Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Covalently Linked *meso*-Tetraaryl Triphyrin(2.1.1)-Ferrocene(s) Conjugates: Synthesis and Properties

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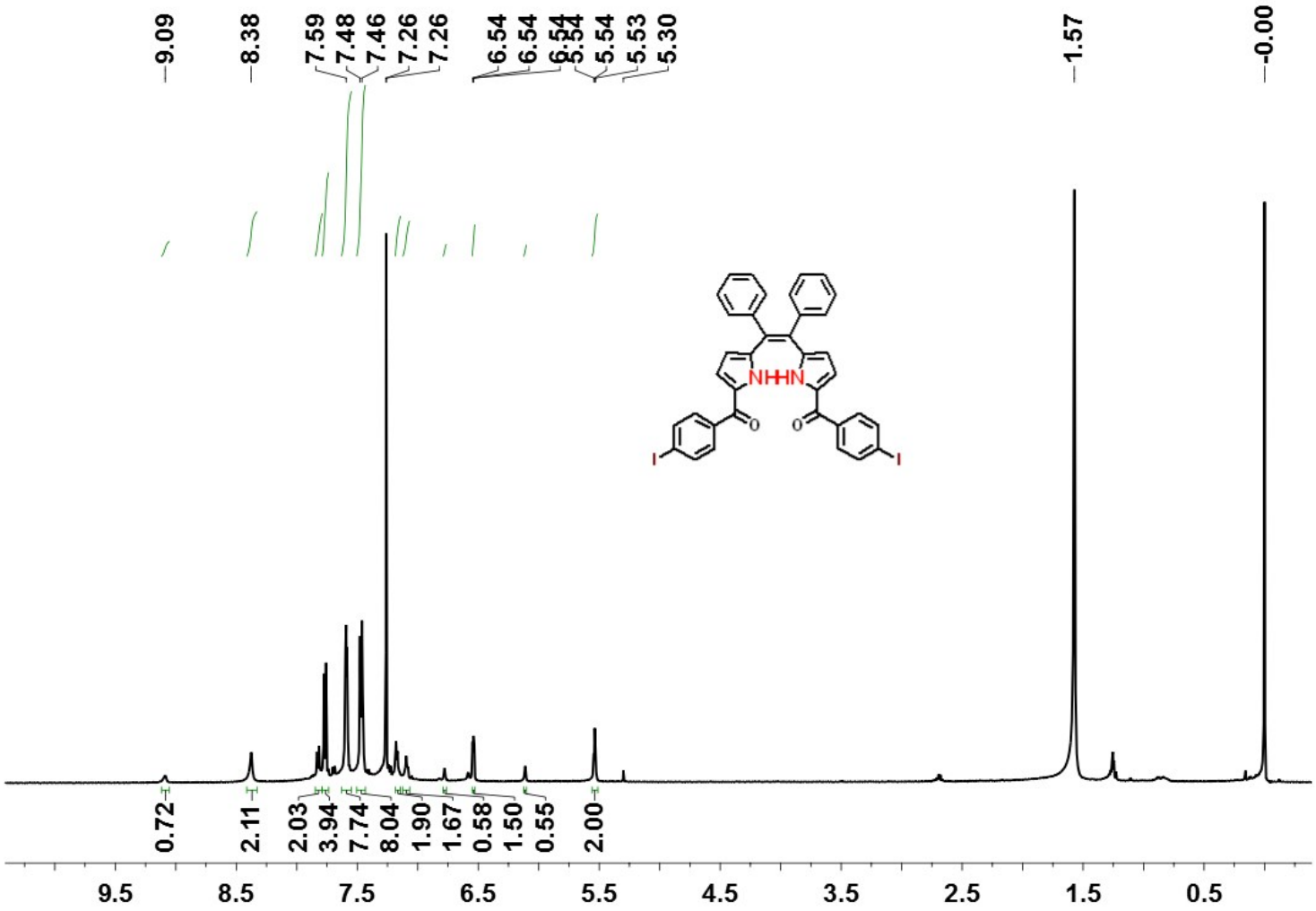

Figure S1. ^{1}H NMR spectrum of the compound **5** (*E/Z* mixture) recorded in $CDCl_3$.

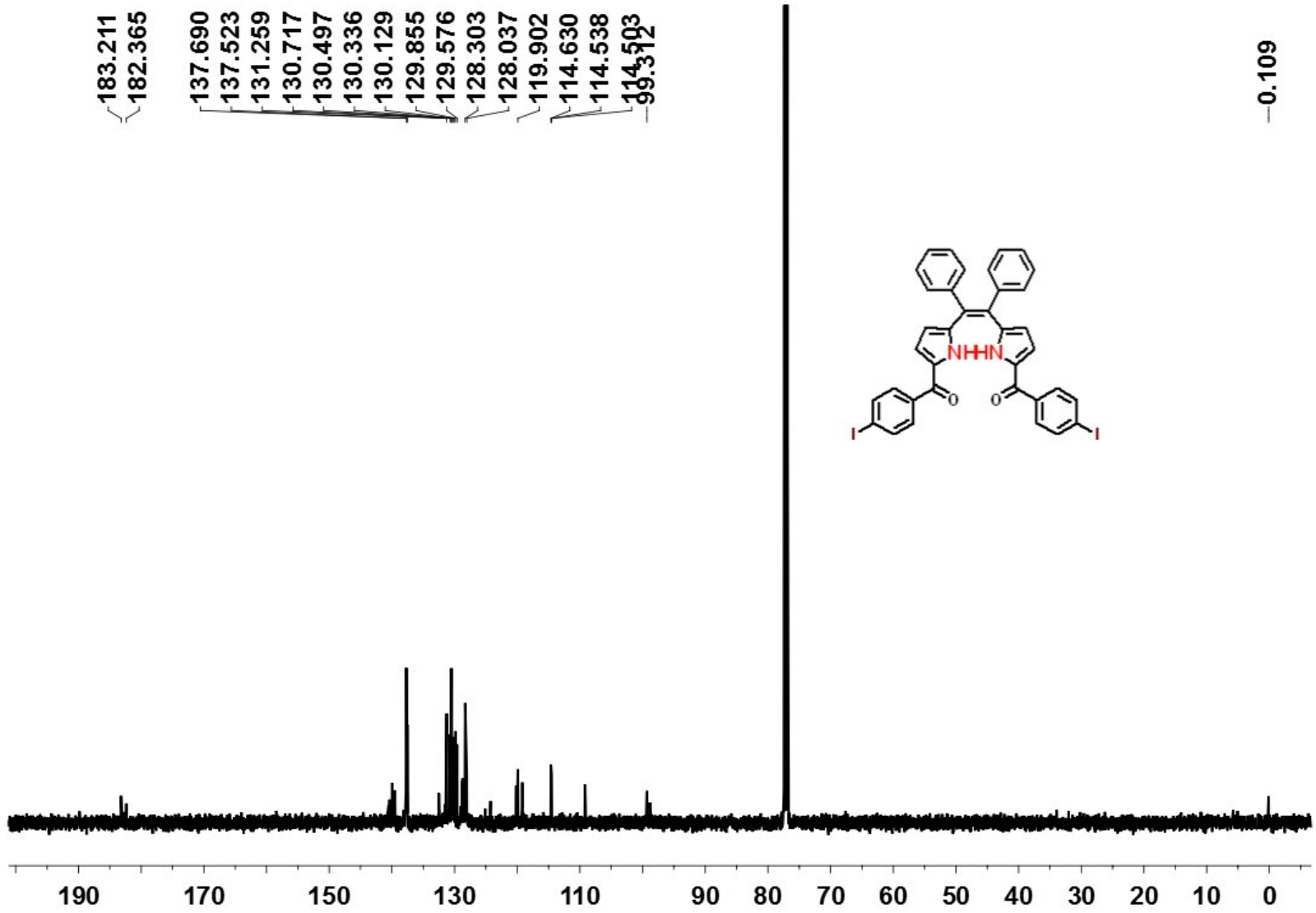

Figure S2. ^{13}C NMR spectrum of the compound **5** (*E/Z* mixture) recorded in $CDCl_3$.

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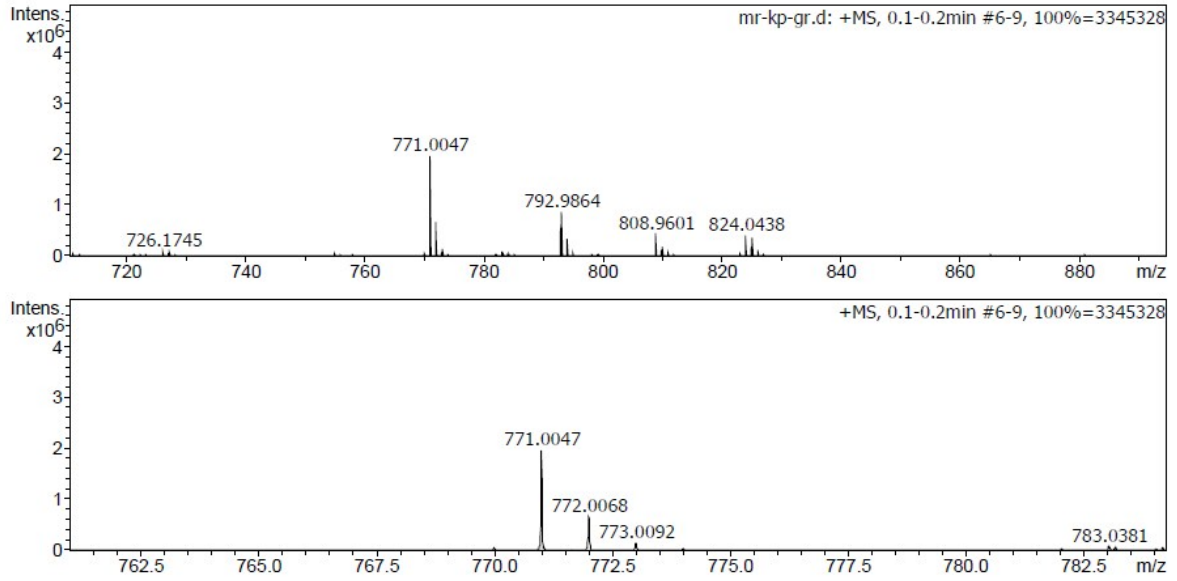
Analysis Info

Analysis Name	D:\Data\DEC 2018\mr-kp-gr.d	Acquisition Date	12/27/2018 3:51:48 PM
Method	Tune_pos_NAICSI-1500B.m	Operator	MR-IN
Sample Name	mr-kp-gr	Instrument	maXis impact 282001.00081
Comment	36H24I2N2O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
771.0047	1	C36H25I2N2O2	771.0000	-6.2	29.1	1	100.00	24.5	even	ok

Figure S3. HR mass spectrum of the compound **5** (*E/Z* mixture).

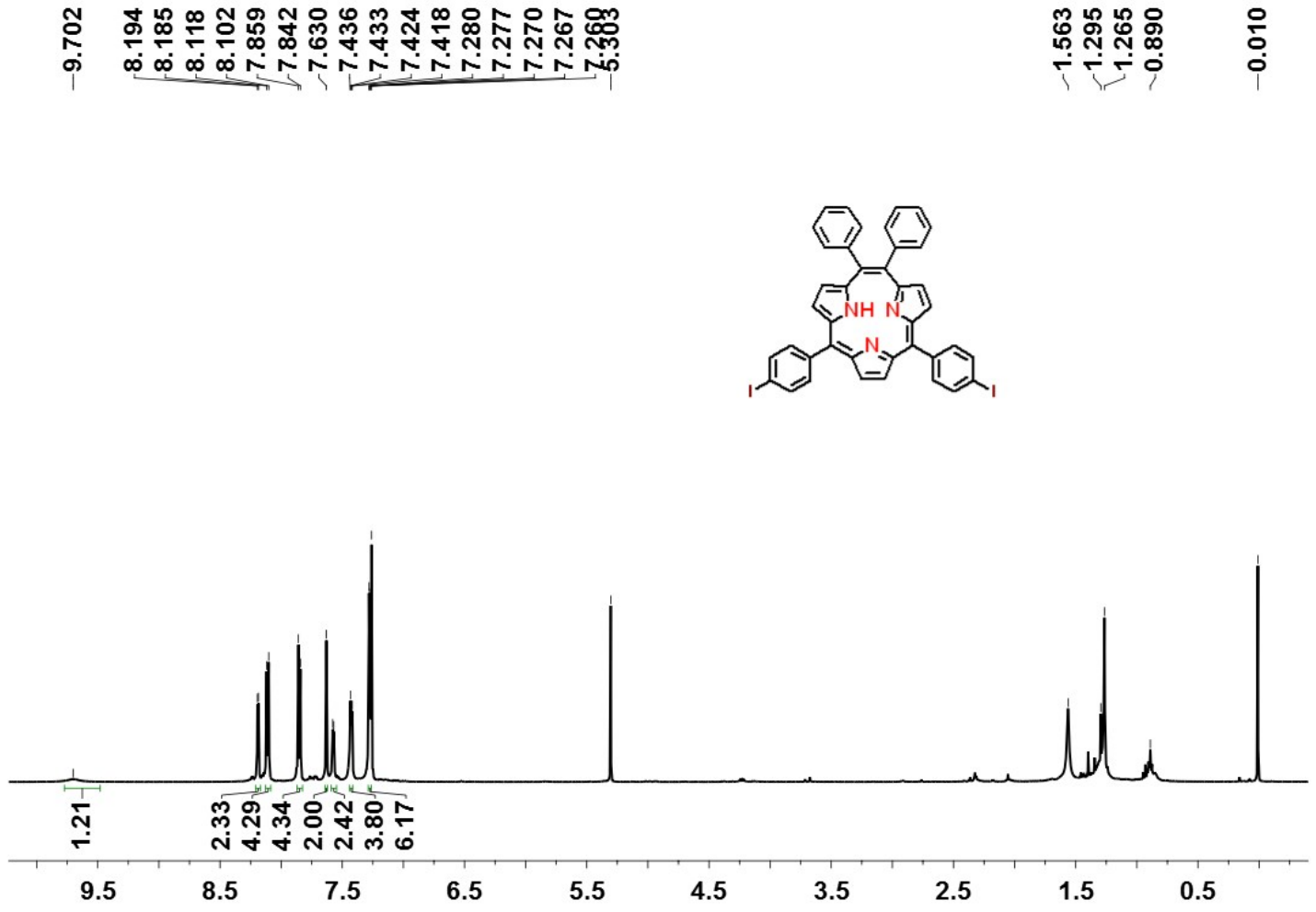


Figure S4. ^{1}H NMR spectrum of the compound **6** recorded in $CDCl_3$.

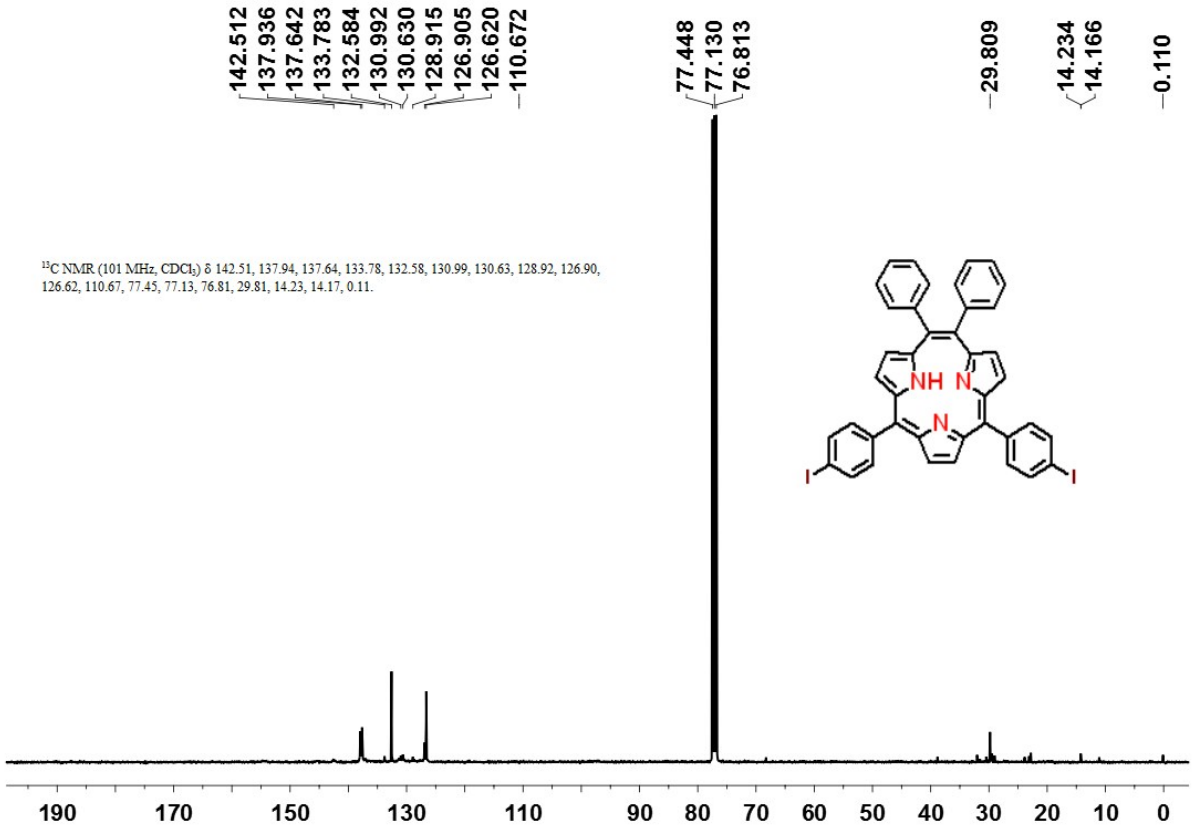


Figure S5. ^{13}C NMR spectrum of the compound **6** recorded in $CDCl_3$.

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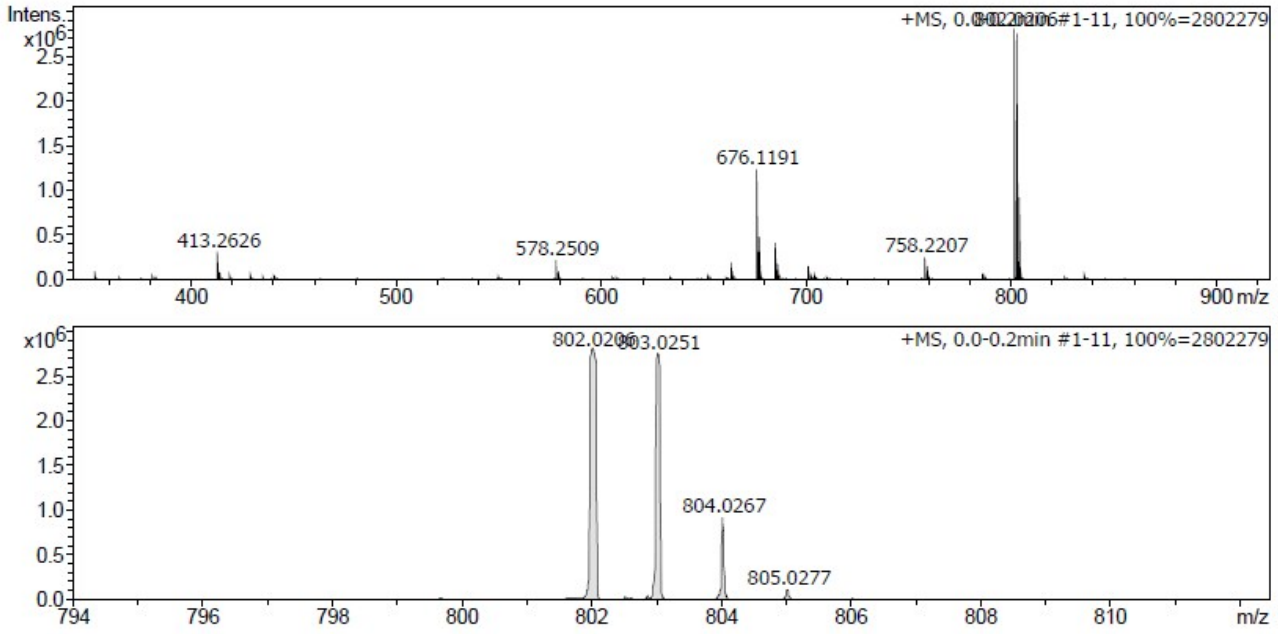
Analysis Info

Analysis Name	D:\Data\FEB 2019\MR-KP-DI-IODO.d	Acquisition Date	2/7/2019 1:25:46 PM
Method	Tune_pos_NAICSI-1500.m	Operator	MR OUT
Sample Name	MR-KP-DI-IODO	Instrument	maXis impact 282001.00081
Comment	C40H25I2N3		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
802.0206	1	C40H26I2N3	802.0211	0.5	290.7	1	100.00	28.5	even	ok

Figure S6. HR mass spectrum of the compound **6**.

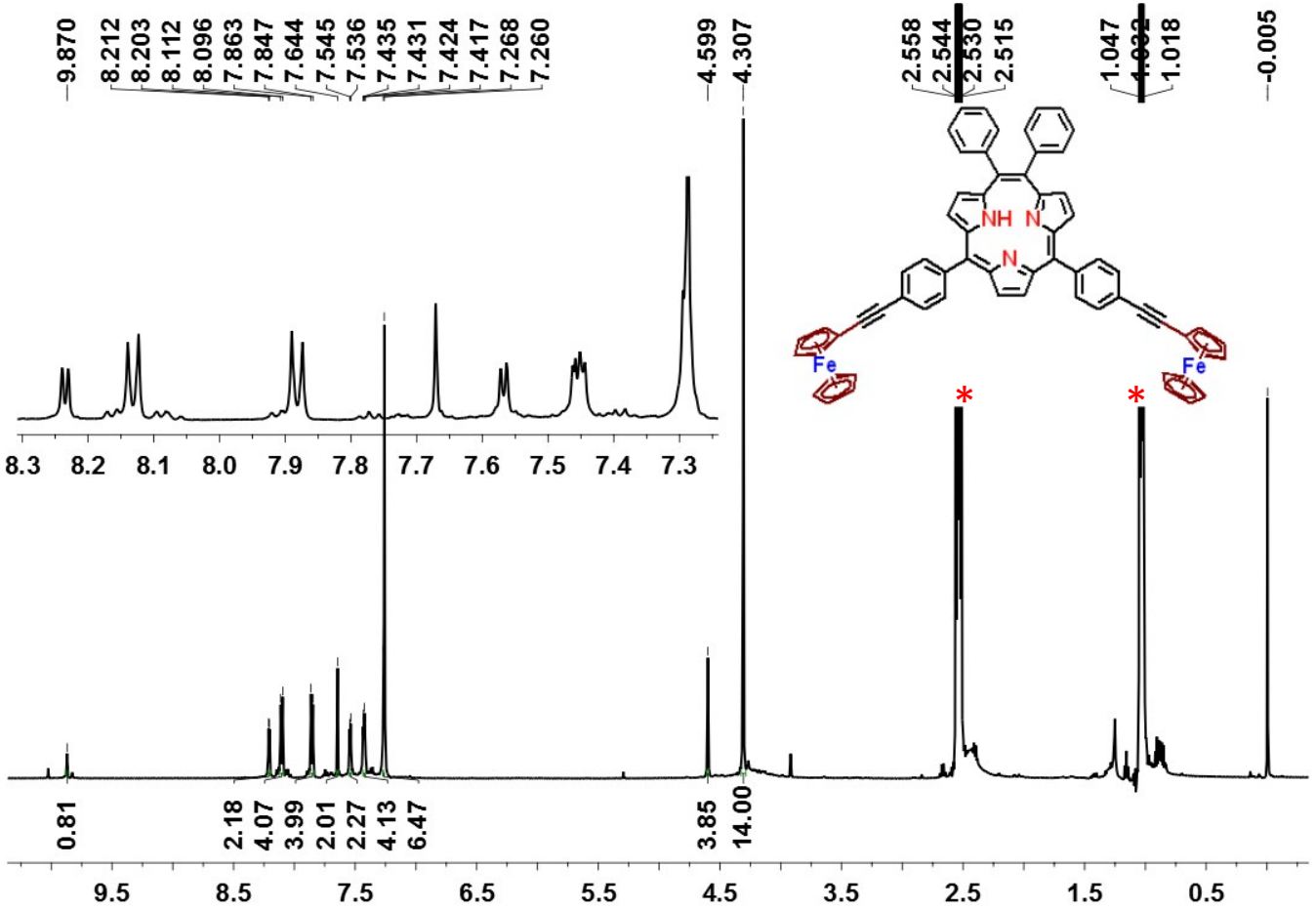


Figure S7. ^{1}H NMR spectrum of the triad **2** recorded in $CDCl_3$; Peaks marked with asterisk (*) were due to triethyl amine added during experiment to avoid protonation of the macrocycle.

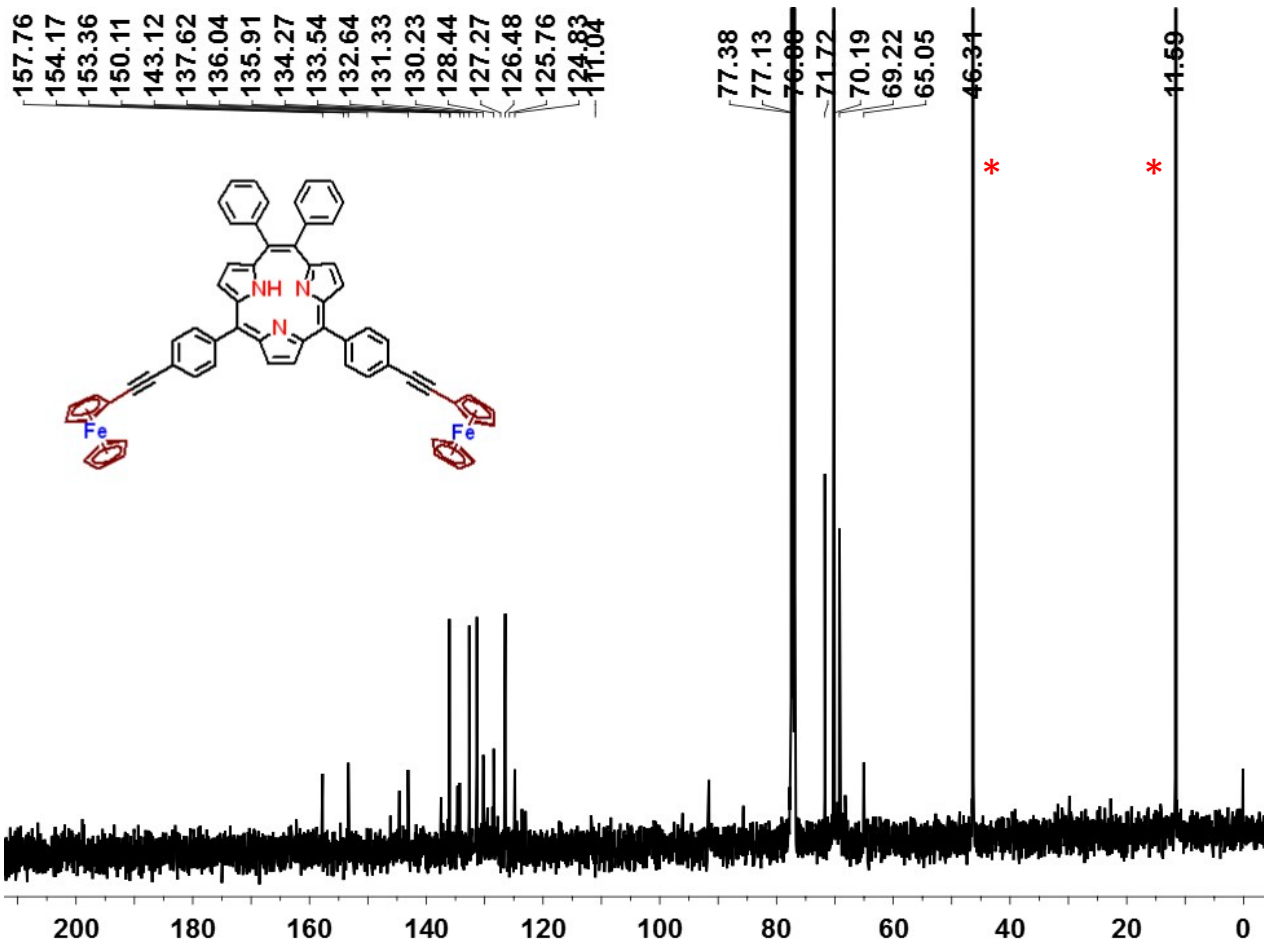


Figure S8. ^{13}C NMR spectrum of the triad **2** recorded in $CDCl_3$; Peaks marked with asterisk (*) were due to triethyl amine added during experiment to avoid protonation of the macrocycle.

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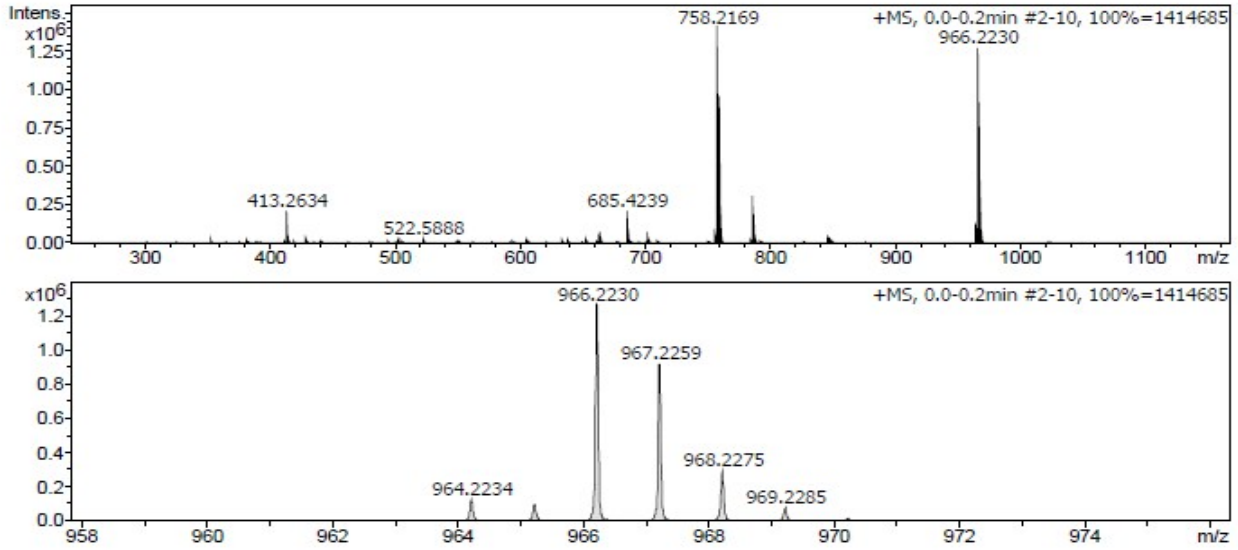
Analysis Info

Analysis Name	D:\Data\FEB 2019\MR-KP-FE-TRIAD-RE1.d	Acquisition Date	2/7/2019 1:04:51 PM
Method	Tune_pos_NAICSI-1500.m	Operator	MR OUT
Sample Name	MR-KP-FE-TRIAD-RE1	Instrument	maXis impact 282001.00081
Comment	C64H43N3Fe2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
966.2230	1	C64H44Fe2N3	966.2232	-0.2	20.0	1	100.00	44.5	even	ok
	2	C61H44Fe2N3O2	962.2130	-1.0	560.4	2	0.00	41.5	even	ok

Figure S9. HR mass spectrum of the triad **2**.

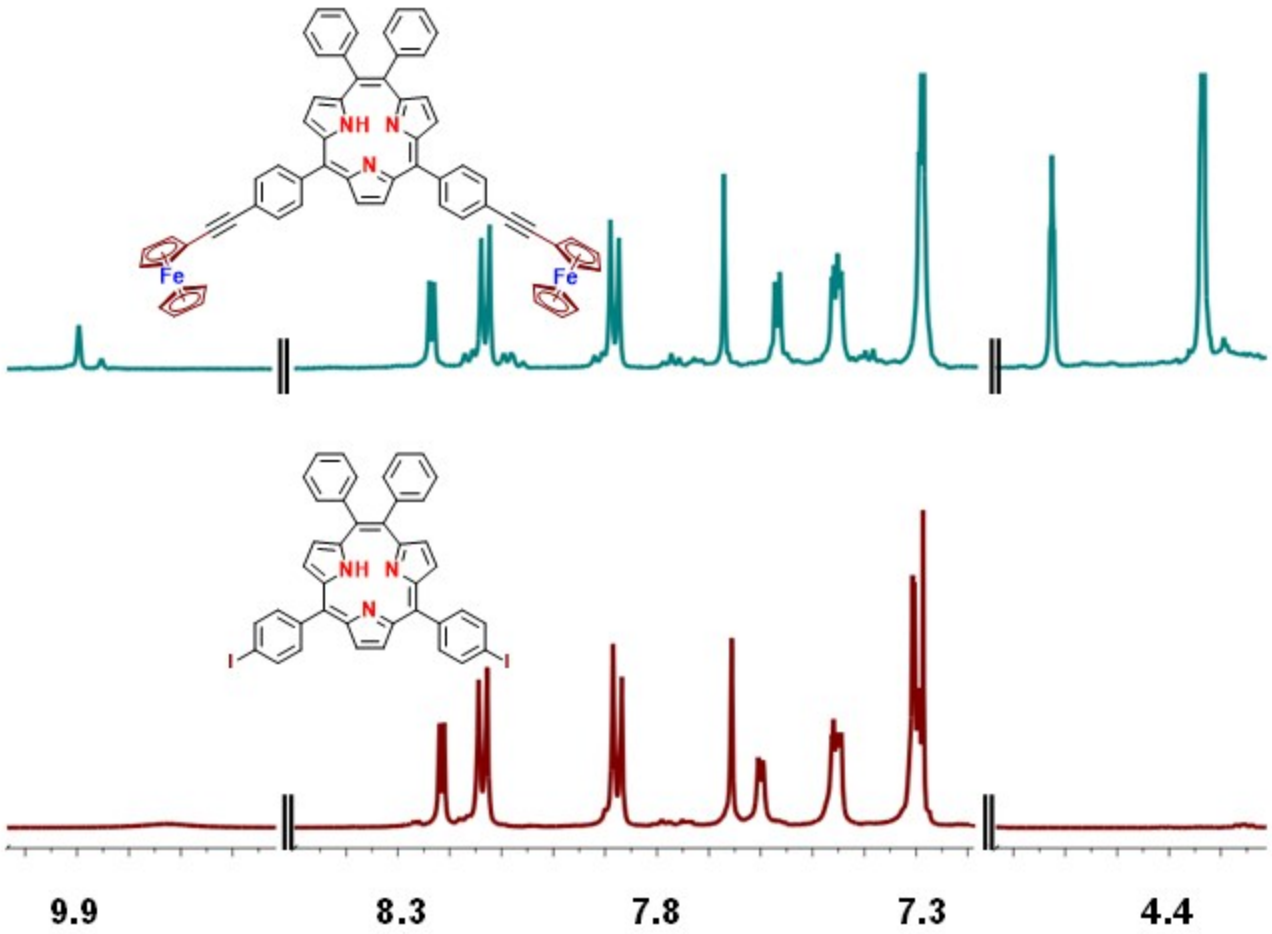


Figure S10. Comparison of partial ^{1}H NMR spectra of the compound **6** and triad **2** recorded in $CDCl_3$.

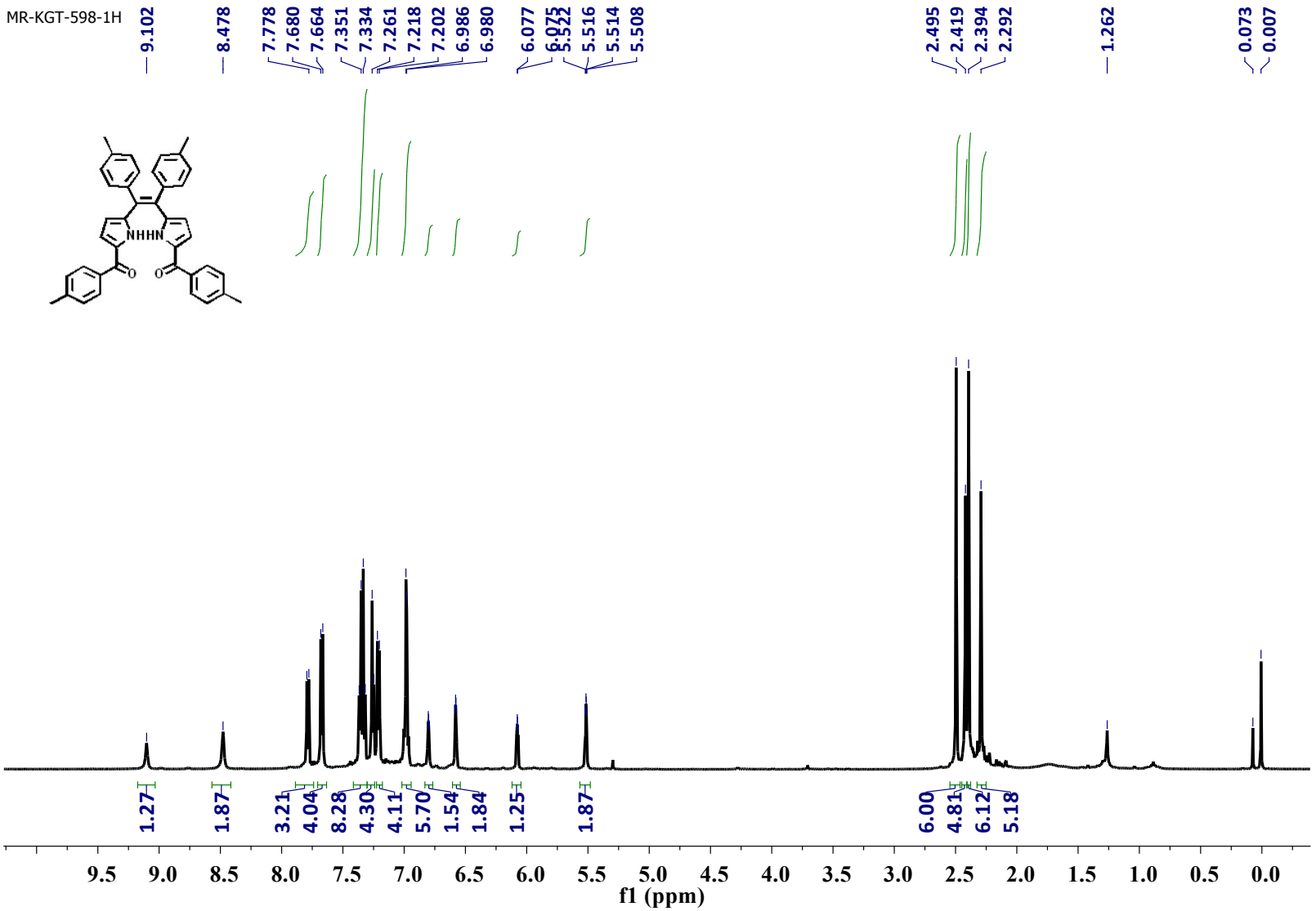


Figure S11. ^{1}H NMR spectrum of the compound **8** recorded in $CDCl_3$.

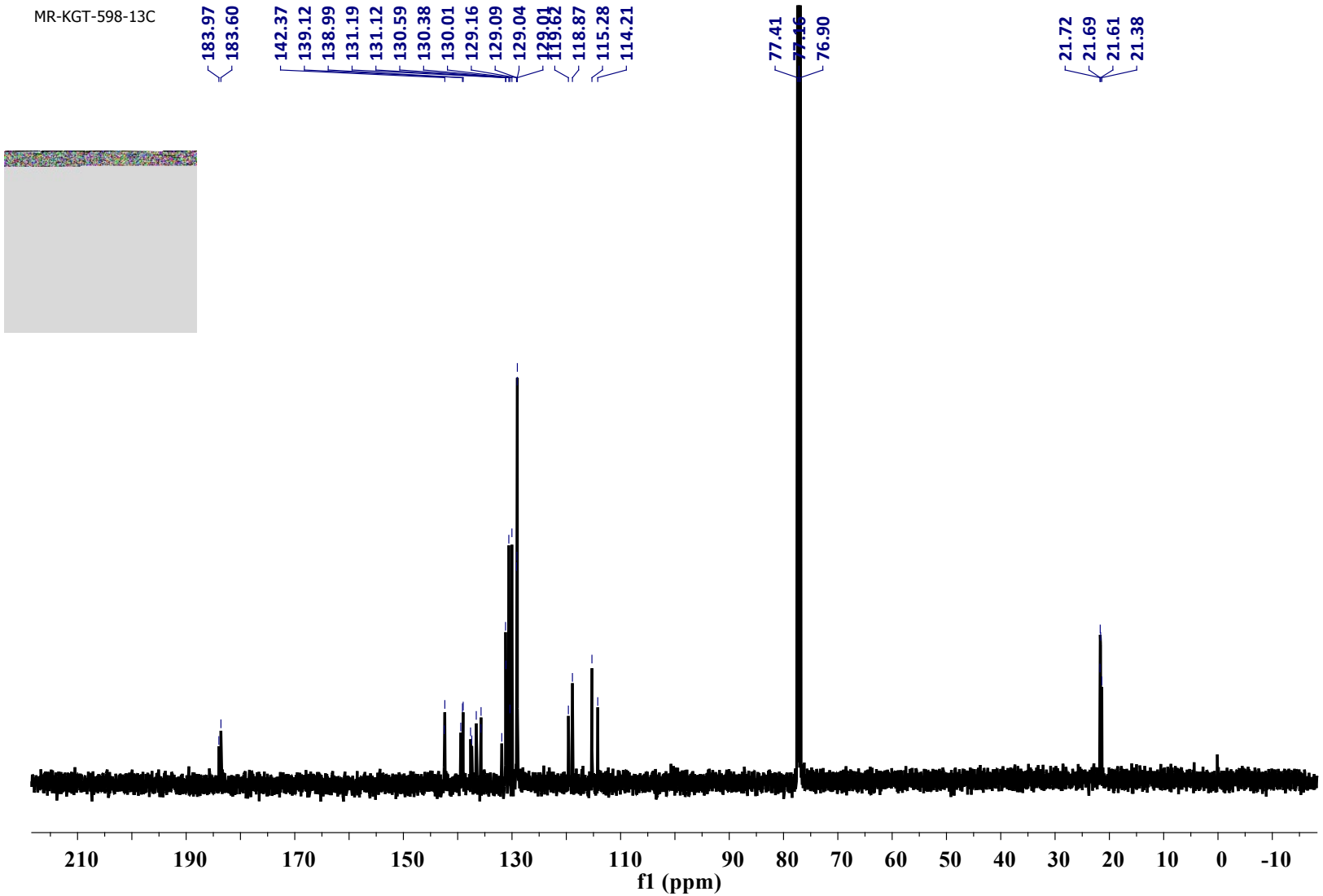
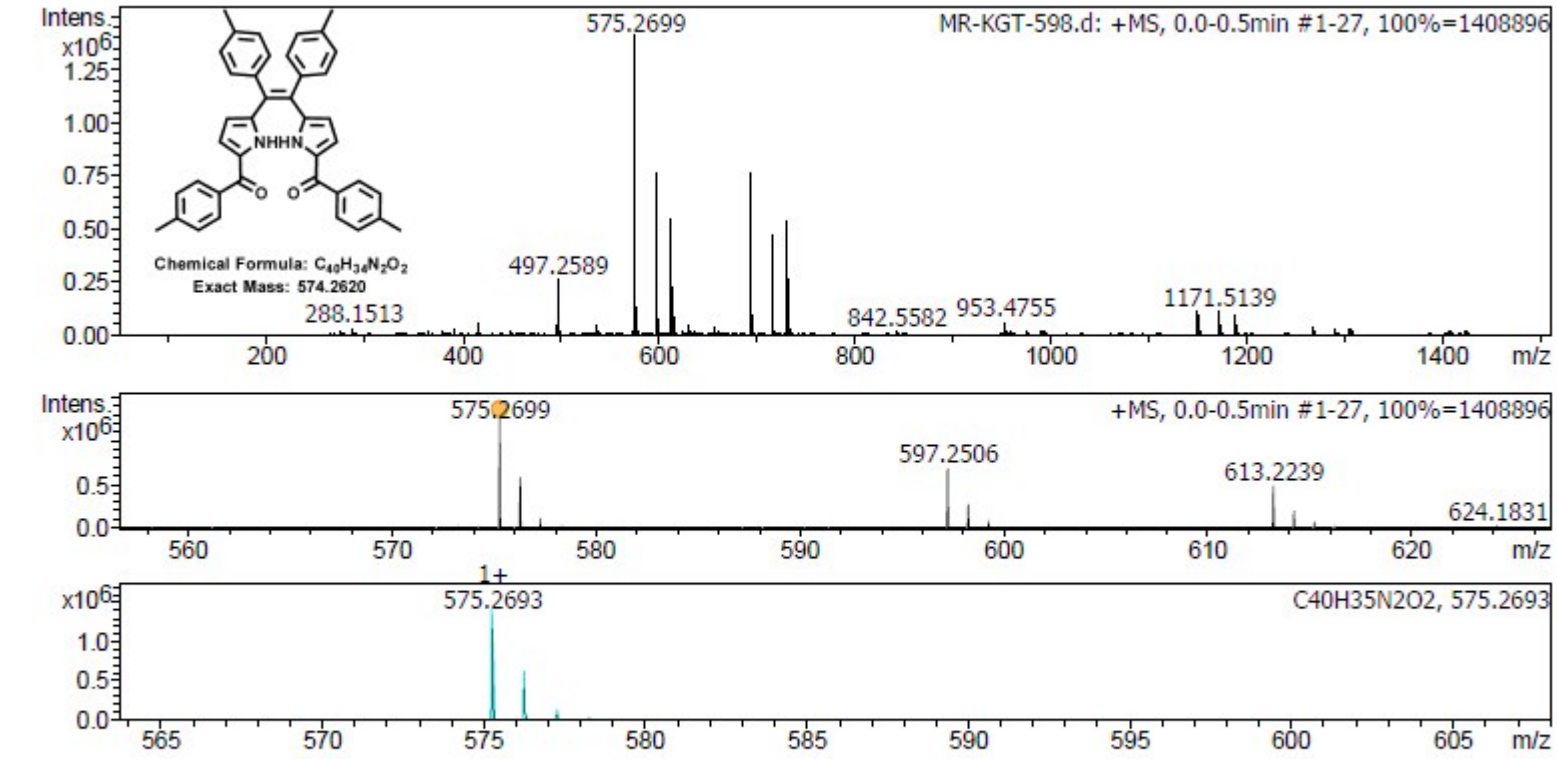


Figure S12. ^{13}C NMR spectrum of the compound **8** recorded in $CDCl_3$.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
575.2699	1	C40H35N2O2	575.2693	1.1	9.7	1	100.00	24.5	even	ok

Figure S13. HR mass spectrum of the compound **8**

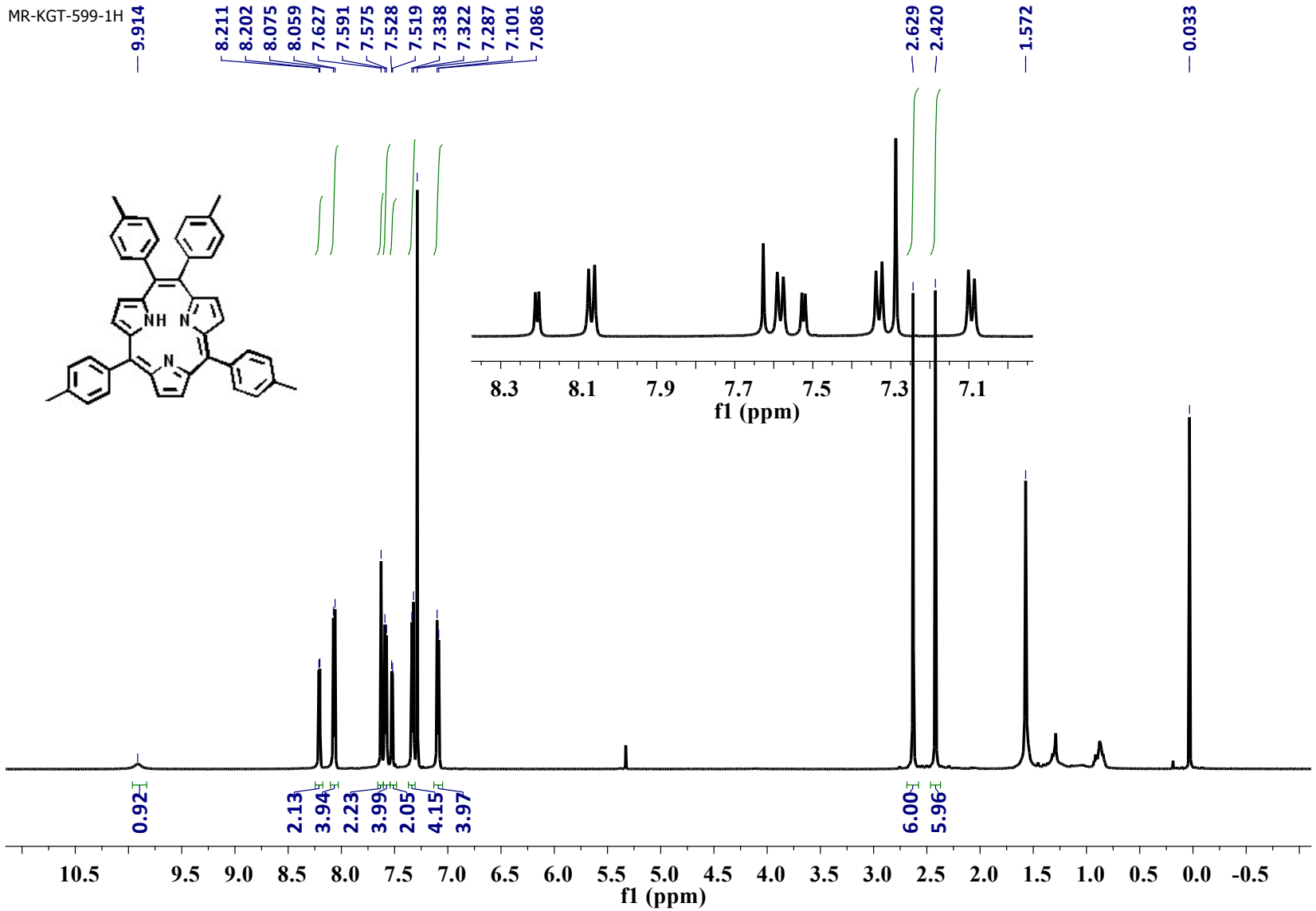


Figure S14. ^{1}H NMR spectrum of the compound **9** recorded in $CDCl_3$.

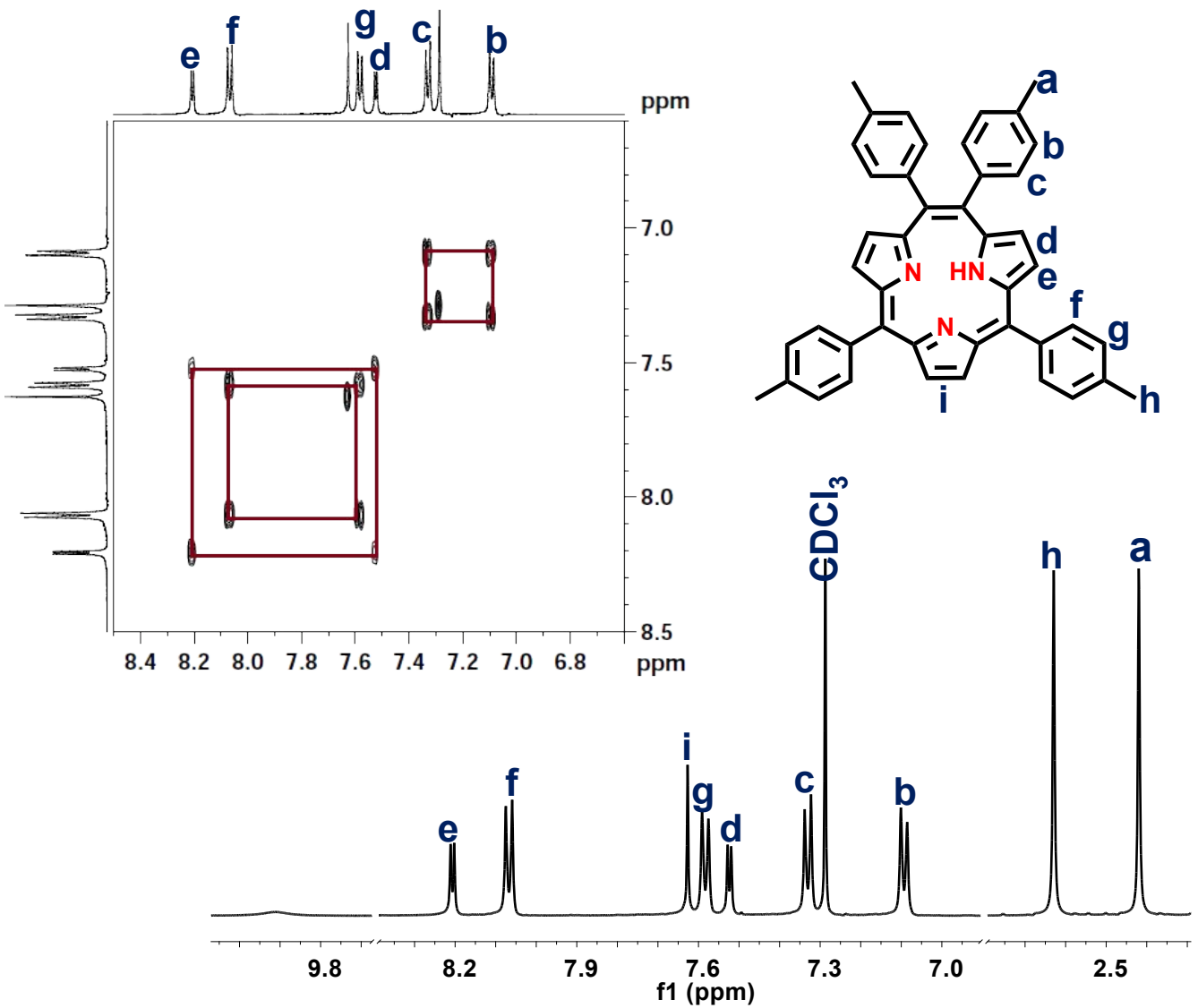


Figure S15. Partial ^{1}H (a) and ^{1}H-^{1}H (b) NMR spectra of the compound **9** recorded in $CDCl_3$.

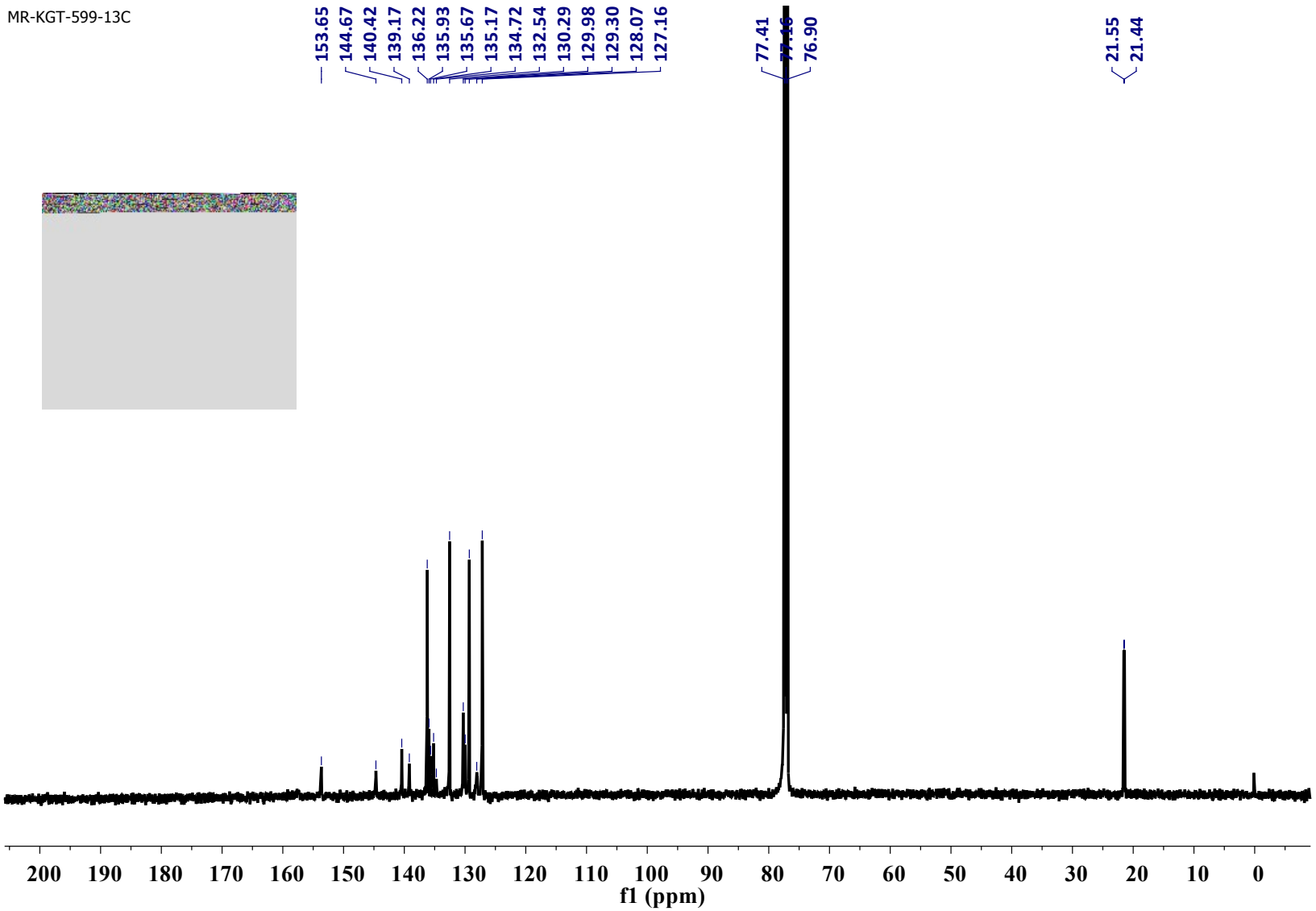
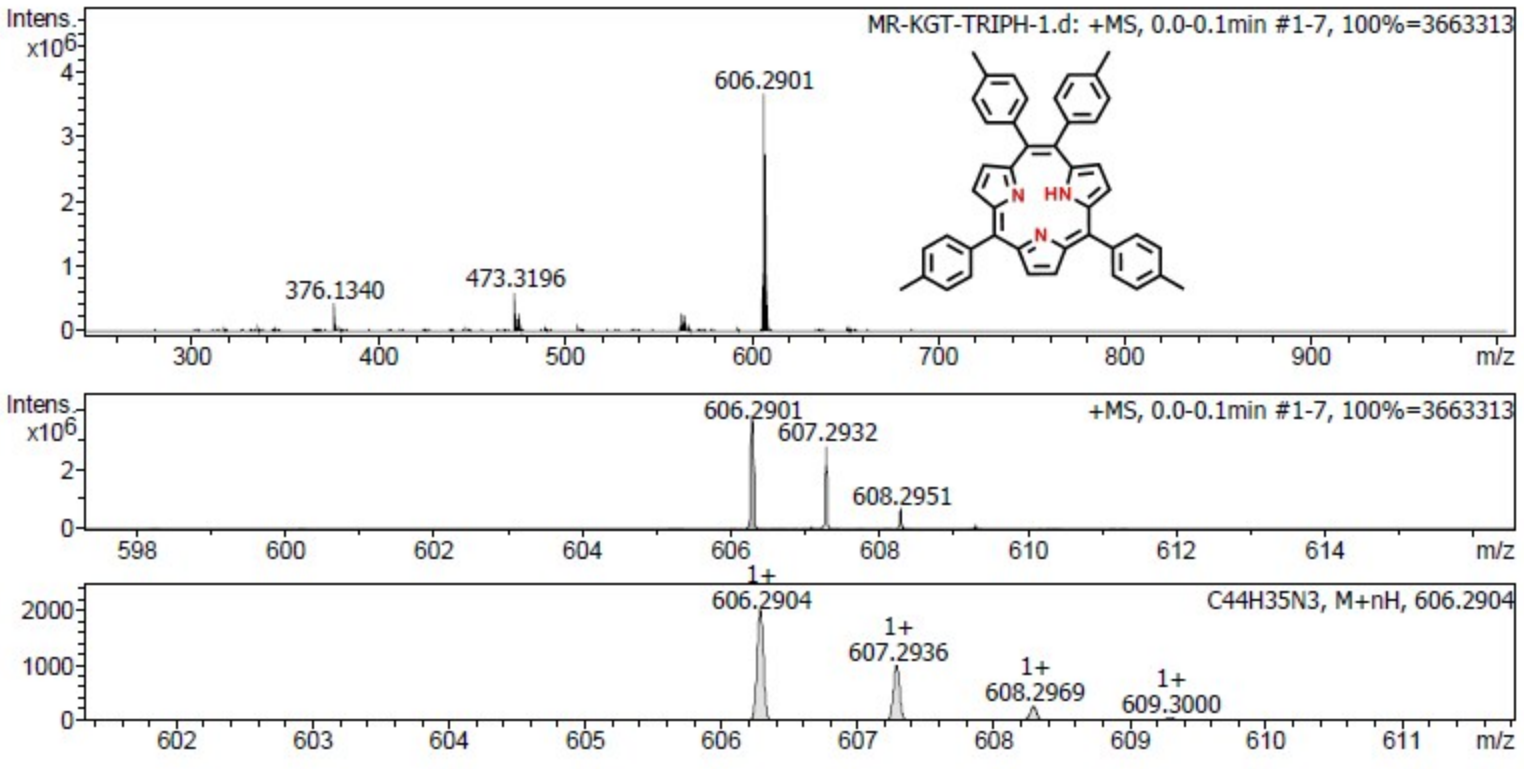


Figure S16. ^{13}C NMR spectrum of the compound **9** recorded in $CDCl_3$.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
606.2901	1	C44H36N3	606.2904	0.5	130.4	1	100.00	28.5	even	ok

Figure S17. HR mass spectrum of the compound **9**.

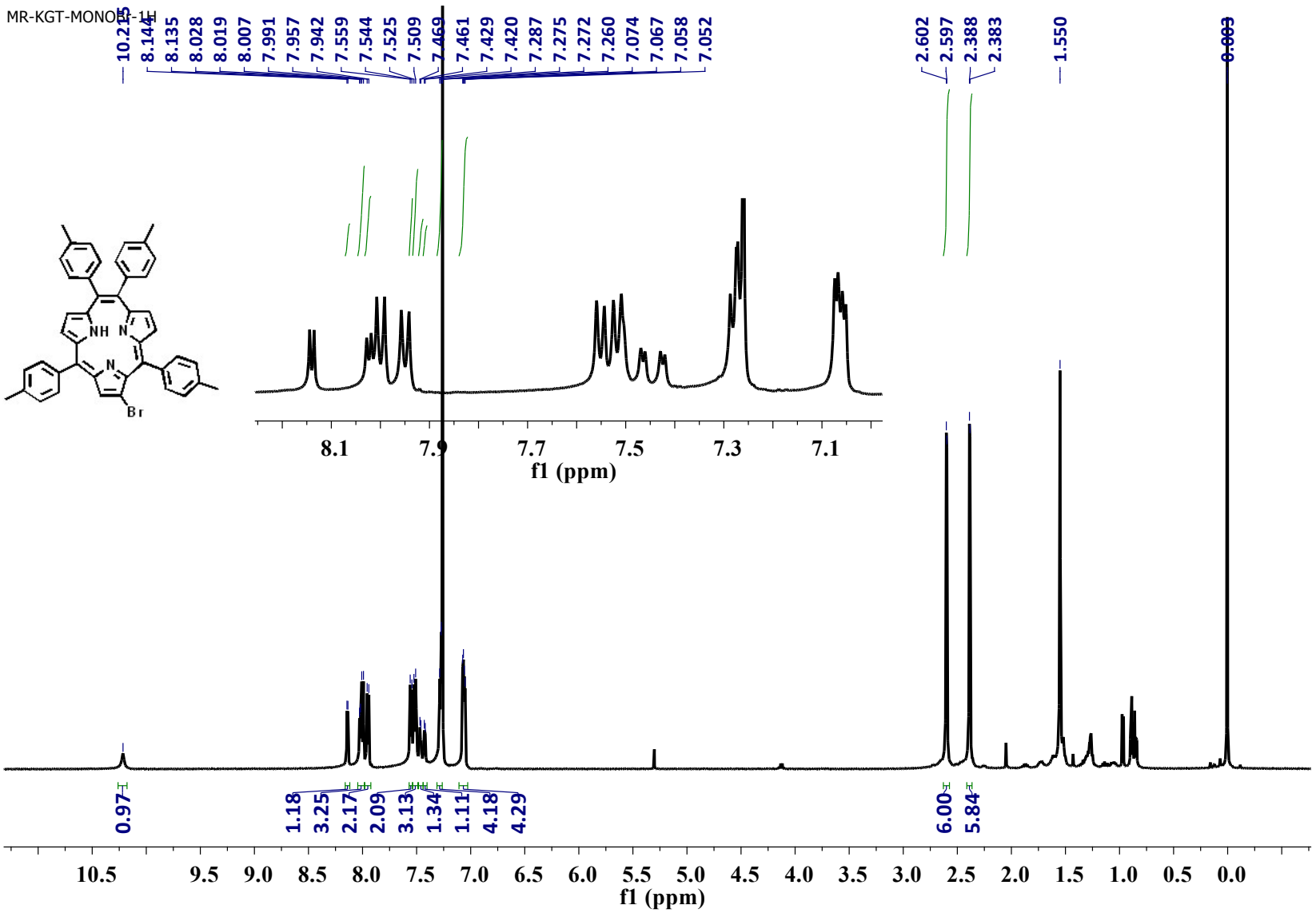


Figure S18. ^{1}H NMR spectrum of the compound **10** recorded in $CDCl_3$.

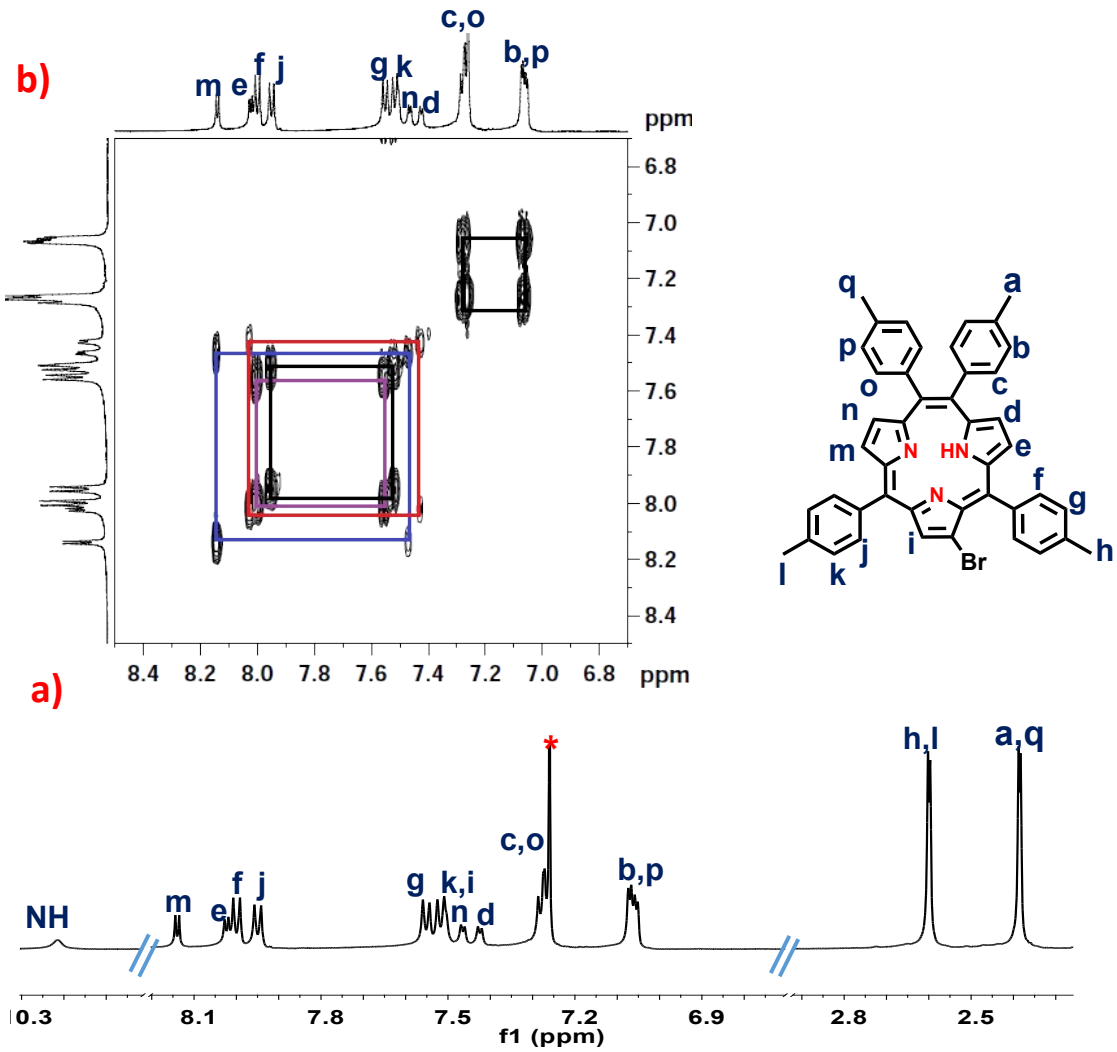


Figure S19. Partial ^{1}H (a) and ^{1}H-^{1}H (b) NMR spectra of the compound **10** recorded in $CDCl_3$.

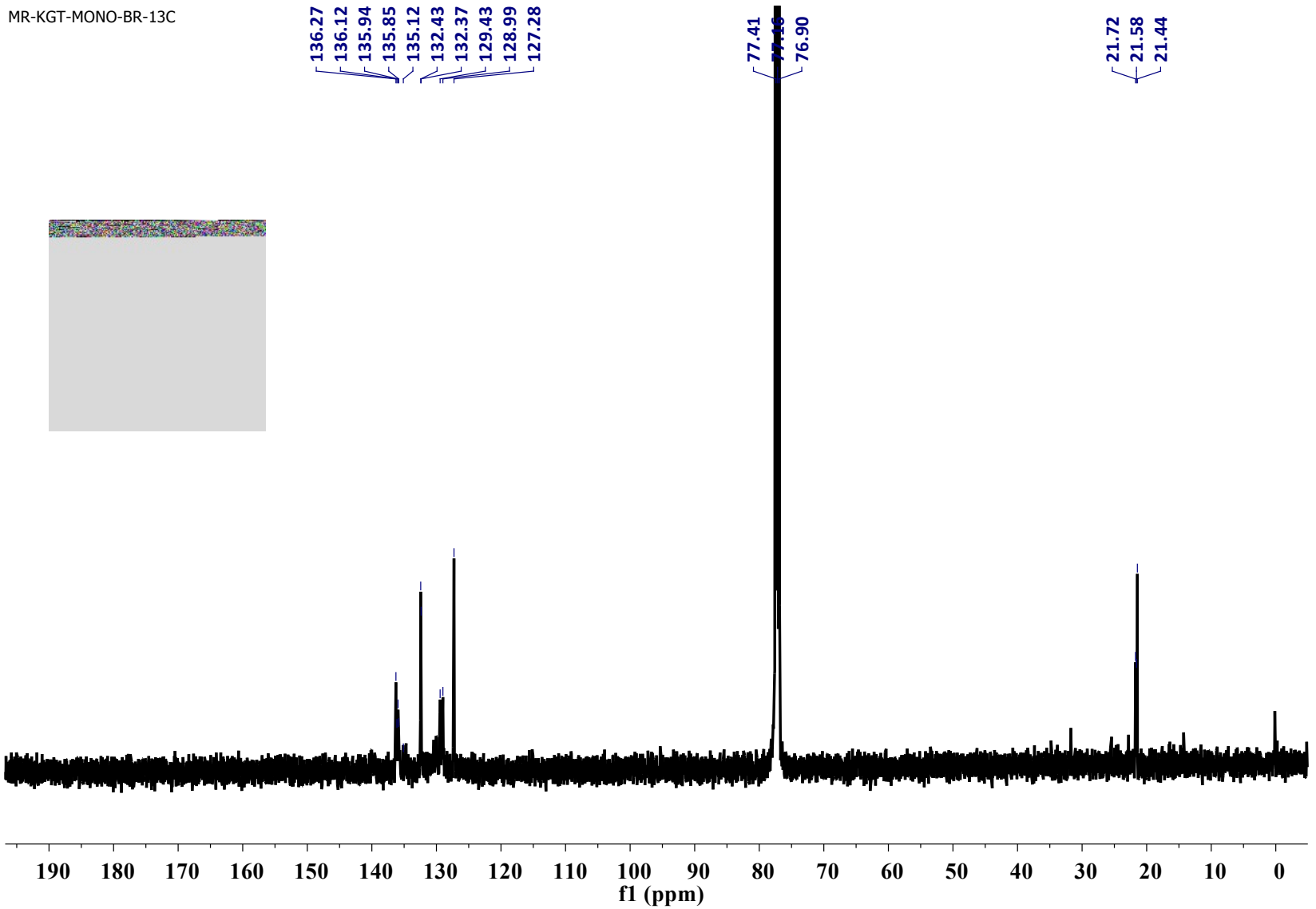
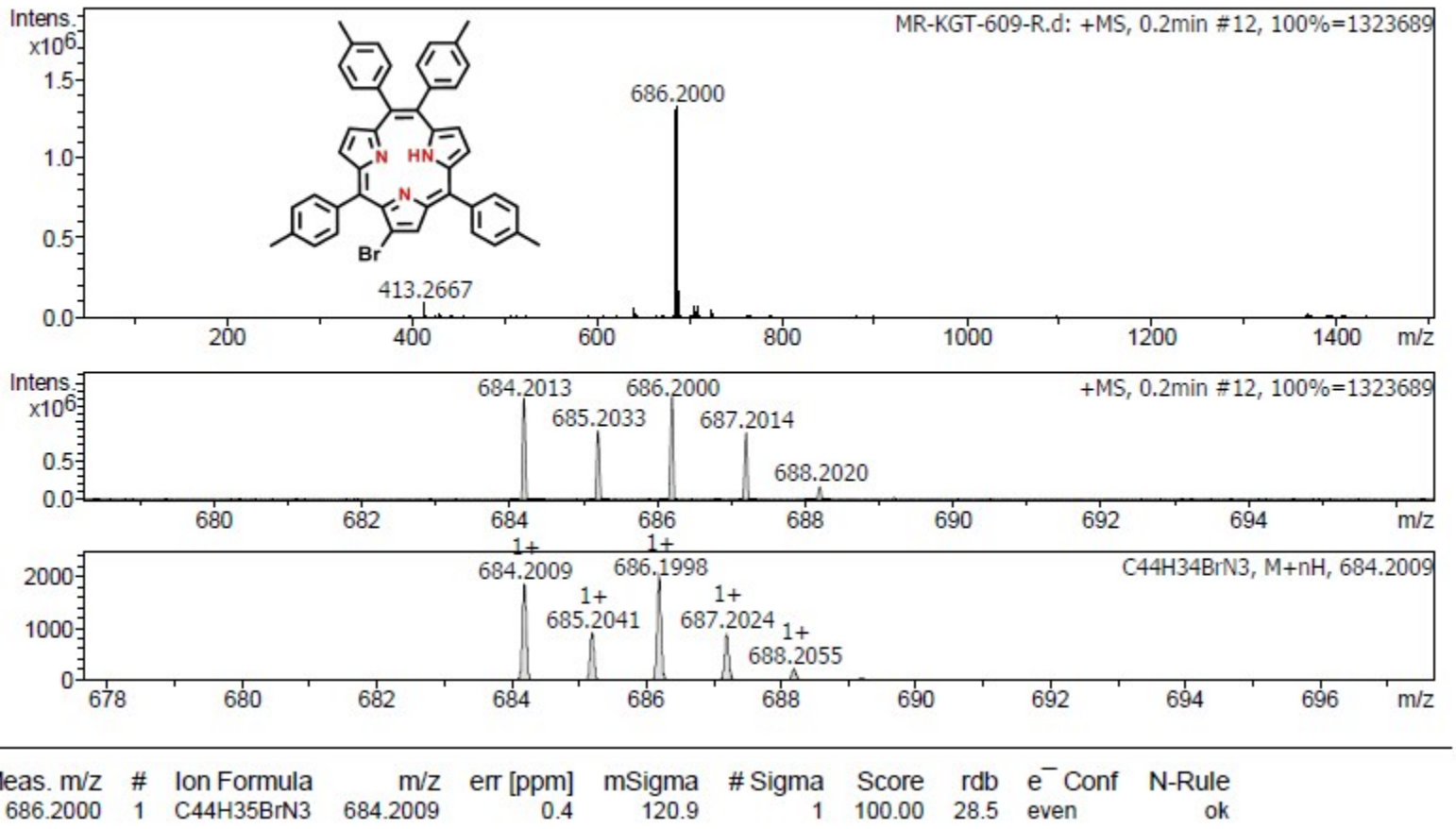


Figure S20. ^{13}C NMR spectrum of the compound **10** recorded in $CDCl_3$.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
686.2000	1	C44H35BrN3	684.2009	0.4	120.9	1	100.00	28.5	even	ok

Figure S21. HR mass spectrum of the compound **10**.

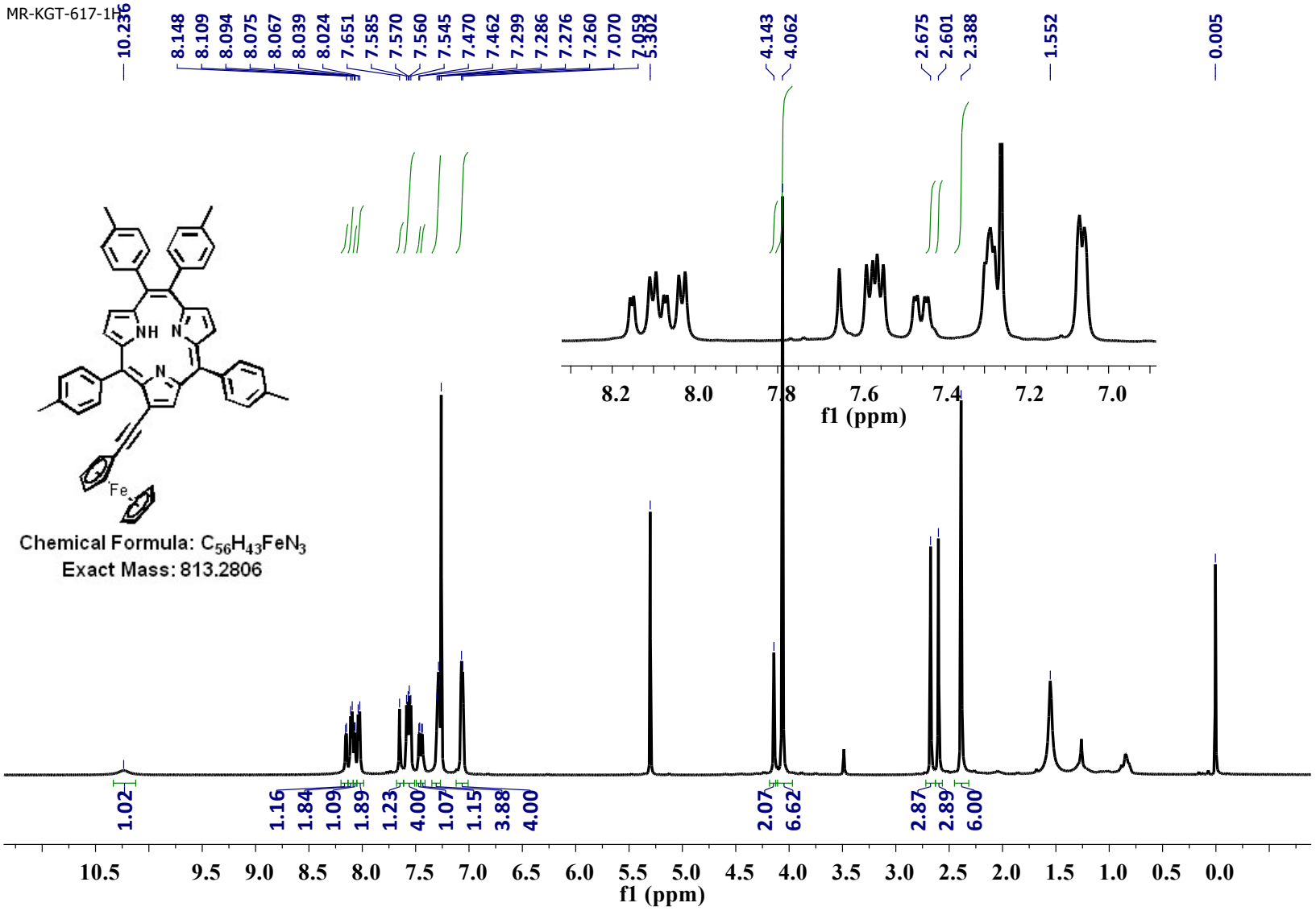


Figure S22. ^{1}H NMR spectrum of the dyad **3** recorded in $CDCl_3$.

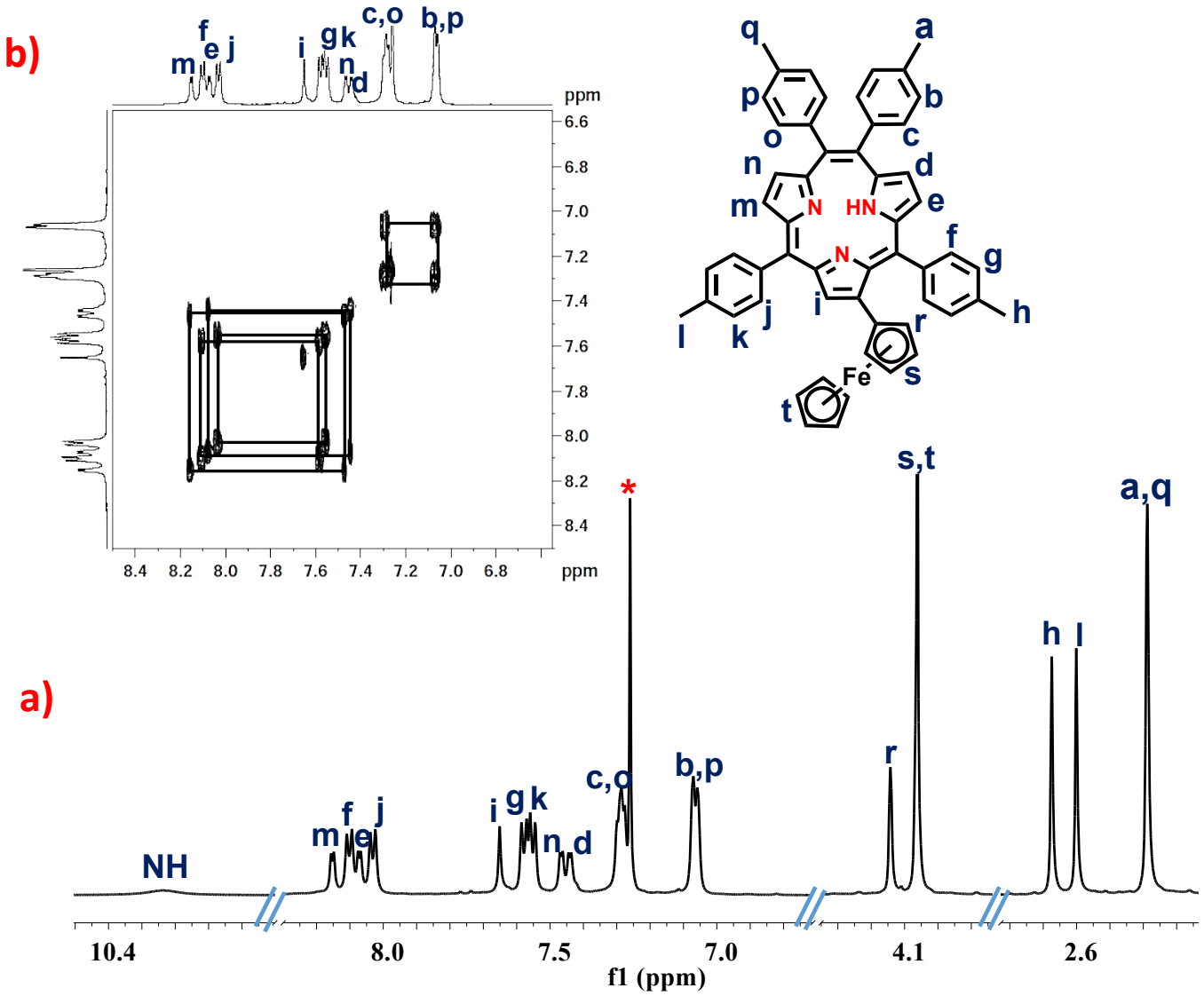


Figure S23. Partial ^{1}H NMR (a) and ^{1}H-^{1}H COSY (b) spectra of the dyad **3** recorded in $CDCl_3$.

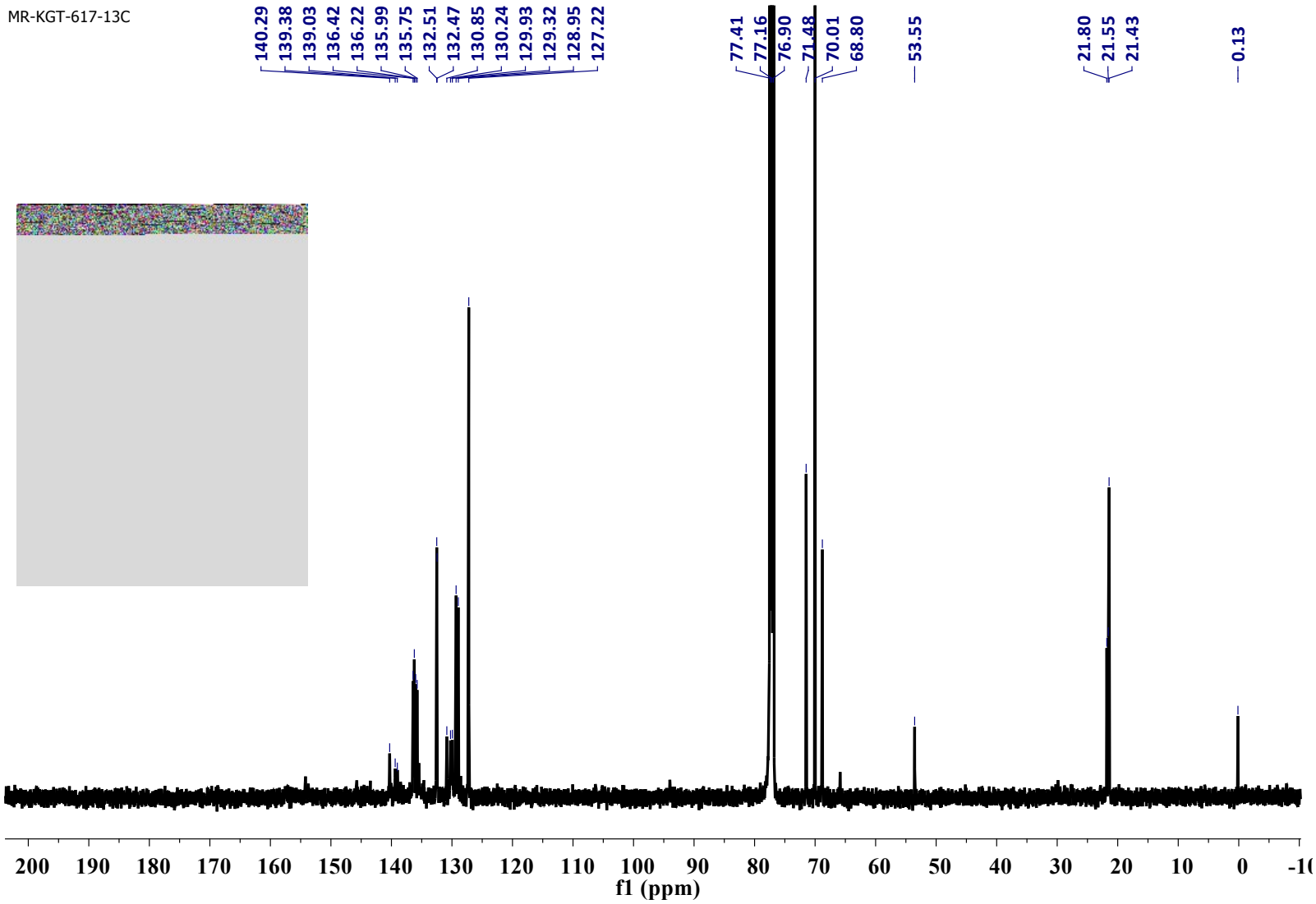


Figure S24. ^{13}C NMR spectrum of the dyad **3** recorded in $CDCl_3$.

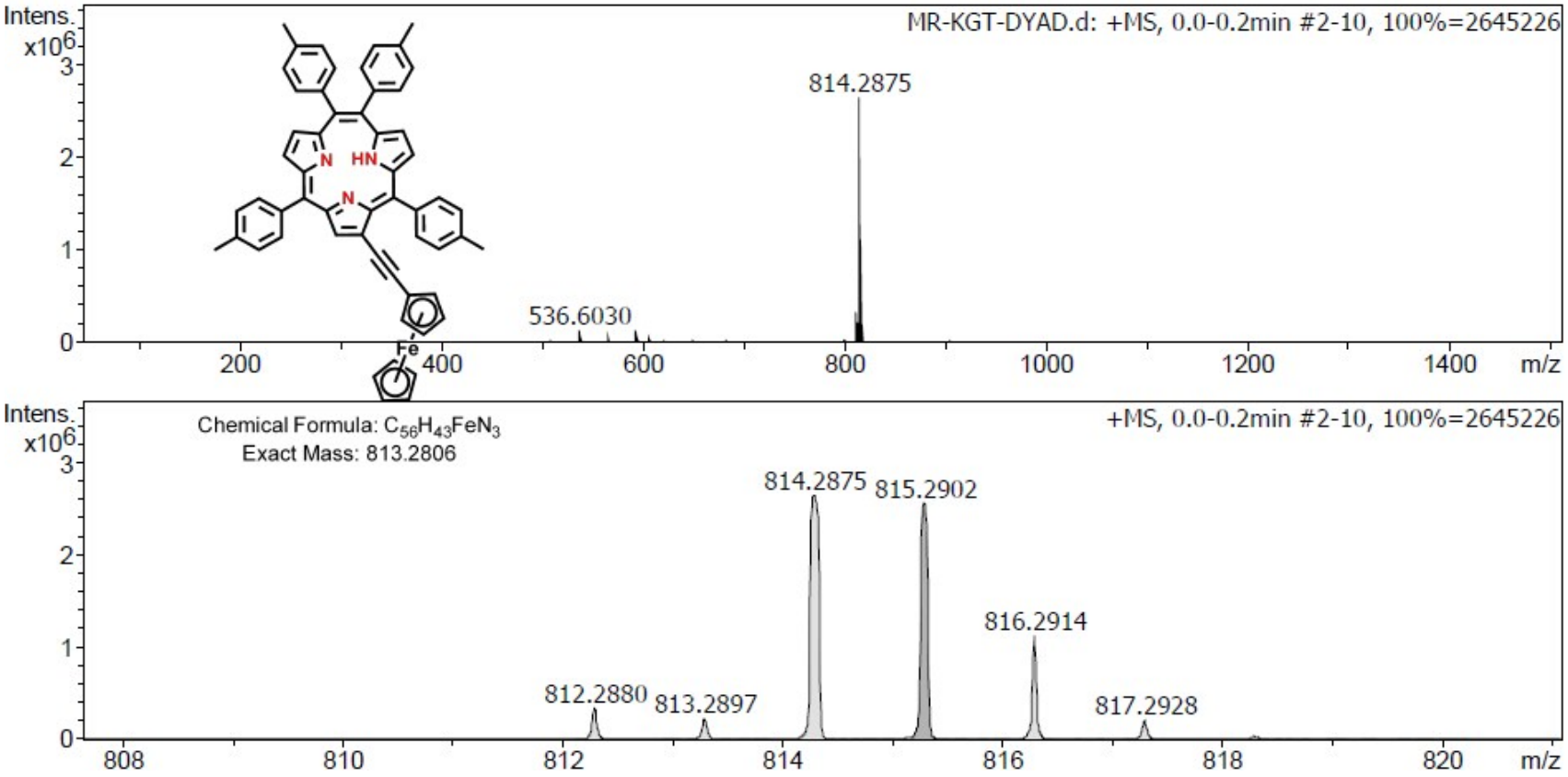


Figure S25. HR mass spectrum of the dyad **3**.

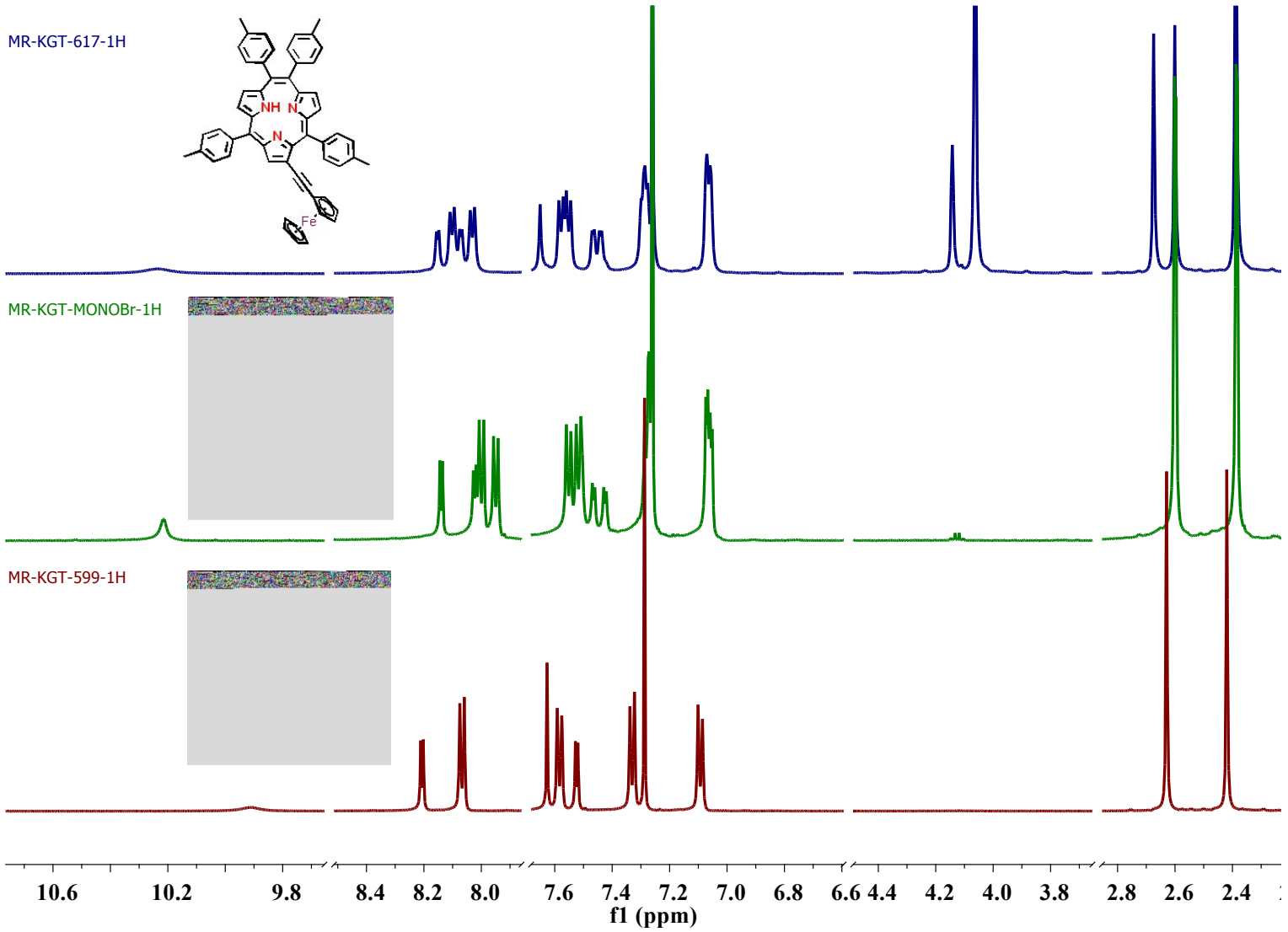


Figure S26. Comparision of ^{1}H NMR spectra of the triphyrin **9**, monobromo triphyrin **10** and dyad **3** recorded in $CDCl_3$.

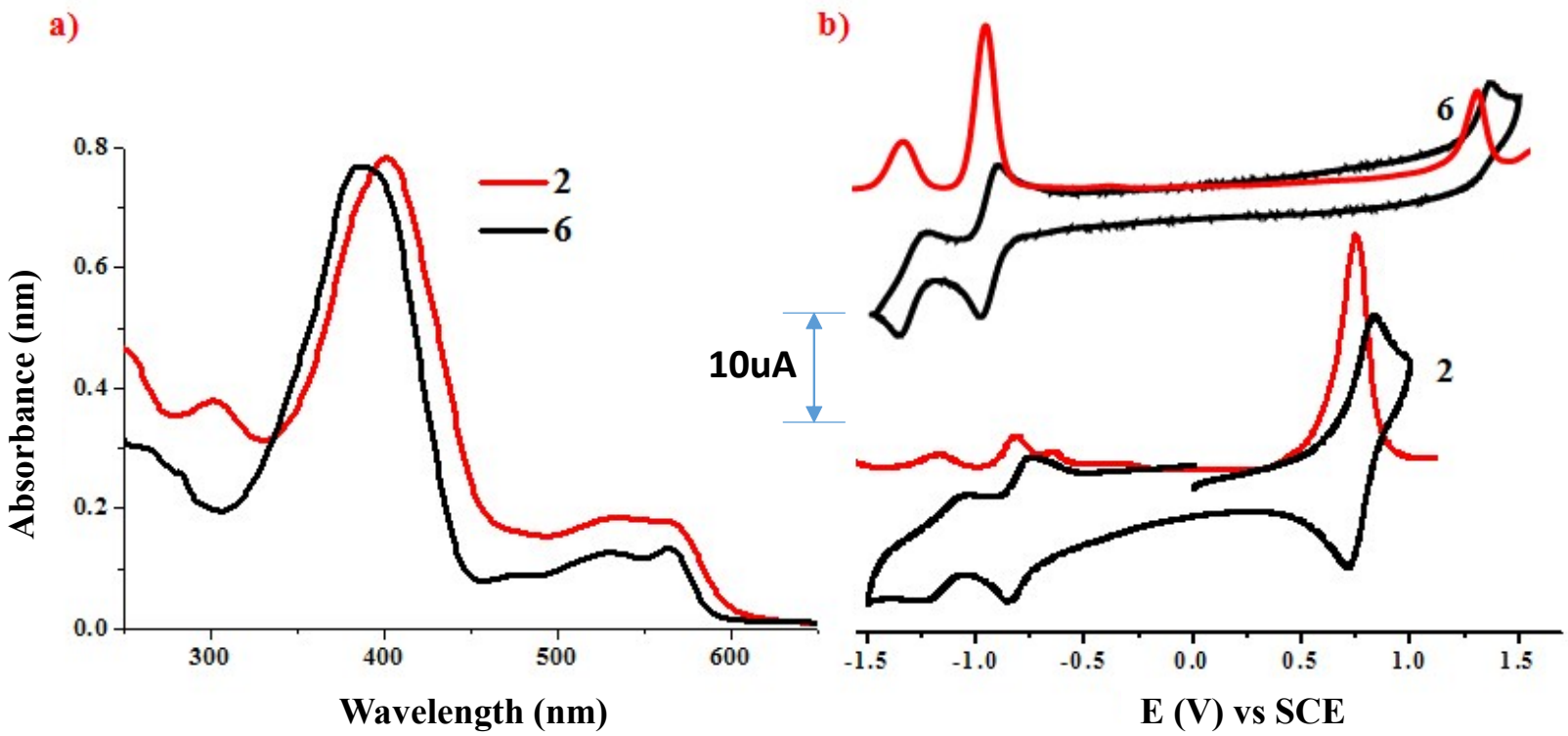


Figure S27. (a) comparison of absorption spectra of the triphyrin(2.1.1) **6** (red solid line) and triphyrin(2.1.1)-ferrocene triad **2** (black solid line) recorded in $CHCl_3$ (10 μM), and (b) comparison of cyclic voltammograms (black solid lines) and differential pulse voltammograms (red solid lines) of the triphyrin(2.1.1) **6** and triphyrin(2.1.1)-ferrocene triad **2** recorded in CH_2Cl_2 with TBAP as a supporting electrolyte (0.1 M) at scan rate of 50 mVs^{-1}.

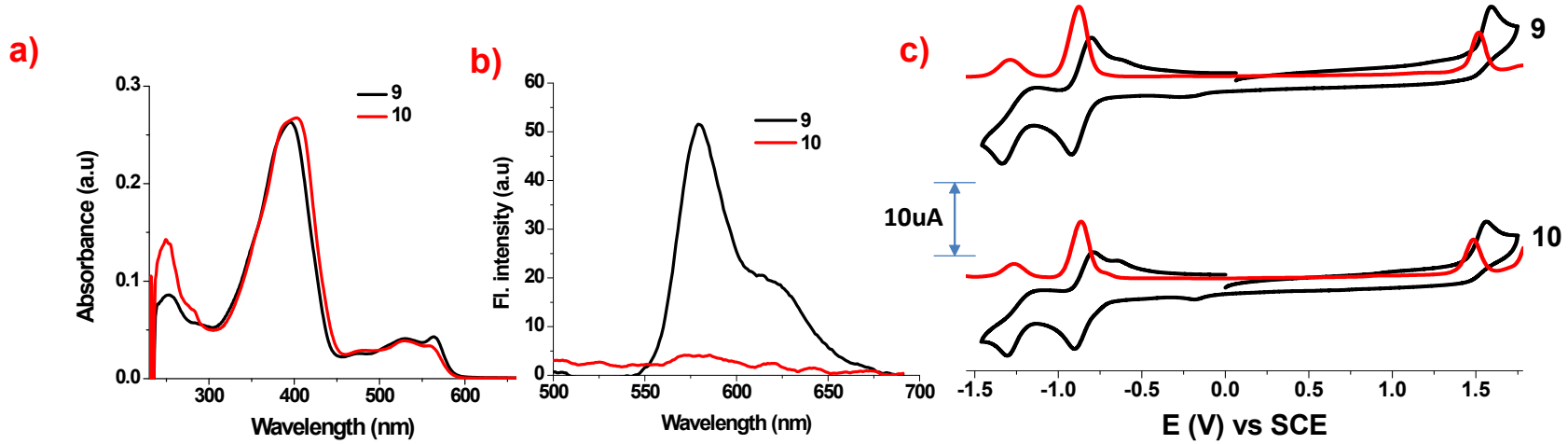


Figure S28. Comparison of absorption (a) and emission (b) spectra of the triphyrin(2.1.1) **9** and monobromo triphyrin(2.1.1) **10** recorded in $CHCl_3$ (1 μM), and (c) comparison of cyclic voltammograms (black solid lines) and differential pulse voltammograms (red solid lines) of the triphyrin(2.1.1) **9** and monobromo triphyrin(2.1.1) **10** recorded in CH_2Cl_2 with TBAP as a supporting electrolyte (0.1 M) at scan rate of 50 mVs^{-1}.

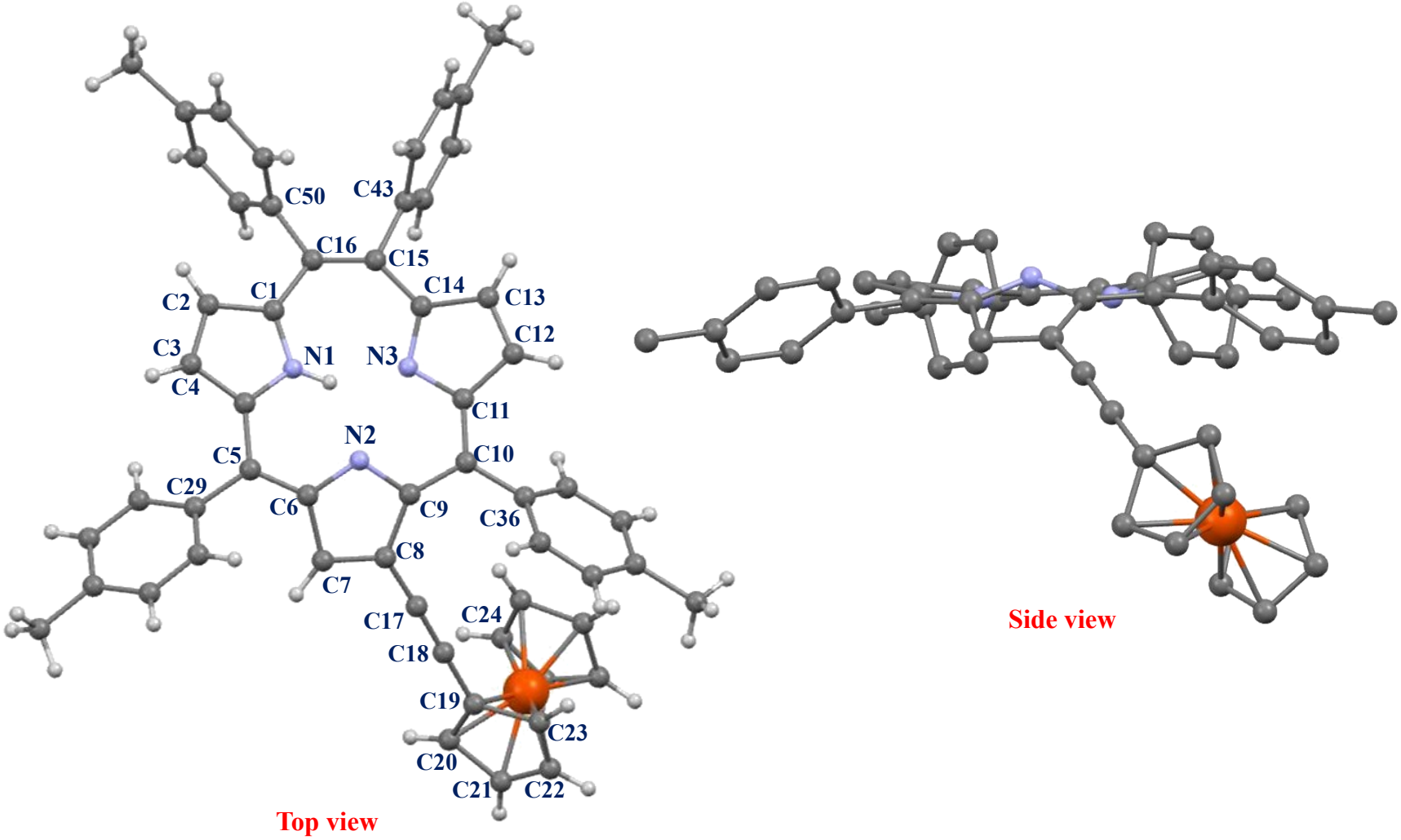


Figure S29. Crystal structure of the dyad **3**; Hydrogens in the side view were omitted for clarity.

Table S1. Crystal data and structure refinement for the dyad **3.**

Identification code	MR-KGT-617_Mo
Empirical formula	$C_{56}H_{43}FeN_3$
Formula weight	813.826
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.3859(10)
b/Å	17.6141(10)
c/Å	22.8451(19)
α/°	90
β/°	94.387(8)
γ/°	90
Volume/Å^3	4167.0(6)
Z	4
ρ_{calc}g/cm^3	1.292
μ/mm^{-1}	0.405
F(000)	1692.0
Crystal size/mm^3	0.116 × 0.106 × 0.048
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.576 to 62.386
Index ranges	$-14 \leq h \leq 15$, $-24 \leq k \leq 24$, $-32 \leq l \leq 32$
Reflections collected	56659
Independent reflections	12392 [R_{int} = 0.2662, R_{sigma} = 0.3106]
Data/restraints/parameters	12392/0/545
Goodness-of-fit on F^2	1.106
Final R indexes [I>=2σ (I)]	R_1 = 0.1807, wR_2 = 0.3922
Final R indexes [all data]	R_1 = 0.4362, wR_2 = 0.5288
Largest diff. peak/hole / e Å^{-3}	1.26/-0.87

Table S2. Bond lengths for the dyad **3.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C19	1.968(18)	C20	C19	1.48(2)	C9	C10	1.437(12)
Fe1	C20	2.015(15)	C20	C21	1.37(2)	C10	C11	1.395(11)
Fe1	C21	1.990(15)	C21	C22	1.31(2)	C10	C36	1.464(11)
Fe1	C22	2.025(15)	C22	C23	1.458(18)	C11	C12	1.453(12)
Fe1	C23	2.026(13)	C25	C24	1.49(3)	C13	C12	1.345(11)
Fe1	C24	1.950(19)	C25	C26	1.38(2)	C14	C13	1.452(13)
Fe1	C25	2.05(2)	C26	C27	1.347(19)	C15	C14	1.425(11)
Fe1	C26	2.071(17)	C28	C24	1.43(4)	C15	C16	1.369(12)
Fe1	C27	2.030(12)	C28	C27	1.41(2)	C15	C43	1.527(11)
Fe1	C28	2.026(16)	C29	C34	1.411(12)	C17	C18	1.291(18)
N1	C1	1.334(10)	C30	C29	1.387(12)	C19	C18	1.448(18)
N1	C4	1.364(11)	C30	C31	1.381(12)	C19	C23	1.417(18)
N2	C6	1.346(11)	C32	C31	1.386(12)	C46	C47	1.364(14)
N2	C9	1.360(10)	C32	C35	1.518(13)	C46	C49	1.559(12)
N3	C11	1.383(10)	C33	C32	1.395(13)	C48	C47	1.368(13)
N3	C14	1.354(10)	C33	C34	1.352(12)	C50	C16	1.501(11)
C1	C2	1.460(12)	C36	C37	1.411(11)	C50	C51	1.375(12)
C1	C16	1.476(12)	C37	C38	1.336(12)	C50	C55	1.377(11)
C2	C3	1.412(12)	C39	C38	1.401(13)	C51	C52	1.380(13)
C4	C3	1.441(12)	C39	C42	1.543(12)	C53	C52	1.372(13)
C4	C5	1.466(11)	C40	C39	1.377(12)	C53	C54	1.393(13)
C5	C6	1.357(12)	C41	C36	1.393(12)	C53	C56	1.574(13)
C5	C29	1.464(12)	C41	C40	1.385(12)	C55	C54	1.373(12)
C6	C7	1.496(13)	C43	C44	1.379(12)	C8	C17	1.350(17)
C8	C7	1.358(15)	C43	C48	1.394(12)	C9	C8	1.485(13)
C46	C45	1.417(13)	C44	C45	1.403(12)			

Table S3. Bond angles for the dyad **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C19	Fe1	C20	43.7(6)	C16	C15	C14	131.8(8)	C25	Fe1	C22	115.2(9)	C28	C27	Fe1	69.5(8)
C19	Fe1	C21	68.7(7)	C16	C15	C43	117.2(7)	C25	Fe1	C26	39.0(7)	C24	C28	Fe1	66.1(10)
C19	Fe1	C22	67.5(5)	C1	C16	C50	109.6(8)	C25	Fe1	C27	67.3(7)	C27	C28	Fe1	69.8(8)
C19	Fe1	C23	41.5(5)	C15	C16	C1	126.9(8)	C27	Fe1	C26	38.3(6)	C27	C28	C24	97.0(18)
C19	Fe1	C25	164.8(8)	C15	C16	C50	123.4(8)	C28	Fe1	C22	159.8(8)	C30	C29	C5	123.6(8)
C19	Fe1	C26	156.2(9)	C18	C17	C8	174.5(16)	C28	Fe1	C23	120.9(7)	C30	C29	C34	117.5(9)
C19	Fe1	C27	124.7(6)	C17	C18	C19	179.4(15)	C28	Fe1	C25	74.9(10)	C34	C29	C5	118.8(9)
C19	Fe1	C28	107.6(8)	C18	C19	Fe1	121.5(10)	C28	Fe1	C26	69.4(8)	C31	C30	C29	120.4(9)
C20	Fe1	C21	40.1(6)	C18	C19	C20	122.7(13)	C28	Fe1	C27	40.7(6)	C30	C31	C32	121.5(9)
C20	Fe1	C22	67.2(8)	C18	C19	C23	125.9(15)	C1	N1	C4	109.2(7)	C31	C32	C35	122.1(10)
C20	Fe1	C23	72.6(8)	C20	C19	Fe1	69.8(10)	C6	N2	C9	110.1(7)	C33	C32	C31	118.0(10)
C20	Fe1	C25	122.1(8)	C23	C19	Fe1	71.4(9)	C14	N3	C11	108.7(8)	C33	C32	C35	119.9(9)
C20	Fe1	C26	157.5(8)	C23	C19	C20	111.2(13)	N1	C1	C2	109.8(8)	C34	C33	C32	120.8(9)
C20	Fe1	C27	162.4(6)	C19	C20	Fe1	66.5(9)	N1	C1	C16	124.8(8)	C33	C34	C29	121.7(9)
C20	Fe1	C28	123.9(8)	C21	C20	Fe1	69.0(10)	C2	C1	C16	125.4(8)	C37	C36	C10	121.3(8)
C21	Fe1	C22	38.2(6)	C21	C20	C19	102.9(16)	C3	C2	C1	105.5(8)	C41	C36	C10	121.3(8)
C21	Fe1	C23	69.9(6)	C20	C21	Fe1	70.9(9)	C2	C3	C4	106.0(8)	C41	C36	C37	117.3(8)
C21	Fe1	C25	103.7(9)	C22	C21	Fe1	72.3(9)	N1	C4	C3	109.5(8)	C38	C37	C36	122.0(9)
C21	Fe1	C26	121.9(8)	C22	C21	C20	112.5(16)	N1	C4	C5	122.9(8)	C37	C38	C39	120.1(9)
C21	Fe1	C27	157.0(7)	C21	C22	Fe1	69.5(10)	C3	C4	C5	127.5(10)	C38	C39	C42	120.2(9)
C21	Fe1	C28	160.5(6)	C21	C22	C23	112.2(16)	C4	C5	C29	120.9(8)	C40	C39	C38	119.6(9)
C22	Fe1	C26	106.6(7)	C23	C22	Fe1	68.9(7)	C6	C5	C4	117.7(8)	C40	C39	C42	120.1(9)
C22	Fe1	C27	124.6(8)	C19	C23	Fe1	67.0(9)	C6	C5	C29	121.2(8)	C39	C40	C41	119.9(9)
C23	Fe1	C22	42.2(6)	C22	C23	Fe1	68.9(8)	N2	C6	C5	121.4(8)	C40	C41	C36	120.9(9)
C23	Fe1	C25	150.0(8)	C22	C23	C19	101.1(15)	N2	C6	C7	110.9(8)	C44	C43	C15	120.1(8)
C23	Fe1	C26	118.3(9)	C25	C24	Fe1	71.6(10)	C5	C6	C7	126.7(9)	C44	C43	C48	118.8(8)
C23	Fe1	C27	106.8(6)	C28	C24	Fe1	71.8(14)	C8	C7	C6	102.0(10)	C48	C43	C15	121.1(9)
C24	Fe1	C19	128.9(6)	C28	C24	C25	116(2)	C7	C8	C9	111.6(9)	C43	C44	C45	121.7(8)
C24	Fe1	C20	110.7(9)	C24	C25	Fe1	64.6(12)	C17	C8	C7	120.9(11)	C44	C45	C46	119.1(9)
C24	Fe1	C21	124.5(12)	C26	C25	Fe1	71.4(11)	C17	C8	C9	127.3(13)	C45	C46	C49	120.5(10)
C24	Fe1	C22	155.7(12)	C26	C25	C24	99(2)	N2	C9	C8	105.3(9)	C47	C46	C45	116.8(9)
C24	Fe1	C23	162.1(11)	C25	C26	Fe1	69.6(13)	N2	C9	C10	118.9(8)	C47	C46	C49	122.7(9)
C24	Fe1	C25	43.8(8)	C27	C26	Fe1	69.2(8)	C10	C9	C8	134.0(9)	C48	C47	C46	124.9(9)
C24	Fe1	C26	65.6(7)	C27	C26	C25	112.2(19)	C9	C10	C36	119.6(8)	C47	C48	C43	118.6(10)
C24	Fe1	C27	64.5(10)	C26	C27	Fe1	72.5(10)	C11	C10	C9	118.5(8)	C51	C50	C16	120.5(8)
C24	Fe1	C28	42.1(11)	C26	C27	C28	115.7(17)	C11	C10	C36	121.9(9)	C51	C50	C55	117.6(8)
C12	C13	C14	106.6(9)	C52	C53	C56	122.8(10)	N3	C11	C10	123.6(9)	C55	C50	C16	121.8(7)
N3	C14	C13	109.1(8)	C54	C53	C56	117.7(10)	N3	C11	C12	107.0(7)	C50	C51	C52	121.5(10)
N3	C14	C15	123.9(9)	C53	C54	C55	118.9(10)	C10	C11	C12	129.4(8)	C53	C52	C51	119.9(9)
C13	C12	C11	108.6(8)	C52	C53	C54	119.5(9)	C15	C14	C13	127.0(8)	C50	C55	C54	122.3(9)

Table S4. Cartesian coordinates of the S_0 optimized geometry of the triad **2**

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
N	-1.24982	1.26905	-0.25923	H	2.71011	-1.18774	1.76049	H	-10.36752	11.58168	-0.44286
N	-3.47464	0.05739	-0.83023	C	4.12121	-2.85293	-1.43911	H	-9.45478	9.17119	-1.25169
N	-1.34337	-1.29987	-0.38959	H	4.51087	-3.31844	-2.34020	Fe	-7.57855	11.25904	-0.84984
H	-1.61198	-0.27199	-0.33254	C	-4.88848	-5.62698	0.83757	C	-6.81803	13.08349	-1.49685
C	-1.09114	3.52132	-0.68110	H	-4.60736	-6.39307	1.55300	C	-5.75273	12.16199	-1.25935
H	-1.38631	4.54055	-0.88772	C	4.97149	2.60900	-0.35689	C	-7.66918	12.52492	-2.49759
C	0.04594	1.57777	-0.41779	C	4.53657	1.94633	-1.50641	H	-6.97188	14.02312	-0.98415
C	-5.45303	0.81787	0.05415	H	5.15541	1.94145	-2.39935	C	-5.94547	11.03504	-2.11403
H	-6.19511	1.50489	0.43830	C	-3.74588	4.70713	0.57286	H	-4.95784	12.28168	-0.53603
C	-1.99394	2.40341	-0.42864	H	-2.86008	4.56114	1.18199	C	-7.13017	11.25819	-2.87869
C	-4.12516	1.16892	-0.46187	C	2.92748	1.96865	0.76676	H	-8.58054	12.96771	-2.87547
C	2.48701	1.28690	-0.37751	H	2.29493	1.98605	1.64979	H	-5.33494	10.14279	-2.13632
C	1.08942	-0.78202	-0.38937	C	2.92272	-2.13937	-1.49176	H	-7.56077	10.57404	-3.59685
C	-0.04246	-1.67126	-0.44157	H	2.38258	-2.05505	-2.43068	C	-8.55442	-8.93691	0.70989
C	-4.22603	-1.00450	-0.48351	C	-6.09317	-5.76838	0.11754	C	-9.88582	-9.07500	0.17501
C	0.17394	3.01184	-0.68392	C	-4.46745	5.88823	0.68410	C	-10.44405	-10.28293	0.67834
H	1.09495	3.54505	-0.86943	H	-4.13725	6.66640	1.36475	C	-9.47139	-10.90949	1.51617
C	-0.03127	-3.10839	-0.56623	C	-5.34391	3.87607	-1.03484	C	-8.30700	-10.09166	1.53568
H	0.85356	-3.72239	-0.63209	H	-5.67539	3.10030	-1.71757	H	-10.35848	-8.37668	-0.50086
C	-2.18615	-2.38045	-0.48345	C	4.30397	-2.36543	0.91663	H	-11.42297	-10.67492	0.43940
C	-5.51579	-0.54765	0.04293	H	4.83552	-2.45306	1.86007	H	-9.58623	-11.85857	2.02121
H	-6.31640	-1.17095	0.41775	C	-6.06835	5.05542	-0.93168	H	-7.38460	-10.29351	2.06142
C	2.40265	-1.52428	-0.34342	H	-6.96837	5.19642	-1.52144	Fe	-8.71650	-10.68730	-0.41128
C	-4.16296	3.67460	-0.29142	C	-5.64381	6.08752	-0.06848	C	-8.29283	-12.57824	-1.16504
C	-3.41381	2.40967	-0.41058	H	5.93152	3.11723	-0.34946	C	-9.23162	-11.91229	-2.00968
C	-3.60717	-2.28463	-0.43563	H	5.74908	-3.52245	-0.19159	C	-7.10287	-11.78947	-1.12015
C	1.13185	0.62649	-0.38264	C	-6.38884	7.29430	0.04069	H	-8.46517	-13.49999	-0.62645
C	3.30549	1.29022	-1.51592	C	-7.03991	8.31831	0.13298	C	-8.62211	-10.71165	-2.48660
H	2.97078	0.77945	-2.41327	C	-7.81437	9.49992	0.24380	H	-10.23945	-12.24150	-2.22253
C	-5.63924	-3.63888	-0.96599	C	-7.56400	10.61354	1.12369	C	-7.30651	-10.63711	-1.93760
H	-5.92295	-2.87270	-1.68028	C	-8.60156	11.56946	0.93689	H	-6.21528	-12.01003	-0.54319
C	4.81630	-2.96742	-0.23403	C	-9.49567	11.07029	-0.05892	H	-9.08648	-9.97310	-3.12539
C	-1.33844	-3.53622	-0.60019	C	-9.01543	9.80325	-0.49314	H	-6.60675	-9.82398	-2.07450
H	-1.68307	-4.55324	-0.71711	H	-6.72117	10.69777	1.79491	C	-6.93502	-6.89838	0.31152
C	-4.07966	-4.51287	0.65628	H	-8.67950	12.52409	1.43853	C	-7.67413	-7.84860	0.48964
H	-3.17690	-4.40649	1.24837	C	-4.43355	-3.49347	-0.25023	H	-7.37210	-4.84793	-1.35782
C	4.16278	2.61807	0.78069	C	-6.45163	-4.75065	-0.79127	C	3.10629	-1.65184	0.86229

Table S4. Cartesian coordinates of the S_0 optimized geometry of the dyad **3**

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-1.04993	-1.52366	0.01855	C	-0.34794	-3.61888	6.93704	H	6.49661	-1.69622	9.05788
C	1.07459	-1.14810	-0.32676	H	-0.25931	-4.42694	6.21607	H	5.35451	-0.75841	10.02235
N	0.07997	-1.05806	0.57059	C	3.79083	-0.94736	3.49301	H	5.32031	-2.52812	10.07536
C	2.43112	-1.00636	0.10861	H	4.49867	-0.78161	4.29165	C	-7.58932	-2.56212	-1.03024
C	-2.13445	-1.83337	0.88968	C	3.98980	-0.74760	2.15859	H	-8.26432	-1.91154	-0.46001
C	2.74027	-1.09215	1.48975	H	4.87998	-0.36374	1.68046	H	-7.69740	-2.29056	-2.08536
C	-1.89495	-1.94347	2.28816	C	4.71407	-1.53887	-0.81929	H	-7.94303	-3.58956	-0.90503
C	2.41180	-1.41489	3.64393	H	4.86124	-2.25267	-0.01536	C	6.62237	-0.27150	-3.87751
N	1.84043	-1.50359	2.43329	C	5.70575	-1.36605	-1.78151	H	6.20730	-0.06402	-4.86861
C	-0.71968	-2.05940	4.21161	H	6.62715	-1.93832	-1.70523	H	7.25881	0.58107	-3.60811
C	1.74872	-1.72833	4.88737	C	4.32037	0.21953	-2.93606	H	7.27112	-1.14878	-3.95692
C	0.39209	-2.02384	5.12646	H	4.15764	0.91148	-3.75896	C	-1.68043	-2.40168	-2.36350
C	2.67528	-1.71153	6.07723	C	3.32299	0.04943	-1.98049	C	-2.41005	-2.88130	-3.21284
C	-3.50264	-2.06207	0.37550	H	2.39924	0.61429	-2.05756	Fe	-3.58615	-5.44626	-4.62090
C	3.50109	-0.82930	-0.89481	C	0.54768	-1.59973	-1.60202	C	-3.27894	-3.42517	-4.18984
C	5.53232	-0.48088	-2.85415	H	1.10554	-1.78556	-2.50918	C	-2.95565	-3.70868	-5.56556
C	-6.16151	-2.40682	-0.56273	C	-0.79942	-1.85071	-1.40977	C	-4.66192	-3.78127	-3.99725
N	-0.64751	-1.94394	2.86518	C	-2.83394	-2.08390	3.37119	C	-4.12506	-4.21098	-6.20373
C	4.47975	-1.67971	8.26880	H	-3.90851	-2.09720	3.26412	H	-1.98291	-3.57023	-6.01565
C	3.98506	-0.48892	7.72262	C	-2.12054	-2.15896	4.54358	C	-5.17604	-4.25655	-5.23670
H	4.29351	0.46346	8.14766	H	-2.51816	-2.25269	5.54250	H	-5.18994	-3.70681	-3.05773
C	3.10089	-0.50240	6.64357	C	-4.08080	-1.14392	-0.51981	H	-4.19506	-4.53455	-7.23313
H	2.73352	0.43554	6.23621	H	-3.50187	-0.28483	-0.84363	H	-6.17922	-4.62221	-5.40767
C	3.17061	-2.90430	6.62027	C	-5.38521	-1.31165	-0.97210	C	-4.27740	-7.39115	-4.36570
H	2.85725	-3.85347	6.19577	H	-5.81094	-0.57941	-1.65371	C	-3.25272	-7.36180	-5.35957
C	4.05428	-2.88650	7.69813	C	-5.57682	-3.33545	0.30880	C	-3.72150	-6.90111	-3.14443
H	4.42042	-3.82737	8.10254	H	-6.14900	-4.20327	0.62780	H	-5.30292	-7.69763	-4.52017
C	-0.58908	-1.56811	8.79171	C	-4.27396	-3.16706	0.77477	C	-2.06360	-6.85400	-4.75211
H	-0.68234	-0.75550	9.50854	H	-3.83848	-3.90810	1.43754	H	-3.36675	-7.64262	-6.39769
C	-0.89697	-2.87652	9.18948	H	0.29211	-1.76047	2.39455	C	-2.35339	-6.57098	-3.38334
C	-0.76718	-3.89579	8.23892	C	-1.37811	-3.16870	10.59146	H	-4.25141	-6.77020	-2.21113
H	-0.99726	-4.92112	8.51897	H	-2.44573	-2.94018	10.70199	H	-1.11883	-6.68216	-5.24921
C	-0.16521	-1.28833	7.49419	H	-1.24167	-4.22282	10.85001	H	-1.67333	-6.12884	-2.66810
H	0.06746	-0.26609	7.21226	H	-0.84208	-2.56671	11.33231				
C	-0.03056	-2.31151	6.54556	C	5.46037	-1.66434	9.41801				