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Supporting Information

Ferrocenyl end capped molecular rods*:* synthesis, structure, and properties

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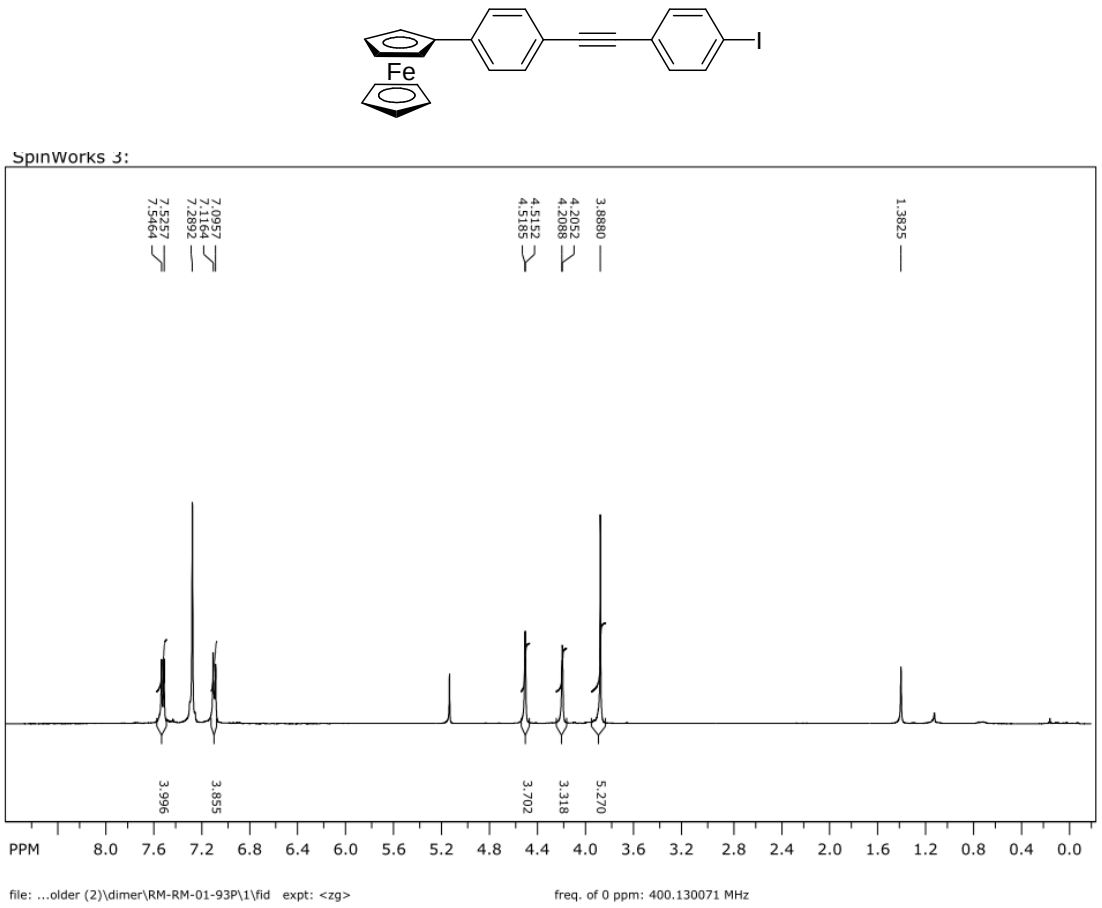


Fig. S-1: ^{1}H-NMR spectrum of compound **21** recorded in $CDCl_3$.

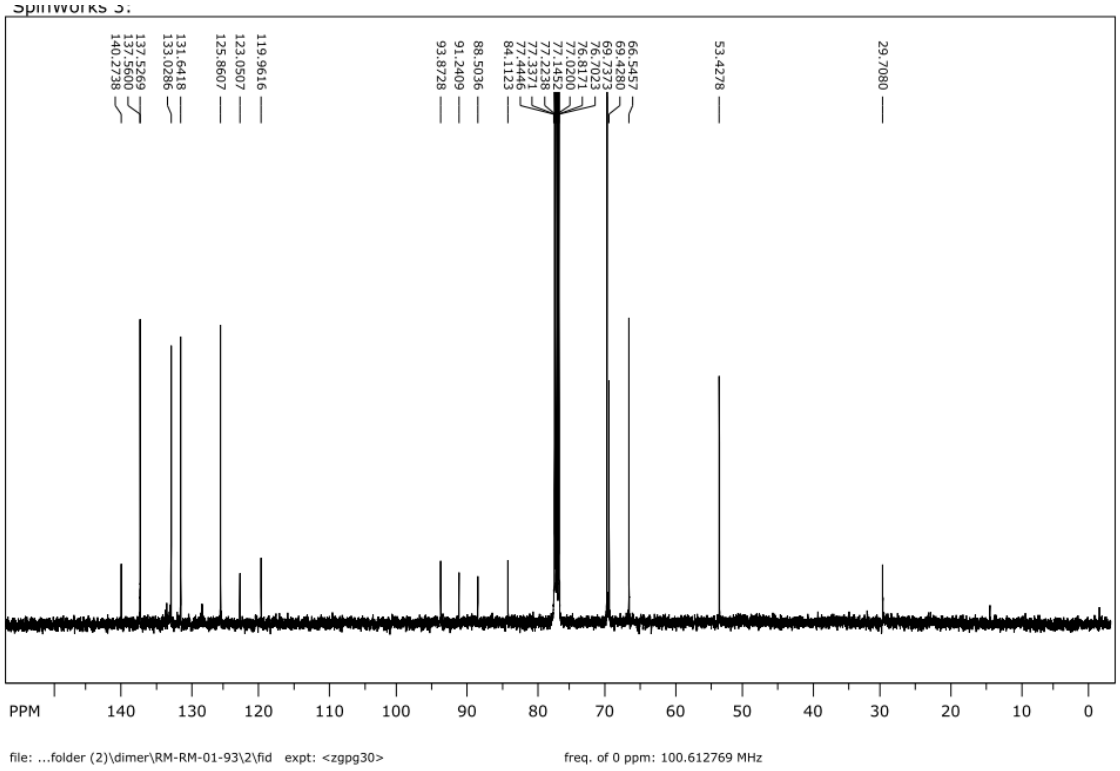


Fig. S-2: ^{13}C-NMR spectrum of compound **21** recorded in $CDCl_3$.

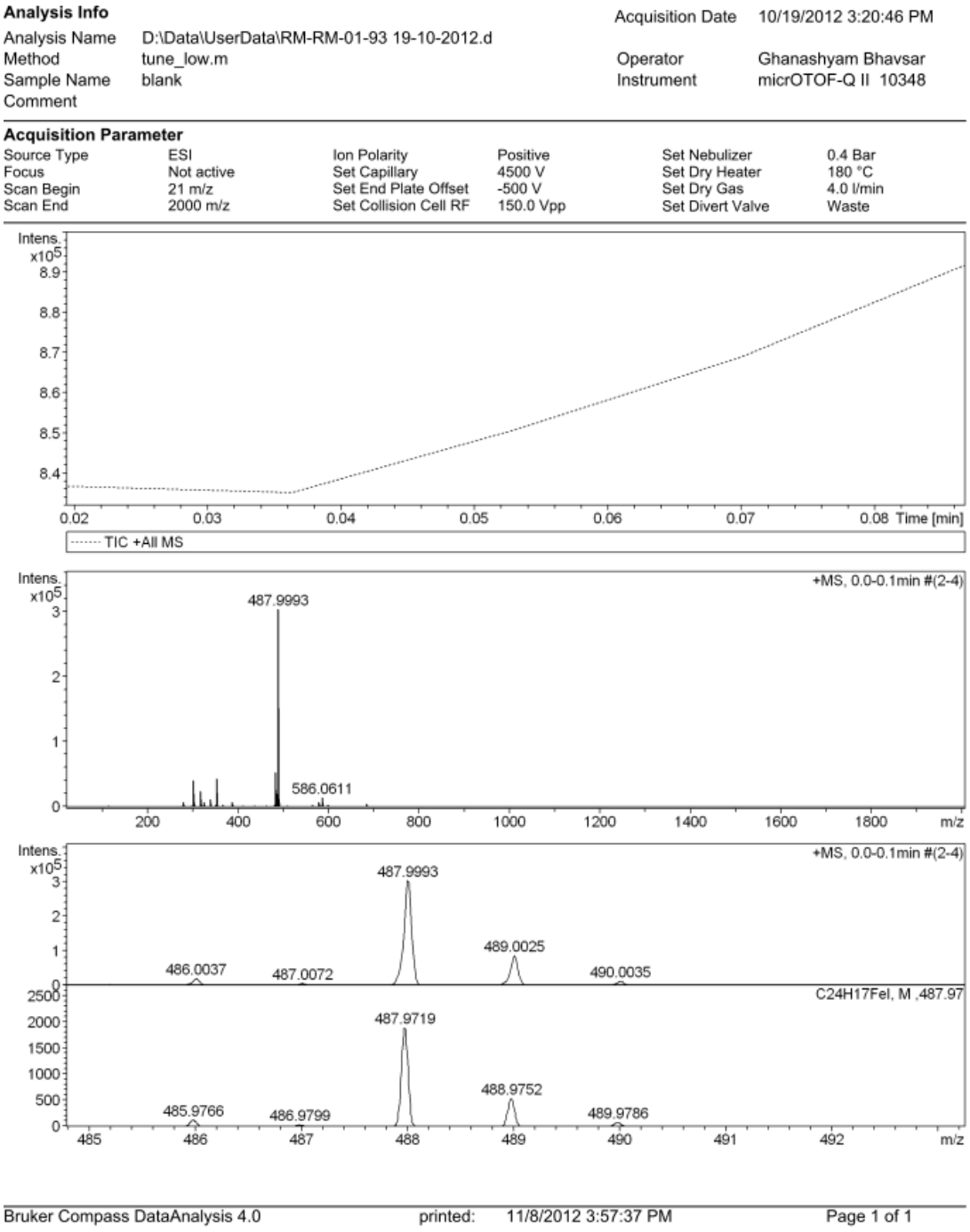


Fig. S-3: HRMS mass spectrum of compound **21.**

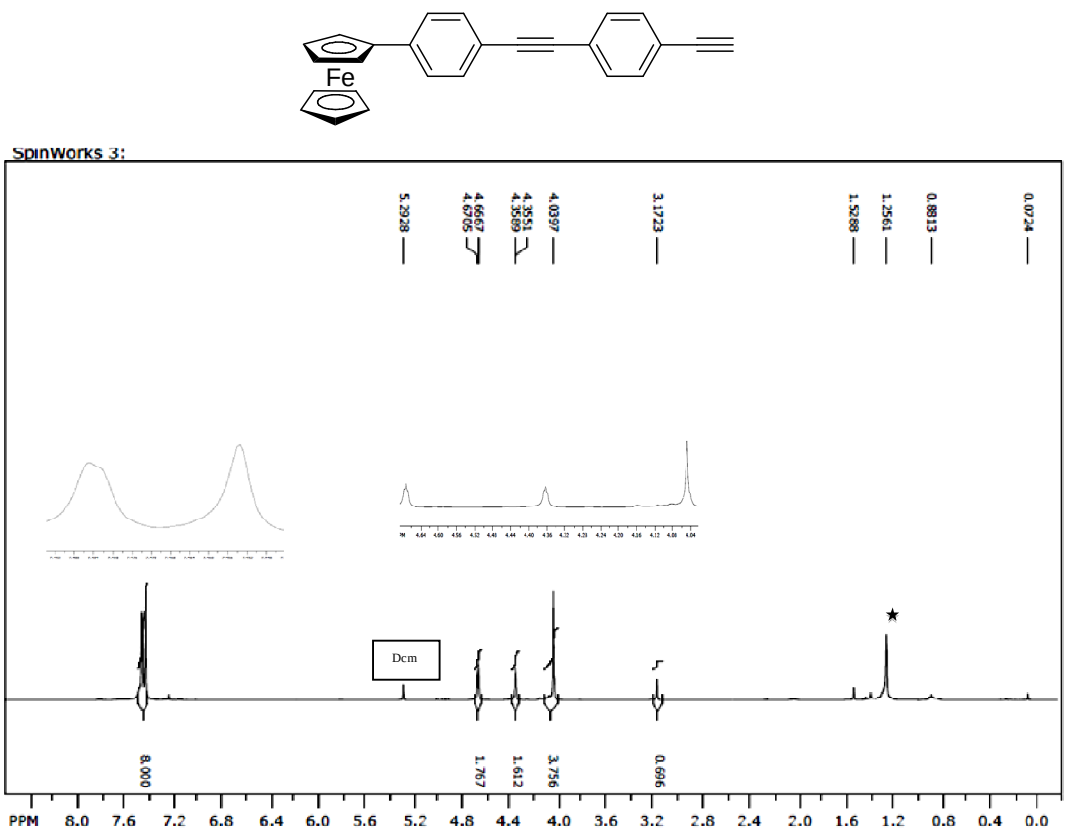


Fig. S-4: ^{1}H-NMR spectrum of compound **22** recorded in $CDCl_3$. ⋆ indicates hexane as residual solvent

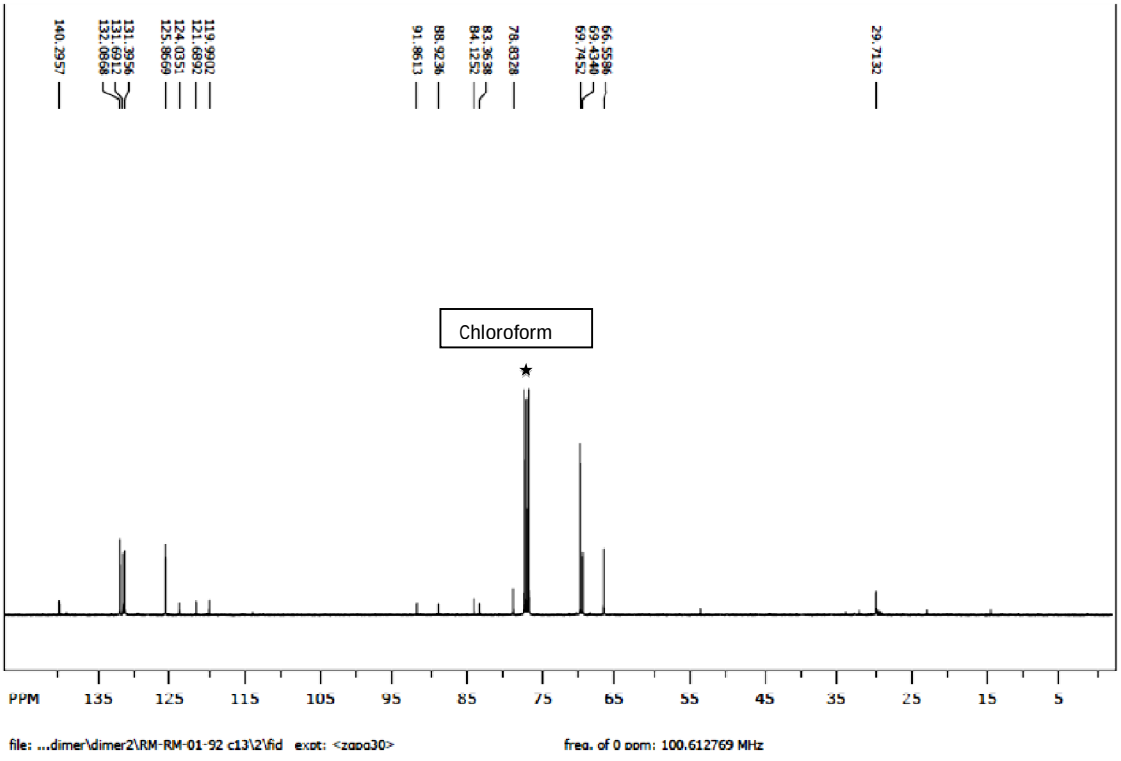


Fig. S-5: ^{13}C-NMR spectrum of compound **22** recorded in $CDCl_3$

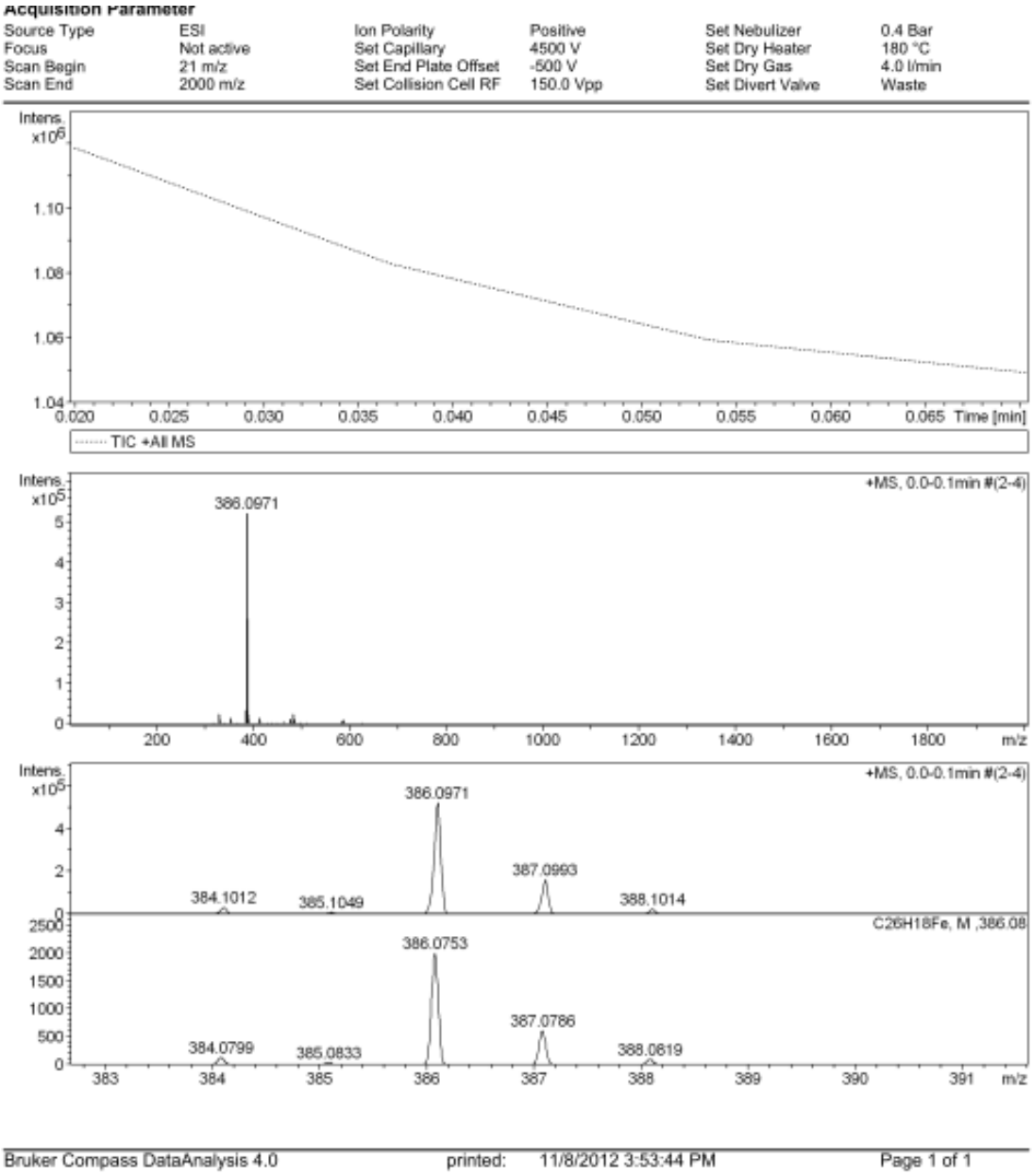
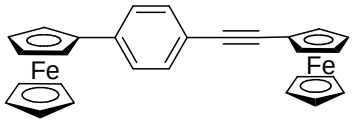


Fig. S-6: HRMS mass spectrum of compound **22**



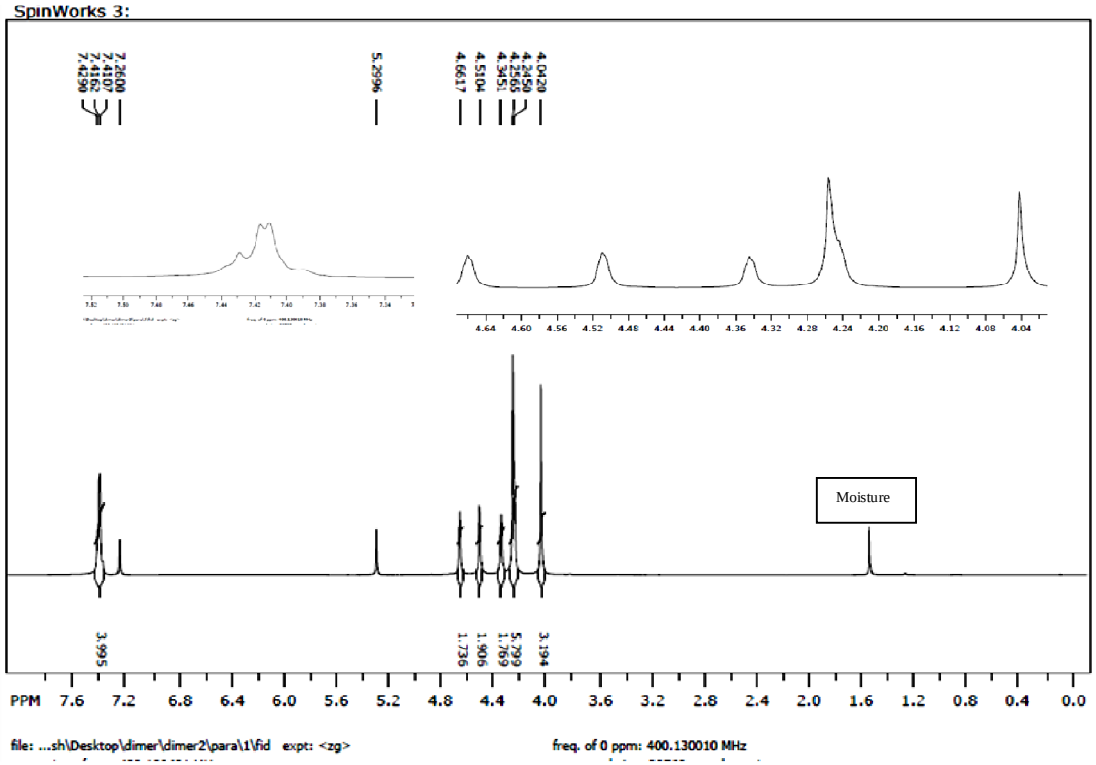


Fig. S-7: ^{1}H-NMR spectrum of compound **1** recorded in $CDCl_3$

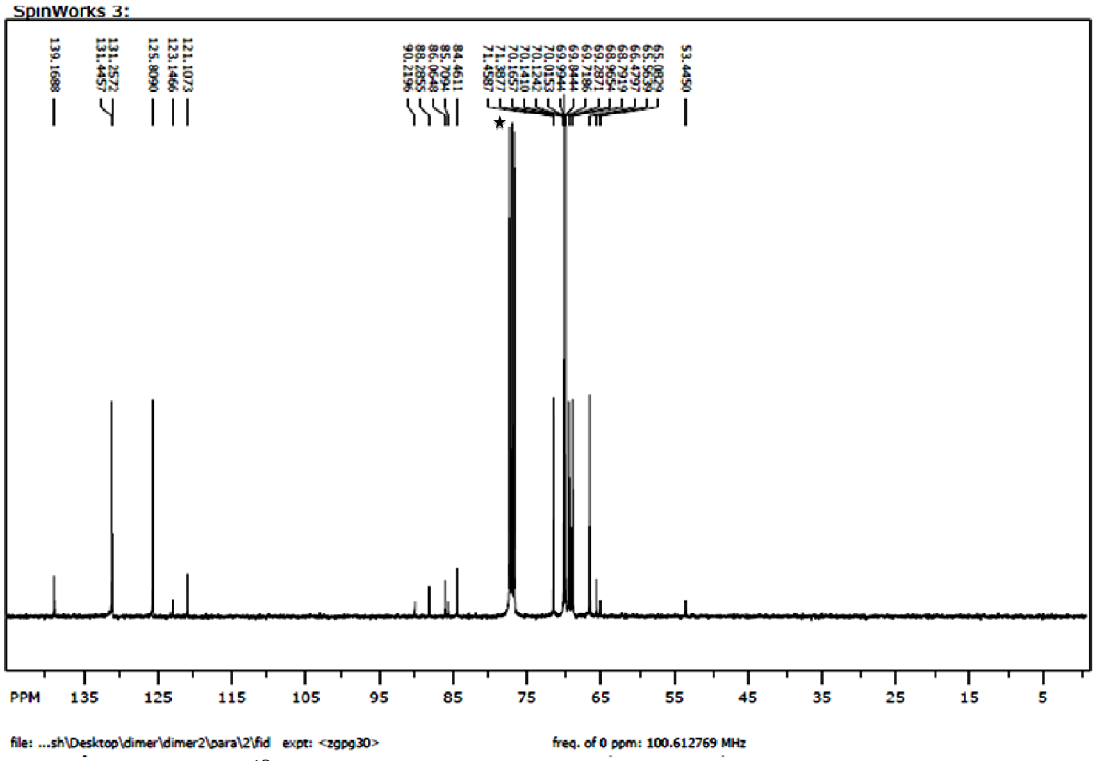


Fig. S-8: ^{13}C-NMR spectrum of compound **1** recorded in $CDCl_3$

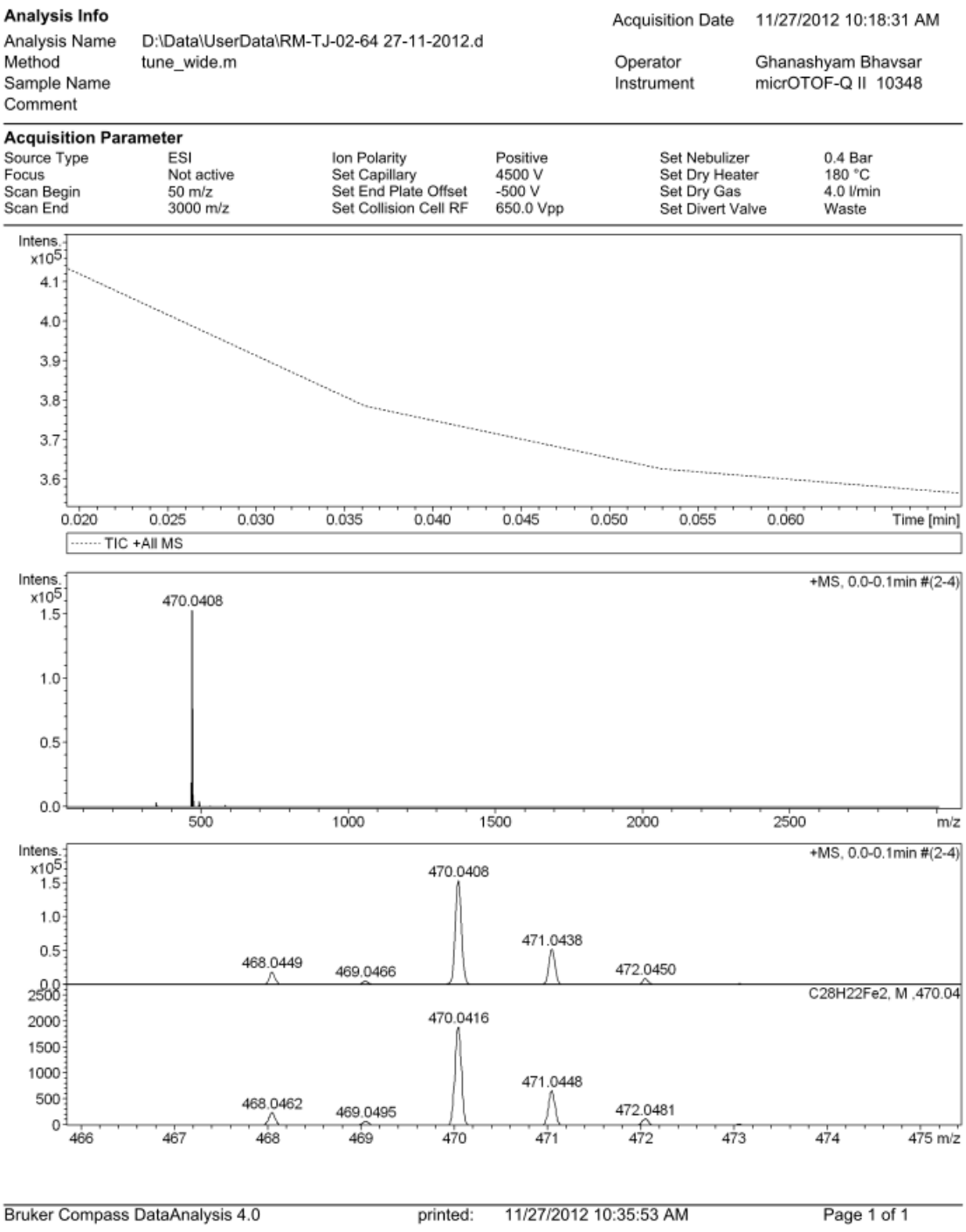


Fig. S-9: HRMS mass spectrum of compound **1**

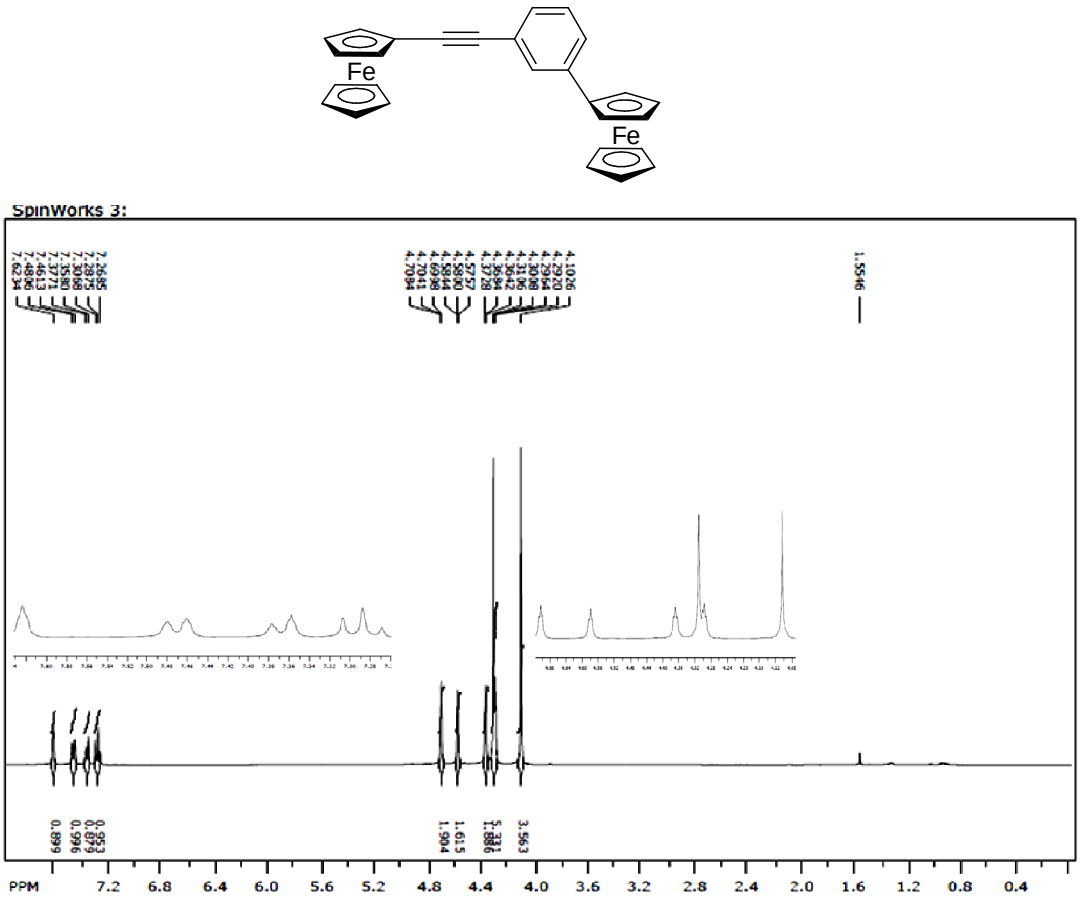


Fig. S-10: ^{1}H-NMR spectrum of compound **2** recorded in $CDCl_3$

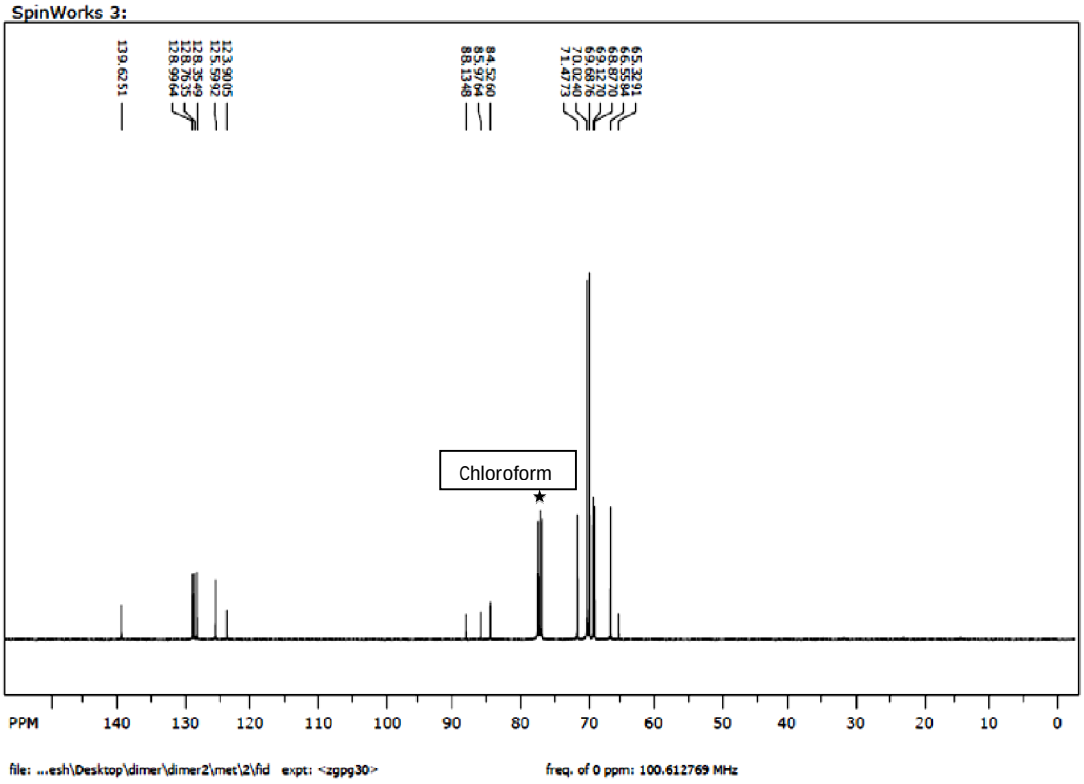


Fig. S-11: ^{13}C-NMR spectrum of compound **2** recorded in $CDCl_3$

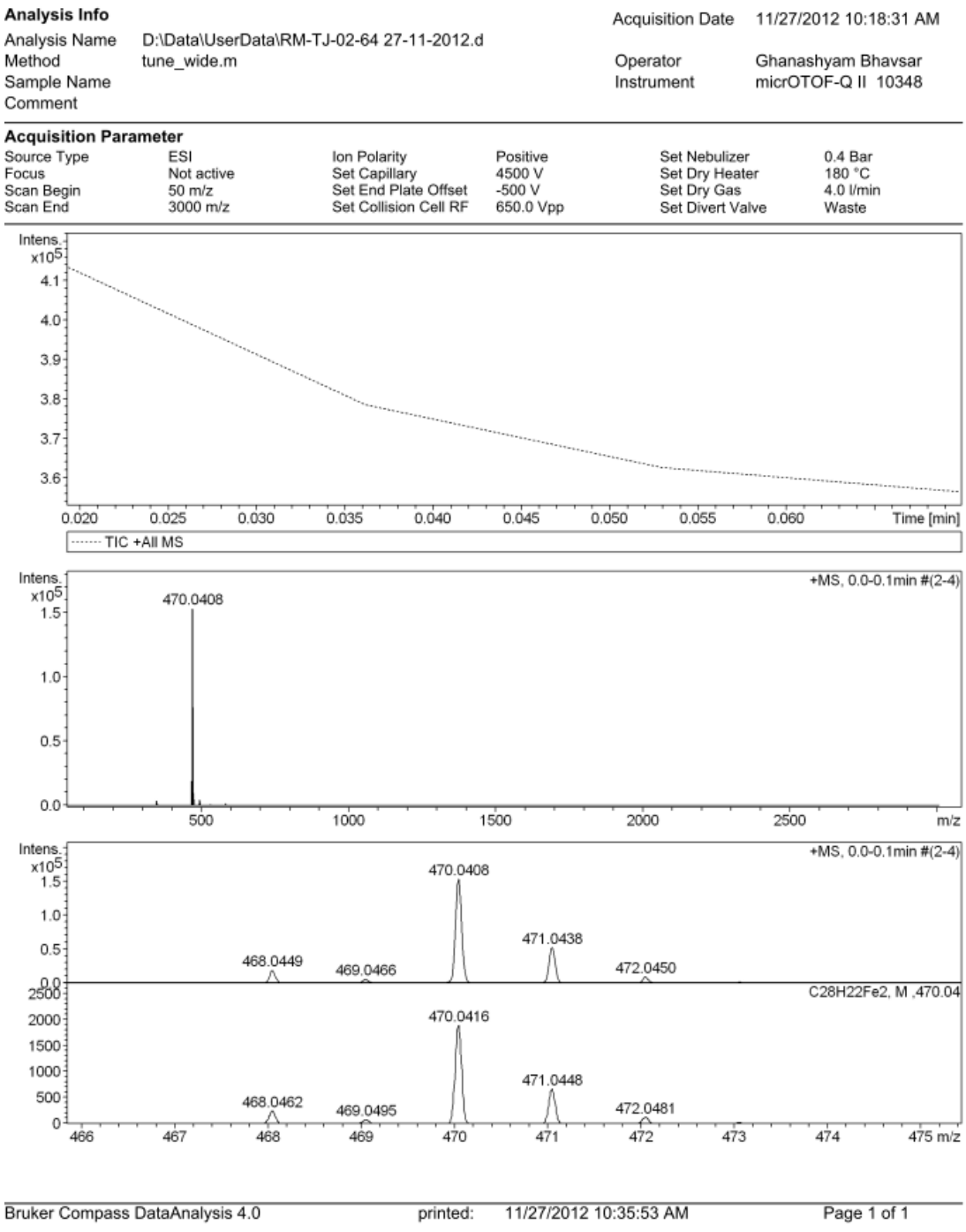
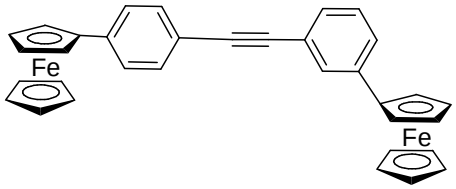


Fig. S-12: HRMS mass spectrum of compound **2**



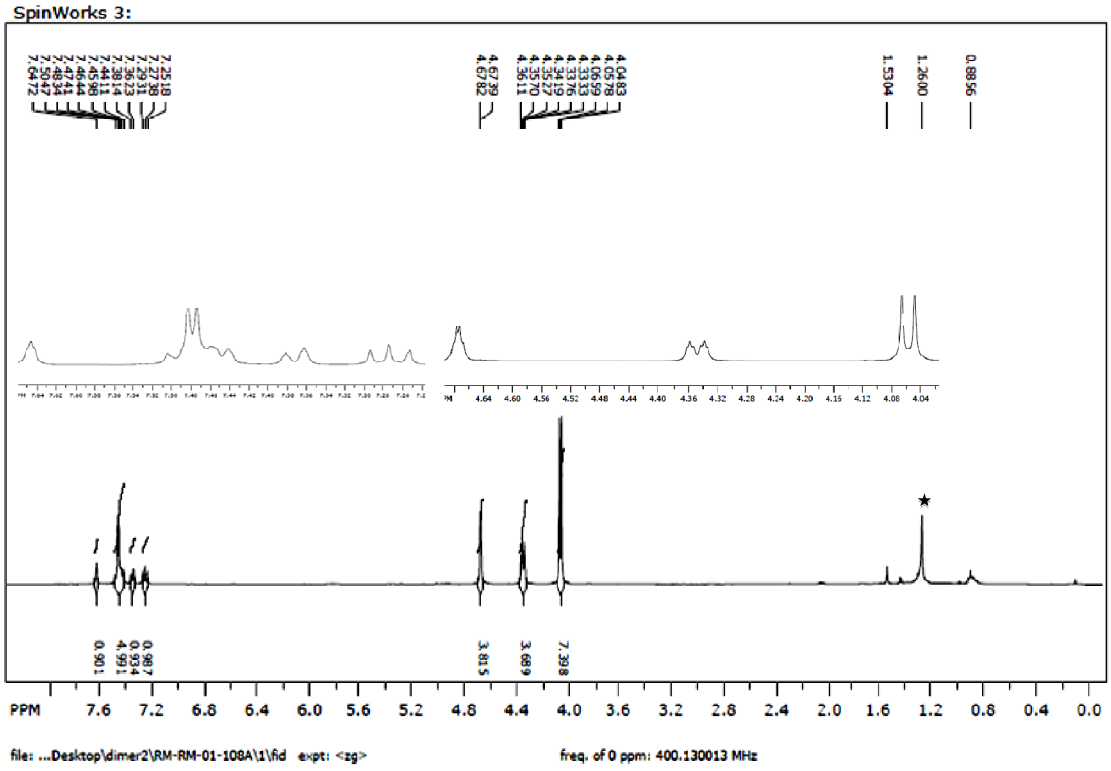


Fig. S-13: ^{1}H-NMR spectrum of compound **3** recorded in $CDCl_3$. indicates hexane as residual solvent

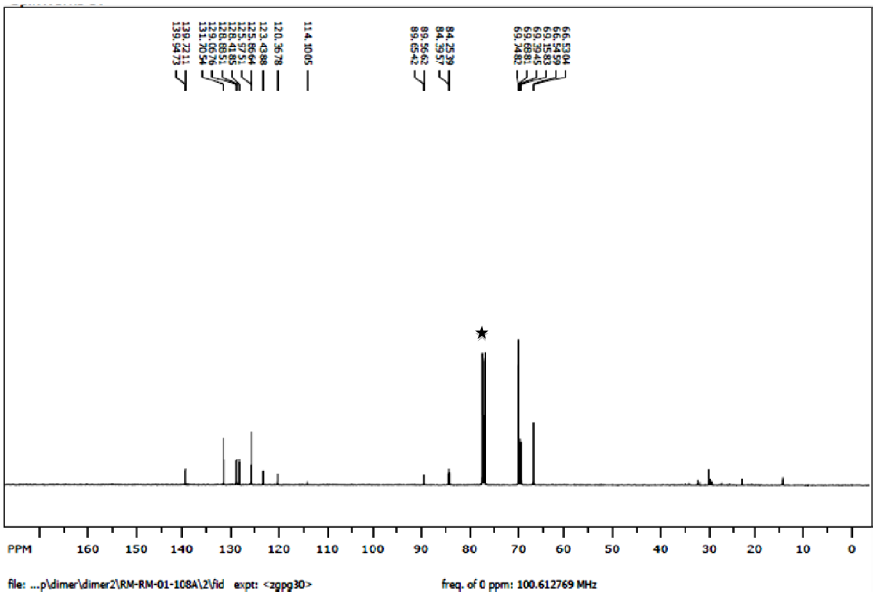


Fig. S-14: ^{13}C-NMR spectrum of compound **3** recorded in $CDCl_3$

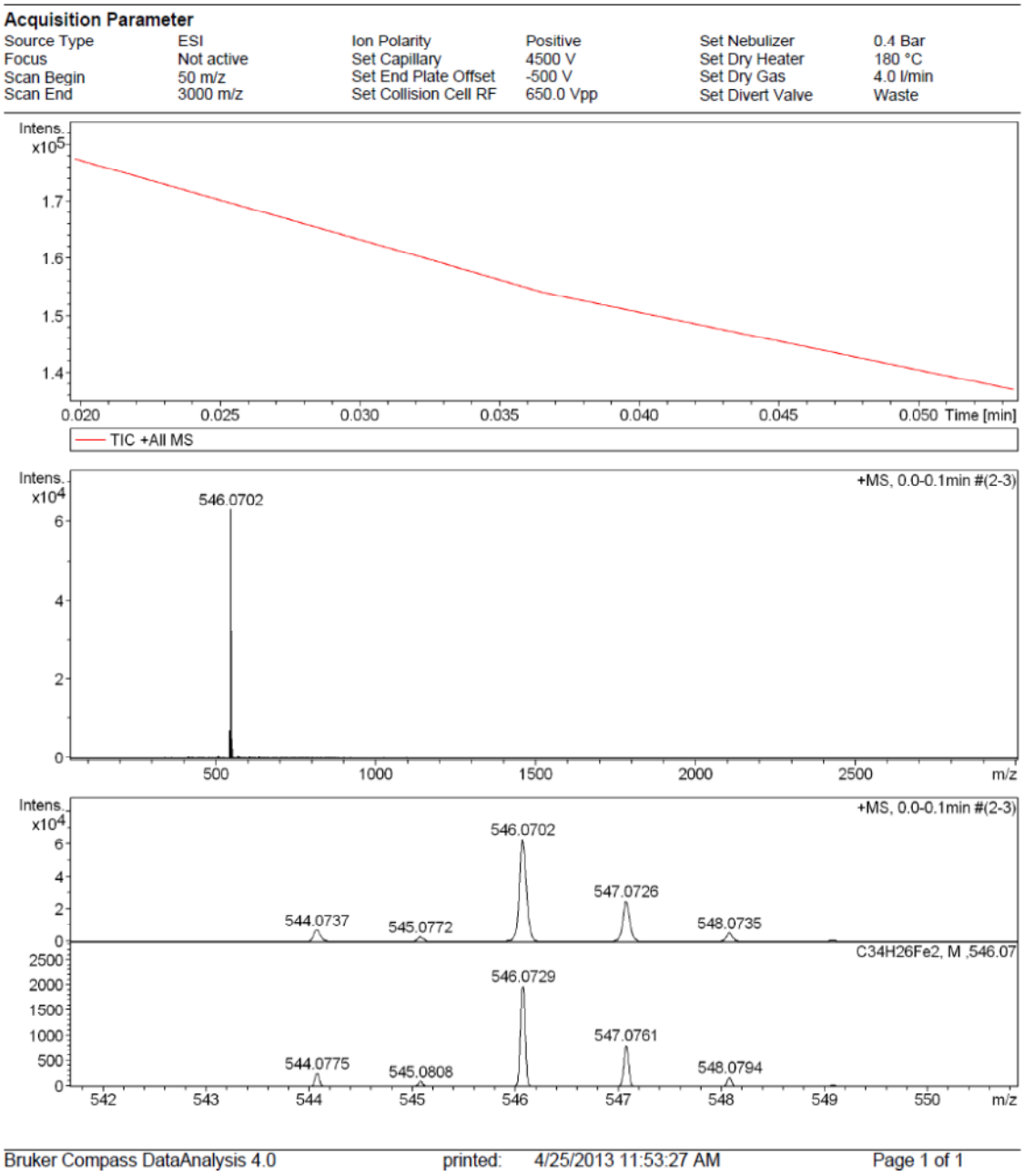


Fig. S-15: HRMS mass spectrum of compound **3**

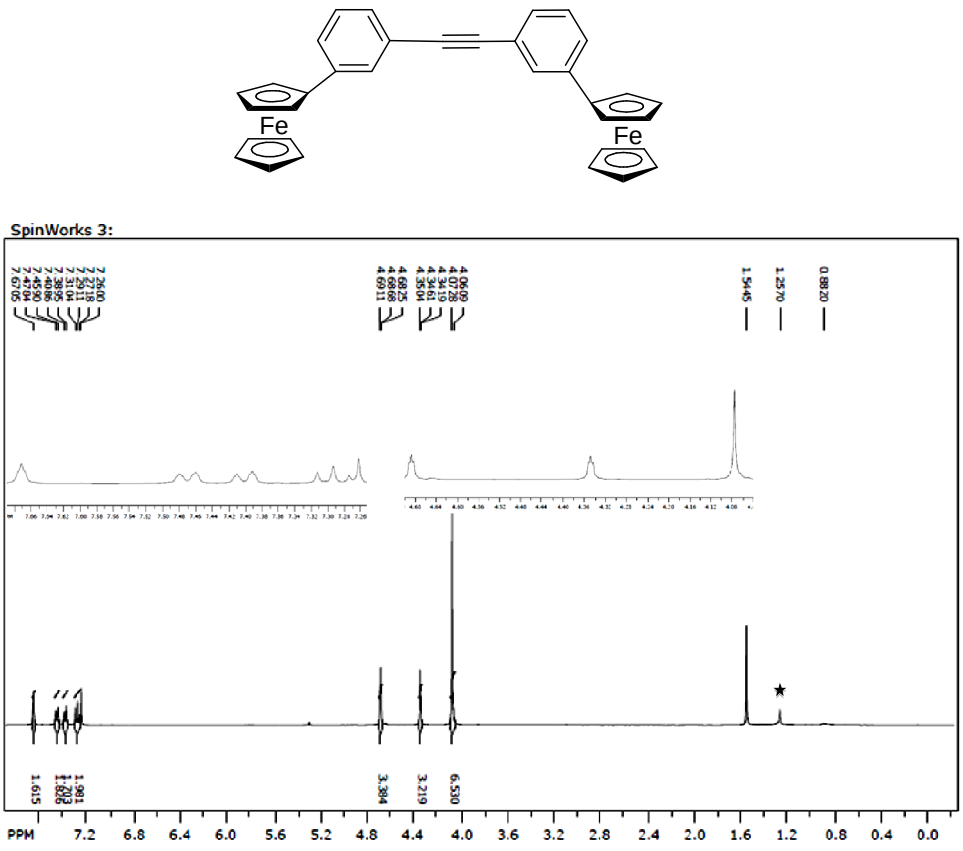


Fig. S-16: ^{1}H-NMR spectrum of compound **4** recorded in $CDCl_3$. ⋆indicates hexane as residual solvent

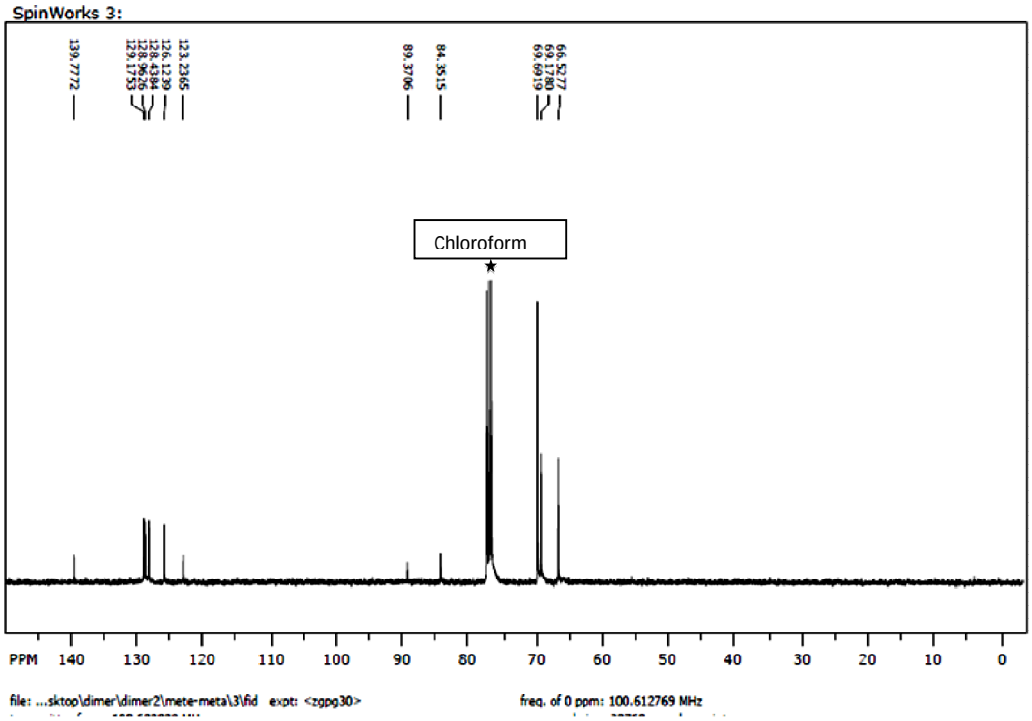


Fig. S-17: ^{13}C-NMR spectrum of compound **4** recorded in $CDCl_3$

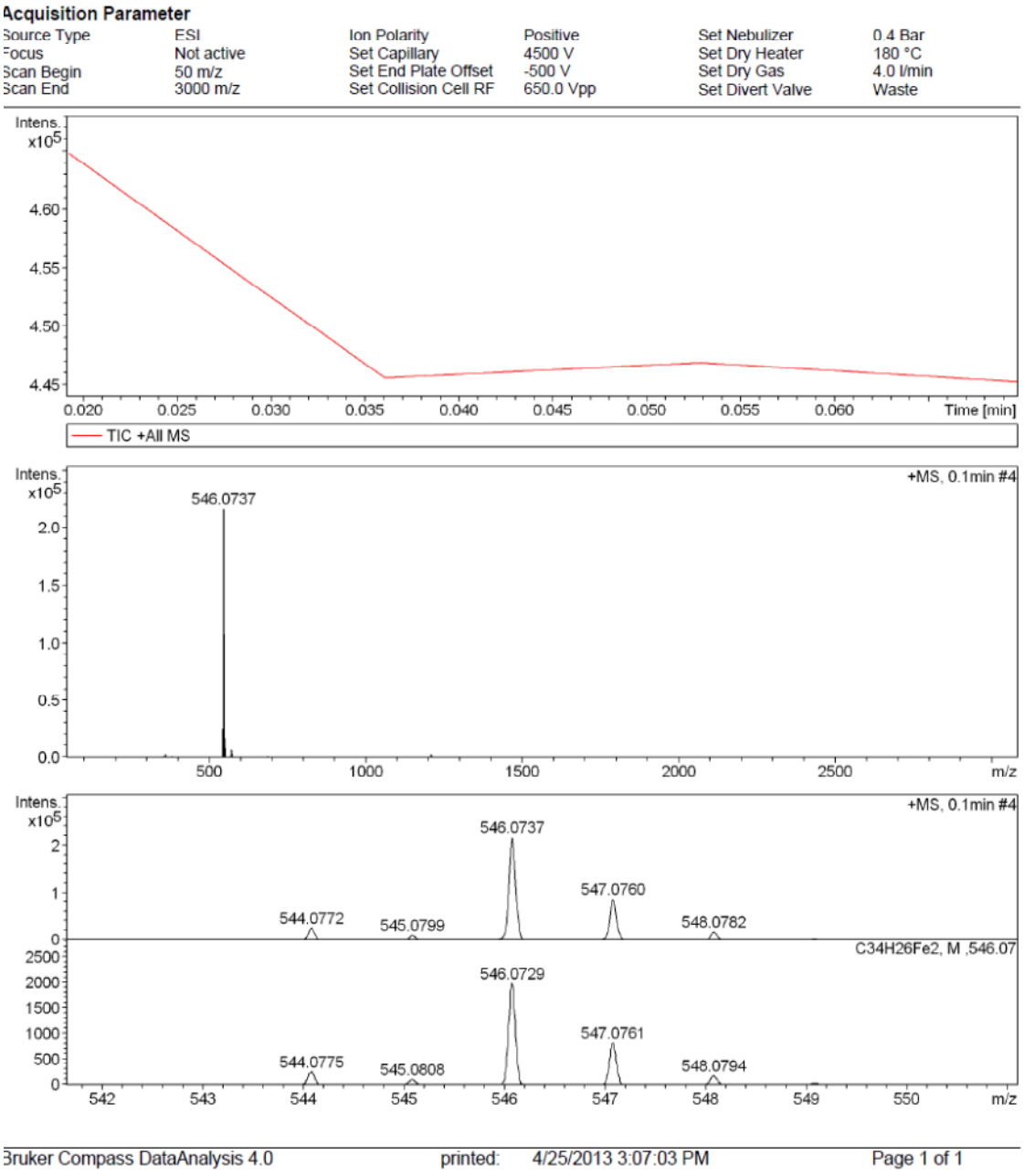
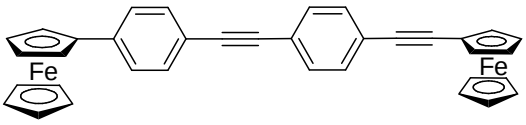


Fig. S-18: HRMS mass spectrum of compound **4**



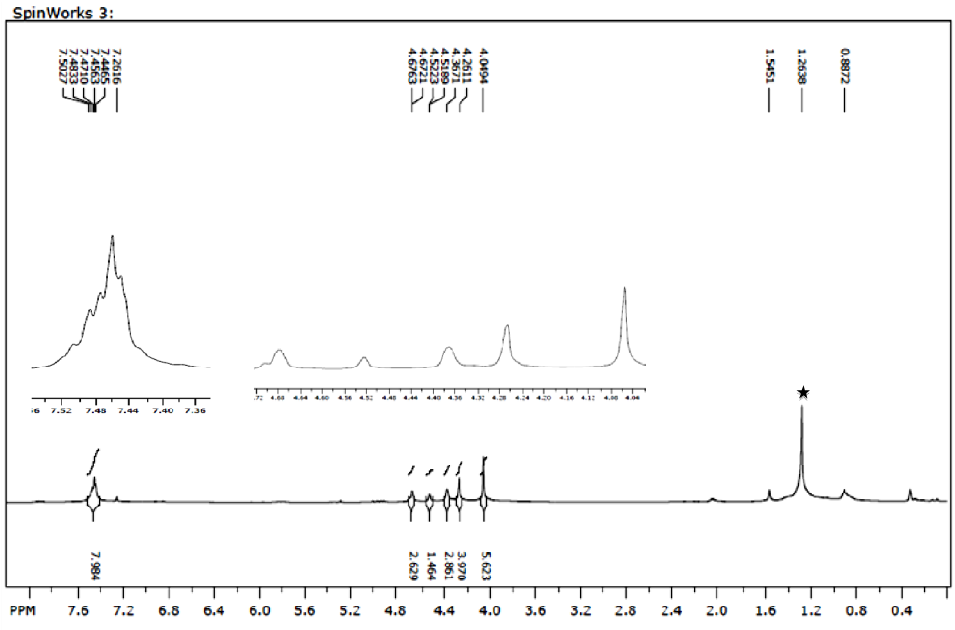


Fig. S-19: ^{1}H-NMR spectrum of compound **5** recorded in $CDCl_3$. ★ indicates hexane as residual solvent

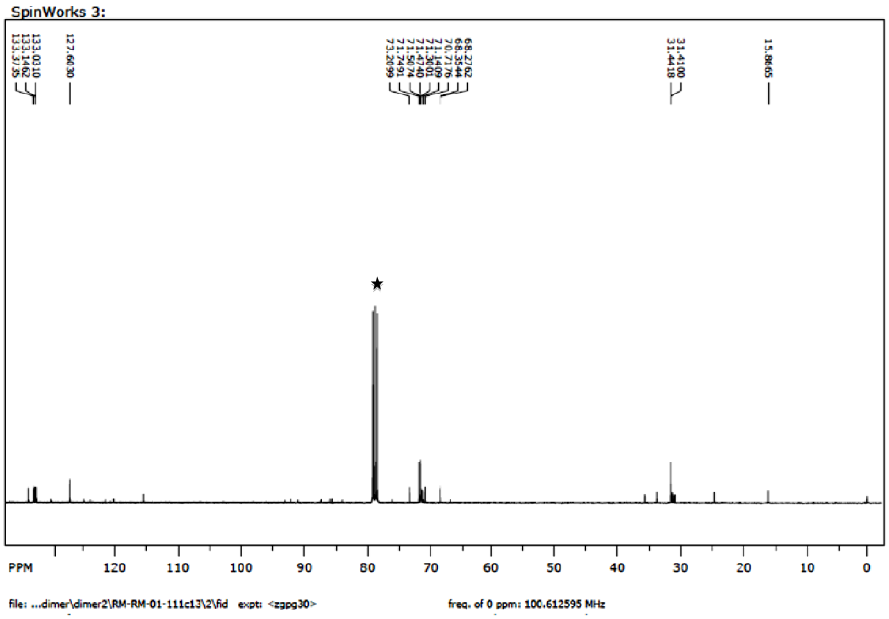


Fig. S-20: ^{13}C-NMR spectrum of compound **5** recorded in $CDCl_3$

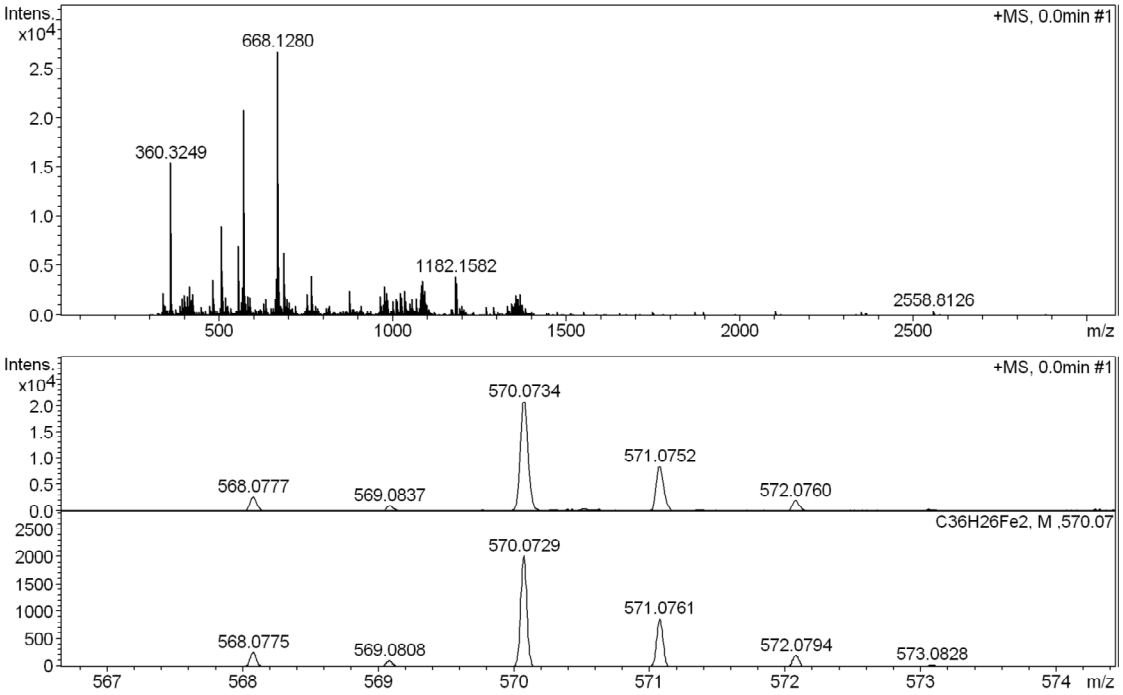


Fig. S-21: HRMS mass spectrum of compound **5**

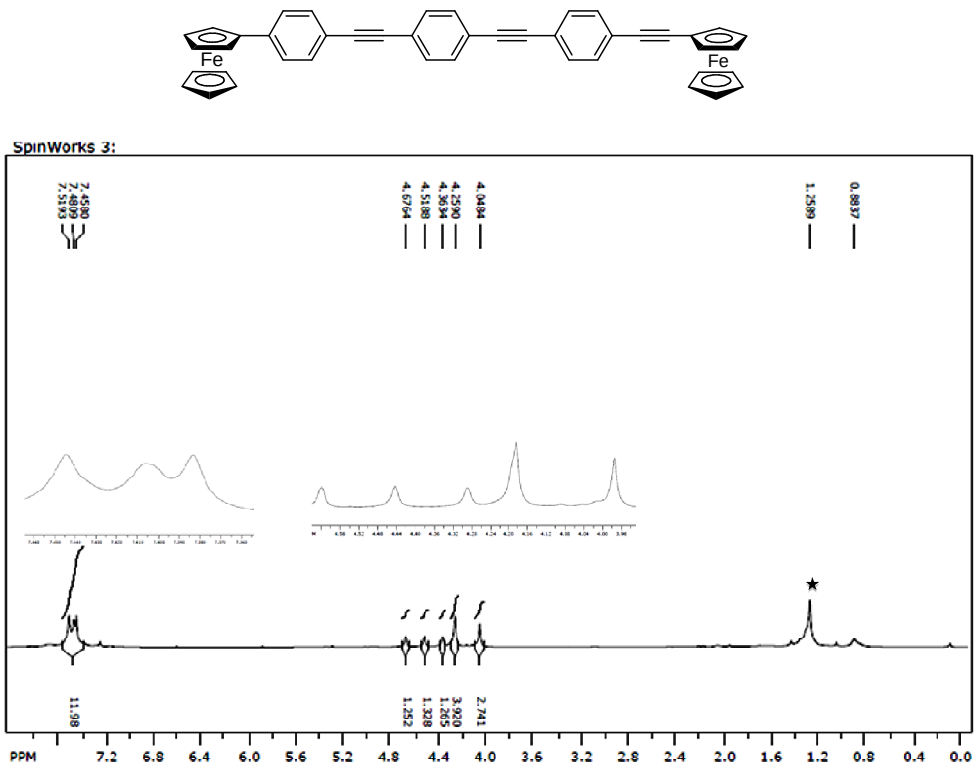


Fig. S-22: ^{1}H-NMR spectrum of compound **6** recorded in $CDCl_3$. ★ indicates hexane as residual solvent

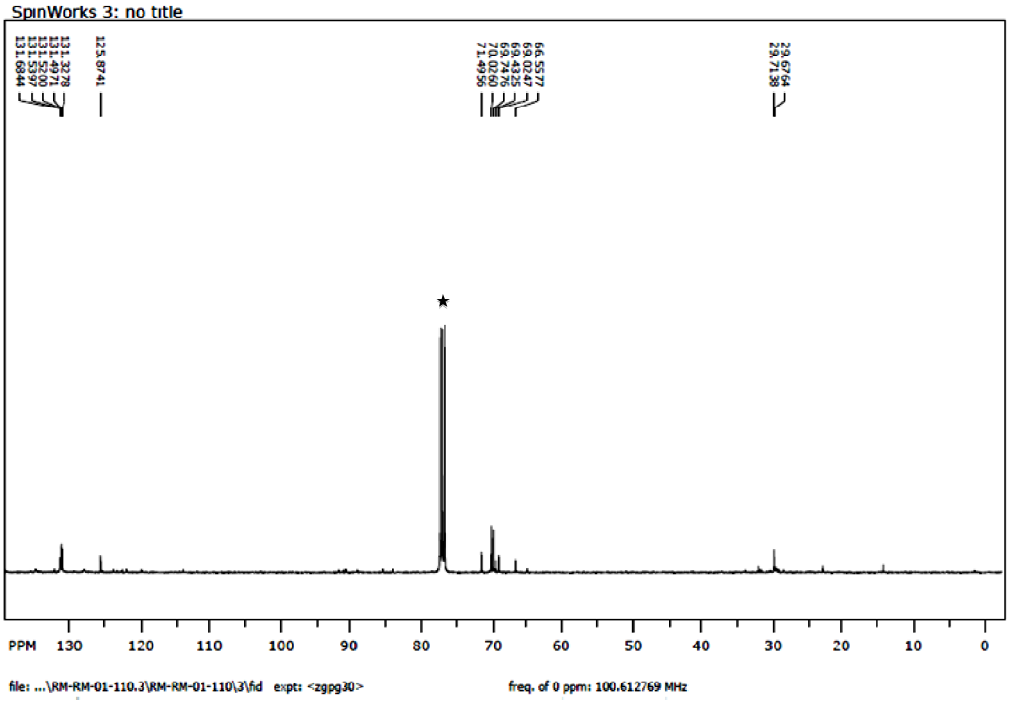


Fig. S-23: ^{13}C-NMR spectrum of compound **6** recorded in $CDCl_3$

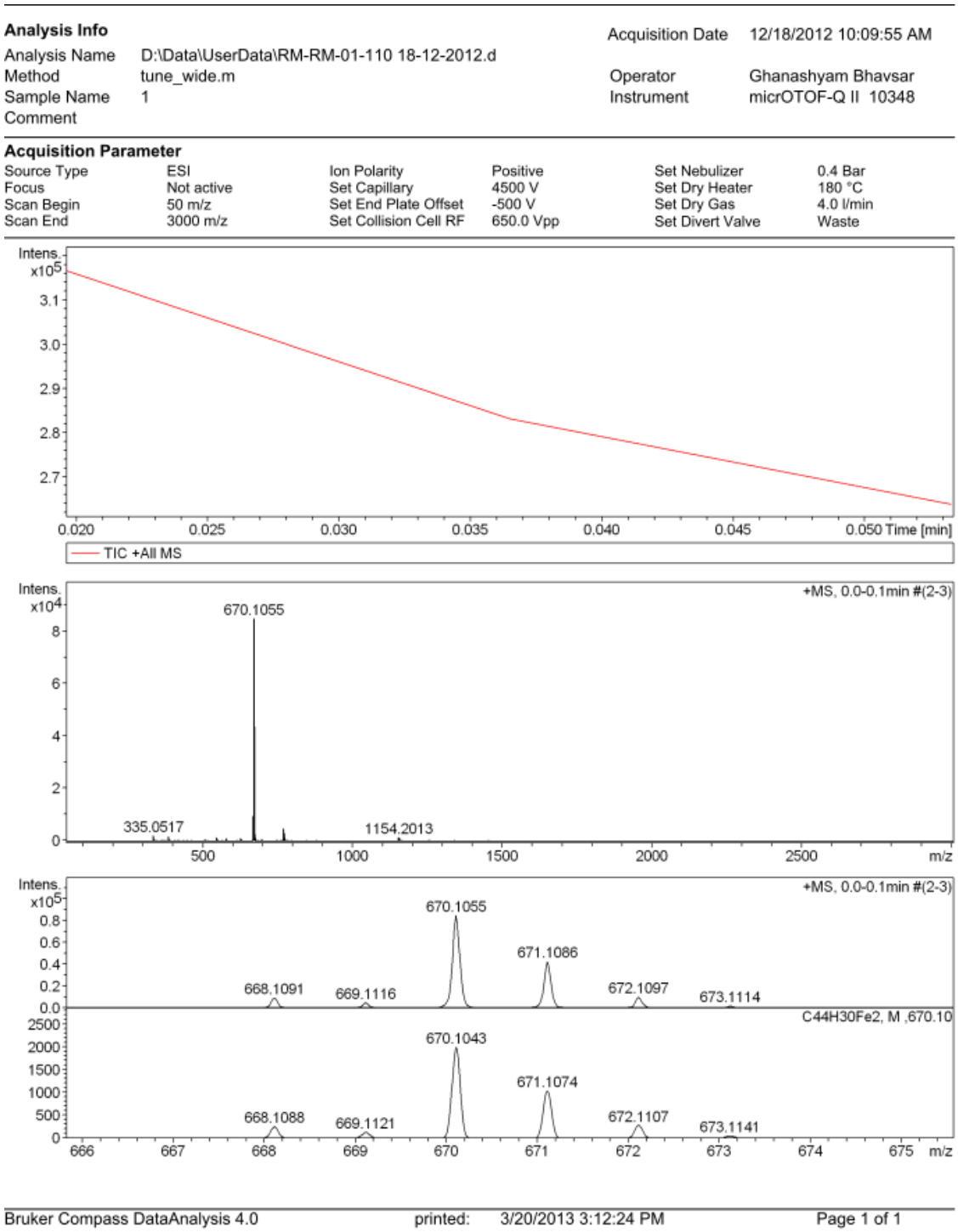
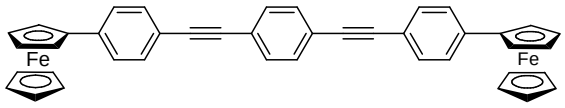


Fig. S-24: HRMS mass spectrum of compound **6**



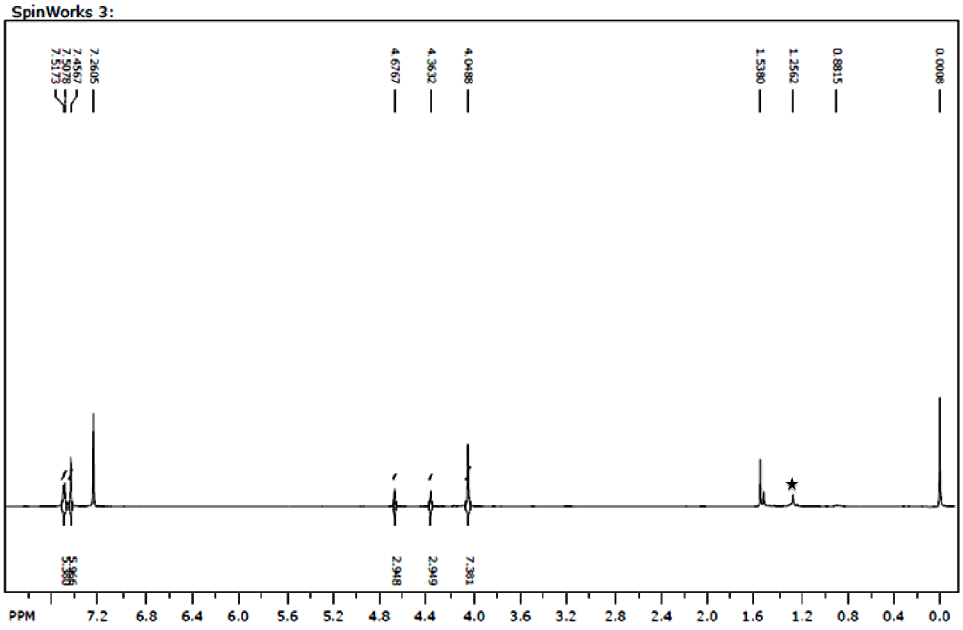


Fig. S-25: ^{1}H-NMR spectrum of compound **7** recorded in $CDCl_3$. ⋆ indicates hexane as residual solvent

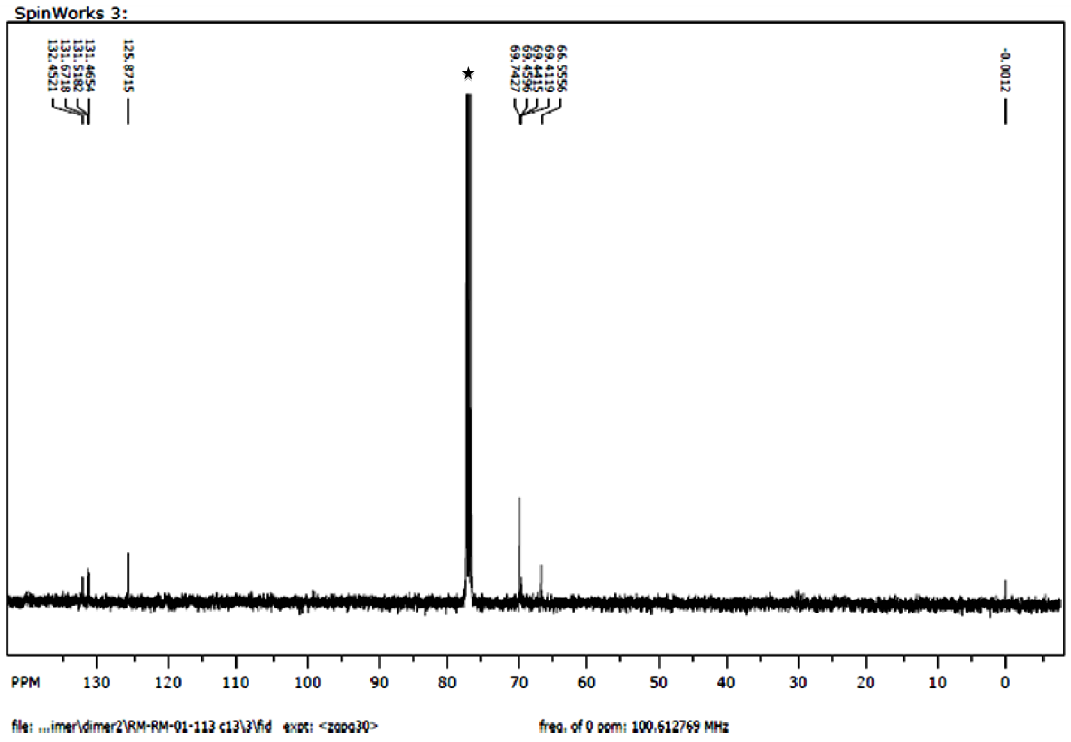


Fig. S-26: ^{13}C-NMR spectrum of compound **7** recorded in $CDCl_3$

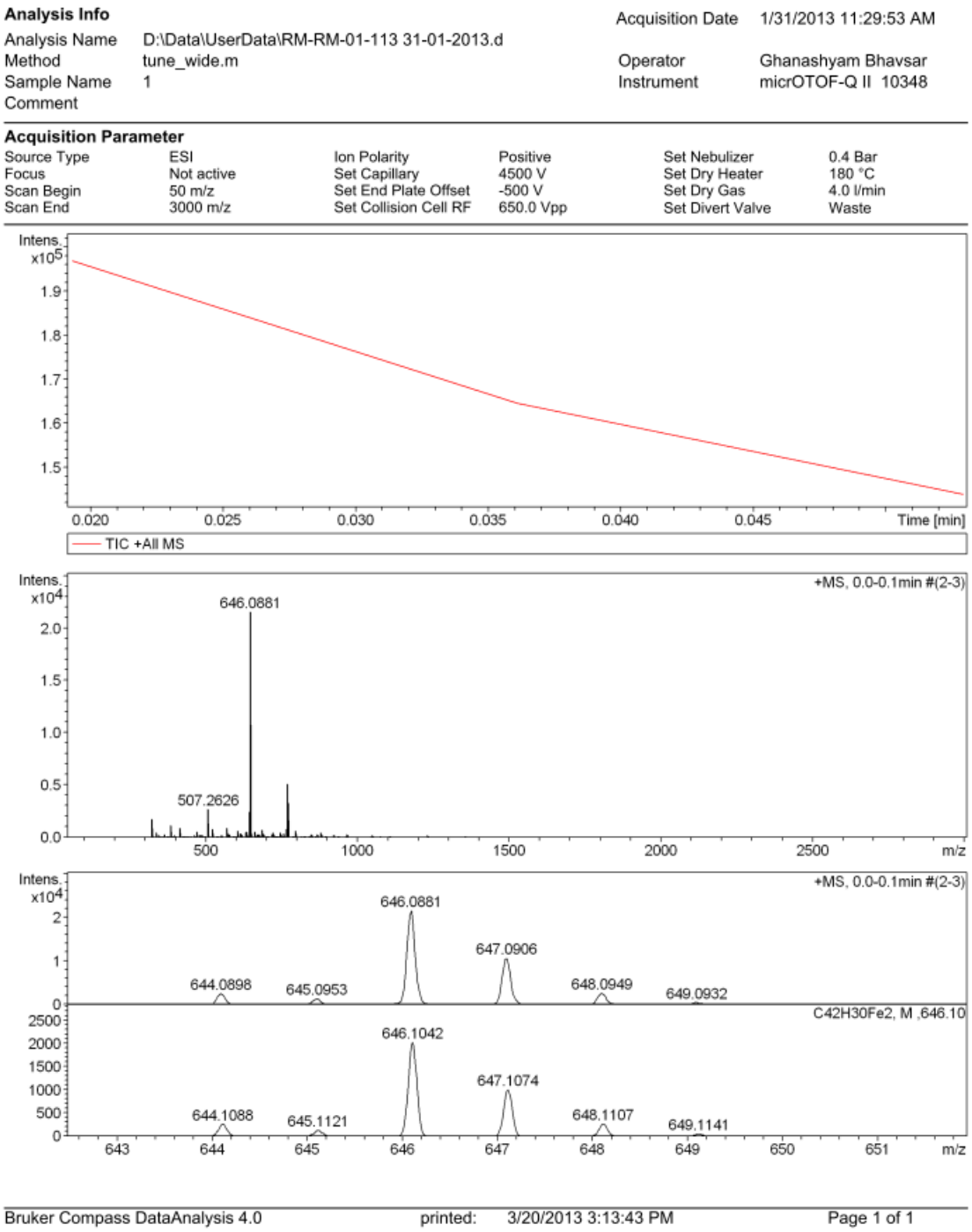
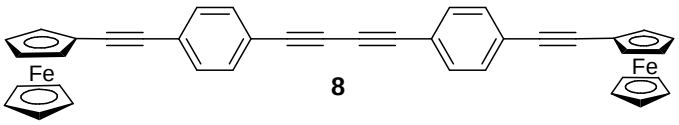


Fig. S-27: HRMS mass spectrum of compound **7**



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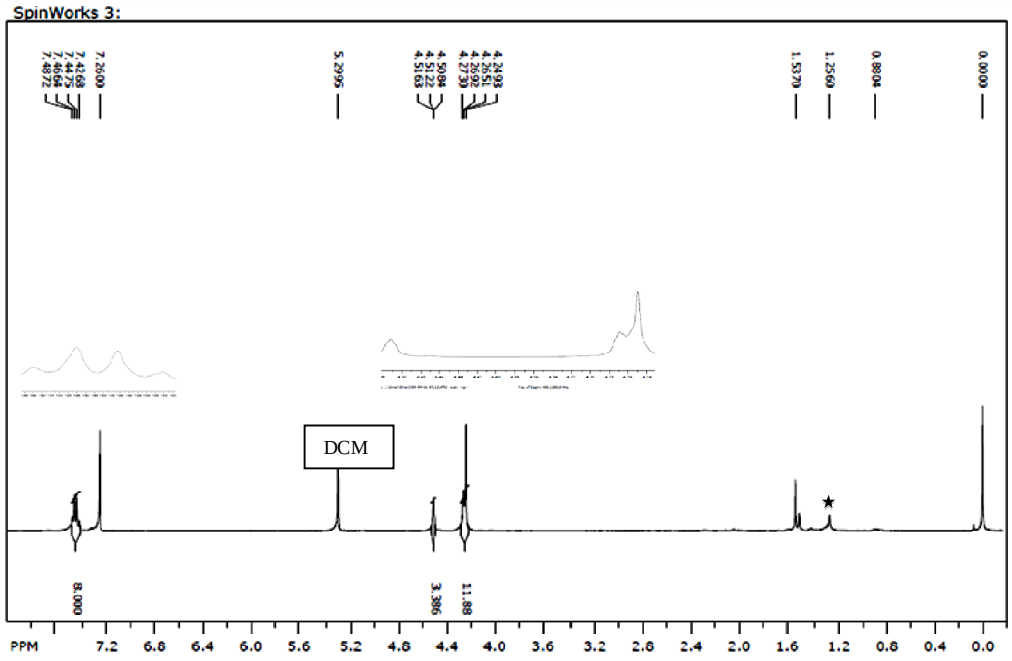


Fig. S-28: ^{1}H-NMR spectrum of compound **8** recorded in $CDCl_3$. ⋆ indicates hexane as residual solvent

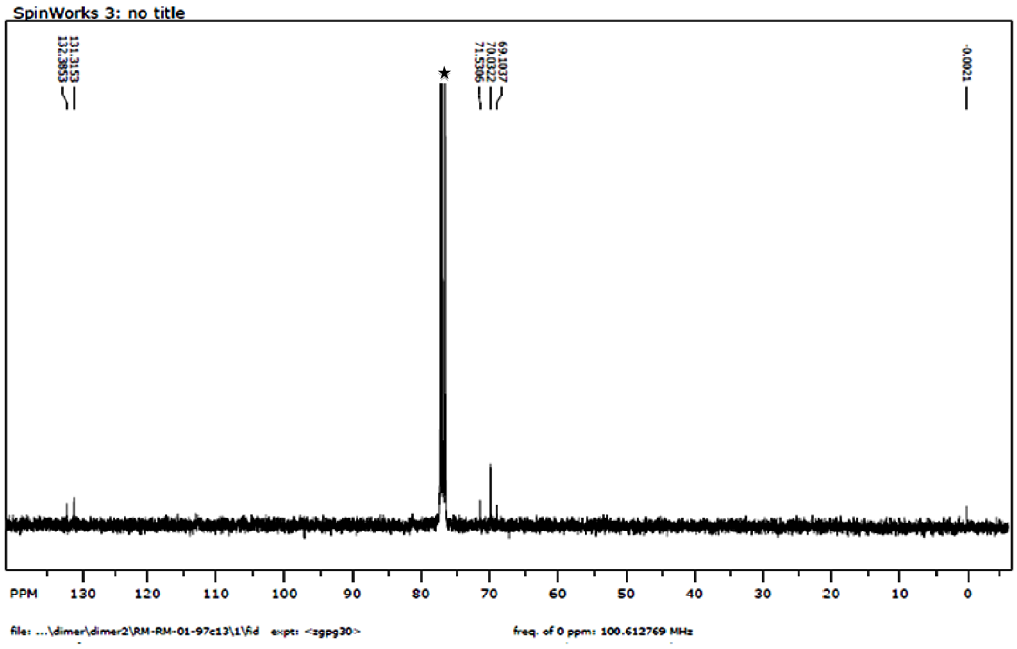


Fig. S-29: ^{13}C-NMR spectrum of compound **8** recorded in $CDCl_3$

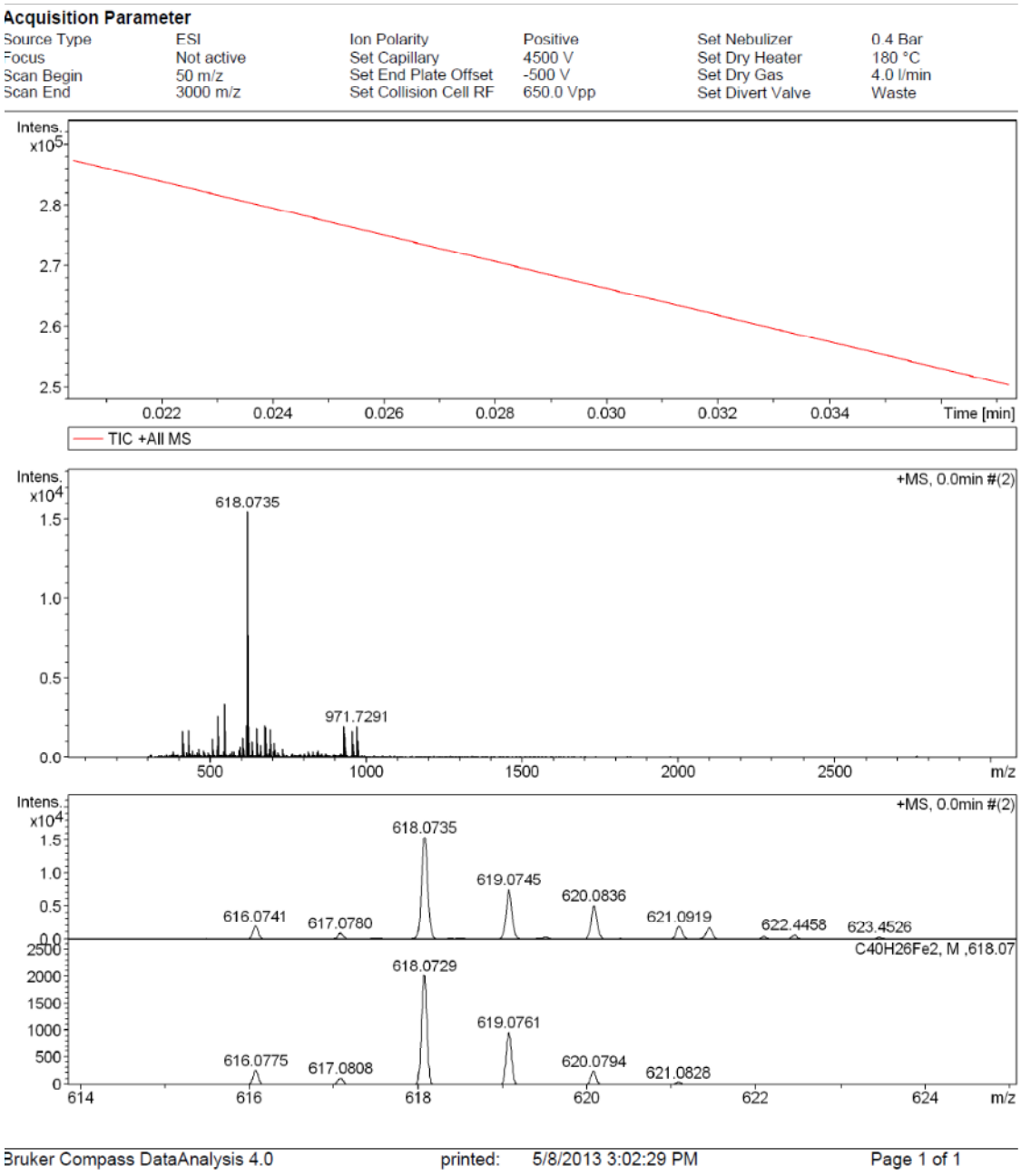
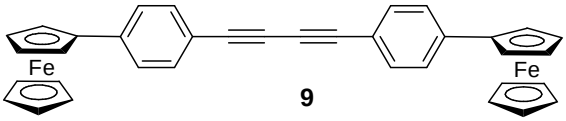


Fig. S-30: HRMS mass spectrum of compound **8**



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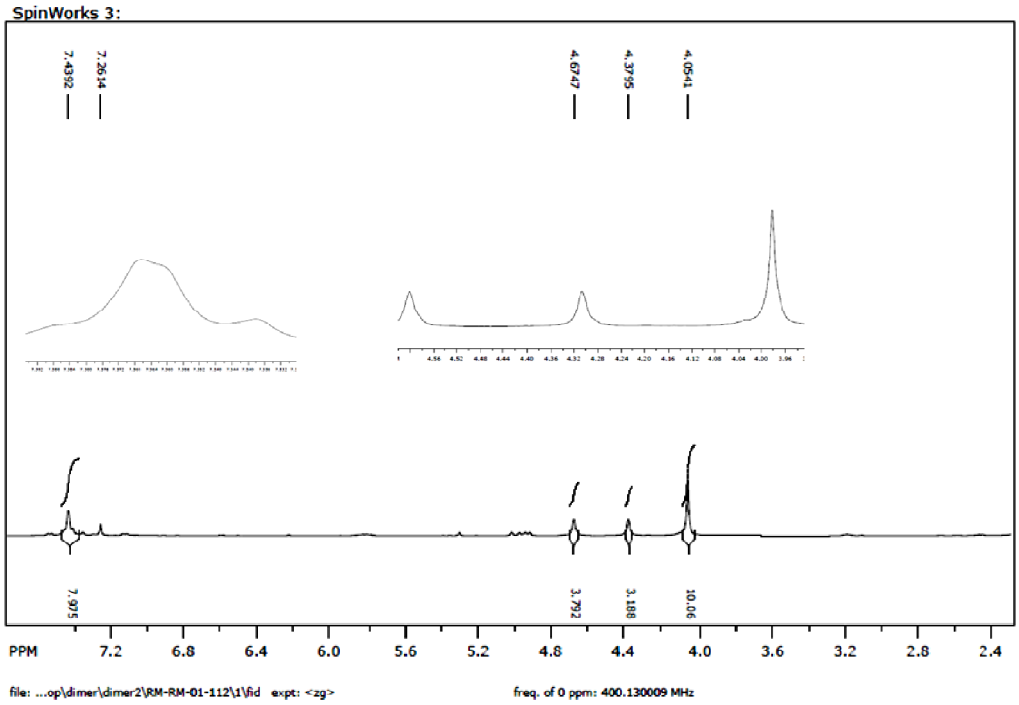


Fig. S-31: ^{1}H-NMR spectrum of compound **9** recorded in $CDCl_3$

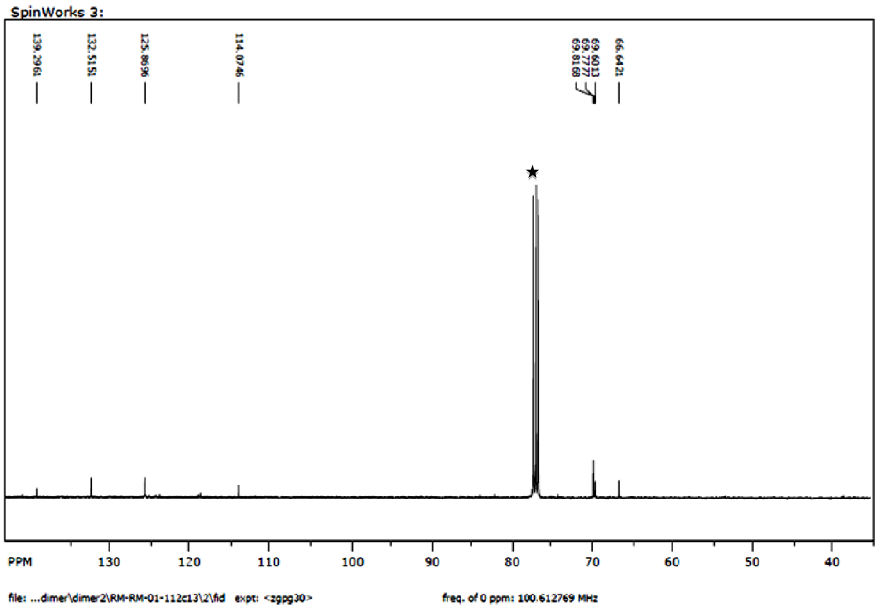


Fig. S-32: ^{13}C-NMR spectrum of compound **9** recorded in $CDCl_3$

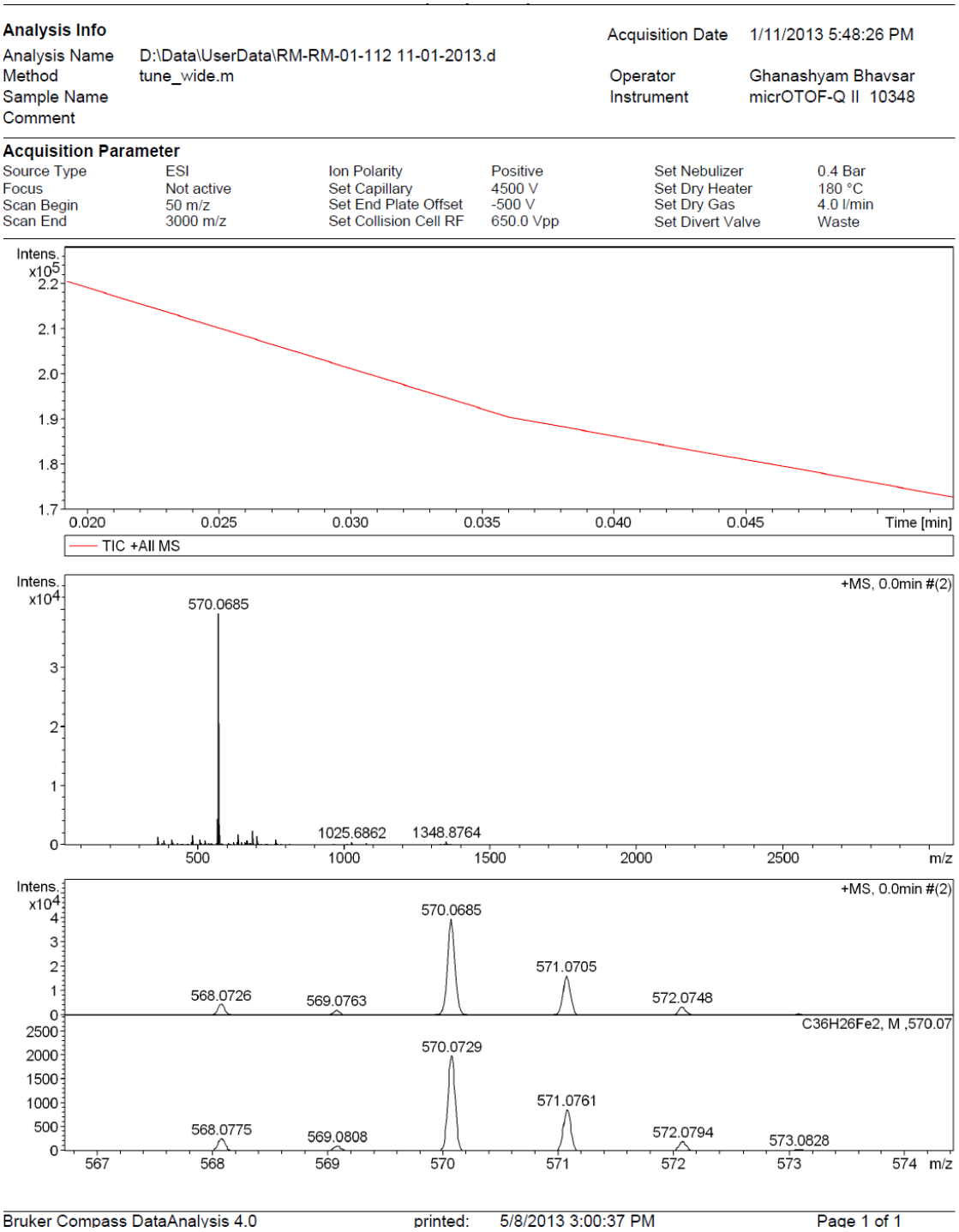
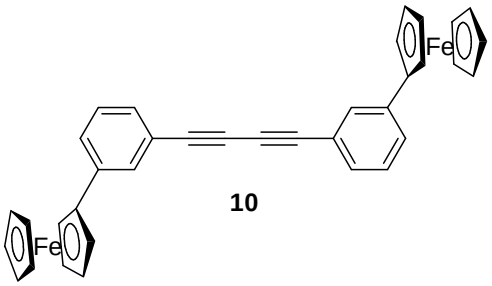


Fig. S-33: HRMS mass spectrum of compound **9**



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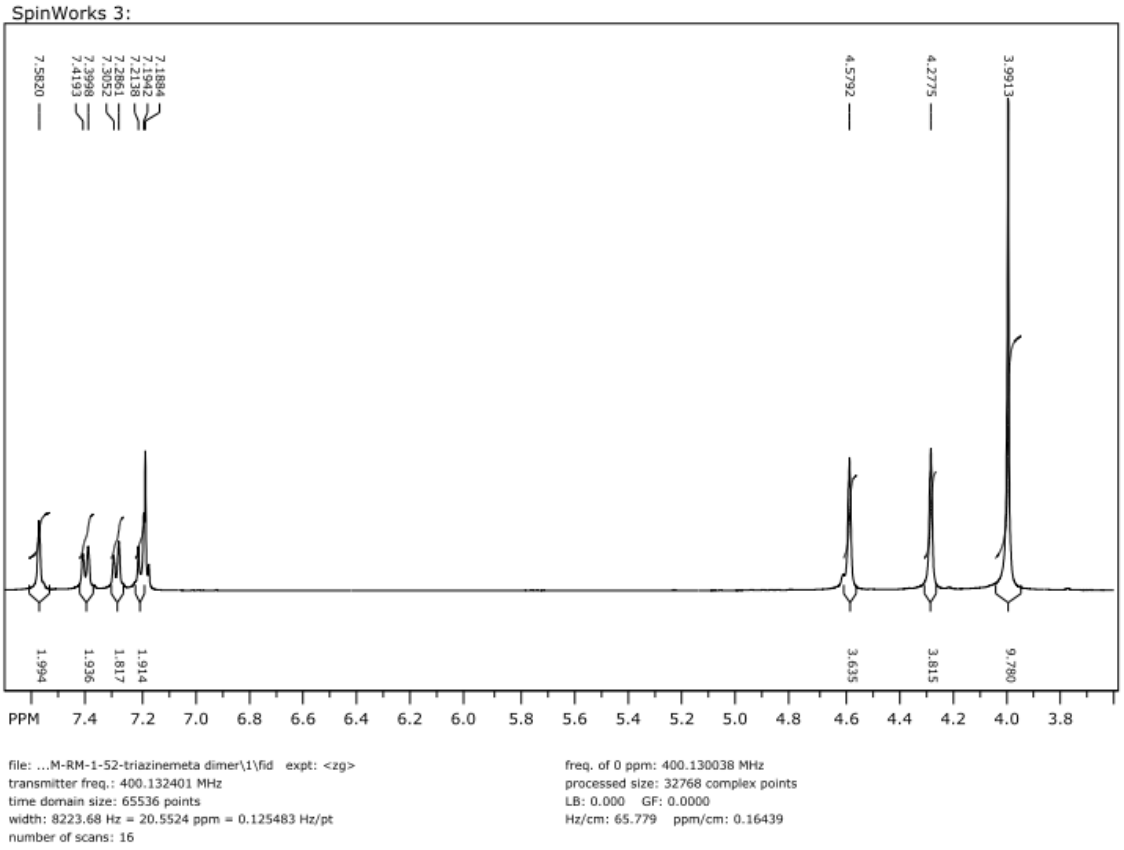


Fig. S-34: ^{1}H-NMR spectrum of compound **10** recorded in $CDCl_3$

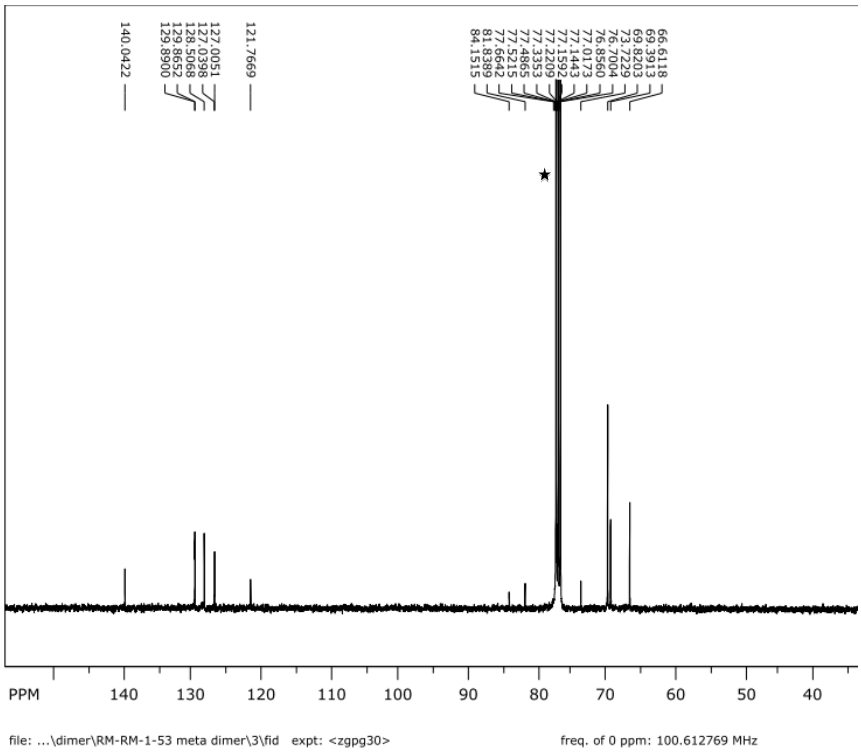


Fig. S-35: ^{13}C-NMR spectrum of compound **10** recorded in $CDCl_3$

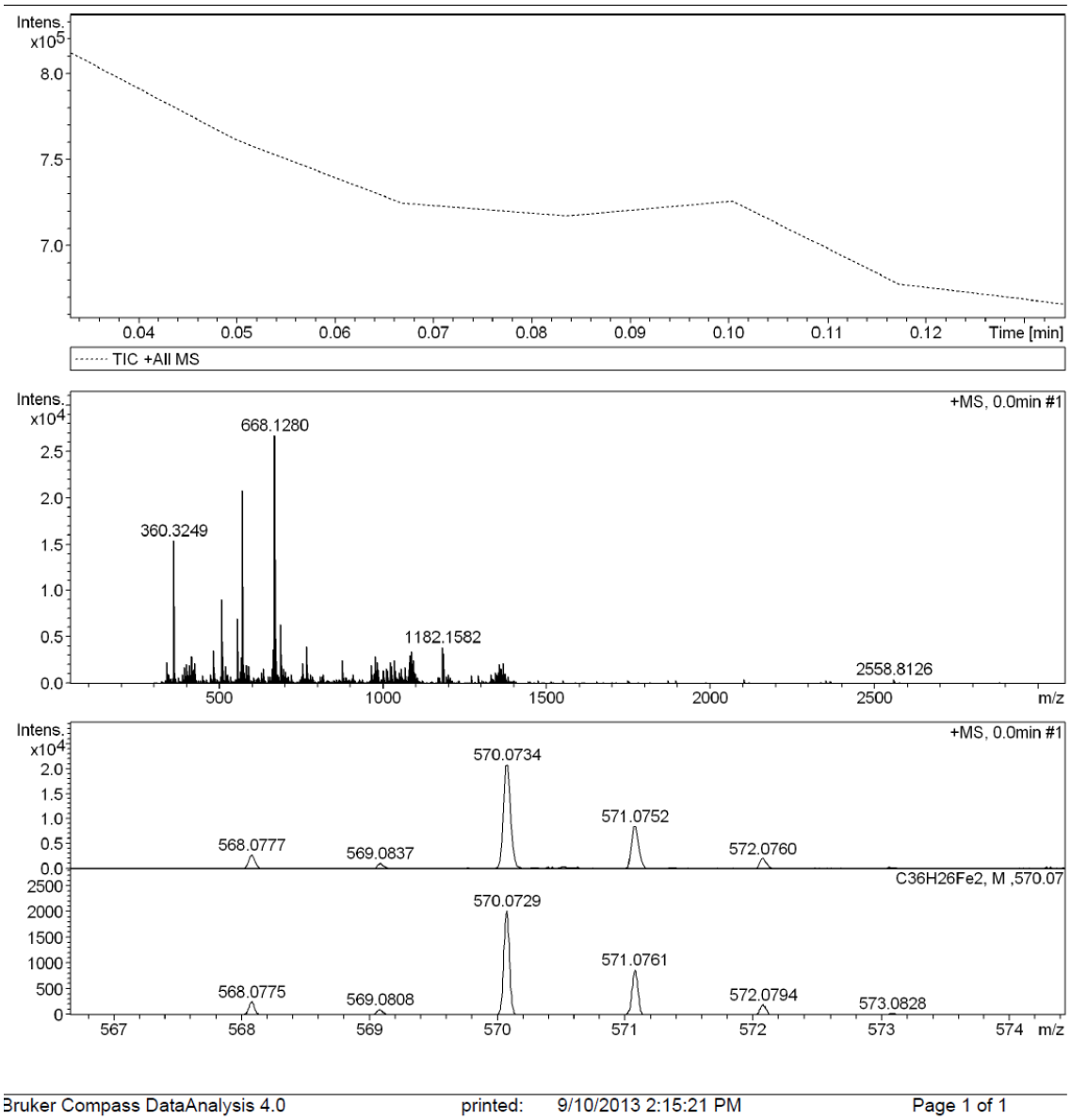
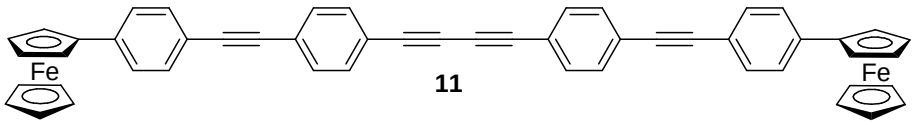


Fig. S-36: HRMS mass spectrum of compound **10**



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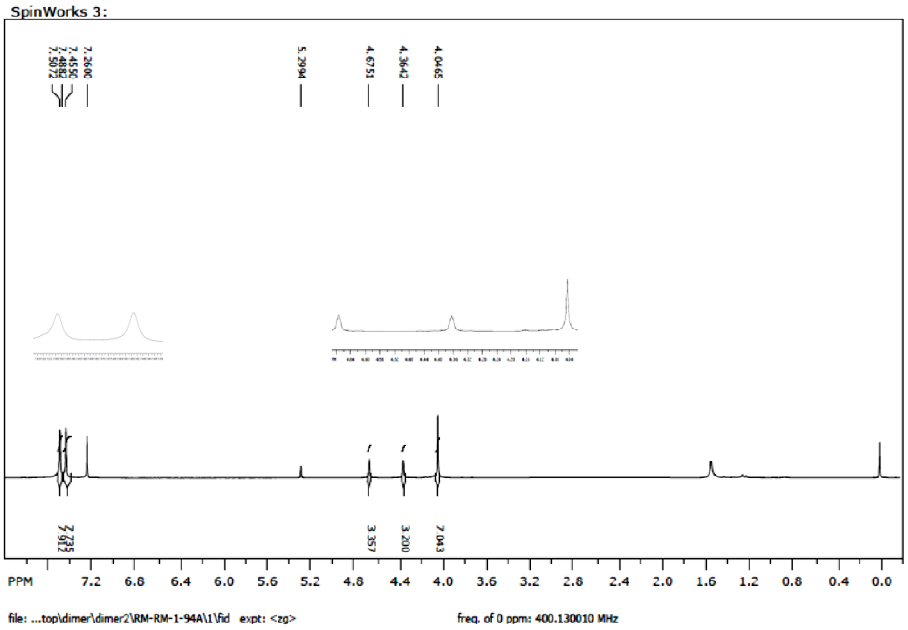


Fig. S-37: ^{1}H-NMR spectrum of compound **11** recorded in $CDCl_3$

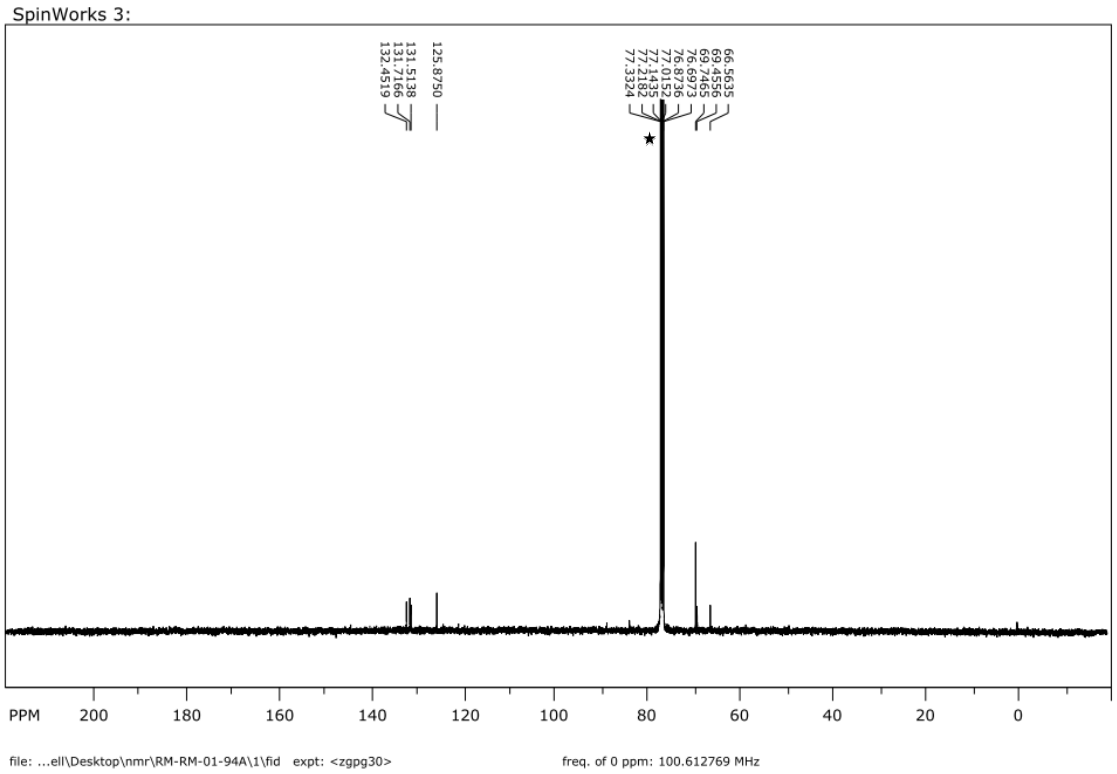


Fig. S-38: ^{13}C-NMR spectrum of compound **11** recorded in $CDCl_3$

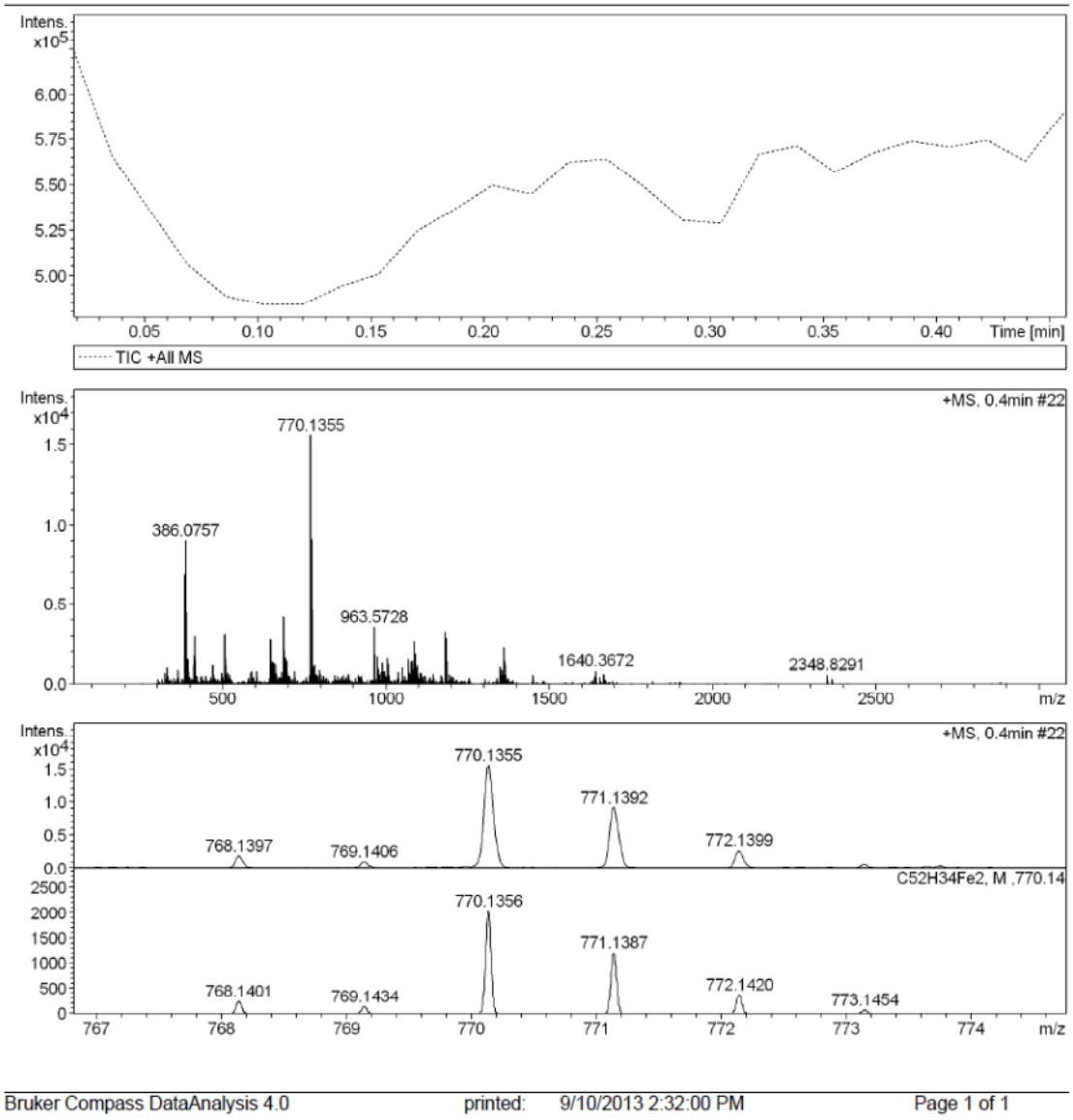


Fig. S-39: HRMS mass spectrum of compound **11**.

The selected bond lengths, and bond angles of ferrocenyl phenylethnyl rods 2, 4, 10, 14, and 19

Table S1. The selected bond lengths, and bond angles of compounds 14, and 19

Compound 14				Compound 19			
Bond lengths (Å)		**Bond angles °**		**Bond lengths (Å)**		**Bond angles °**	
C(5)-C(6)	1.377(3)	C(21)-Fe(1)-C(15)	41.58(1)	C(6)-I(1)	2.096(2)	C(7)-C(6)-I(1)	117.46(15)
C(7)-C(8)	1.394(3)	C(20)-Fe(1)-C(13)	121.971)	C(24)-I(2)	2.101(2)	C(5)-C(6)-I(1)	121.52(15)
C(8)-C(9)	1.385(3)	C(14)-Fe(1)-C(10)	40.74(8)	C(7)-C(8)	1.388(3)	Fe(1)-C(10)-H(10)	125.8
C(7)-C(10)	1.474(3)	C(19)-Fe(1)-C(10)	159.47(0)	C(9)-Fe(1)	2.048(2)	C(16)-Fe(1)-C(15)	40.47(9)
Fe(1)-C(18)	2.044(2)	C(2)-Si(1)-C(1)	108.92(0)	C(11)Fe(1)	2.048(2)	C(28)-Fe(2)-C(27)	41.09(9)
Fe(1)-C(11)	2.043(2)	C(2)-Si(1)-C(17)	108.03(1)	C(13)Fe(1)	2.048(2)	C(28)-Fe(2)-C(34)	157.40(9)
Si(1)-C(17)	1.862(3)	Si(1)-C(1)-H(1B)	109.5	C(10)C(11	1.414(3)	C(8)-C(3)-C(2)	119.57(19)

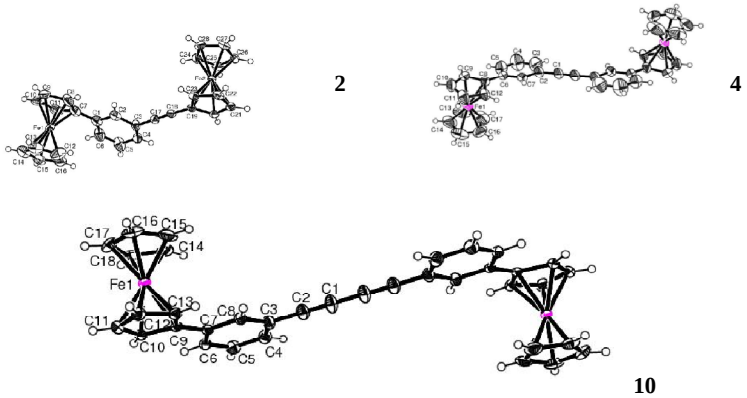
Table S2. The selected bond lengths, and bond angles of compounds 2, and 4

Compound 2				Compound 4			
Bond lengths (Å)		**Bond angles °**		**Bond lengths (Å)**		**Bond angles °**	
C(2)-C(3)	1.423(7)	C(7)-Fe(1)-C(11)	42.7(2)	C(1)-C(2)	1.425(15)	C(16)-Fe(1)-C(10)	156.5(7)
C(1)-C(6)	1.408(8)	C(2)-C(1)-C(6)	118.1(5)	[a]C(1)-C(1)#1	1.20(2)	C(9)-Fe(1)-C(10)	40.6(4)
C(7)-C(9)	1.389(7)	Fe(1)-C(8)-H(8)	128.9	C(6)-C(7)	1.393(12)	C(9)-Fe(1)-C(14	122.0(5)
C(13)-C(14)	1.441(8)	C(8)-C(9)-Fe(1)	68.2(3)	C(10)C(11)	1.412(16)	C(3)-C(2)-C(7)	118.9(10)
Fe(1)-C(14)	2.103(6)	Fe(1)-C(9)-H(9)	127.5	C(13)C(17)	1.40(2)	C(7)-C(6)-C(8)	119.8(8)

[a]The C(1)#1 atom is C1 at (-x, 3-y, -z)

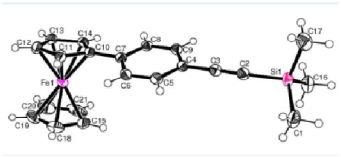
Table S3. The selected bond lengths, and bond angles of compound 10

Compound 10			
Bond lengths (Å)		**Bond angles °**	
C(1)-C(2)	1.201(7)	C(15)-Fe(1)-C(9)	118.4(2)
C(2)-C(3)	1.433(7)	C(2)-C(1)-C(1)#1	179.4(9)
C(7)-C(9)	1.474(7)	C(1)-C(2)-C(3)	177.8(6)
C(25)-C(27)	1.476(6)	C(20)-C(19)-(19)#2	179.2(8)
C(20)-C(21)	1.437(7)	C(19)-C(20)-C(21)	178.3(6)
C(19)-C(19)#2	1.374(11)	C(28)-C(27)-Fe(2)	69.5(3)
C(1)-C(1)#1	1.384(10)	C(6)-C(7)-C(9)	121.8(4)

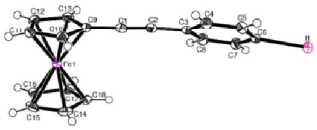


2 **4**

10



14



19

Figure S40. ORTEP structures of the ferrocenyl phenylethynyl rods **2, 4**, **10**, **14**, and **19** (50 % probability chosen for the ellipsoids).

X-ray crystallography

Single crystal X-ray structural studies of the ferrocenyl phenylethynyl rods **2, 4**, **10, 14,** and **19** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 293(2) K using graphite-monochromoated Mo Kα radiation (λ_α = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97 and refined by full matrix least-squares with SHELXL-97, refining on $F^{2.1}$. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropic ally. The remaining hydrogen atoms were placed in geometrically constrained positions and refined with isotropic temperature factors, generally 1.2U_{eq} of their parent atoms. The crystal and refinement data are summarized in Table 5, Table 6, and Table 7. The compound **10** squeeze has been applied and details have been included in CIF. The CCDC of ferrocenyl phenylethnyl compound **2 (**CCDC 942659), compound **4 (**CCDC 942660), compound **10 (**CCDC 942658), compound **14 (**CCDC 942661), compound **19 (**CCDC943231), contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S5. Crystallographic data and structure refinement detail for compounds 14, 19

Compound	**14**	**19**
Empirical formula	C_{21} H_{22} Fe Si_1	C_{18} H_{13} Fe I
Formula weight	358.33	412.03
Crystal system	Monoclinic	Triclinic
Space group	P 21/n	P -1
Unit cell dimensions		
a (A°)	a = 11.0972(4) A	a = 10.2384(3) A
b (A°)	b = 13.1305(3) A	b = 10.6457(4) A
c (A°)	c = 13.4256(4) A	c = 14.4194(5) A
Volume	1805.13(9) A^3	1445.82(9) A^3
Z, Calculated density	4, 1.318 Mg/m^3	4, 1.893 Mg/m^3
Absorption coefficient	0.899 mm^-1	3.164 mm^-1
Max. and min. transmission	752	800
F (000)		
Crystal size	0.23 x 0.18 x 0.13 mm	0.36 x 0.32 x 0.28 mm
Theta range for data collection	3.10 to 24.99 deg.	2.98 to 25.00 deg.
Completeness to theta	24.99 99.8 %	25.00 99.8 %
		10272 / 5081 [R(int) = 0.0191]

Reflections collected / unique	13235 / 3174 [R(int) = 0.0385]	5081 / 0 / 361
Data / restraints / parameters	3174 / 0 / 211	1.032
Goodness-of-fit on F^2	1.029	Full-matrix least-squares on F^2
Refinement method	Full-matrix least-squares on F^2	R1 = 0.0178, wR2 = 0.0443
Final R indices [I>2sigma (I)]	R1 = 0.0327, wR2 = 0.0803	R1 = 0.0190, wR2 = 0.0452
R indices (all data)	R1 = 0.0366, wR2 = 0.0841	0.433 and -0.553 e.A^-3
Largest diff. peak and hole	0.448 and -0.331 e.A^-3	

Table S6. Crystallographic data and structure refinement detail for compounds 2, 4

Compound	**2**	**4**
Empirical formula	C_{28} H_{22} Fe_2	C_{34} H_{26} Fe_2
Formula weight	470.16	546.25
Crystal system	Monoclinic	Monoclinic
Space group	P 21/n	P 21/c
Unit cell dimensions		a = 10.1907(12) A
a (A°)	a = 14.6452(3) A	b = 7.5711(3) A
b (A°)	b = 10.2825(2) A	c = 20.759(3) A
c (A°)	c = 14.8003(3) A	
Volume	2067.90(7) A^3	1287.9(2) A^3
Z, Calculated density	4, 1.510 Mg/m^3	

		2, 1.409 Mg/m^3
Absorption coefficient	1.415 mm^-1	1.147 mm^-1
Max. and min. transmission	968	
F (000)		564
Crystal size	0.23 x 0.18 x 0.13 mm	0.23 x 0.16 x 0.13 mm
Theta range for data collection	2.97 to 25.00 deg.	2.95 to 25.00 deg.
Completeness to theta	25.00 99.8 %	25.00 99.7 %
Reflections collected / unique	16462 / 3642 [R(int) = 0.0259]	9242 / 2255 [R(int) = 0.0448]
Data / restraints / parameters	3642 / 0 / 271	2255 / 0 / 163
Goodness-of-fit on F^2	1.055	1.055
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Final R indices [I>2sigma (I)]	R1 = 0.0587, wR2 = 0.1534	R1 = 0.0986, wR2 = 0.2692
R indices (all data)		
Largest diff. peak and hole	1.647 and -0.626 e.A^-3	2.269 and -0.817 e.A^-3

Table S7. Crystallographic data and structure refinement detail for compound 10

Compound	**10**
Empirical formula	C_{36} H_{26} Fe_2
Formula weight	570.27
Crystal system	Triclinic,
Space group	P -1
Unit cell dimensions	
a (A°)	a = 5.9624(2) A
b (A°)	b = 13.0786(7) A
c (A°)	c = 19.7678(10) A
Volume	1532.17(12) A^3
Z, Calculated density	2, 1.236 Mg/m^3
Absorption coefficient	0.967 mm^-1
Max. and min. transmission	588
F (000)	0.28 x 0.21 x 0.18 mm
Crystal size	3.12 to 25.00 deg.
Theta range for data collection	25.00 99.8 %t
Completeness to theta	10430 / 5374 [R(int) = 0.0359]
Reflections collected / unique	5374 / 0 / 343
Data / restraints / parameters	1.506

Goodness-of-fit on F^2	
Refinement method	Full-matrix least-squares on F^2
Final R indices [I>2sigma (I)]	R1 = 0.0642, wR2 = 0.1901
R indices (all data)	
Largest diff. peak and hole	1.202 and -0.485 e.A^-3

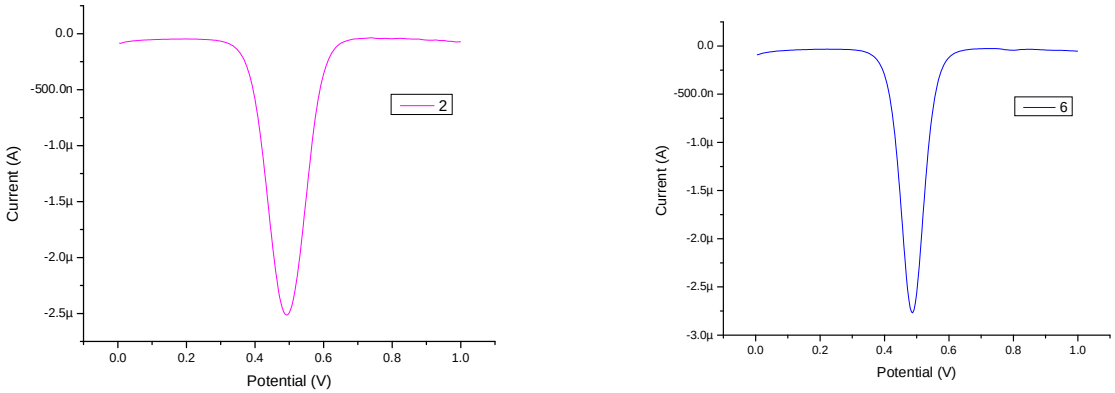


Figure S41. Differential pulse voltammograms (DPVs) of the compounds **2, 6**

DFT Calculations.

DFT calculation data of ferrocenyl phenylethnyl rods **1**-**4**, and **9**-**10.**

Calculation method: B3LYP/6-31+G** for C, H, and Lanl2DZ for Fe with Gaussian 09[1]

Table S8. Data for ferrocenyl phenylethnyl Compound 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.763461	0.814627	0.326225
2	6	0	-1.598081	0.465444	0.303005
3	6	0	-0.233266	0.061602	0.277006
4	6	0	0.394743	-0.449382	1.430204
5	6	0	0.528942	0.156873	-0.906276
6	6	0	1.725871	-0.848060	1.397102
7	1	0	-0.176924	-0.537650	2.348628
8	6	0	1.859455	-0.238294	-0.927790
9	1	0	0.063316	0.550944	-1.804135
10	6	0	2.490798	-0.748210	0.221960
11	1	0	2.176547	-1.261688	2.294076
12	1	0	2.427248	-0.136505	-1.847639
13	6	0	-4.118959	1.228797	0.360743
14	26	0	-5.795614	0.062137	-0.063941
15	6	0	-5.000197	1.174232	1.499420
16	6	0	-4.870333	1.797514	-0.729486
17	6	0	-6.259857	1.713560	1.114344
18	6	0	-6.179956	2.097884	-0.259004
19	6	0	-5.152312	-1.832932	-0.620372
20	6	0	-5.942410	-1.259134	-1.661498

21	6	0	-7.240739	-0.987050	-1.131748
22	6	0	-7.252028	-1.391953	0.237244
23	6	0	-5.960731	-1.914407	0.553478
24	1	0	-4.737749	0.775461	2.468940
25	1	0	-4.493038	1.950191	-1.730623
26	1	0	-7.135710	1.786899	1.744025
27	1	0	-6.984866	2.512412	-0.849983
28	1	0	-4.107951	-2.104357	-0.691828
29	1	0	-5.606780	-1.039940	-2.665769
30	1	0	-8.060436	-0.524365	-1.664171
31	1	0	-8.081387	-1.288576	0.923408
32	1	0	-5.641080	-2.277374	1.520544
33	6	0	3.896314	-1.190186	0.194929
34	26	0	5.596385	0.001568	-0.077314
35	6	0	4.781904	-1.302574	1.320362
36	6	0	4.639662	-1.612816	-0.960594
37	6	0	6.038374	-1.798272	0.864800
38	6	0	5.949674	-1.991297	-0.546376
39	6	0	4.988479	1.980119	-0.260419
40	6	0	5.673171	1.565437	-1.442935
41	6	0	6.996186	1.173958	-1.073024
42	6	0	7.128186	1.346061	0.338131
43	6	0	5.887359	1.844089	0.840175
44	1	0	4.549066	-1.018044	2.337084
45	1	0	4.265576	-1.643186	-1.974437
46	1	0	6.915200	-1.961135	1.476132
47	1	0	6.744124	-2.336327	-1.193708

48	1	0	3.954871	2.292449	-0.201624
49	1	0	5.254303	1.526522	-2.439106
50	1	0	7.753664	0.784326	-1.739241
51	1	0	8.003047	1.108788	0.927869
52	1	0	5.658179	2.051054	1.876522

Total energy (Sum of electronic and zero-point energies): -1327.0748935 Hartree

Table S9. Data for ferrocenyl phenylethnyl Compound 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.444564	0.896902	0.580762
2	6	0	-1.339020	1.110879	0.120881
3	6	0	-3.731051	0.656651	1.126924
4	26	0	-5.339788	-0.276358	0.184130
5	6	0	-4.144913	-0.509239	1.865664
6	6	0	-4.864913	1.543549	1.064420
7	6	0	-5.501330	-0.329050	2.258229
8	6	0	-5.945014	0.935623	1.764013
9	6	0	-4.737630	-0.848745	-1.719620
10	6	0	-5.831085	0.065020	-1.805383
11	6	0	-6.943297	-0.511582	-1.119114
12	6	0	-6.536249	-1.781200	-0.608622
13	6	0	-5.172412	-1.989193	-0.979337

14	1	0	-3.523281	-1.370054	2.067118
15	1	0	-4.880197	2.496825	0.555562
16	1	0	-6.101394	-1.042692	2.805753
17	1	0	-6.939288	1.346260	1.872868
18	1	0	-3.738779	-0.680502	-2.098373
19	1	0	-5.809922	1.037072	-2.278466
20	1	0	-7.912932	-0.052941	-0.981621
21	1	0	-7.143672	-2.452123	-0.016698
22	1	0	-4.565692	-2.845071	-0.717476
23	6	0	-0.040471	1.365580	-0.410093
24	6	0	0.274289	2.620209	-0.967250
25	6	0	0.944704	0.359557	-0.391871
26	6	0	1.546785	2.846916	-1.486154
27	1	0	-0.480343	3.399524	-0.986747
28	6	0	2.228605	0.584934	-0.903071
29	1	0	0.687836	-0.612813	0.014702
30	6	0	2.516613	1.846593	-1.454241
31	1	0	1.787842	3.816271	-1.913370
32	1	0	3.510790	2.045732	-1.842104
33	6	0	3.238456	-0.491815	-0.882957
34	26	0	5.049676	-0.524362	0.166244
35	6	0	3.281423	-1.606396	0.020831
36	6	0	4.348386	-0.642828	-1.782576
37	6	0	4.390290	-2.432275	-0.326278
38	6	0	5.049960	-1.836460	-1.442717
39	6	0	5.266065	1.277903	1.178585
40	6	0	6.380181	1.066239	0.311027

41	6	0	7.022931	-0.146754	0.705359
42	6	0	6.305337	-0.684557	1.816376
43	6	0	5.219608	0.196108	2.108791
44	1	0	2.610037	-1.769251	0.852485
45	1	0	4.605160	0.033814	-2.585726
46	1	0	4.700126	-3.329367	0.191772
47	1	0	5.941710	-2.207469	-1.928890
48	1	0	4.553507	2.088606	1.112108
49	1	0	6.670608	1.698186	-0.517092
50	1	0	7.881760	-0.595885	0.225607
51	1	0	6.525226	-1.613190	2.324984
52	1	0	4.473687	0.052377	2.878402

Total energy (Sum of electronic and zero-point energies): -1327.0741035 Hartree

Table S10. Data for ferrocenyl phenylethnyl Compound 3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.162847	2.927543	0.525953
2	6	0	-4.225439	3.897967	0.169631
3	6	0	-4.784623	1.582257	0.672422
4	6	0	-2.894033	3.554146	-0.037949
5	1	0	-4.537443	4.933029	0.063248

6	6	0	-3.441722	1.241286	0.460367
7	6	0	-2.486338	2.211971	0.109412
8	1	0	-3.126763	0.207088	0.550986
9	6	0	-5.777414	0.565544	1.072455
10	26	0	-6.415539	-1.113317	-0.002427
11	6	0	-5.519561	-0.640986	1.808130
12	6	0	-7.193642	0.618799	0.843495
13	6	0	-6.758681	-1.307688	2.036198
14	6	0	-7.794572	-0.529227	1.437913
15	6	0	-5.368560	-1.200995	-1.797403
16	6	0	-6.766544	-1.063754	-2.051468
17	6	0	-7.433839	-2.182642	-1.466128
18	6	0	-6.447811	-3.011682	-0.850500
19	6	0	-5.171321	-2.404562	-1.055122
20	1	0	-4.548073	-0.980962	2.139363
21	1	0	-7.711298	1.380405	0.276970
22	1	0	-6.885725	-2.251867	2.547735
23	1	0	-8.844867	-0.784291	1.405707
24	1	0	-4.599401	-0.495265	-2.080005
25	1	0	-7.239955	-0.240740	-2.568996
26	1	0	-8.501449	-2.354615	-1.460934
27	1	0	-6.637836	-3.920810	-0.296605
28	1	0	-4.224952	-2.776635	-0.687009
29	1	0	-6.192516	3.216565	0.712191
30	1	0	-2.161273	4.306171	-0.310852
31	6	0	-1.125592	1.845480	-0.103270
32	6	0	0.039632	1.546386	-0.287274

33	6	0	1.404594	1.207657	-0.504774
34	6	0	1.850125	-0.126332	-0.395276
35	6	0	2.349632	2.198200	-0.838286
36	6	0	3.183935	-0.448176	-0.605925
37	1	0	1.136501	-0.902245	-0.136811
38	6	0	3.681467	1.865326	-1.053716
39	1	0	2.023282	3.228771	-0.934930
40	6	0	4.131123	0.538356	-0.938181
41	1	0	4.383222	2.644535	-1.334828
42	1	0	3.505571	-1.479335	-0.495396
43	6	0	5.542833	0.196974	-1.185146
44	26	0	6.931942	-0.540319	0.195977
45	6	0	6.056226	-1.078586	-1.604760
46	6	0	6.668918	1.082163	-1.077063
47	6	0	7.468388	-0.970128	-1.763964
48	6	0	7.847708	0.365894	-1.435600
49	6	0	5.981800	-0.772360	2.029824
50	6	0	7.050432	0.166870	2.147164
51	6	0	8.263872	-0.498171	1.793555
52	6	0	7.945143	-1.848506	1.457098
53	6	0	6.534422	-2.017927	1.602966
54	1	0	5.467771	-1.968931	-1.777318
55	1	0	6.633919	2.108044	-0.737667
56	1	0	8.136578	-1.768889	-2.054902
57	1	0	8.855784	0.756699	-1.422912
58	1	0	4.932501	-0.563530	2.187200
59	1	0	6.953079	1.207569	2.424041

60	1	0	9.246794	-0.049011	1.754916
61	1	0	8.644265	-2.600758	1.118309
62	1	0	5.979534	-2.923042	1.397528

Total energy (Sum of electronic and zero-point energies): -1558.1339724 Hartree

Table S11. Data for ferrocenyl phenylethnyl Compound 4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.705695	2.696089	1.114314
2	6	0	-4.022341	3.901145	0.946108
3	6	0	-4.044444	1.466640	0.954980
4	6	0	-2.668519	3.909618	0.627499
5	1	0	-4.551157	4.841266	1.074594
6	6	0	-2.680310	1.481510	0.632869
7	6	0	-1.979245	2.689470	0.469730
8	1	0	-2.150230	0.546087	0.488403
9	6	0	-4.766615	0.194181	1.152436
10	26	0	-5.135723	-1.298998	-0.265851
11	6	0	-4.196817	-1.057239	1.568383
12	6	0	-6.177874	-0.021571	0.999733
13	6	0	-5.243384	-2.018550	1.679279

14	6	0	-6.469091	-1.378307	1.326798
15	6	0	-4.326449	-0.699339	-2.084171
16	6	0	-5.730725	-0.915995	-2.220626
17	6	0	-6.002443	-2.277060	-1.883554
18	6	0	-4.765742	-2.901833	-1.539300
19	6	0	-3.729916	-1.926293	-1.662804
20	1	0	-3.149699	-1.236574	1.768660
21	1	0	-6.893340	0.710808	0.652211
22	1	0	-5.123242	-3.057314	1.954438
23	1	0	-7.441593	-1.848342	1.277014
24	1	0	-3.811092	0.240138	-2.229640
25	1	0	-6.463504	-0.171433	-2.499462
26	1	0	-6.977597	-2.743962	-1.861928
27	1	0	-4.640347	-3.924283	-1.210181
28	1	0	-2.681491	-2.082580	-1.449075
29	1	0	-5.755492	2.706739	1.390347
30	1	0	-2.132760	4.844323	0.499908
31	6	0	-0.592051	2.680508	0.140564
32	6	0	0.591584	2.680416	-0.140311
33	6	0	1.978735	2.689372	-0.469643
34	6	0	2.679815	1.481428	-0.632773
35	6	0	2.667925	3.909543	-0.627649
36	6	0	4.043897	1.466577	-0.955100
37	1	0	2.149759	0.546010	-0.488174
38	6	0	4.021681	3.901089	-0.946518
39	1	0	2.132144	4.844230	-0.500054
40	6	0	4.705057	2.696039	-1.114708

41	1	0	4.550445	4.841210	-1.075225
42	1	0	5.754801	2.706695	-1.390930
43	6	0	4.766099	0.194143	-1.152417
44	26	0	5.135944	-1.298691	0.265857
45	6	0	4.196258	-1.057458	-1.567911
46	6	0	6.177465	-0.021411	-1.000374
47	6	0	5.242887	-2.018647	-1.679092
48	6	0	6.468682	-1.378174	-1.327266
49	6	0	4.327324	-0.698910	2.084424
50	6	0	5.731715	-0.915205	2.220315
51	6	0	6.003606	-2.276274	1.883410
52	6	0	4.766917	-2.901403	1.539810
53	6	0	3.730902	-1.926088	1.663541
54	1	0	3.149065	-1.236873	-1.767714
55	1	0	6.893009	0.711006	-0.653080
56	1	0	5.122865	-3.057521	-1.953889
57	1	0	7.441195	-1.848203	-1.277659
58	1	0	3.811823	0.240484	2.229929
59	1	0	6.464446	-0.170426	2.498707
60	1	0	6.978855	-2.742964	1.861486
61	1	0	4.641633	-3.923959	1.210979
62	1	0	2.682427	-2.082726	1.450315

Total energy (Sum of electronic and zero-point energies): -1558.1331584 Hartree

Table S12. Data for ferrocenyl phenylethnyl Compound 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.670713	-0.107398	0.354497
2	6	0	1.877814	-0.300216	0.351620
3	6	0	3.279140	-0.523658	0.337749
4	6	0	3.993808	-0.734490	1.534792
5	6	0	3.995551	-0.543334	-0.878610
6	6	0	5.364938	-0.956167	1.511367
7	1	0	3.457936	-0.731575	2.478464
8	6	0	5.365912	-0.759272	-0.889532
9	1	0	3.460985	-0.381700	-1.809134
10	6	0	6.084634	-0.968537	0.302965
11	1	0	5.893908	-0.751975	-1.837962
12	6	0	-0.670645	0.106884	0.354464
13	6	0	-1.877743	0.299723	0.351582
14	6	0	-3.279052	0.523266	0.337723
15	6	0	-3.995497	0.542899	-0.878618
16	6	0	-3.993659	0.734279	1.534772
17	6	0	-5.365839	0.758960	-0.889516
18	1	0	-3.460975	0.381134	-1.809145
19	6	0	-5.364768	0.956085	1.511370
20	1	0	-3.457756	0.731400	2.478426
21	6	0	-6.084496	0.968399	0.302986
22	1	0	-5.885557	1.140867	2.445670
23	1	0	5.885765	-1.140789	2.445679

24	1	0	-5.893888	0.751647	-1.837919
25	6	0	7.535678	-1.220634	0.290198
26	26	0	9.056009	0.139330	-0.177094
27	6	0	8.442360	-1.071722	1.395119
28	6	0	8.315226	-1.686065	-0.824936
29	6	0	9.747385	-1.453167	0.968596
30	6	0	9.668369	-1.833888	-0.404272
31	6	0	8.190957	1.977294	-0.620133
32	6	0	8.939615	1.504498	-1.740215
33	6	0	10.298117	1.346680	-1.328525
34	6	0	10.388243	1.720934	0.046120
35	6	0	9.085979	2.110870	0.483802
36	1	0	8.187248	-0.695249	2.375835
37	1	0	7.938436	-1.894360	-1.816452
38	1	0	10.645573	-1.421134	1.569795
39	1	0	10.494304	-2.150402	-1.026231
40	1	0	7.124855	2.157236	-0.598606
41	1	0	8.542911	1.279492	-2.720754
42	1	0	11.108934	0.976923	-1.941127
43	1	0	11.279961	1.685006	0.656916
44	1	0	8.818528	2.422896	1.484029
45	6	0	-7.535519	1.220646	0.290247
46	26	0	-9.055967	-0.139163	-0.177054
47	6	0	-8.442159	1.071665	1.395198
48	6	0	-8.315070	1.686180	-0.824825
49	6	0	-9.747188	1.453211	0.968748
50	6	0	-9.668201	1.834032	-0.404102

51	6	0	-8.191333	-1.977162	-0.620810
52	6	0	-8.940429	-1.504075	-1.740474
53	6	0	-10.298726	-1.346128	-1.328148
54	6	0	-10.388293	-1.720626	0.046464
55	6	0	-9.085889	-2.110818	0.483497
56	1	0	-8.187082	0.695070	2.375874
57	1	0	-7.938314	1.894614	-1.816326
58	1	0	-10.645391	1.421145	1.569921
59	1	0	-10.494168	2.150681	-1.025950
60	1	0	-7.125247	-2.157259	-0.599786
61	1	0	-8.544145	-1.278900	-2.721144
62	1	0	-11.109743	-0.976165	-1.940362
63	1	0	-11.279730	-1.684708	0.657673
64	1	0	-8.818037	-2.423118	1.483531

Total energy (Sum of electronic and zero-point energies): -1634.2923487 Hartree

Table S13. Data for ferrocenyl phenylethnyl Compound 10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.595524	0.328652	-1.059815

2	6	0	1.665419	0.918089	-1.052470
3	6	0	2.912015	1.602854	-1.031391
4	6	0	4.117151	0.877894	-0.992888
5	6	0	2.955347	3.013103	-1.031055
6	6	0	5.357641	1.528513	-0.956037
7	1	0	4.075373	-0.205756	-0.971541
8	6	0	4.184332	3.662913	-0.996483
9	1	0	2.027995	3.575258	-1.057940
10	6	0	5.373990	2.933550	-0.963489
11	1	0	4.219537	4.748503	-1.002945
12	1	0	6.325584	3.456053	-0.961392
13	6	0	6.618404	0.760932	-0.935011
14	26	0	7.269006	-0.576175	0.536466
15	6	0	6.831928	-0.546434	-1.490687
16	6	0	7.872160	1.189654	-0.382542
17	6	0	8.196634	-0.906525	-1.291446
18	6	0	8.839909	0.166397	-0.604340
19	6	0	5.850175	-0.643979	2.054172
20	6	0	7.112494	-0.235653	2.581052
21	6	0	8.054620	-1.279124	2.329170
22	6	0	7.374429	-2.332086	1.645924
23	6	0	6.011824	-1.939428	1.475876
24	1	0	6.082704	-1.151956	-1.981549
25	1	0	8.042127	2.114335	0.151675
26	1	0	8.654831	-1.841015	-1.584612
27	1	0	9.869063	0.183982	-0.273181
28	1	0	4.942694	-0.055957	2.050191

29	1	0	7.324319	0.710662	3.059493
30	1	0	9.105994	-1.260908	2.581673
31	1	0	7.819958	-3.251170	1.290679
32	1	0	5.244269	-2.511187	0.972426
33	6	0	-0.595322	-0.327144	-1.059962
34	6	0	-1.665183	-0.916647	-1.052880
35	6	0	-2.911643	-1.601669	-1.032044
36	6	0	-4.116944	-0.876986	-0.993333
37	6	0	-2.954652	-3.011924	-1.032169
38	6	0	-5.357285	-1.527899	-0.956693
39	1	0	-4.075392	0.206666	-0.971662
40	6	0	-4.183490	-3.662026	-0.997821
41	1	0	-2.027174	-3.573861	-1.059234
42	6	0	-5.373307	-2.932941	-0.964598
43	6	0	-6.618247	-0.760653	-0.935453
44	1	0	-4.218449	-4.747622	-1.004644
45	1	0	-6.324780	-3.455664	-0.962689
46	26	0	-7.269256	0.575631	0.536613
47	6	0	-6.832034	0.546927	-1.490526
48	6	0	-7.871932	-1.189911	-0.383243
49	6	0	-8.196836	0.906604	-1.291220
50	6	0	-8.839906	-0.166783	-0.604651
51	6	0	-5.850516	0.643091	2.054433
52	6	0	-7.112751	0.234167	2.581052
53	6	0	-8.055149	1.277499	2.329622
54	6	0	-7.375210	2.330975	1.646915
55	6	0	-6.012488	1.938771	1.476747

56	1	0	-6.082915	1.152848	-1.981053
57	1	0	-8.041728	-2.114888	0.150515
58	1	0	-8.655237	1.841116	-1.584001
59	1	0	-9.869081	-0.184756	-0.273578
60	1	0	-4.942874	0.055318	2.050216
61	1	0	-7.324340	-0.712442	3.059017
62	1	0	-9.106530	1.258873	2.582063
63	1	0	-7.820972	3.250106	1.292086
64	1	0	-5.245060	2.510977	0.973615

Total energy (Sum of electronic and zero-point energies): -1634.2903774 Hartree

1 (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; (b) C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B.* 1988, **37**, 785-789.