Electronic Supplementary Information (ESI) for

A Kinetically Blocked 1,14:11,12-Dibenzopentacene: A Persistent Triplet Diradical of Non-Kekulé Polycyclic Benzenoid Hydrocarbons

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1. *IT*-*T* curve of the monoradical generated by the oxidation of 9 by *p*-chloranil

The ESR signal intensity *I* was estimated by using the pulsed-ESR technique. Fig. S1 shows the temperature dependence of *IT* values at 4-40 K, where *T* denotes the temperature. *I* is proportional to the magnetic susceptibility χ. Namely, *IT* means χ*T* value. It was found that the *IT* value decrease as the temperature is lowered. This behavior indicates an intermolecular antiferromgnetic spin coupling *via* dimerization process at low temperature. The exchange interaction J/k_B was estimated to be −12.0 ±0.8 K based on the singlet-triplet model.

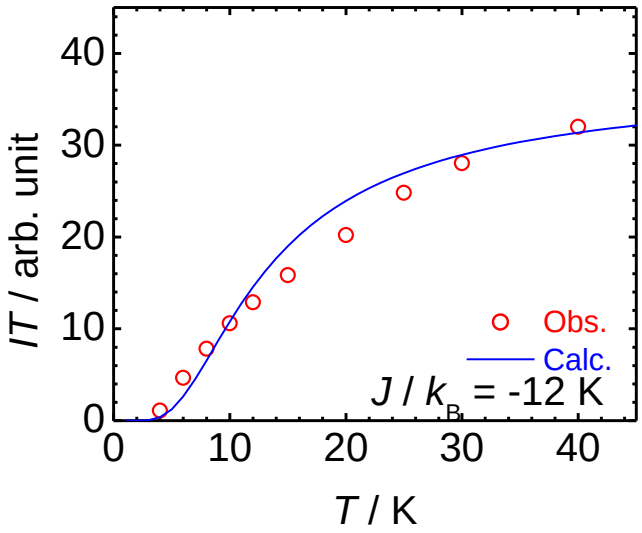


Fig. S1. Temperature dependence of *IT* value for the oxidation product of **9** with *p*-chloranil in toluene. The blue line denotes the calculated *IT* value based on singlet-triplet model using BB equation.

2. Absorption spectrum of dianion 9^{2-}

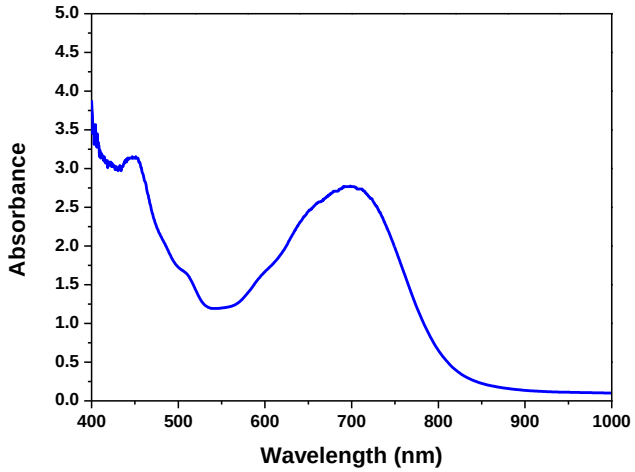


Fig. S2. Absorption spectrum of $\mathbf{9}^{2-}$ after treatment of **9** with lithium diisopropylamide (LDA) in 2-methyl tetrahydrofuran (2-Me-THF) at -78 ^{o}C for 30 min.

3. Concentration dependent *IT*-*T* curves for DP-Mes

The concentration dependent ESR measurements were done by a dilution method. The *in situ* generated triplet diradical solution at -78 ^{o}C starting from 8 mM of precursor **9** (denoted as "1 conc.") was carefully diluted by 1/2 (denoted as "1/2 conc.") and 1/3 (denoted as "1/3 conc.") by adding chilled anhydrous 2-Me-THF (-78 ^{o}C) in an ESR tube under nitrogen protection. Then the solutions with different concentrations were subjected to VT ESR measurements at low temperature. Upon the dilution, there was no obvious change of the ESR spectrum, indicating that there was no significant decomposition of the triplet diradical during the operation. The temperature dependent *IT* values were shown in Fig. S3. The comparison of the absolute signal intensity is difficult, because the measurements error includes amount of sample and signal-to-noise ratio. Therefore, we compared the normalized signal intensity at 70 K on each concentrations.

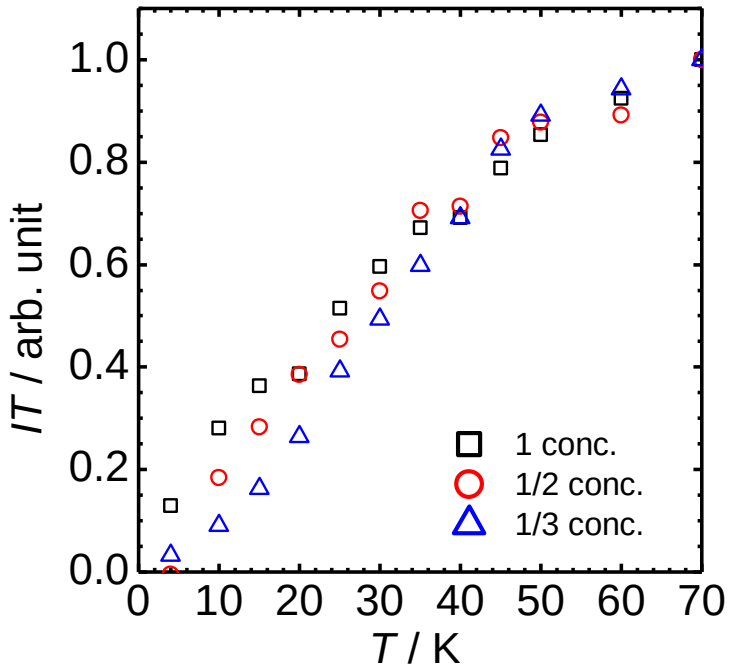
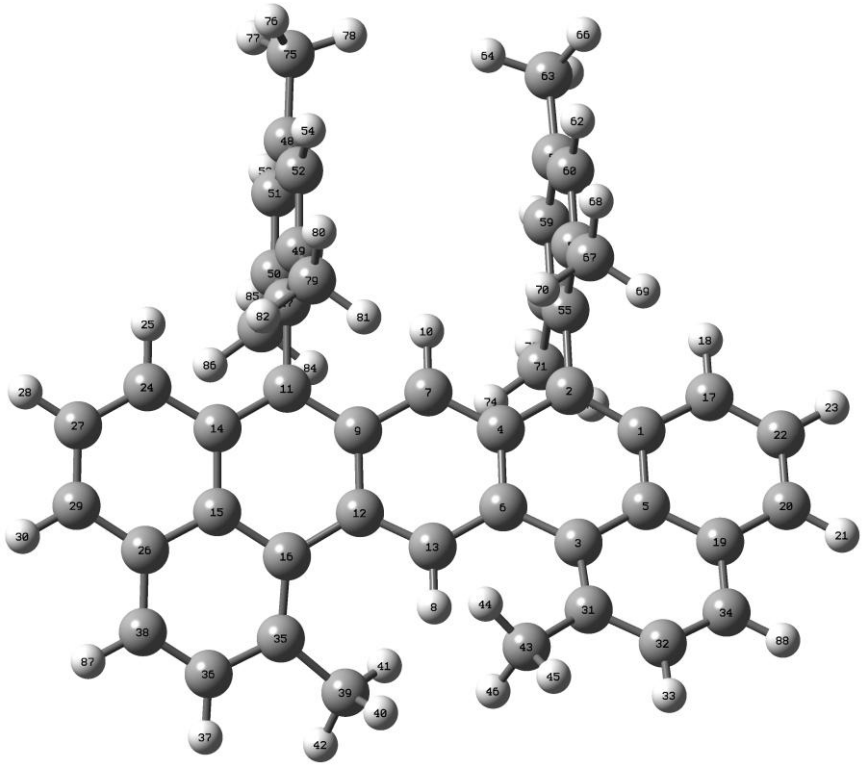


Fig. S3. Temperature dependence of observed *IT* value for the **DP-Mes** at different concentrations. The *in situ* generated diradicals solution was carefully diluted by 1/2 (1/2 conc.) and 1/3 (1/3 conc.) of the original concentration (1 conc.) in an ESR tube at -78 ^{o}C.

4. DFT calculations details

Density functional theory calculations for **DP-Mes** were employed with Gaussian 09 package,[1] utilizing the UCAM-B3LYP level of theory with Pople basis set 6-31G* in the gas phase.

Triplet diradical:



Mulliken atomic spin densities:

1	C	-0.260895
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3	C	-0.206457
4	C	-0.279394
5	C	0.176896
6	C	0.322586
7	C	0.420333
8	H	0.009869
9	C	-0.279394
10	H	-0.016644
11	C	0.560395
12	C	0.322587
13	C	-0.250168
14	C	-0.260895
15	C	0.176896
16	C	-0.206458
17	C	0.365324
18	H	-0.015706
19	C	-0.170391

20	C	0.342589
21	H	-0.015583
22	C	-0.209480
23	H	0.007935
24	C	0.365325
25	H	-0.015706
26	C	-0.170392
27	C	-0.209480
28	H	0.007935
29	C	0.342589
30	H	-0.015583
31	C	0.257502
32	C	-0.160659
33	H	0.006454
34	C	0.228565
35	C	0.257503
36	C	-0.160660
37	H	0.006454
38	C	0.228566
39	C	-0.021735
40	H	0.012762
41	H	0.004877
42	H	0.002783
43	C	-0.021735
44	H	0.004877
45	H	0.002783
46	H	0.012762
47	C	-0.050731
48	C	0.002571
49	C	0.015097
50	C	0.015018
51	C	-0.002130
52	C	-0.002131
53	H	0.000750
54	H	0.000768
55	C	-0.050731
56	C	0.002572
57	C	0.015018
58	C	0.015098
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60	C	-0.002130
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63	C	-0.000185
64	H	0.000127
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66	H	0.000033
67	C	-0.000398
68	H	0.000418
69	H	0.000158

70	H	0.000009
71	C	0.000003
72	H	0.000075
73	H	0.000200
74	H	0.000394
75	C	-0.000185
76	H	0.000024
77	H	0.000034
78	H	0.000127
79	C	0.000003
80	H	0.000200
81	H	0.000394
82	H	0.000075
83	C	-0.000398
84	H	0.000009
85	H	0.000418
86	H	0.000158
87	H	-0.010135
88	H	-0.010135

Sum of Mulliken atomic spin densities = 2.00000 <S**2>= 2.2853

Sum of electronic and zero-point Energies= -1851.448711
Sum of electronic and thermal Energies= -1851.407519
Sum of electronic and thermal Enthalpies= -1851.406575
Sum of electronic and thermal Free Energies= -1851.524191

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C	-0.00000100	0.20580000	0.00002900
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H	-7.09504400	-2.35020300	0.08305800
C	2.59392200	-3.91820600	0.87639600
C	3.85596600	-4.53497000	0.91803000
H	3.91285900	-5.56061100	1.27198700
C	5.00532500	-3.88698700	0.54622600
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H	-2.68155300	6.35057900	1.69710100
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H	-3.56373500	1.34806100	-2.30906600
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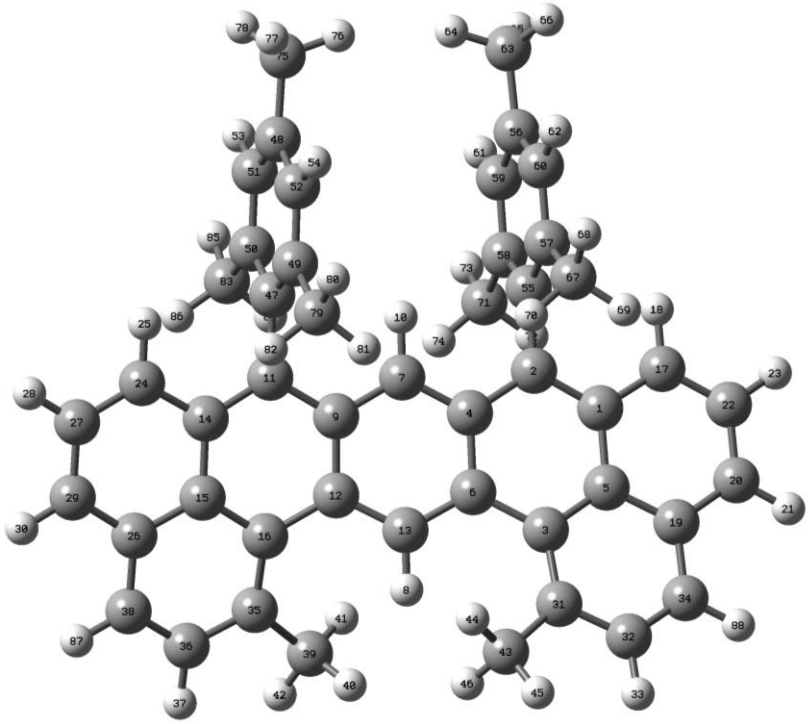
Singlet diradical



Mulliken atomic spin densities:

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1	C	-0.235569
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7	C	0.000018
8	H	0.000000

9	C	0.087148
10	H	-0.000001
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14	C	0.235562
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55	C	-0.047779
56	C	0.002308
57	C	0.014380
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83	C	0.000455
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Sum of Mulliken atomic spin densities = 0.00000 <S**2>= 1.11527

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Sum of electronic and thermal Free Energies= -1851.514791

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C	-6.15248300	-1.80617700	0.12636600
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C	2.60268600	-3.92560500	0.85082600
C	3.86468900	-4.53905600	0.88451900
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C	-2.60301700	-3.92543000	-0.85080300
C	-3.86507300	-4.53878100	-0.88448500
H	-3.92629500	-5.56649700	-1.23158100
C	-5.01235700	-3.88424400	-0.51377200
C	-1.46633000	-4.74573700	-1.41378400
H	-0.92770700	-5.31250000	-0.64529700
H	-0.73588300	-4.13414900	-1.94757400
H	-1.86574500	-5.47991800	-2.11881600
C	1.46592900	-4.74579700	1.41383800
H	0.73549600	-4.13412400	1.94754500
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H	0.92731000	-5.31260400	0.64538100
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C	-2.33471800	4.53170800	0.53393300
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C	-2.51233500	2.55760300	-0.87634800
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C	-2.26098500	3.70001200	1.64729700
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C	2.51252000	2.55739500	0.87635500
C	2.30189200	2.31274200	-1.53172700
C	2.26134400	3.69987700	-1.64727600
C	2.46615200	3.94026400	0.71873900
H	2.16539200	4.14188700	-2.63629700
H	2.53153700	4.57194200	1.60156300

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H	2.69079100	2.73761700	3.01663400
H	3.55735200	1.35137800	2.33611100
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C	2.21292400	1.44889400	-2.76393400
H	3.09938800	0.81595000	-2.87431500
H	2.11991000	2.06151700	-3.66433400
H	1.34757800	0.77946900	-2.71855900
C	-2.24416100	6.02861600	0.67827900
H	-1.20081400	6.36489700	0.64316500
H	-2.66122300	6.36538800	1.63179600
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H	-2.11957000	2.06160000	3.66431300
H	-1.34757200	0.77940500	2.71846200
H	-3.09936200	0.81623700	2.87436400
C	-2.64930400	1.95756300	-2.25237000
H	-1.80503100	1.30023600	-2.48544400
H	-2.69074300	2.73788500	-3.01661100
H	-3.55722500	1.35160000	-2.33607800
H	-5.97226300	-4.39165700	-0.54044300
H	5.97189100	-4.39211500	0.54047200

5. Mass spectrum of DP-Mes solution at room temperature

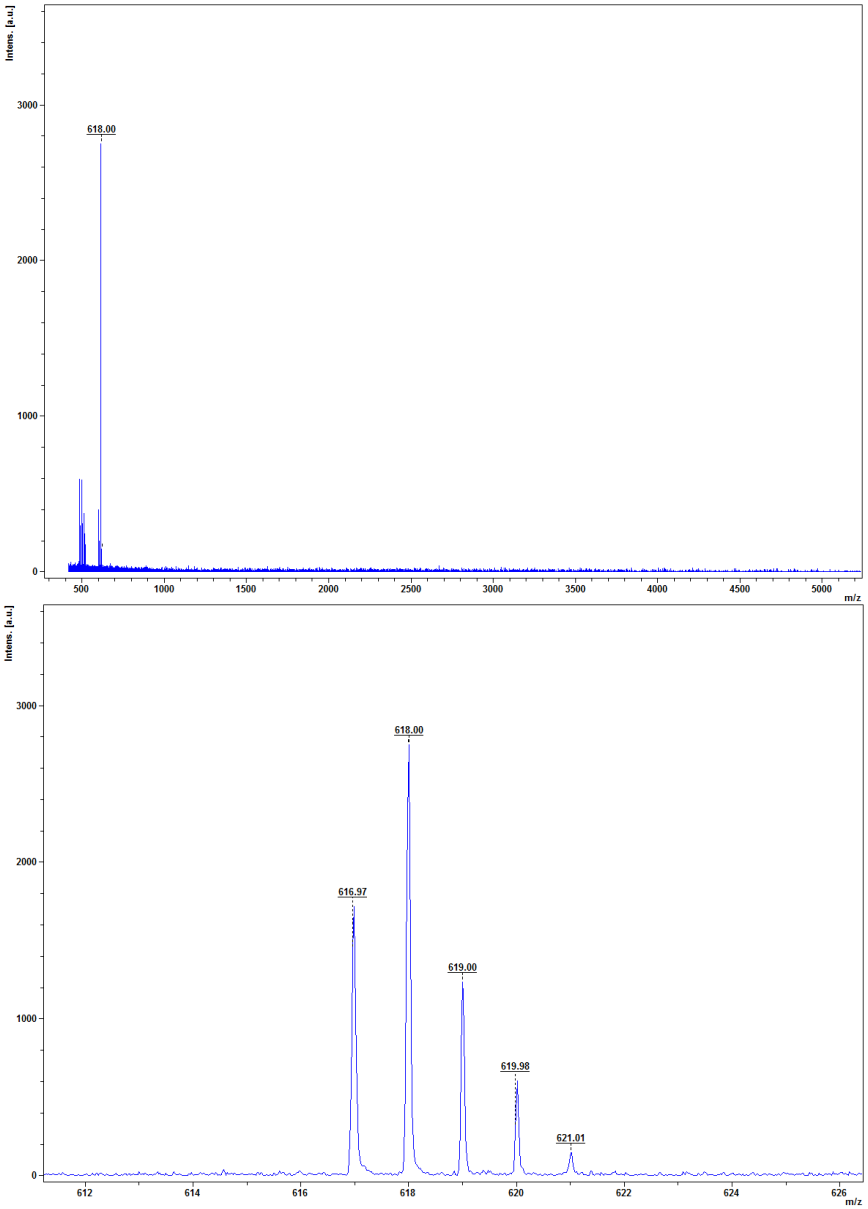


Fig. S4. MALDI-TOF mass spectrum of the products when the solution of **DP-Mes** was briefly warmed up to room temperature.

6. References

(1) Gaussian 09; Revision A.2; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.;

Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, **2009**.

7. Appendix: NMR spectra and HR mass spectra of new compounds

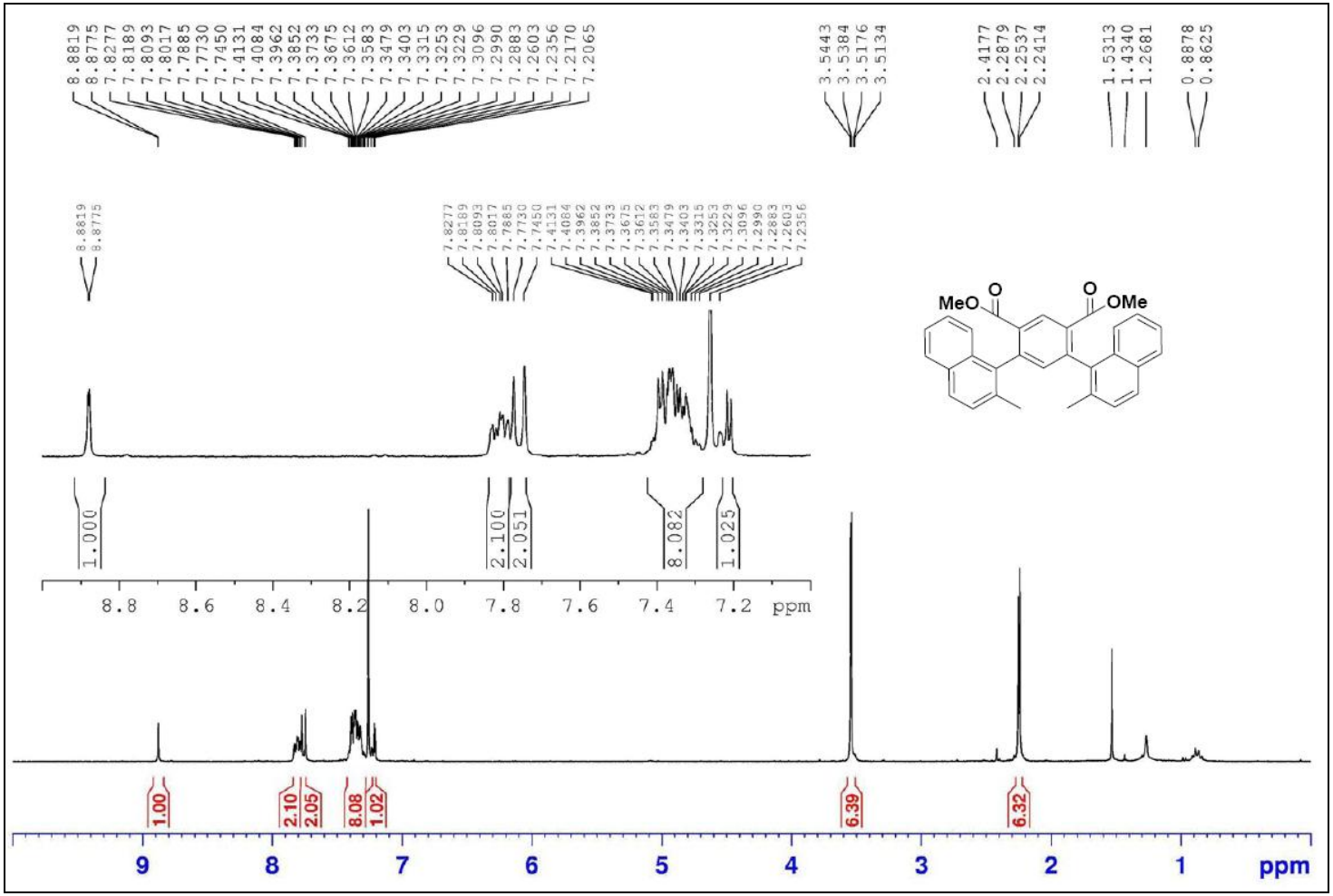


Fig. S5. ^{1}H NMR spectrum of **3** (300MHz, $CDCl_3$, rt)

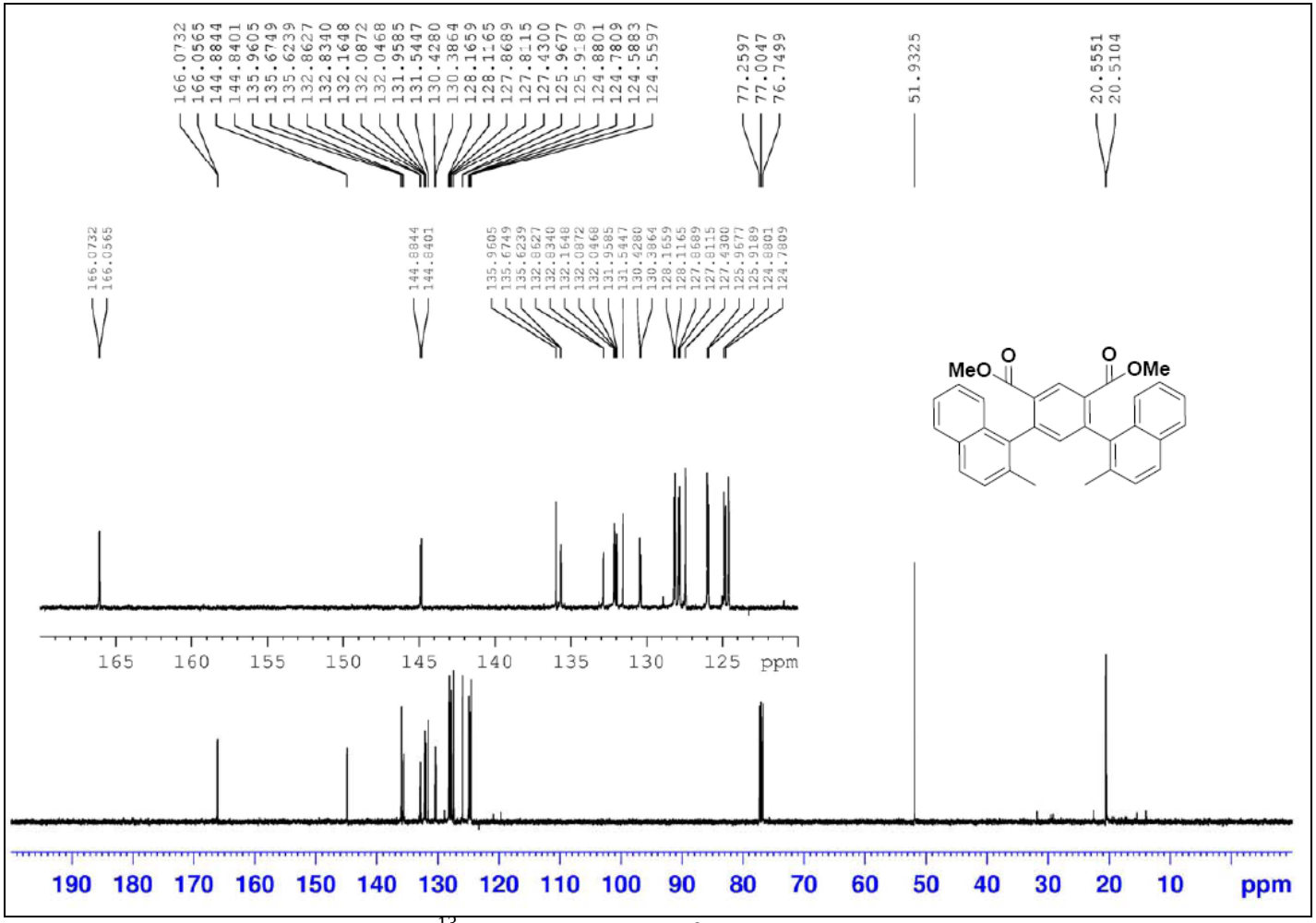


Fig. S6. ^{13}C NMR spectrum of **3** (125MHz, $CDCl_3$, rt)

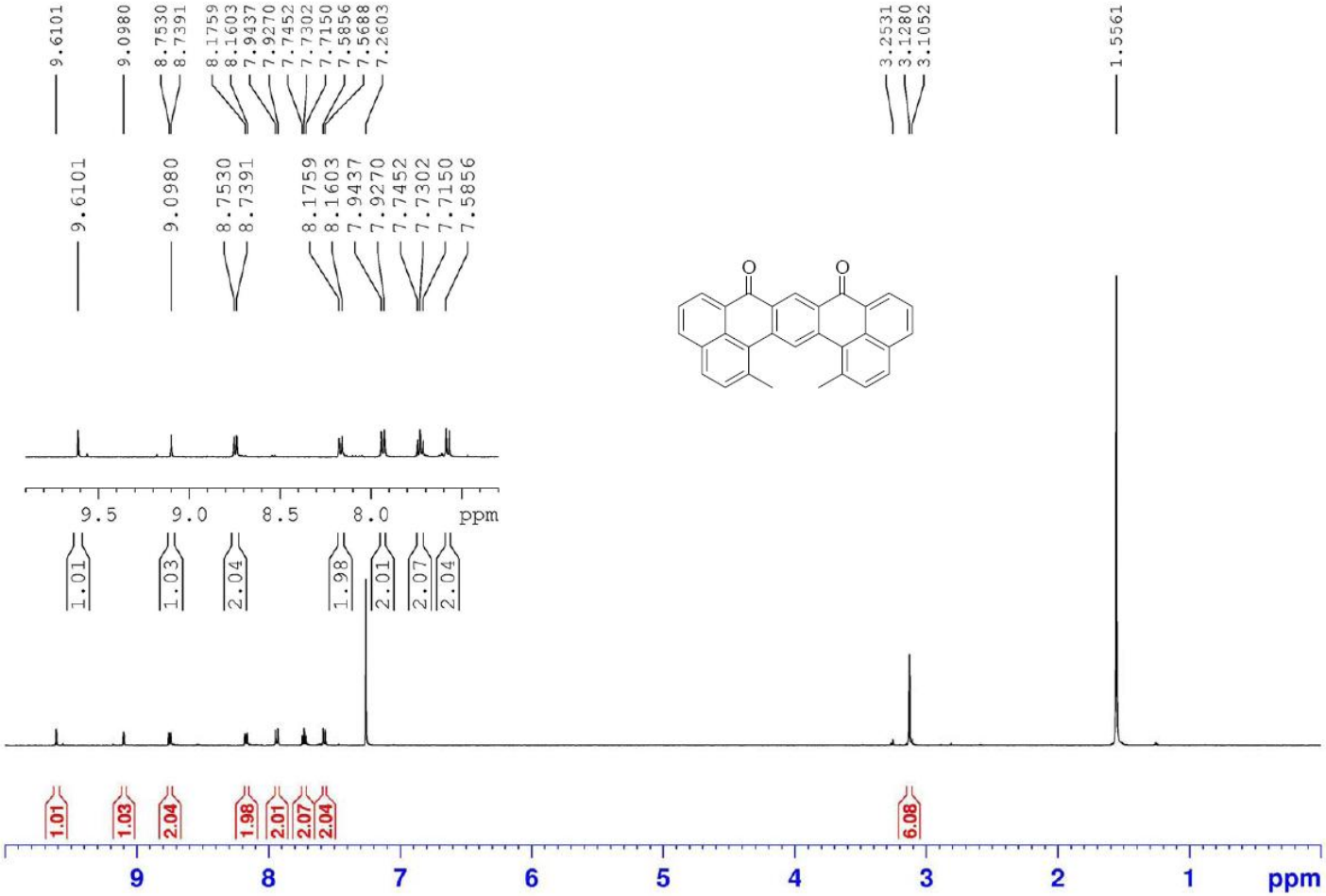


Fig. S7. ^{1}H NMR spectrum of **4** (500 MHz, $CDCl_3$, rt)

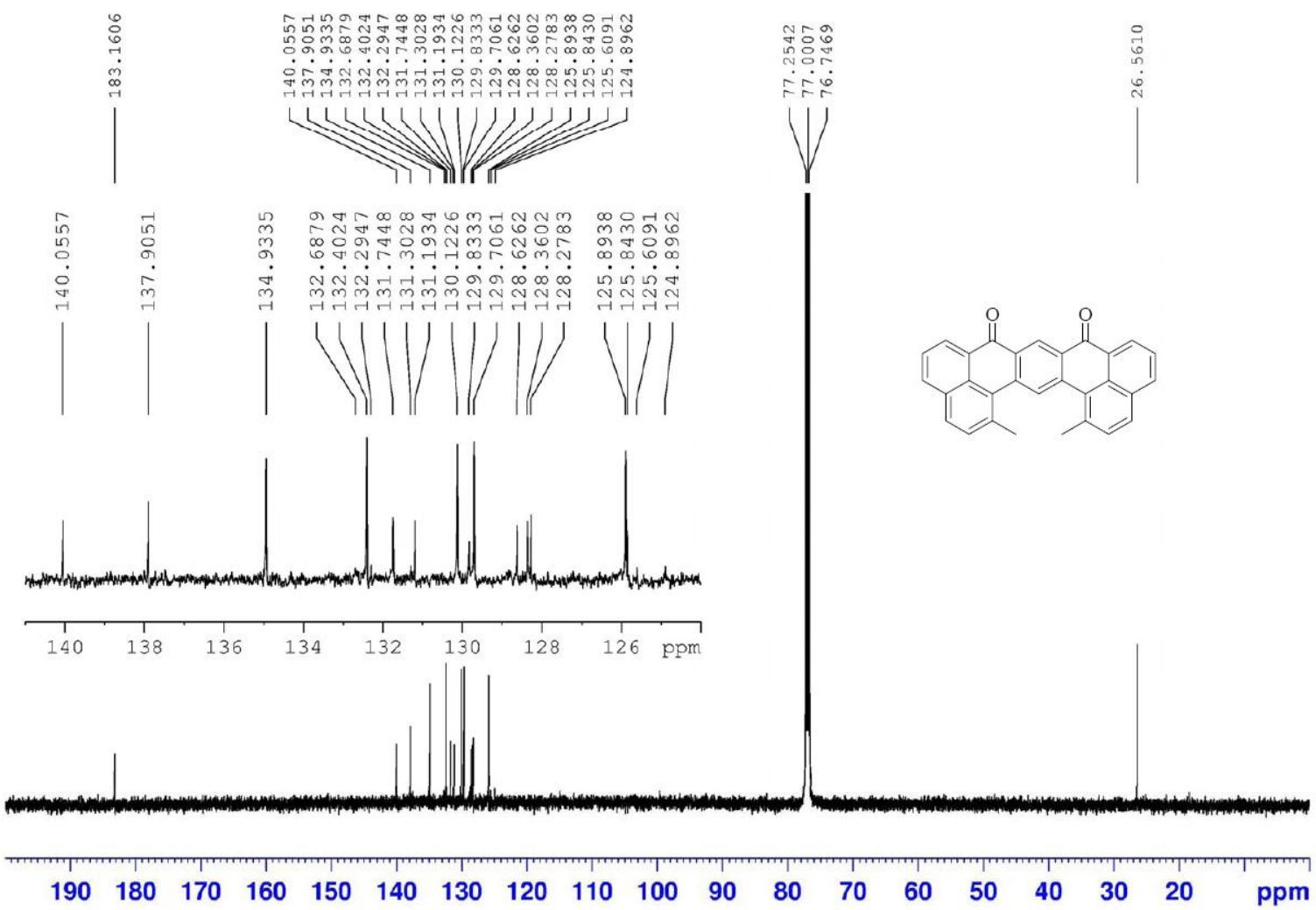


Fig. S8. ^{13}C NMR spectrum of **4** (125 MHz, $CDCl_3$, rt)

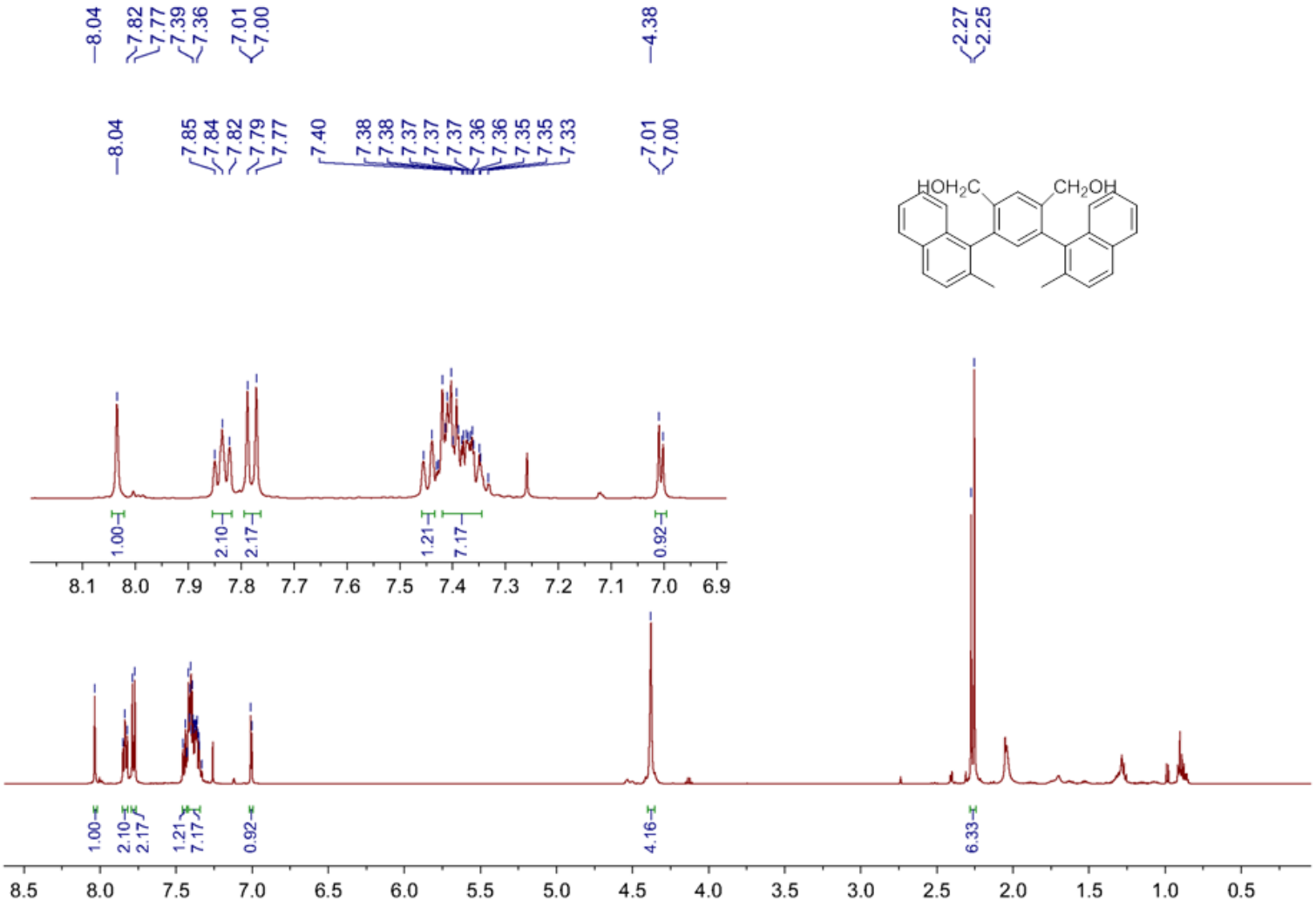


Fig. S9. ^{1}H NMR spectrum of **6** (500MHz, $CDCl_3$, rt)

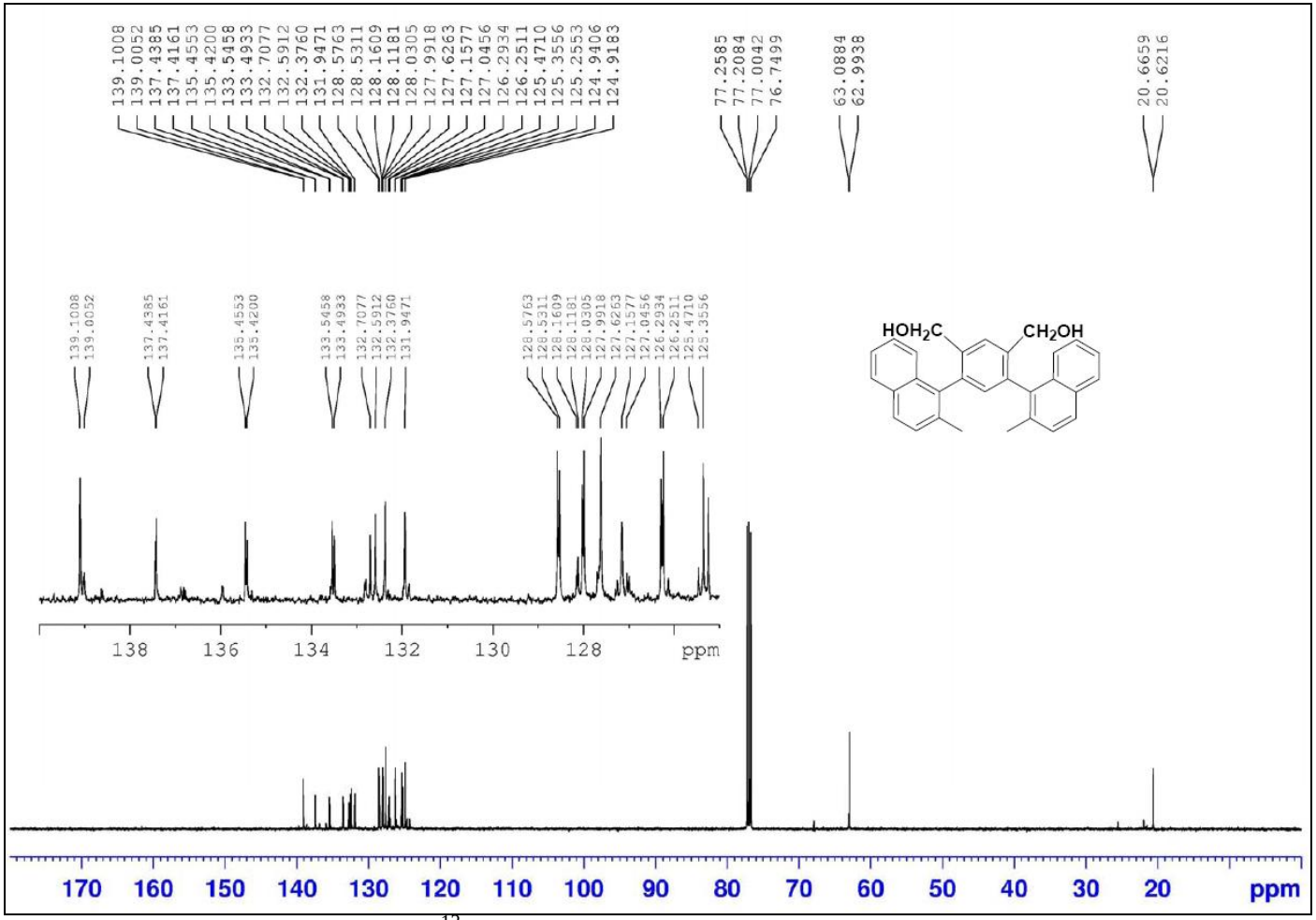


Fig. S10. ^{13}C NMR spectrum of **6** (125 MHz, $CDCl_3$, rt)

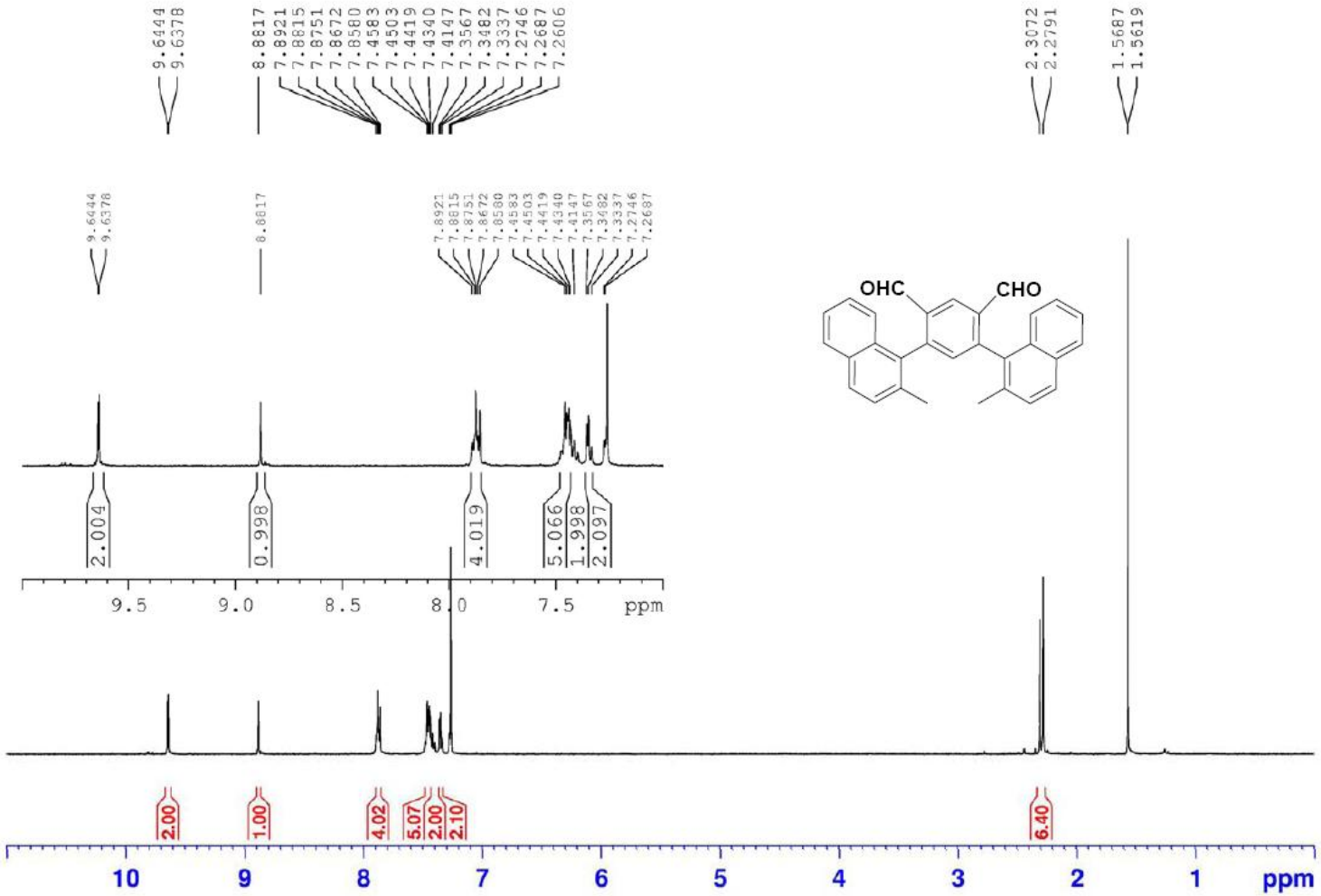


Fig. S11. ^{1}H NMR spectrum of **7** (500MHz, $CDCl_3$, rt)

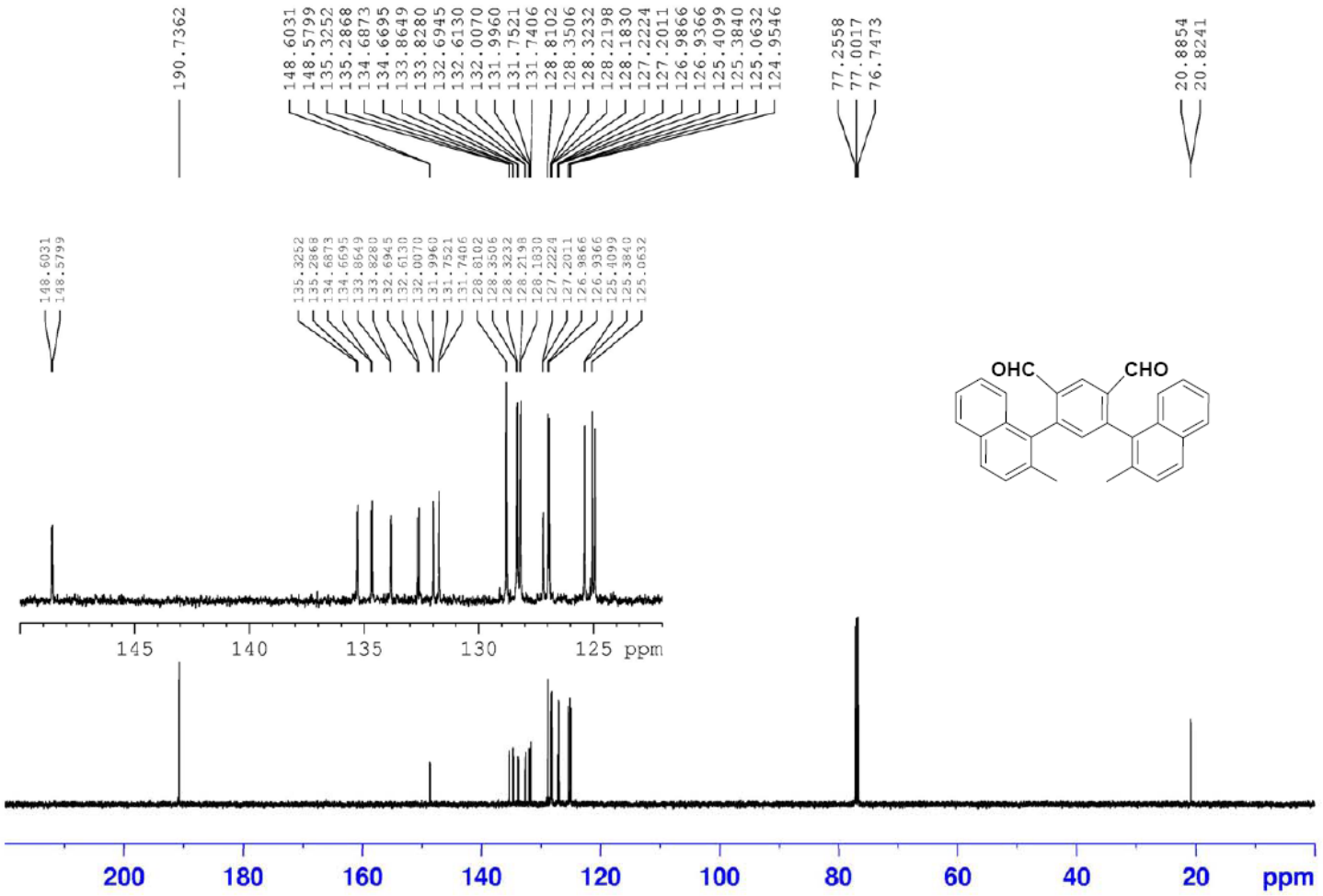


Fig. S12. ^{13}C NMR spectrum of **7** (125 MHz, $CDCl_3$, rt)

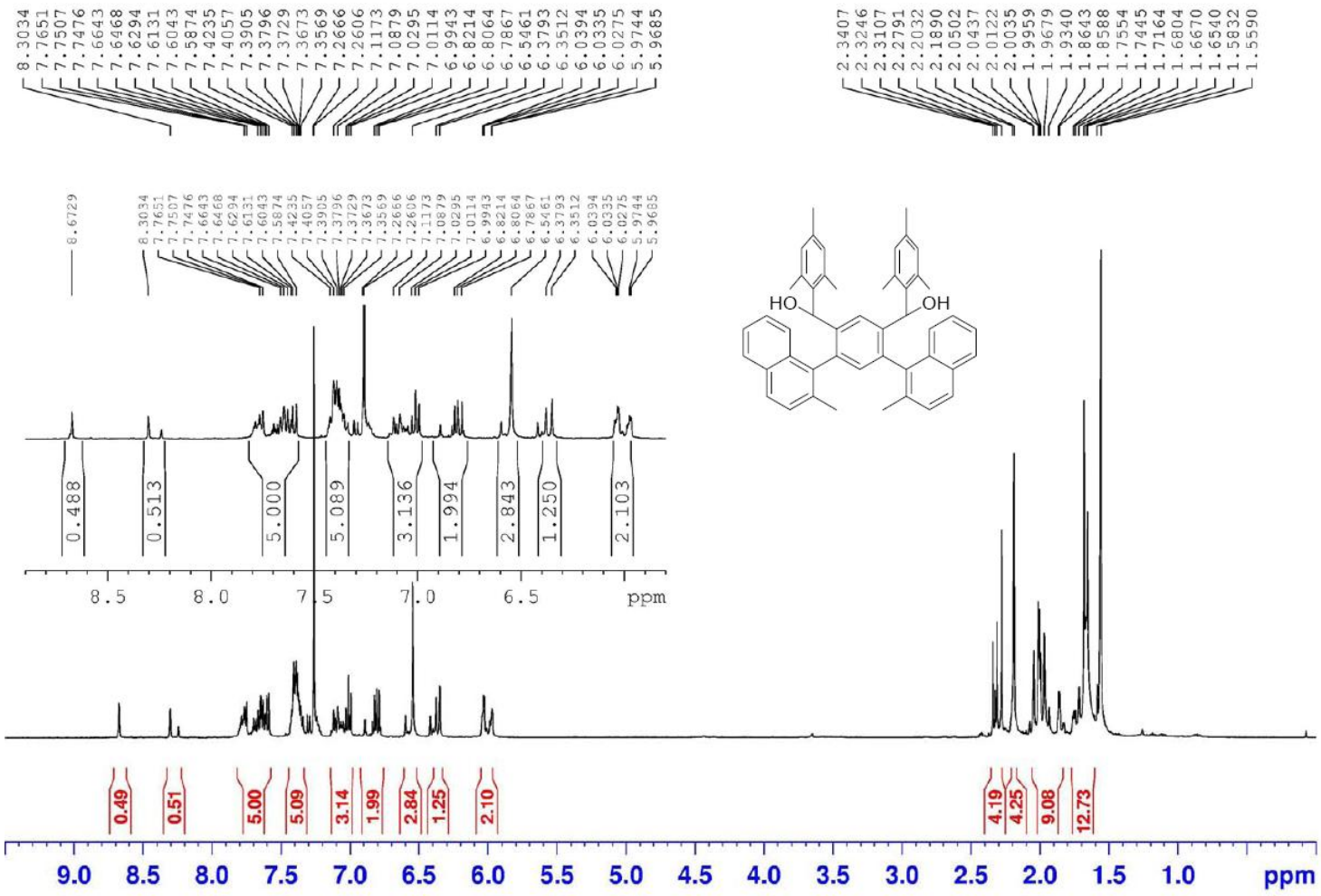


Fig. S13. ^{1}H NMR spectrum of **8** (500MHz, $CDCl_3$, rt)

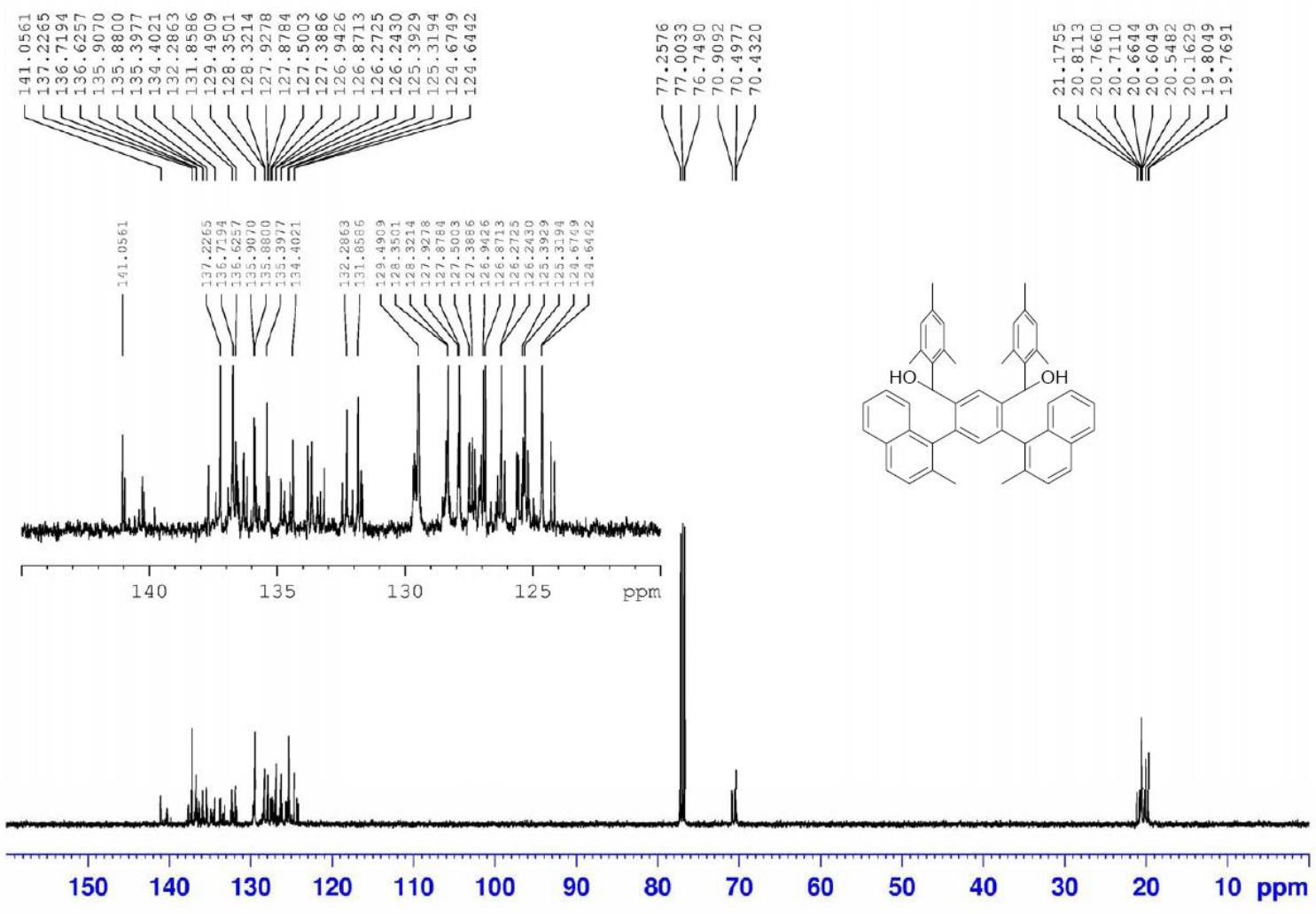


Fig. S14. ^{13}CNMR spectrum of **8** (125 MHz, $CDCl_3$, rt)

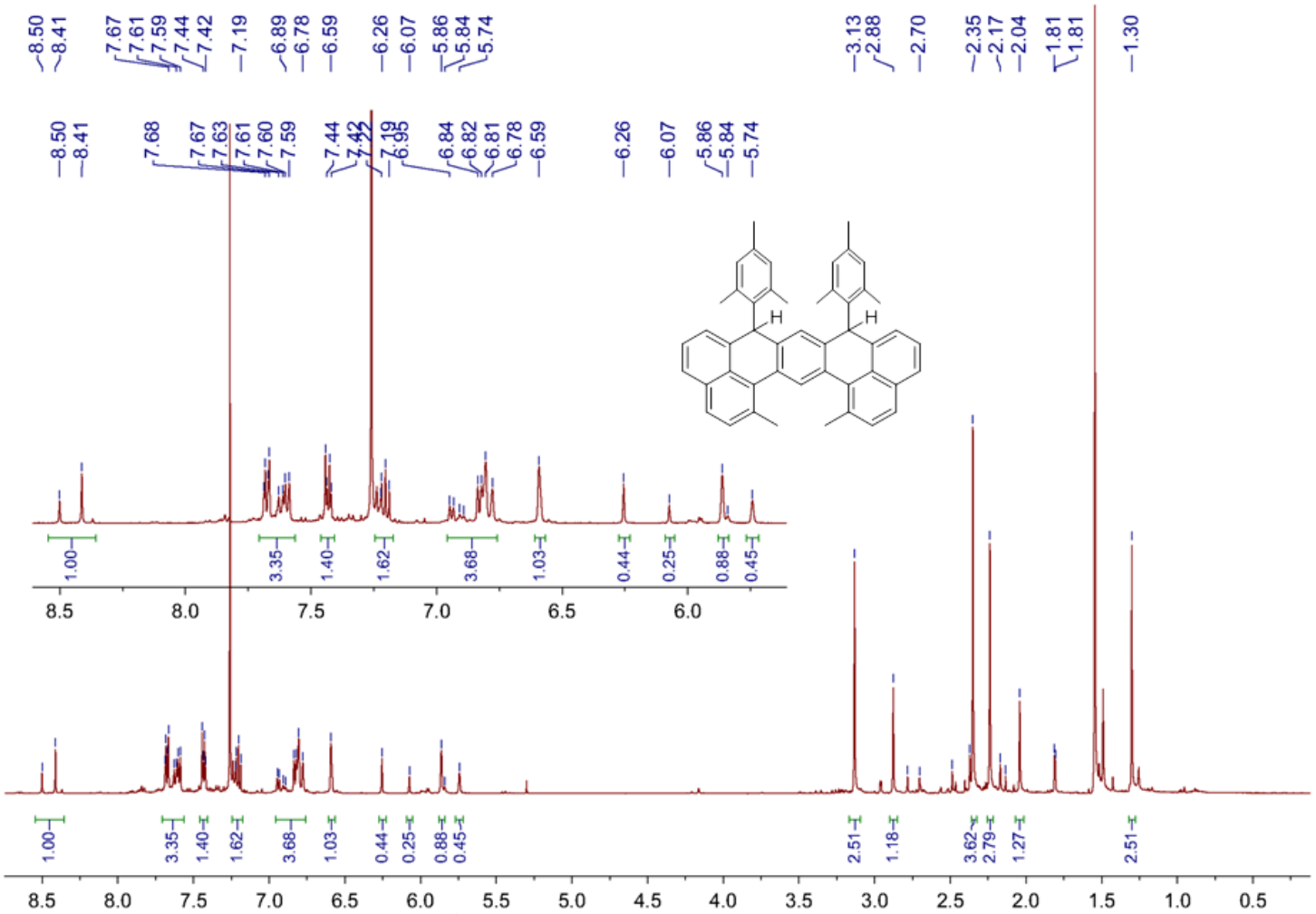


Fig. S15. ^{1}H NMR spectrum of **9** (500MHz, $CDCl_3$, rt)

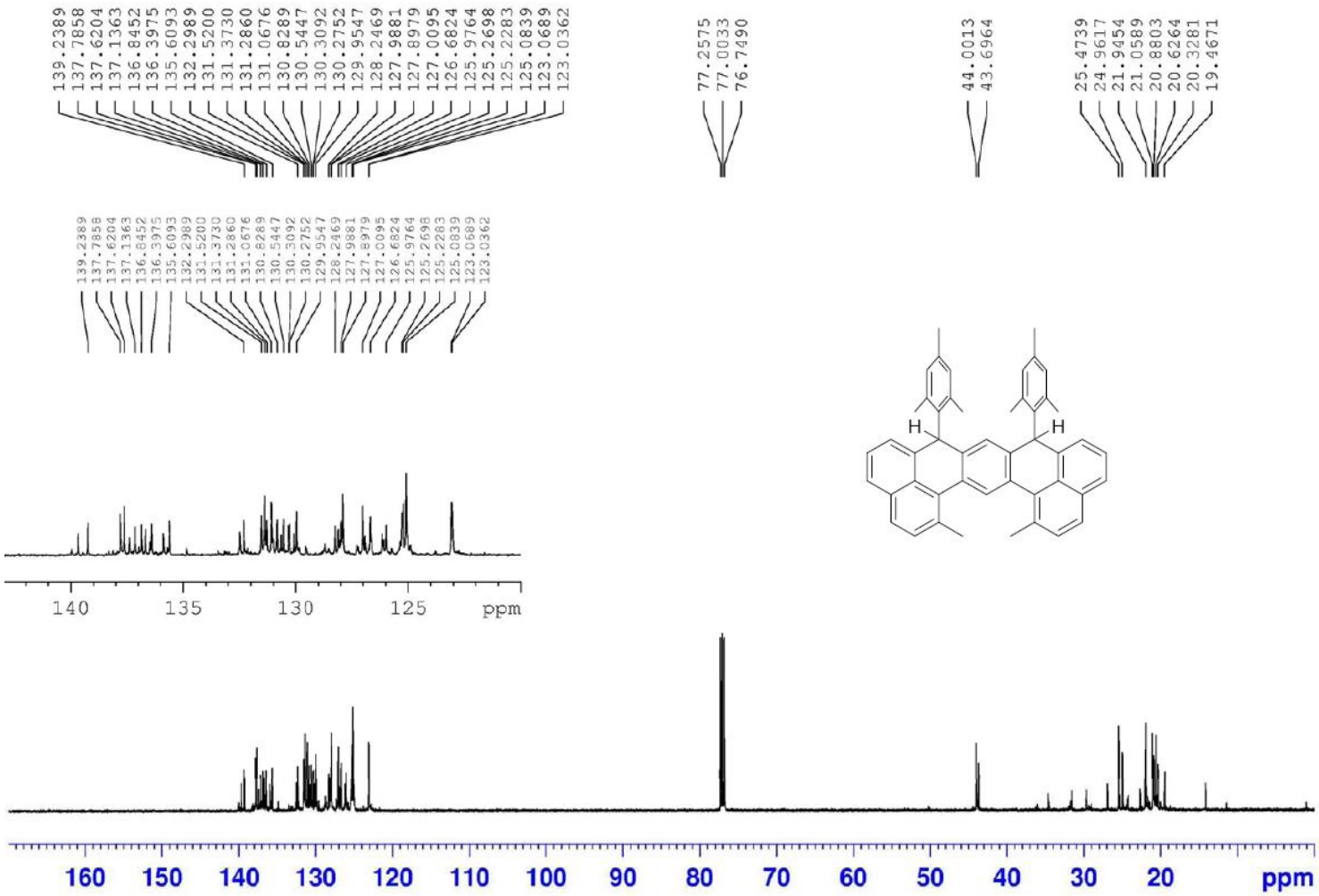
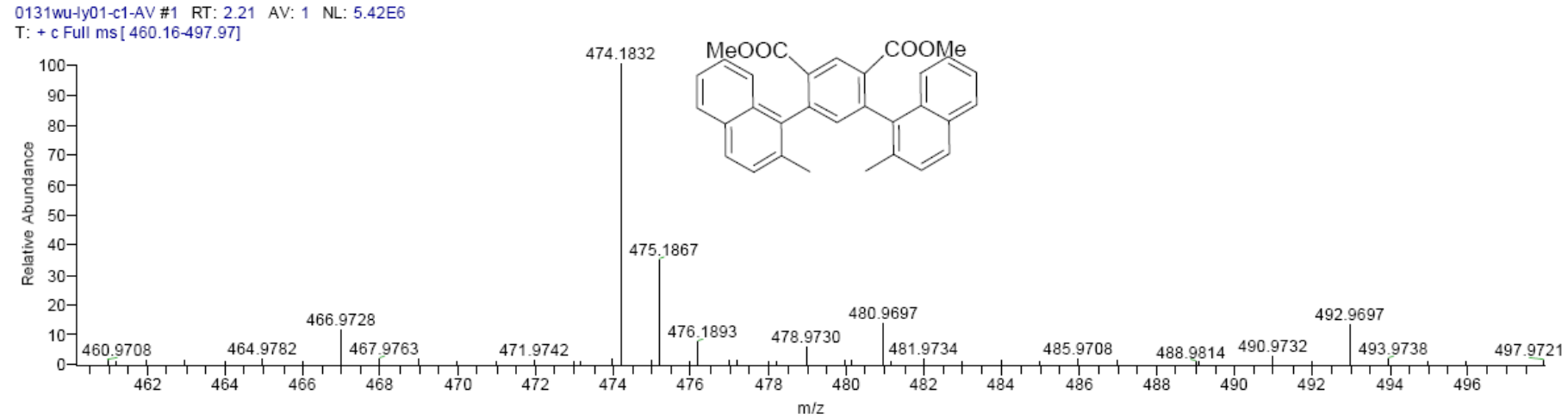


Fig. S16. ^{13}C NMR spectrum of **9** (125 MHz, $CDCl_3$, rt)

A:\31JAN13_EIHR\0131wu-ly01-c1-AV 31/01/2013 04:23:53 PM ly-01
EIHR

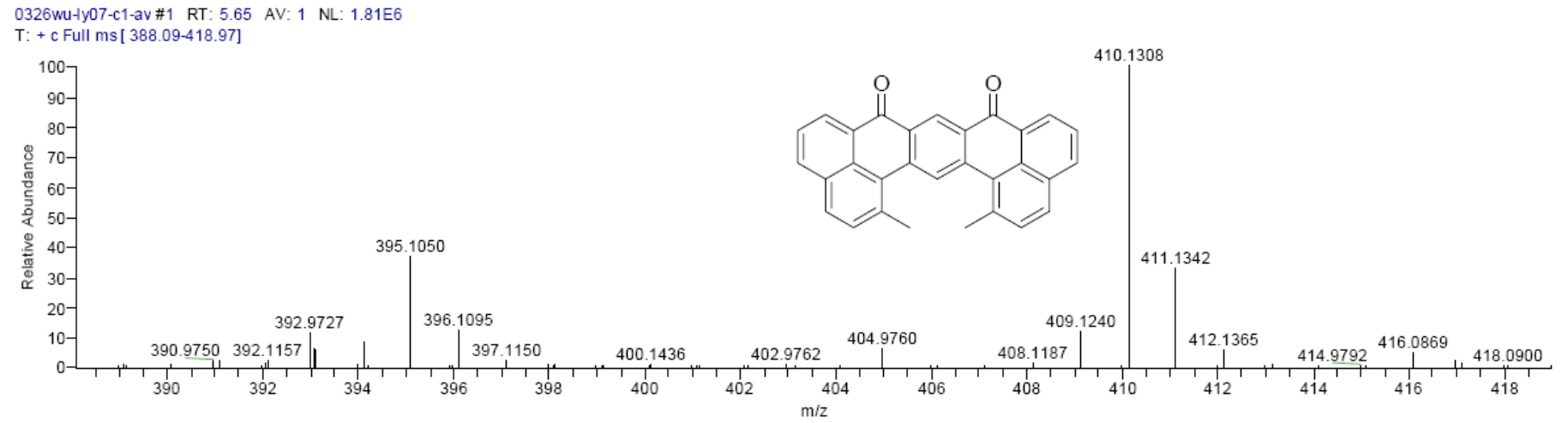


0131wu-ly01-c1-AV#1 RT: 2.21
T: + c Full ms [460.16-497.97]
m/z= 473.99-474.67

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
474.1832	5418415.0	100.00	474.1831	0.12	20.0	$C_{32}H_{26}O_4$

Fig. S17. HR-MS (EI) of compound **3**

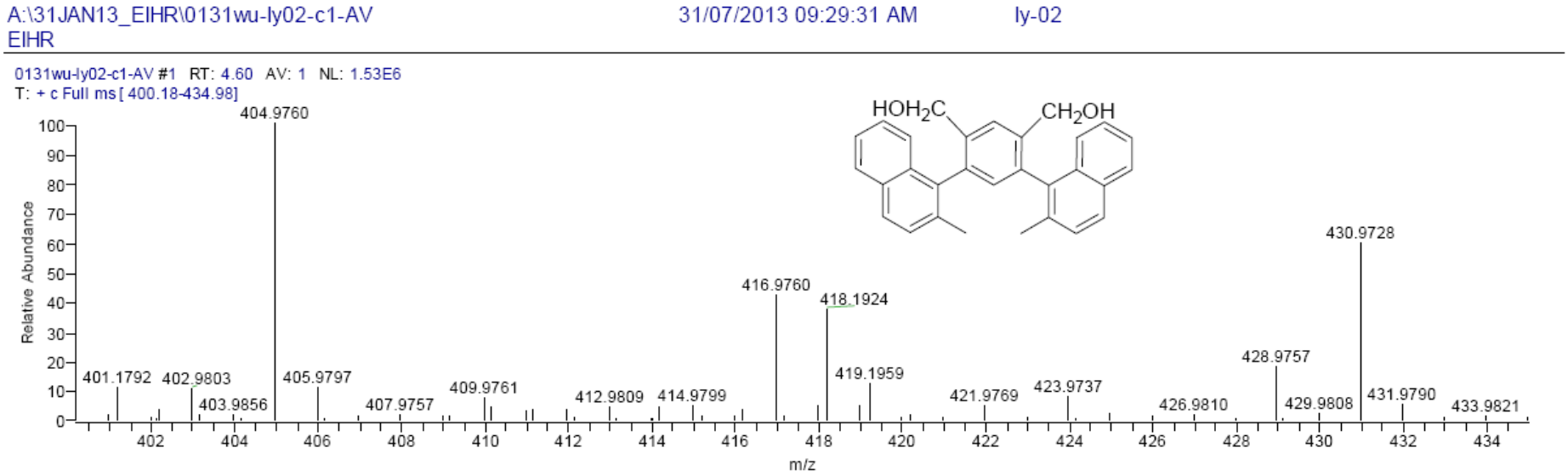
A:\26mar13_eihr\0326wu-ly07-c1-av 26/05/2013 08:59:45 AM ly07
MATRIX:3NBA



0326wu-ly07-c1-av#1 RT: 5.65
T: + c Full ms [388.09-418.97]
m/z= 410.00-410.39

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
410.1308	1812168.0	100.00	410.1307	0.40	22.0	$C_{30}H_{18}O_2$

Fig. S18. HR-MS (EI) of compound **4**

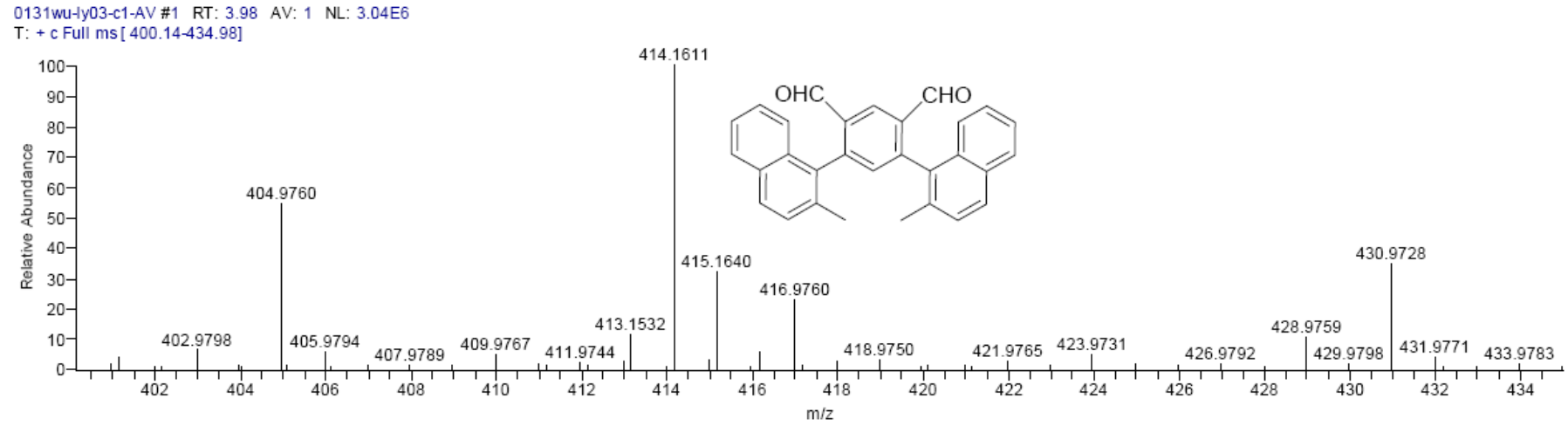


0131wu-ly02-c1-AV#1 RT: 4.60
T: + c Full ms [400.18-434.98]
m/z= 418.06-418.35

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
418.1924	576821.0	100.00	418.1933	-2.07	18.0	$C_{30}H_{26}O_2$

Fig. S19. HR-MS (EI) of compound **6**

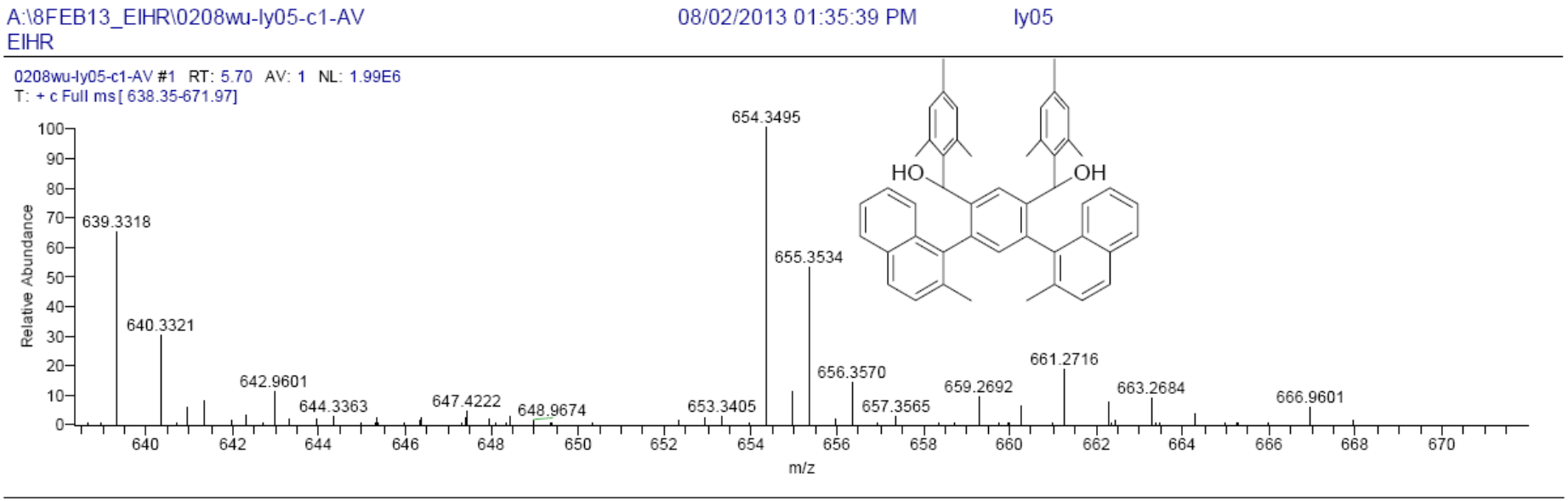
A:\31JAN13_EIHR\0131wu-ly03-c1-AV 31/01/2013 04:46:50 PM ly-03
EIHR



0131wu-ly03-c1-AV#1 RT: 3.98
T: + c Full ms [400.14-434.98]
m/z= 413.97-414.33

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
414.1611	3035843.0	100.00	414.1620	-2.19	20.0	$C_{30}H_{22}O_2$

Fig. S20. HR-MS (EI) of compound **7**

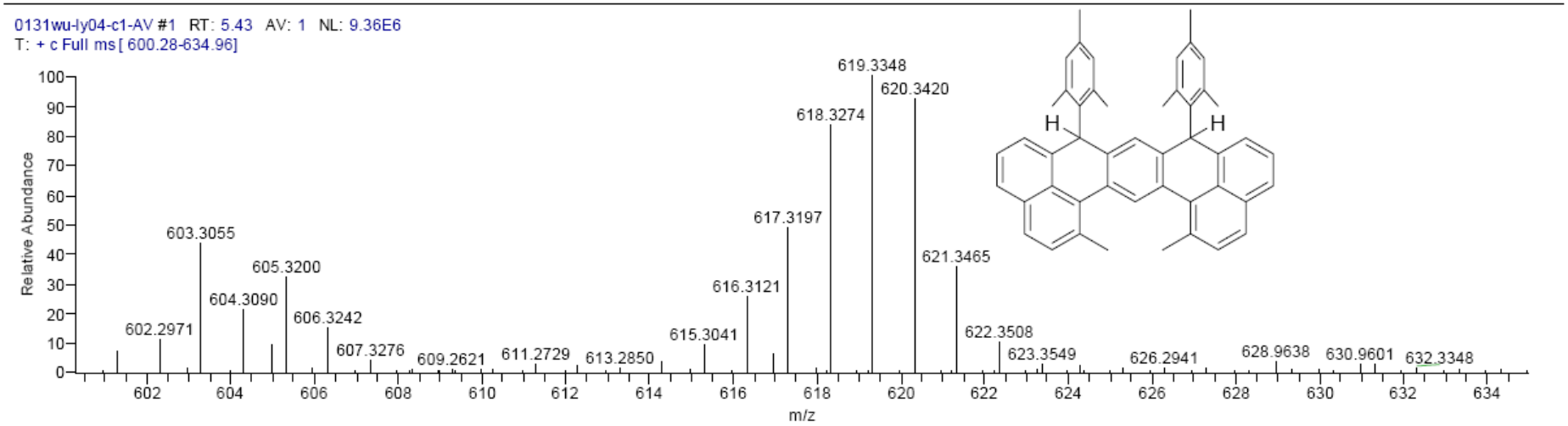


0208wu-ly05-c1-AV#1 RT: 5.70
T: + c Full ms [638.35-671.97]
m/z= 653.95-654.51

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
654.3495	1988868.0	100.00	654.3498	-0.36	26.0	$C_{48}H_{46}O_2$

Fig. S21. HR-MS (EI) of compound **8**

A:\31JAN13_EIHR\0131wu-ly04-c1-AV 31/01/2013 04:14:30 PM ly-04
EIHR



0131wu-ly04-c1-AV#1 RT: 5.43
T: + c Full ms [600.28-634.96]
m/z= 618.14-618.55

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
618.3274	7759725.0	100.00	618.3287	-1.99	28.0	$C_{48}H_{42}$

Fig. S22. HR-MS (EI) of compound **9**