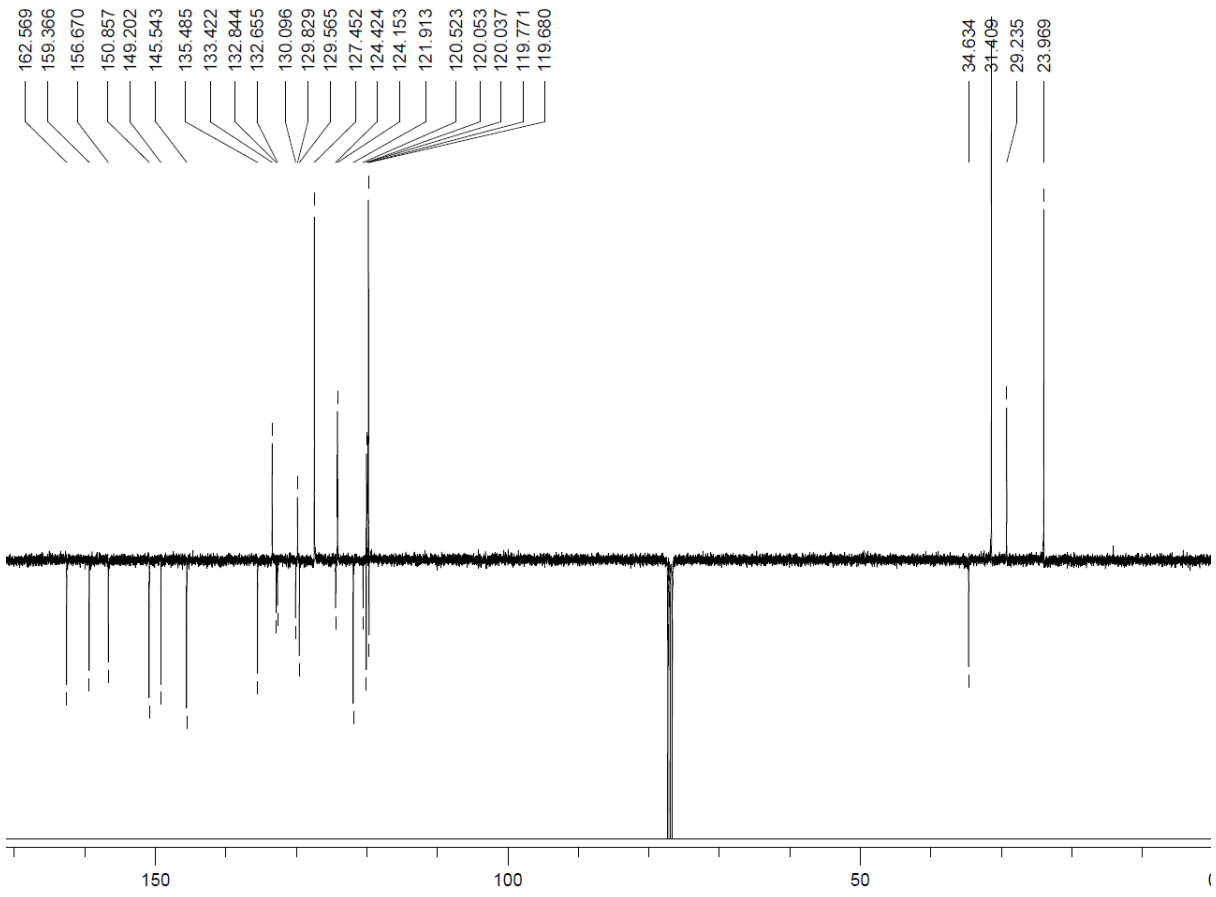


Figure S-4.9: ^{1}H and ^{13}C APT NMR spectra of compound **10**.

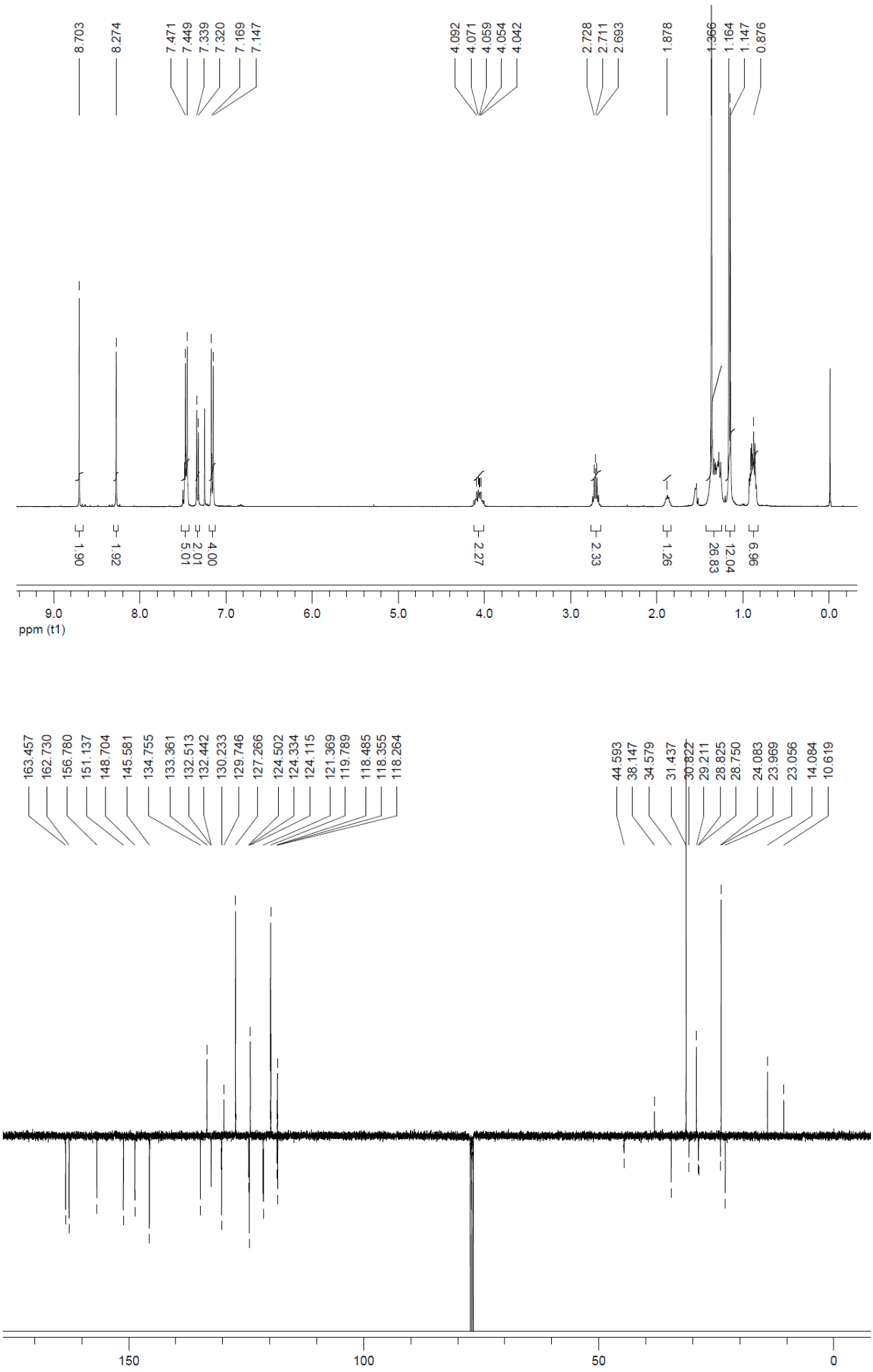


Figure S-4.10: ^{1}H and ^{13}C APT NMR spectra of compound **11**.

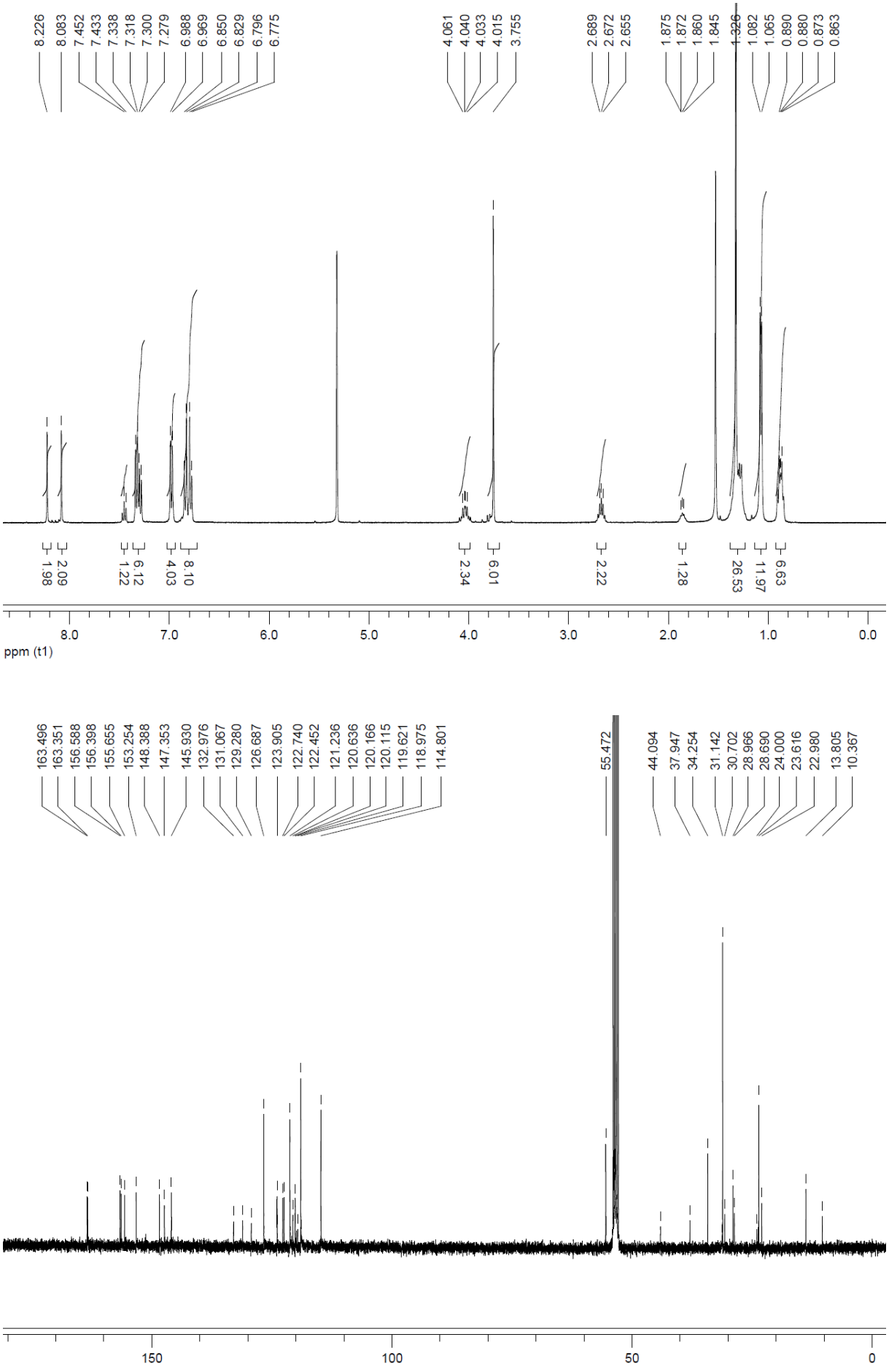


Figure S-4.11: ^{1}H and ^{13}C NMR spectra of compound **12**.

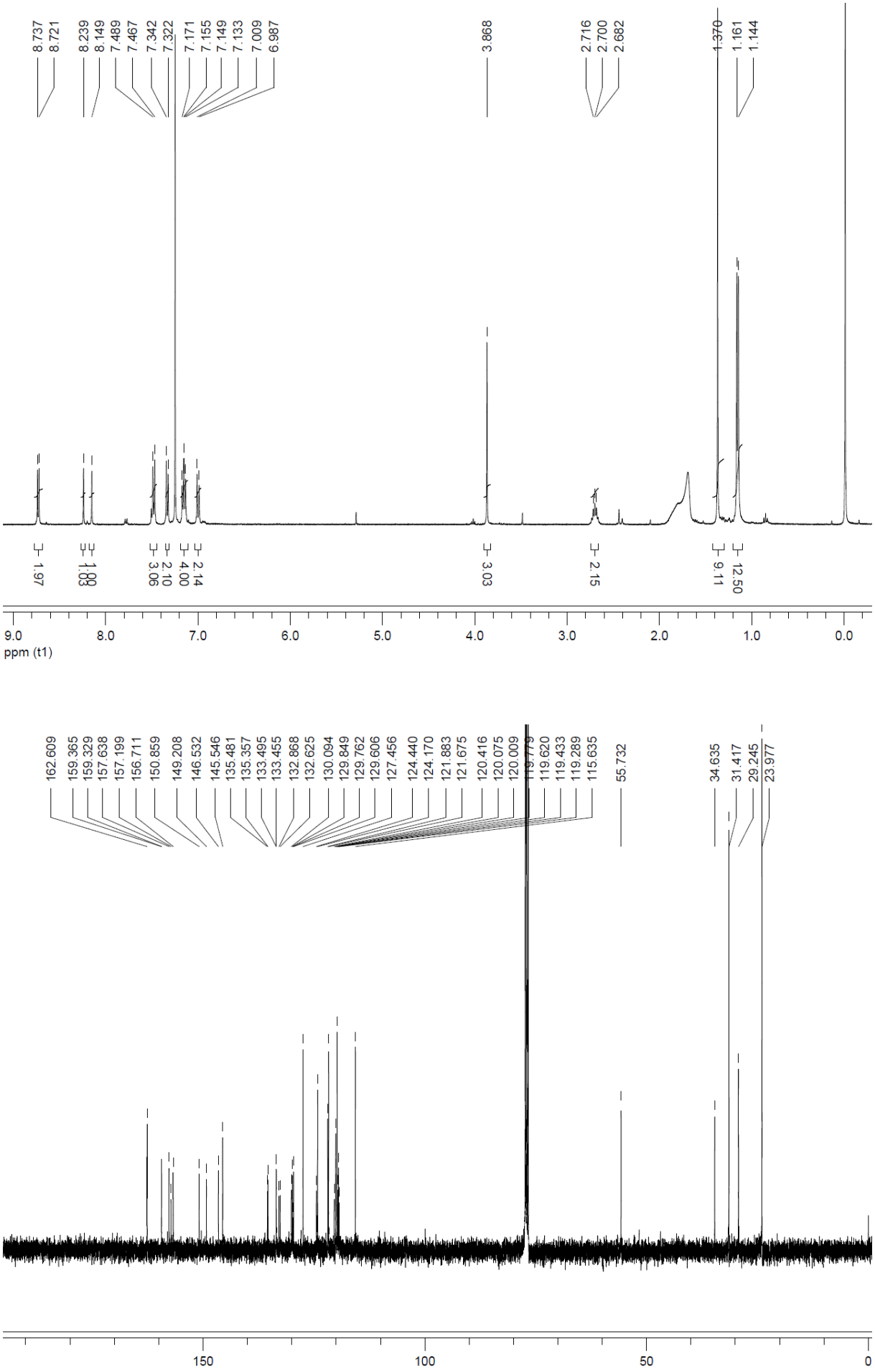


Figure S-4.12: ^{1}H and ^{13}C NMR spectra of compound **13**.

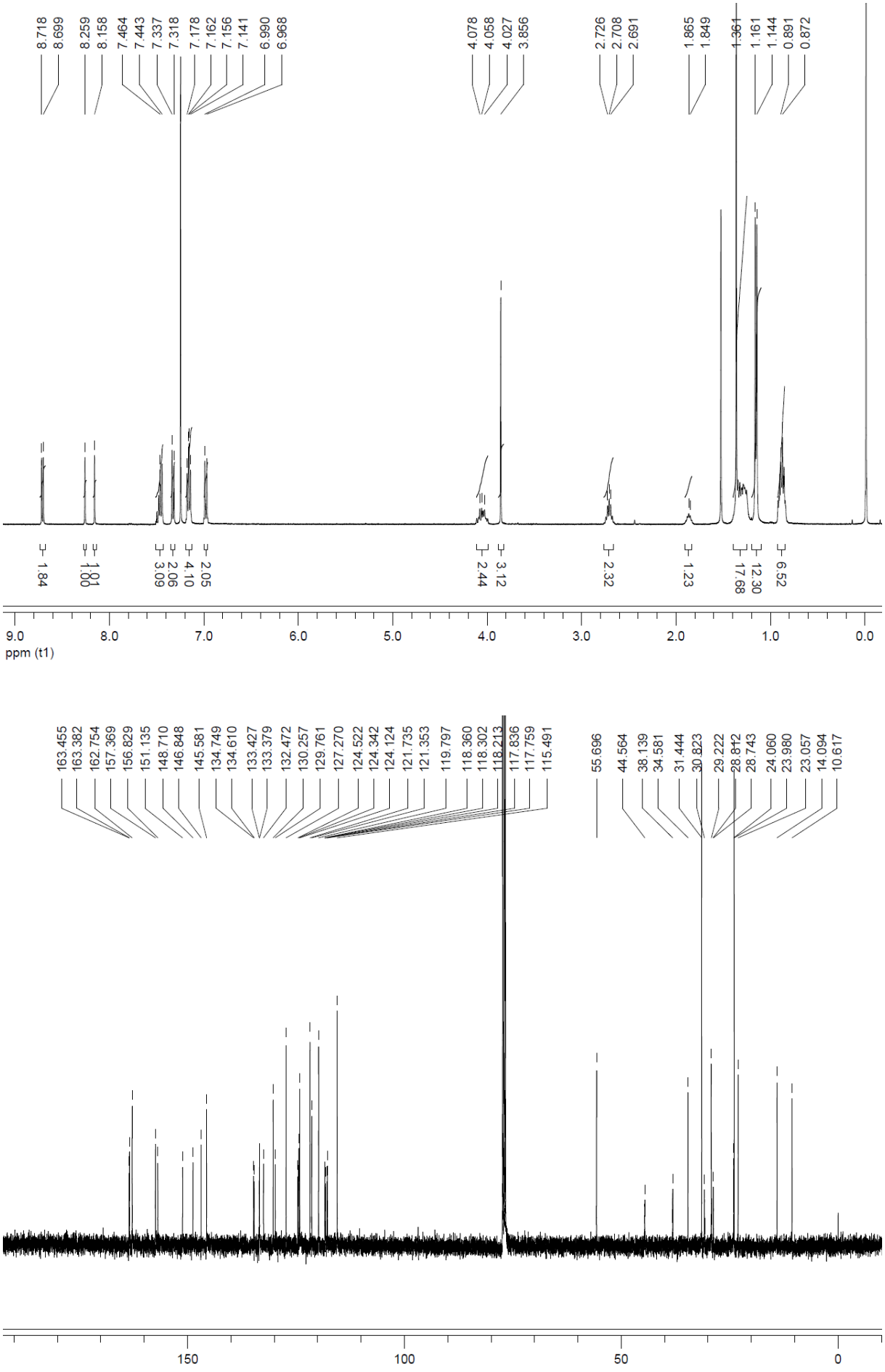


Figure S-4.13: ^{1}H and ^{13}C NMR spectra of compound **14**.

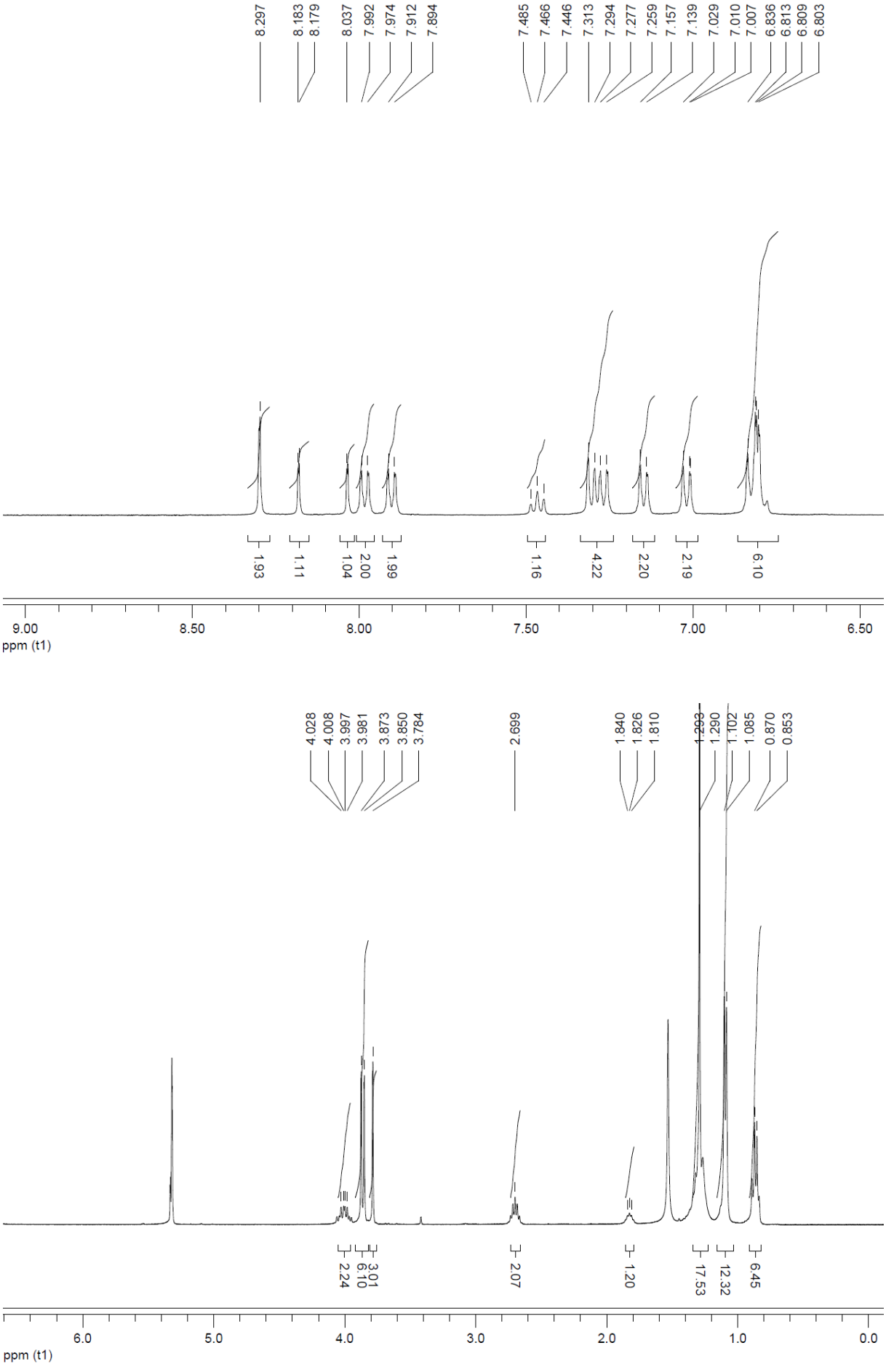


Figure S-4.14: ^{1}H NMR spectrum of compound **15** (aromatic part at the top and aliphatic part at the bottom).

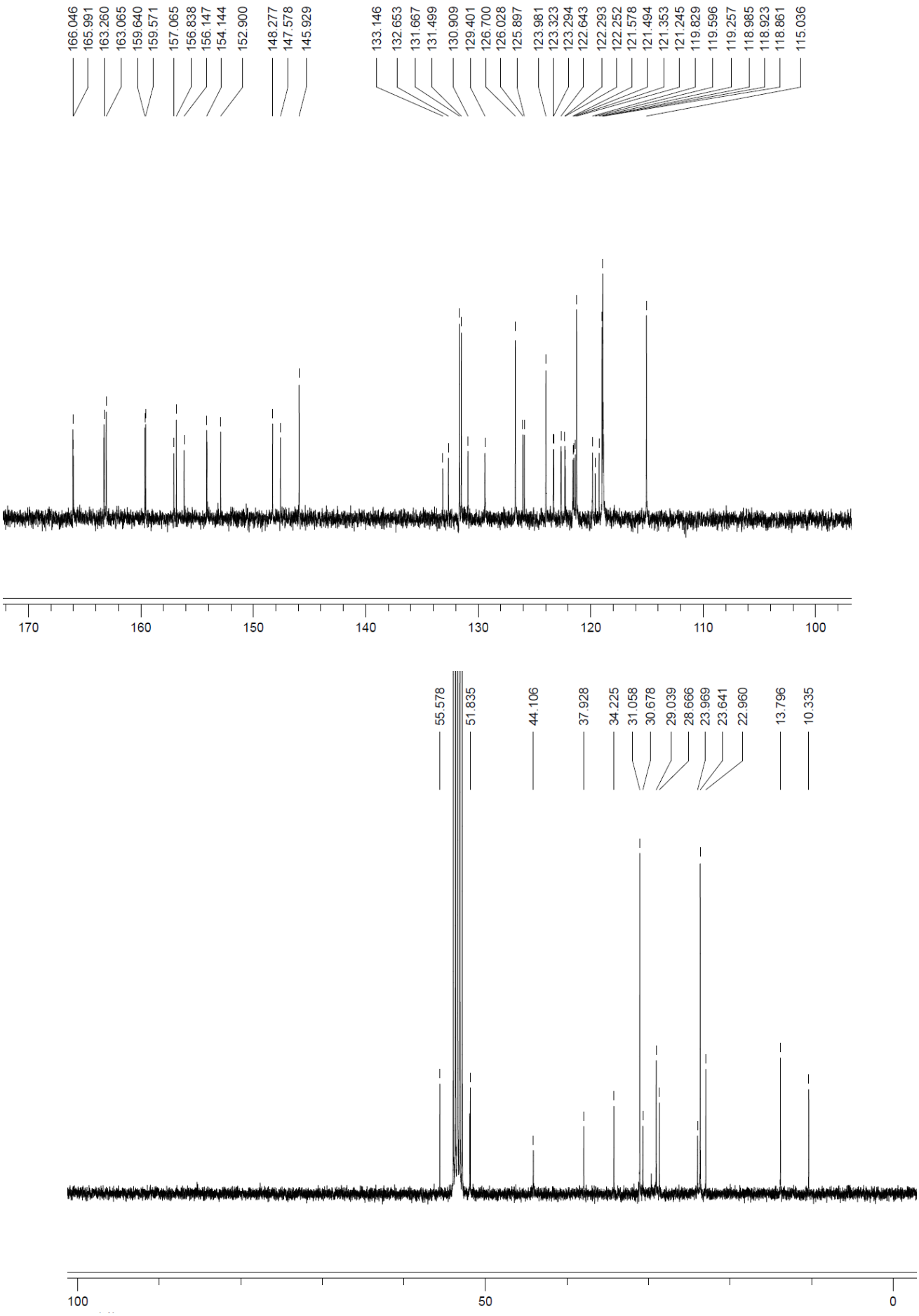
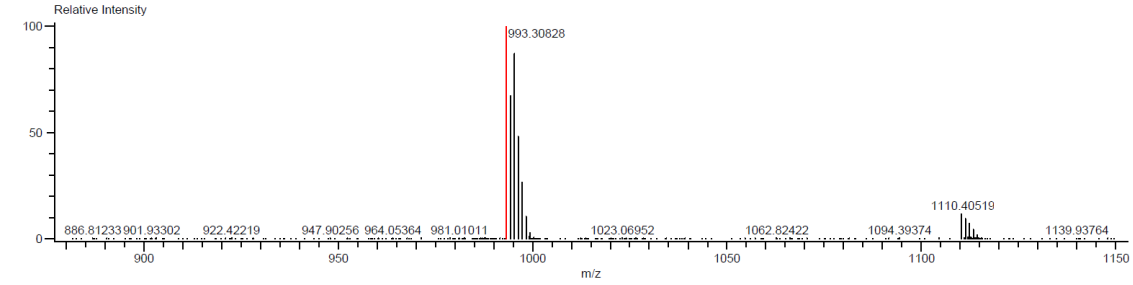


Figure S-4.15: ^{13}C NMR spectrum of compound **15** (aromatic part at the top and aliphatic part at the bottom).

Section 5. High-resolution mass spectra of newly synthesized compounds



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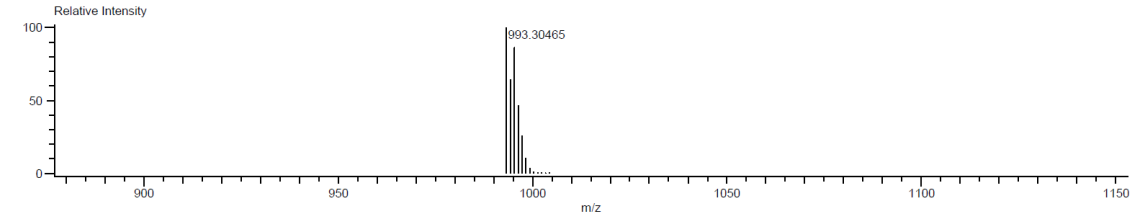
Average Mass:994.94756

Created:2/20/2018 2:15:32 AM
Nominal Mass:993
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
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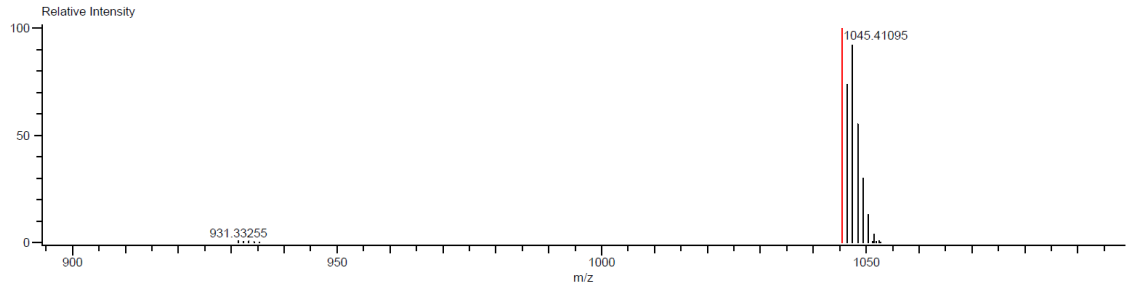
Figure S-5.1: HR mass spectrum of compound **2**.



Composition:$C_{64}H_{65}Cl_2NO_8$
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Description:

Average Mass:1047.10824

Created:2/20/2018 1:59:57 AM
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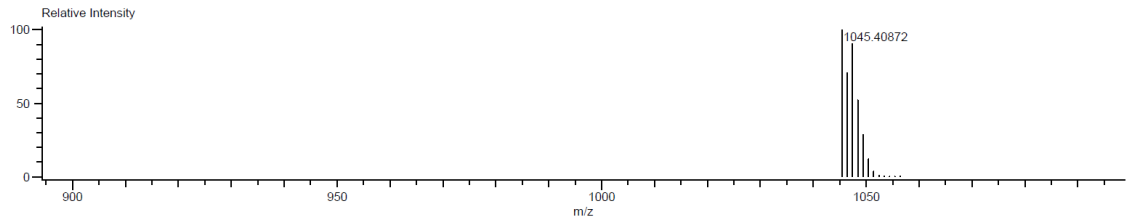
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
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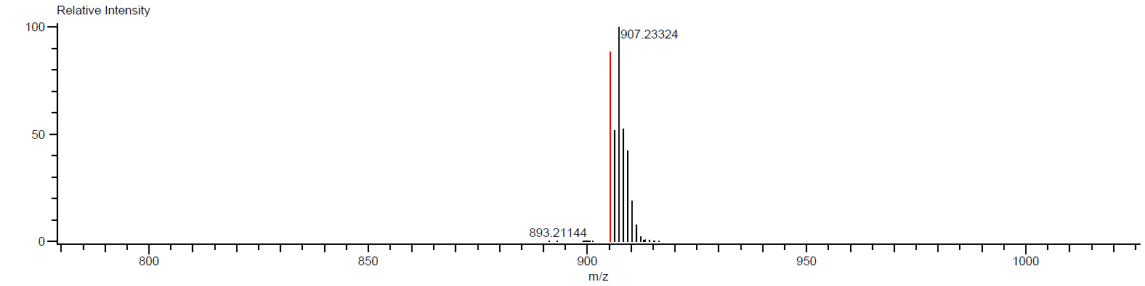
Figure S-5.2: HR mass spectrum of compound **3**.



Composition:$C_{51}H_{46}Cl_3NO_8$
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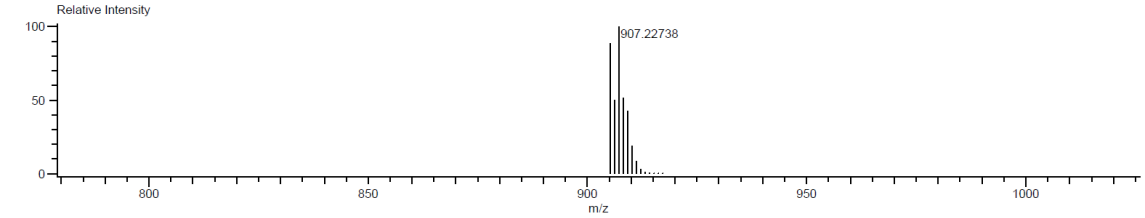
Description:

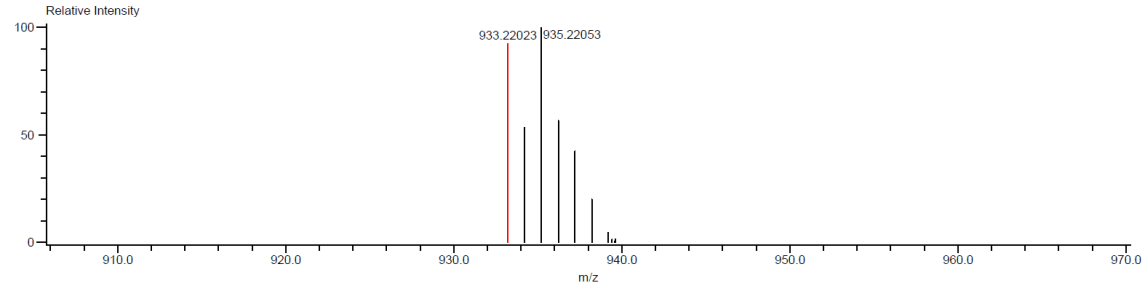
Average Mass:907.27098

Created:2/20/2018 2:29:09 AM
Nominal Mass:905
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
905.23101	802811.30	905.22890	2.33	51	46	3	1	8	28.0

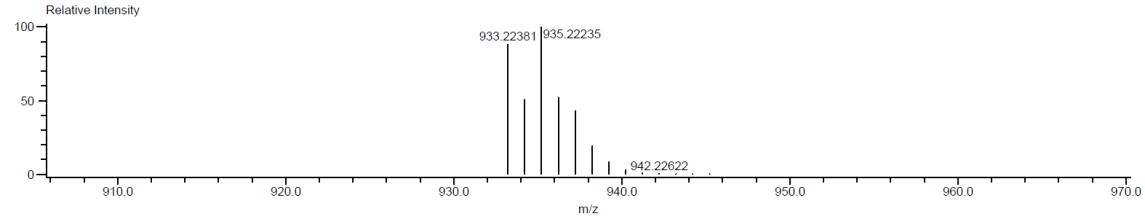
Figure S-5.3: HR mass spectrum of compound **4**.



Composition:$C_{52}H_{46}Cl_3NO_9$
Mono Isotopic Mass:933.22381
Description:

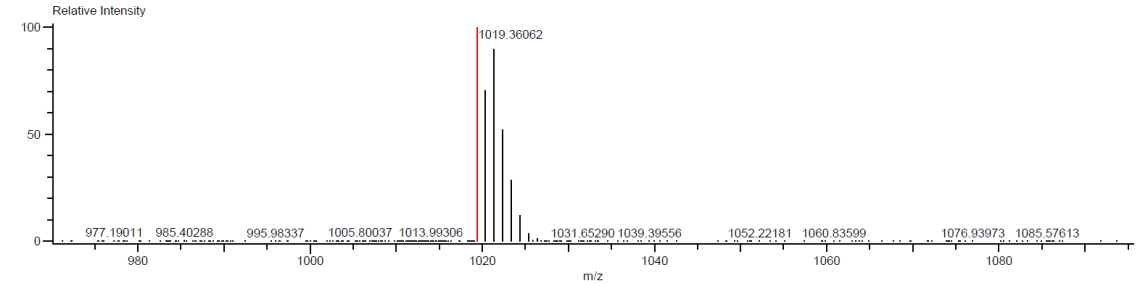
Average Mass:935.28108

Created:2/17/2018 12:01:54 AM
Nominal Mass:933
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
933.22023	43567.16	933.22381	-3.84	52	46	3	1	9	29.0

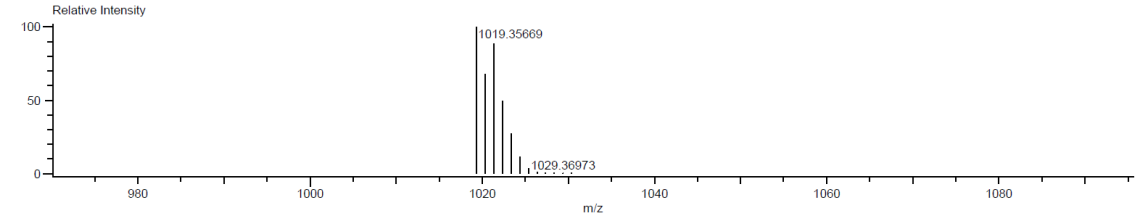
Figure S-5.4: HR mass spectrum of compound **5**.



Composition:$C_{61}H_{59}Cl_2NO_9$
Mono Isotopic Mass:1019.35669
Description:

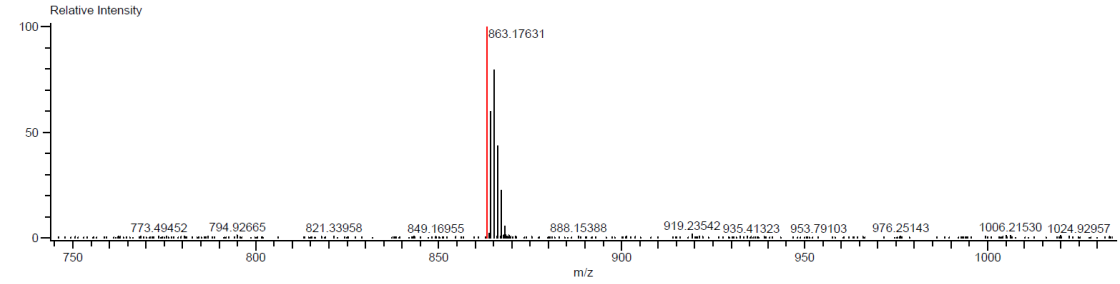
Average Mass:1021.02790

Created:2/20/2018 9:36:16 PM
Nominal Mass:1019
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
1019.36062	1763478.50	1019.35669	3.86	61	59	2	1	9	32.0

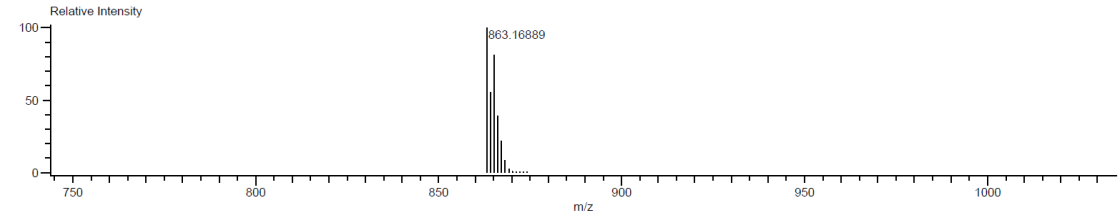
Figure S-5.5: HR mass spectrum of compound **6**.



Composition:$C_{50}H_{35}Cl_2NO_9$
Mono Isotopic Mass:863.16889
Description:

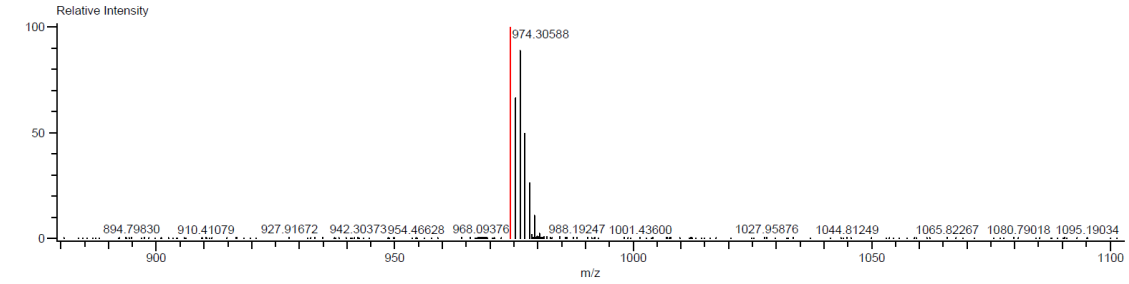
Average Mass:864.71964

Created:2/20/2018 3:46:07 AM
Nominal Mass:863
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
863.17631	80159.63	863.18414	-9.07	54	35	2	1	6	37.0
		863.17827	-2.26	61	31	2	1	1	46.0

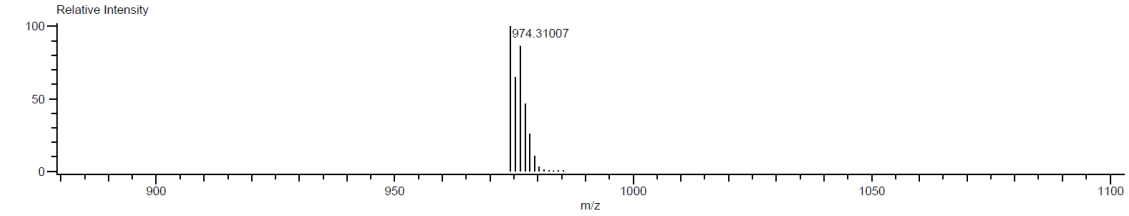
Figure S-5.6: HR mass spectrum of compound **7**.



Composition:$C_{58}H_{52}Cl_2N_2O_8$
Mono Isotopic Mass:974.31007
Description:

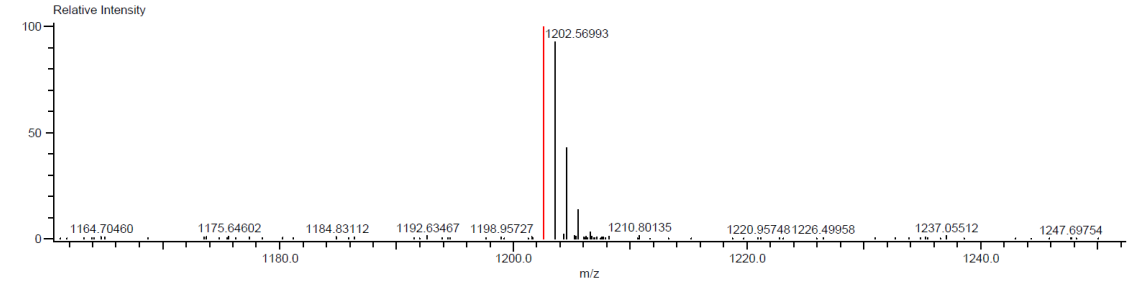
Average Mass:975.94756

Created:2/20/2018 8:30:57 PM
Nominal Mass:974
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
974.30588	133695.25	974.31007	-4.30	58	52	2	2	8	33.0

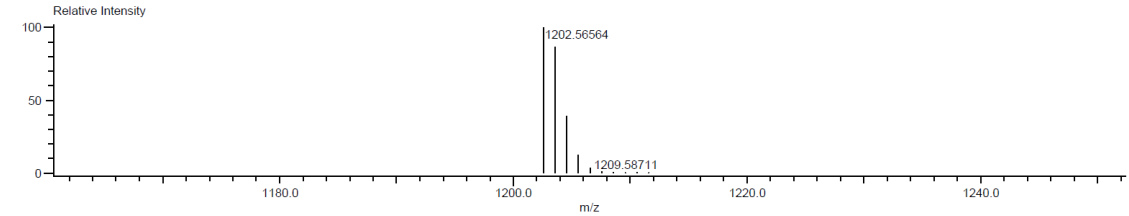
Figure S-5.7: HR mass spectrum of compound **8**.



Composition:$C_{78}H_{78}N_2O_{10}$
Mono Isotopic Mass:1202.56564
Description:

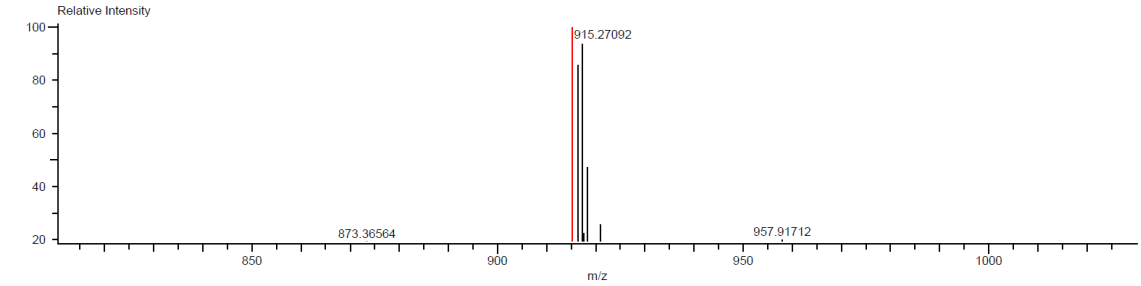
Average Mass:1203.46140

Created:2/20/2018 10:06:14 PM
Nominal Mass:1202
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{14}N	^{16}O	Unsaturation Number
1202.56993	63296.13	1202.56564	3.57	78	78	2	10	41.0

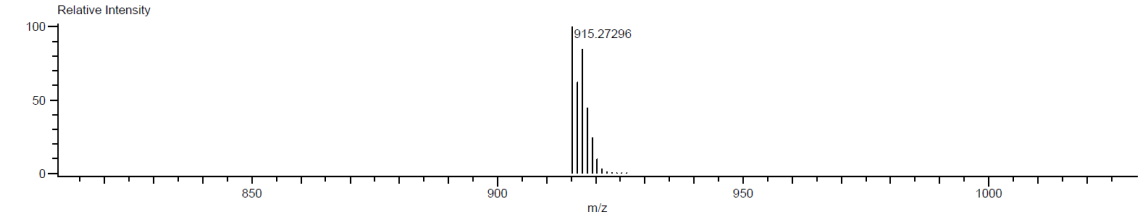
Figure S-5.8: HR mass spectrum of compound **9**.



Composition:$C_{56}H_{47}Cl_2NO_7$
Mono Isotopic Mass:915.27296
Description:

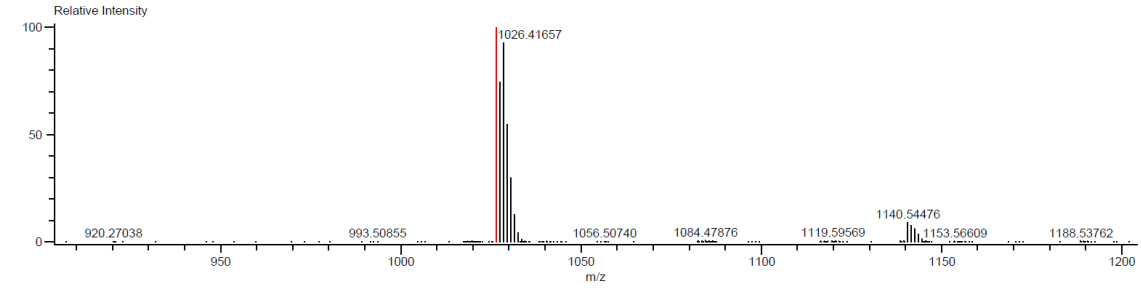
Average Mass:916.88032

Created:2/20/2018 2:49:43 AM
Nominal Mass:915
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
915.27092	3682.00	915.27296	-2.22	56	47	2	1	7	33.0

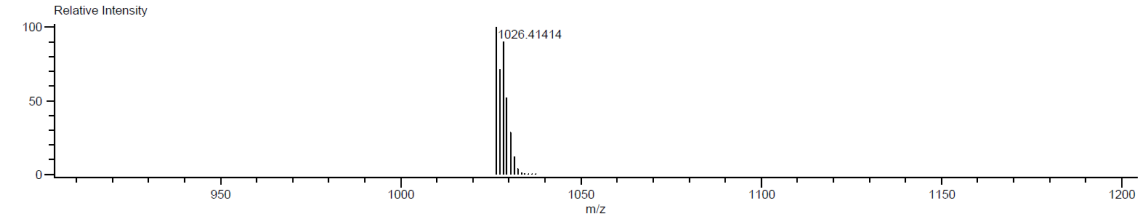
Figure S-5.9: HR mass spectrum of compound **10**.



Composition:$C_{64}H_{64}Cl_2N_2O_6$
Mono Isotopic Mass:1026.41414
Description:

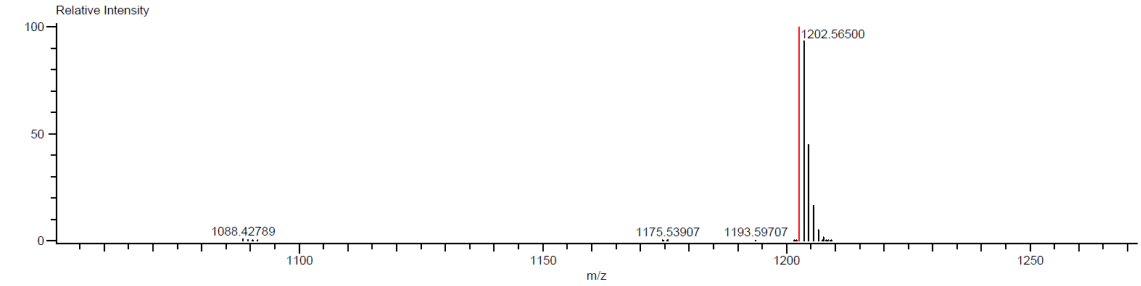
Average Mass:1028.10824

Created:2/20/2018 3:53:21 AM
Nominal Mass:1026
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
1026.41657	785473.24	1026.41414	2.37	64	64	2	2	6	33.0
		1026.42001	-3.35	57	68	2	2	11	24.0
		1026.42589	-9.08	50	72	2	2	16	15.0

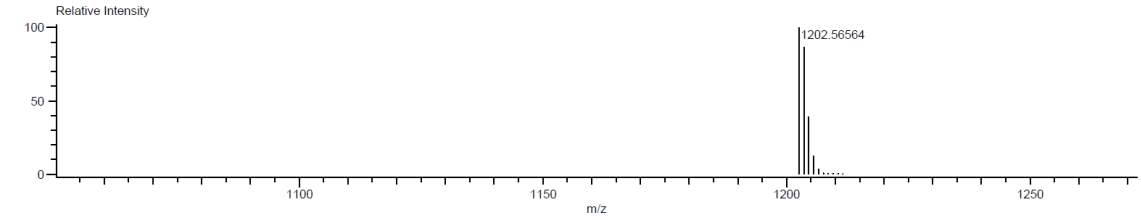
Figure S-5.10: HR mass spectrum of compound **11**.



Composition:$C_{78}H_{78}N_2O_{10}$
Mono Isotopic Mass:1202.56564
Description:

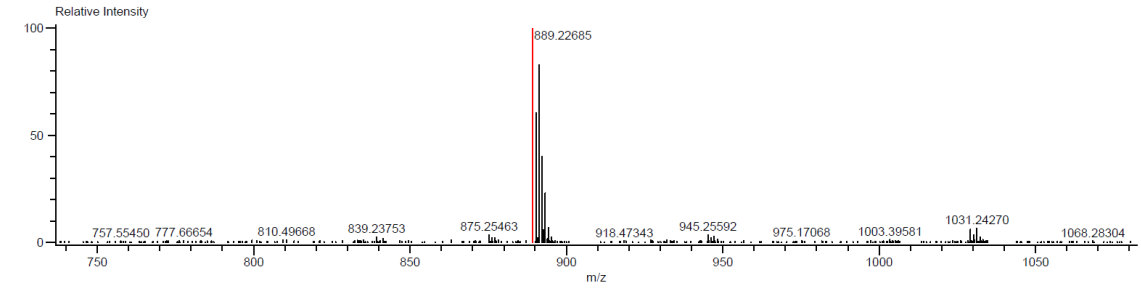
Average Mass:1203.46140

Created:2/20/2018 9:50:32 PM
Nominal Mass:1202
Created by:Accutof



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{14}N	^{16}O	Unsaturation Number
1202.56500	250163.00	1202.56564	-0.54	78	78	2	10	41.0

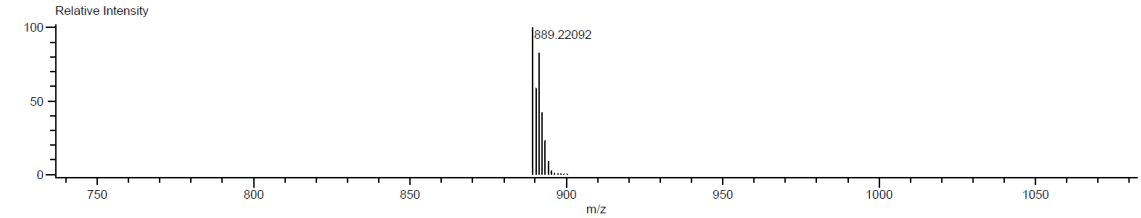
Figure S-5.11: HR mass spectrum of compound **12**.



Composition:$C_{53}H_{41}Cl_2NO_8$
Mono Isotopic Mass:889.22092
Description:

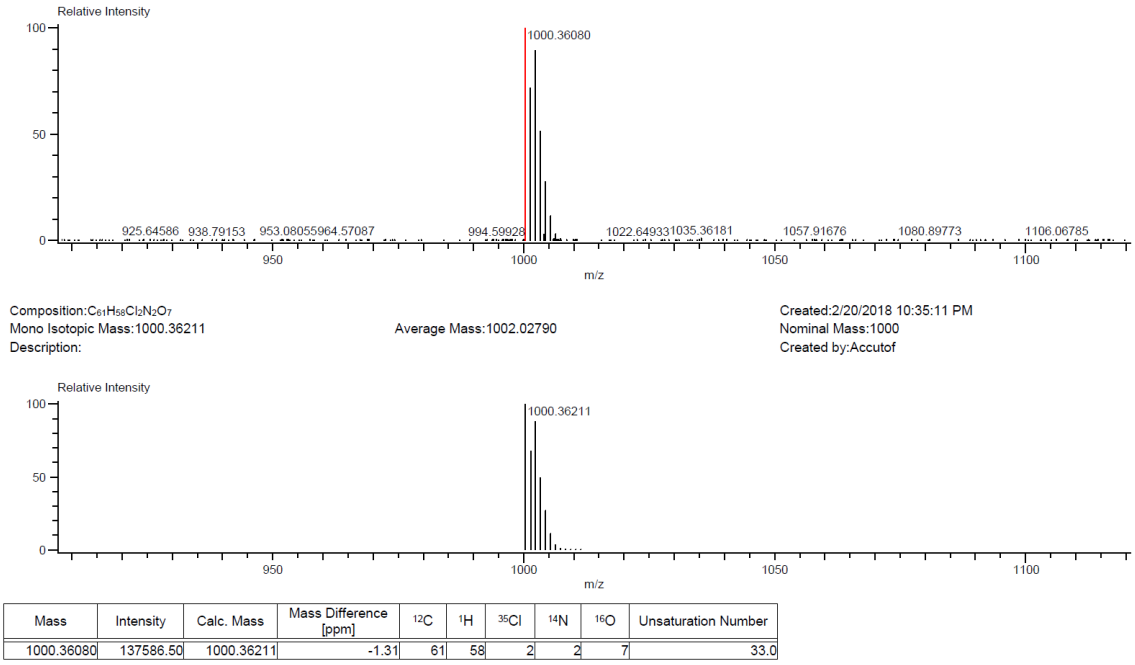
Average Mass:890.79998

Created:2/20/2018 10:19:20 PM
Nominal Mass:889
Created by:Accutof



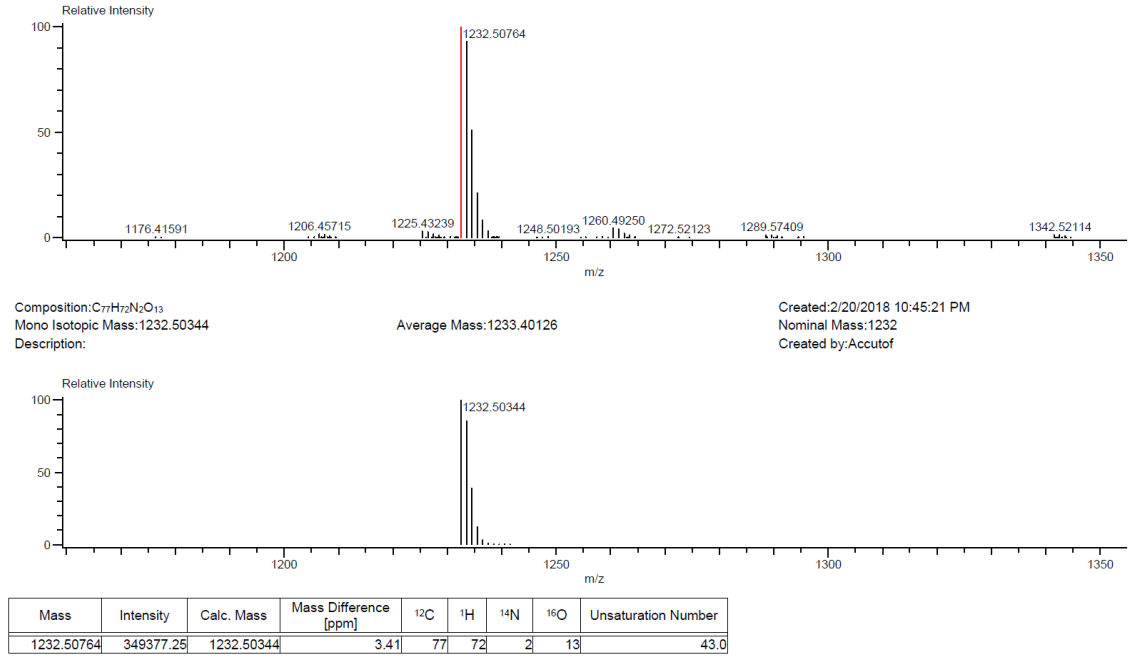
Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
889.22685	72391.66	889.22092	6.67	53	41	2	1	8	33.0
		889.23350	-7.47	54	43	2		8	32.5
		889.22360	3.66	56	39	2	2	5	37.5
		889.22762	-0.87	61	39	2		3	41.5
		889.23030	-3.88	64	37	2	1		46.0

Figure S-5.12: HR mass spectrum of compound **13**.



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{35}Cl	^{14}N	^{16}O	Unsaturation Number
1000.36080	137586.50	1000.36211	-1.31	61	58	2	2	7	33.0

Figure S-5.13: HR mass spectrum of compound **14**.



Mass	Intensity	Calc. Mass	Mass Difference [ppm]	^{12}C	^{1}H	^{14}N	^{16}O	Unsaturation Number
1232.50764	349377.25	1232.50344	3.41	77	72	2	13	43.0

Figure S-5.14: HR mass spectrum of compound **15**.