Supplementary Information

Chiroptical Property of TPE Triangular Macrocycle Crown Ethers from Propeller-Like Chirality Induced by Chiral Acids

Wei-Guo Qiao,[a] Jia-Bin Xiong,[a] Ying-Xue Yuan,[a] Hong-Chao Zhang,[a] Dong Yang,[b] Minghua Liu[b] and Yan-Song Zheng*[a]

[a] Key Laboratory of Material Chemistry for Energy Conversion and Storage, Ministry of Education, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan 430074, China. zyansong@hotmail.com
[b] Beijing National Laboratory for Molecular Science (BNLMS), CAS Key Laboratory of Colloid Interface and Chemical Thermodynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190 , China

Table of Contents

The characterization spectra of compounds 2−8.

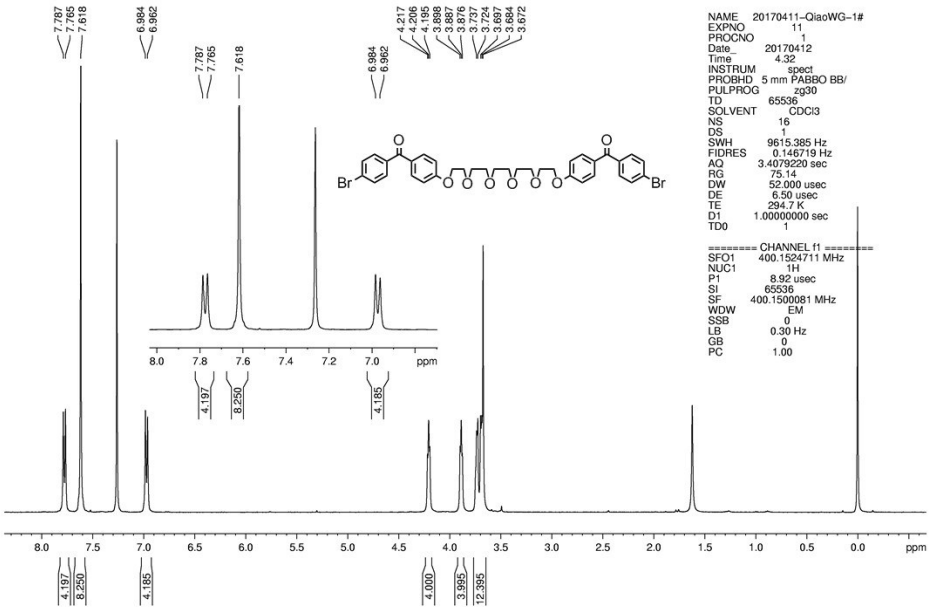


Fig. S1. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

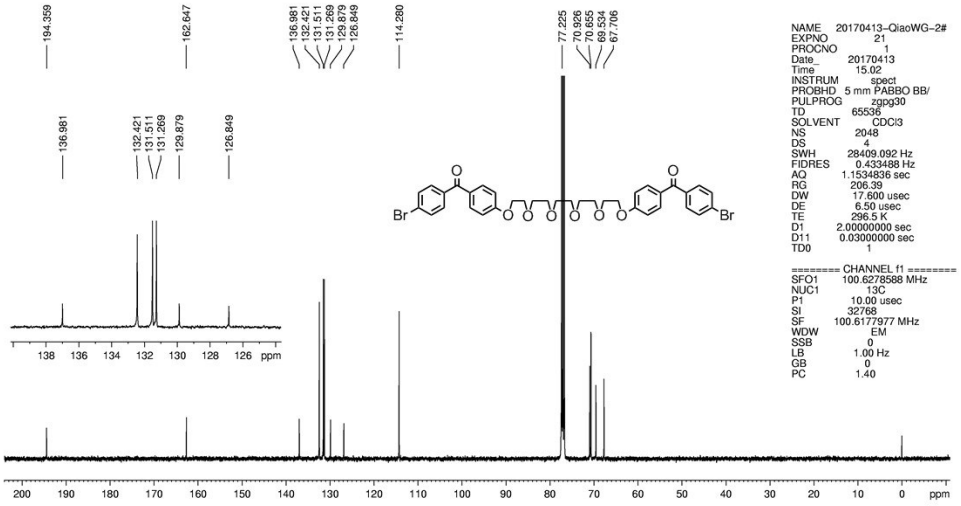


Fig. S2. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

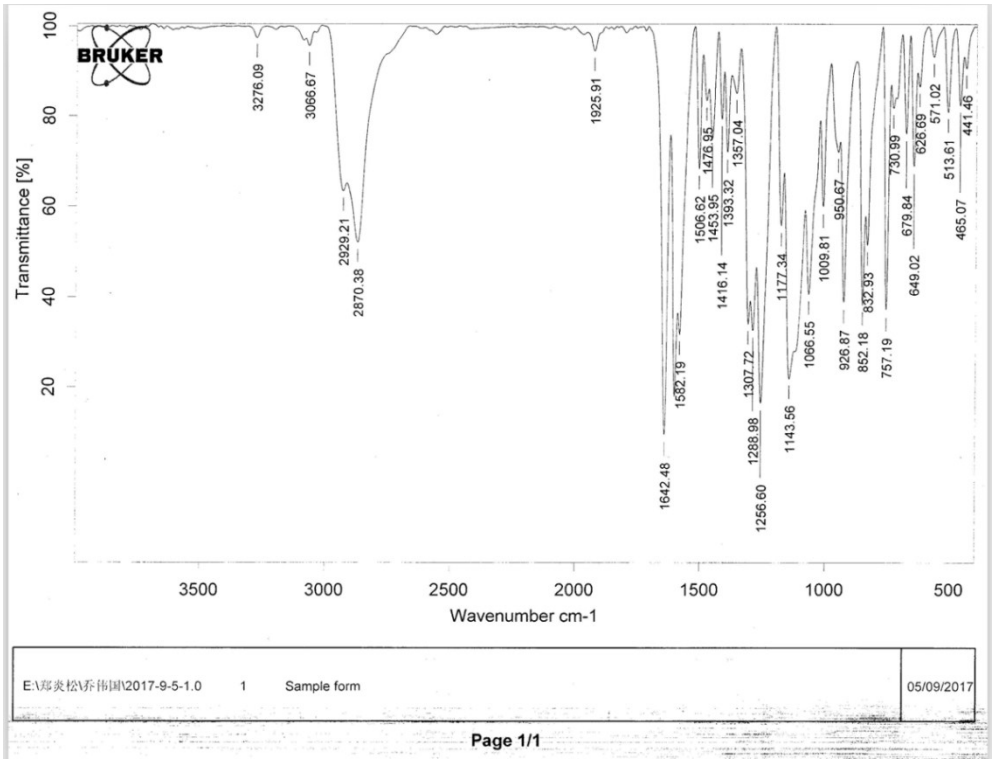


Fig. S3. IR spectrum of compound **2**.

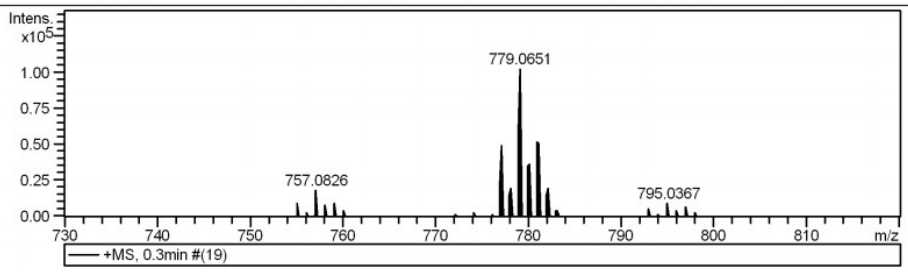
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\ZhengYS\zheng-qiaoweiguo20170911-1.d	Acquisition Date	9/11/2017 9:31:46 AM
Method	tune_wide.m	Operator	BDAL@DE
Sample Name	zheng-qiaoweiguo20170911-1	Instrument / Ser#	micrOTOF 10401
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	755.0830	15423	23.6	10048	0.0490
2	757.0826	14640	44.0	18600	0.0517
3	758.0833	16382	20.3	8546	0.0463
4	759.0809	14310	23.4	9816	0.0530
5	777.0660	16138	128.6	49818	0.0482
6	778.0682	14520	51.6	19917	0.0536
7	779.0651	16155	267.2	102579	0.0482
8	780.0668	14521	97.0	37074	0.0537
9	781.0613	14340	136.7	51990	0.0545
10	782.0632	14625	51.9	19650	0.0535
11	783.0705	14028	11.2	4212	0.0558
12	793.0376	14876	16.7	6004	0.0533
13	795.0367	13540	27.3	9724	0.0587
14	796.0390	13568	11.7	4123	0.0587
15	797.0369	14768	20.6	7239	0.0540

Fig. S4. HRMS spectrum of compound **2**.

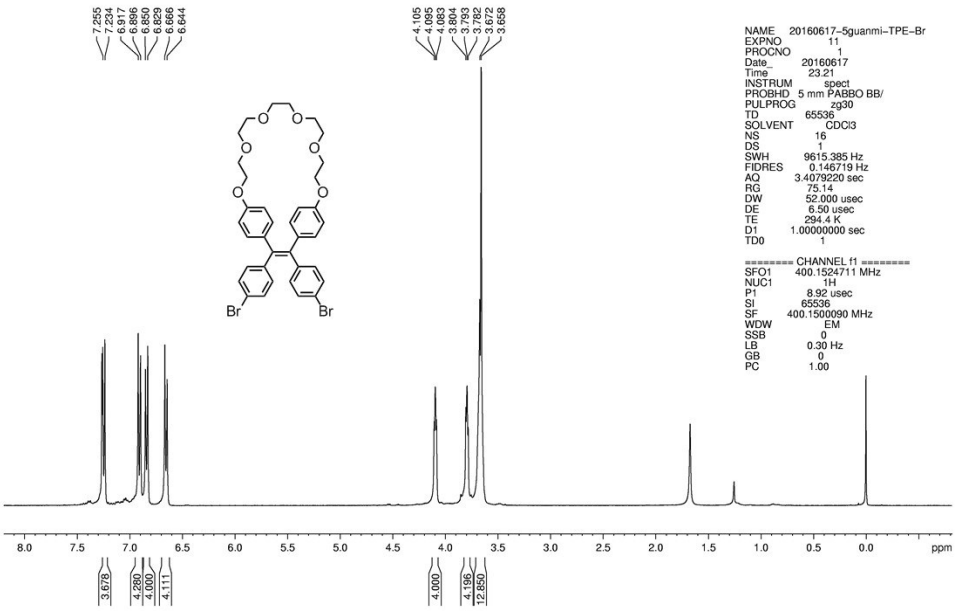


Fig. S5. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

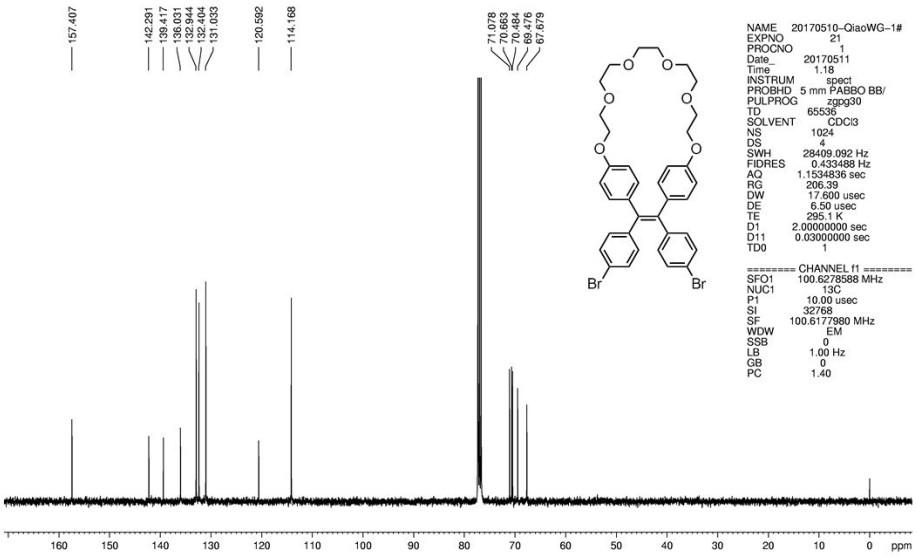


Fig. S6. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

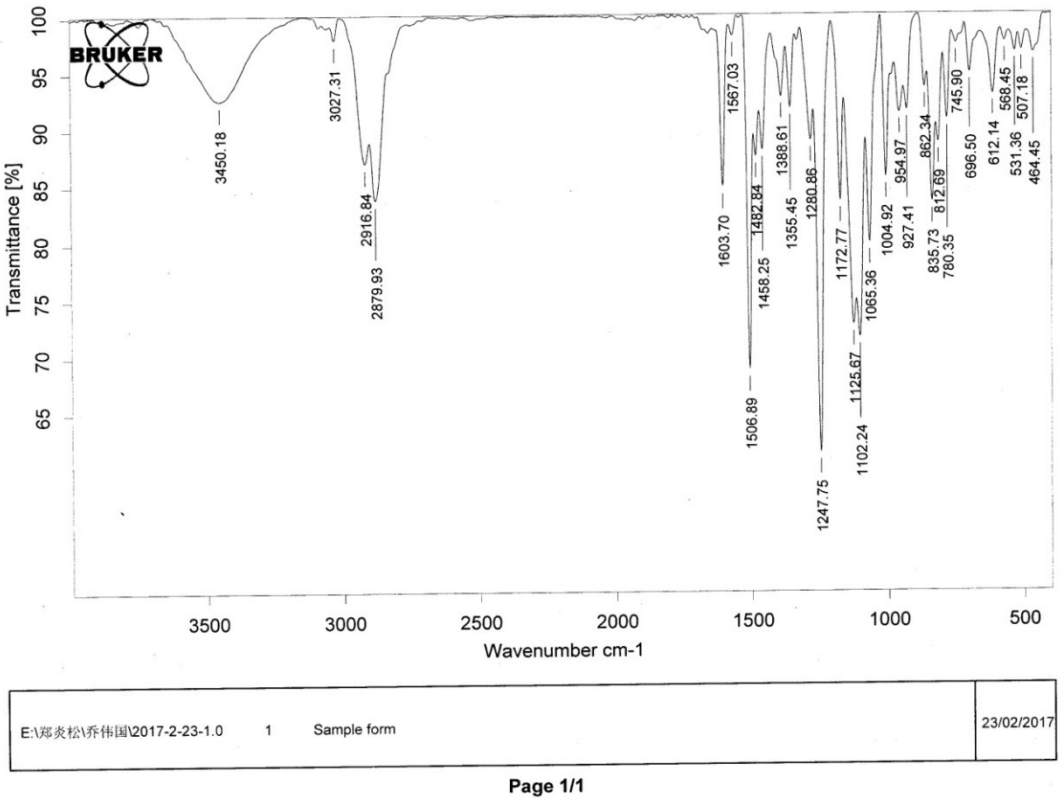


Fig. S7. IR spectrum of compound **3**.

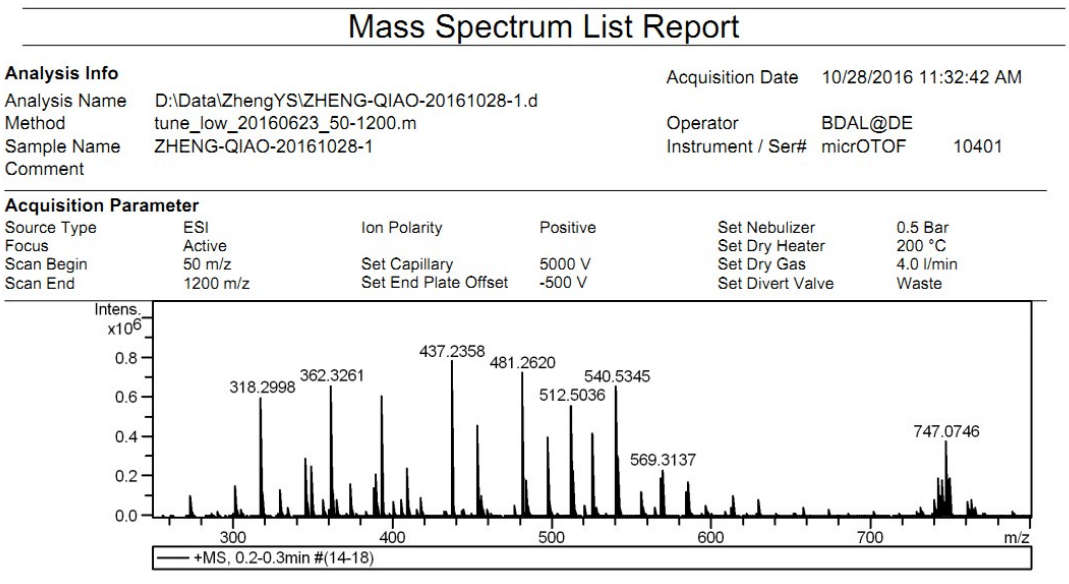


Fig. S8. HRMS spectrum of compound **3**.

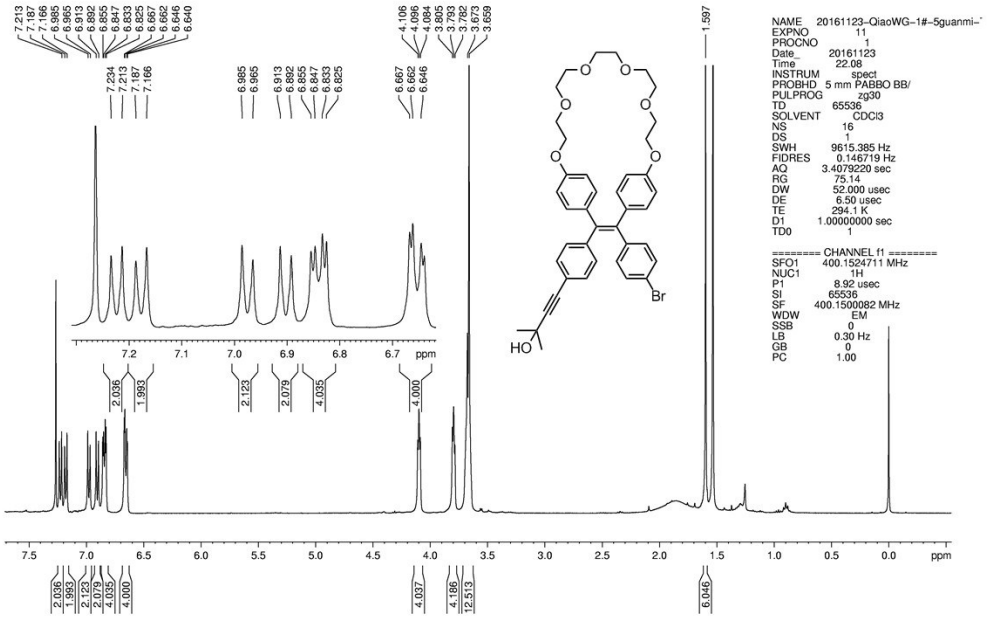


Fig. S9. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

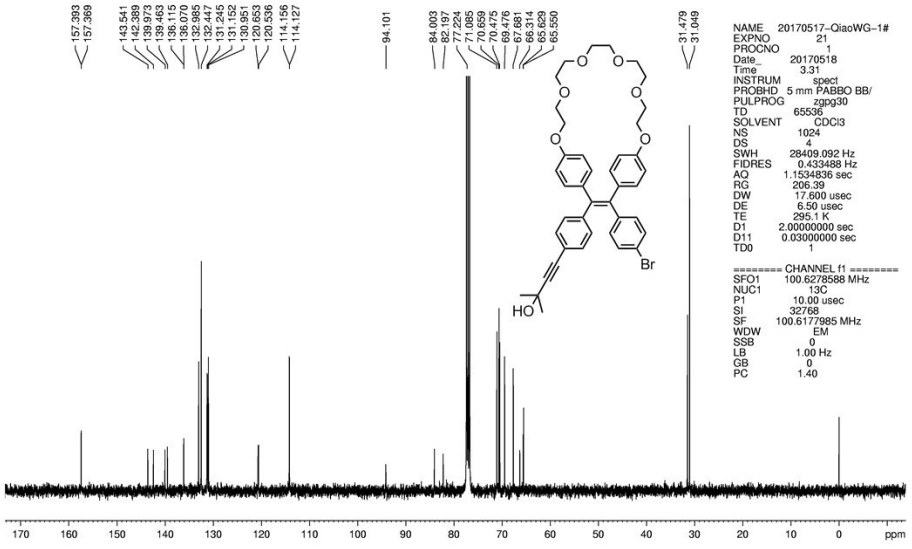


Fig. S10. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

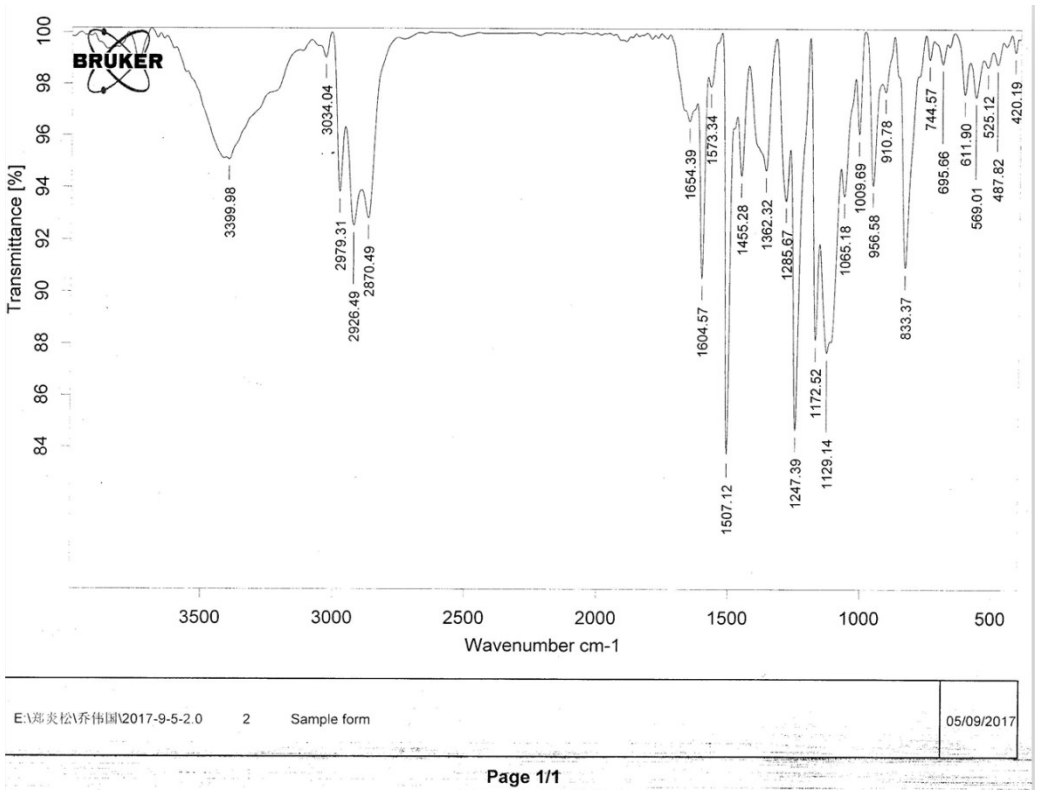


Fig. S11. IR spectrum of compound **4**.

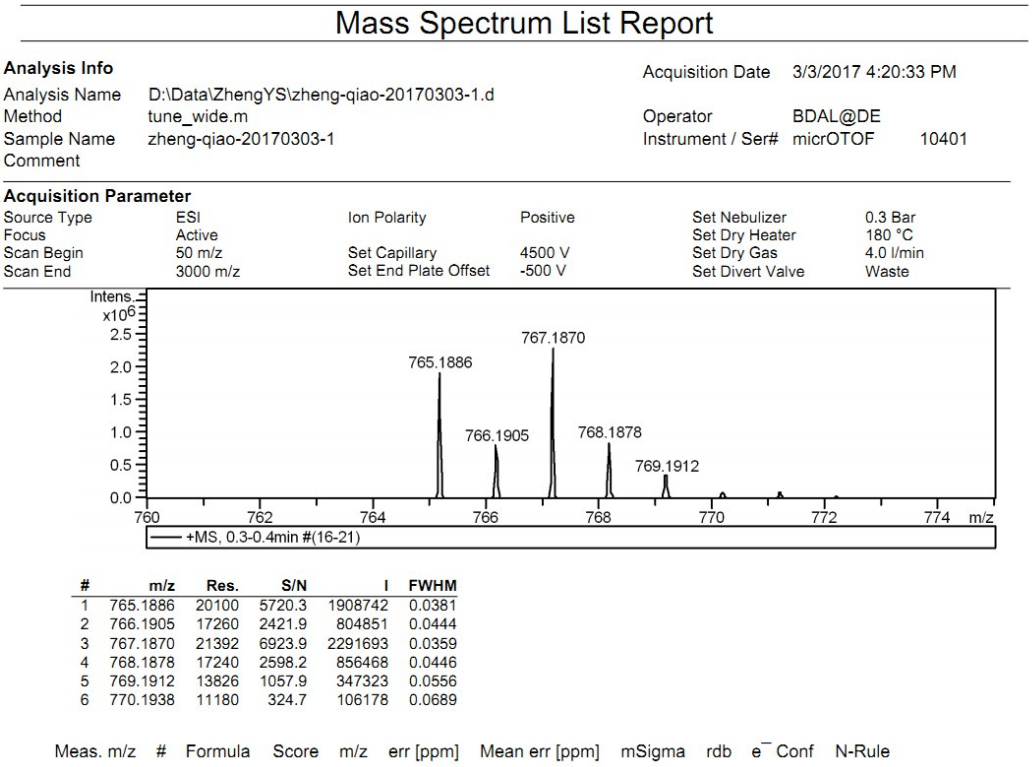


Fig. S12. HRMS spectrum of compound **4**.

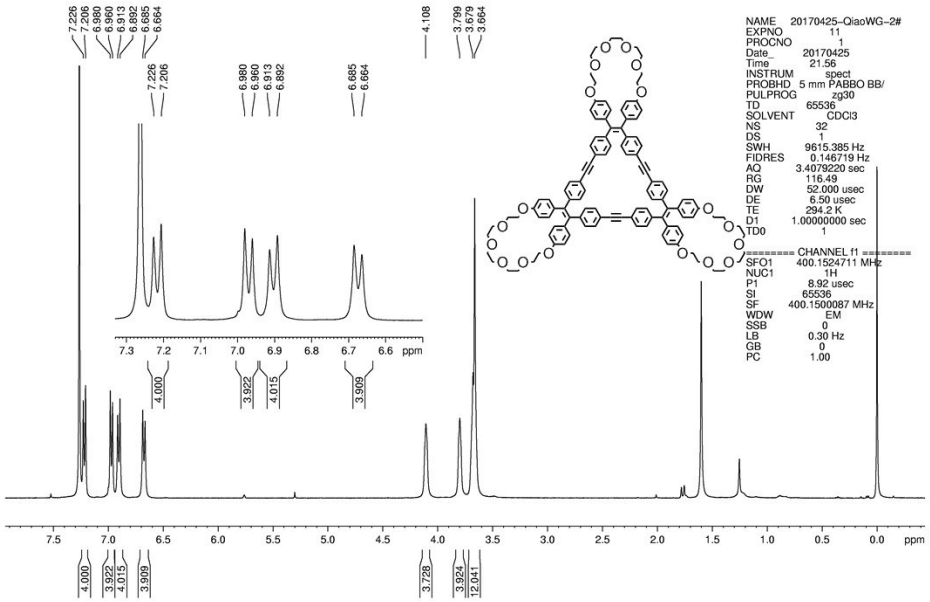


Fig. S13. ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

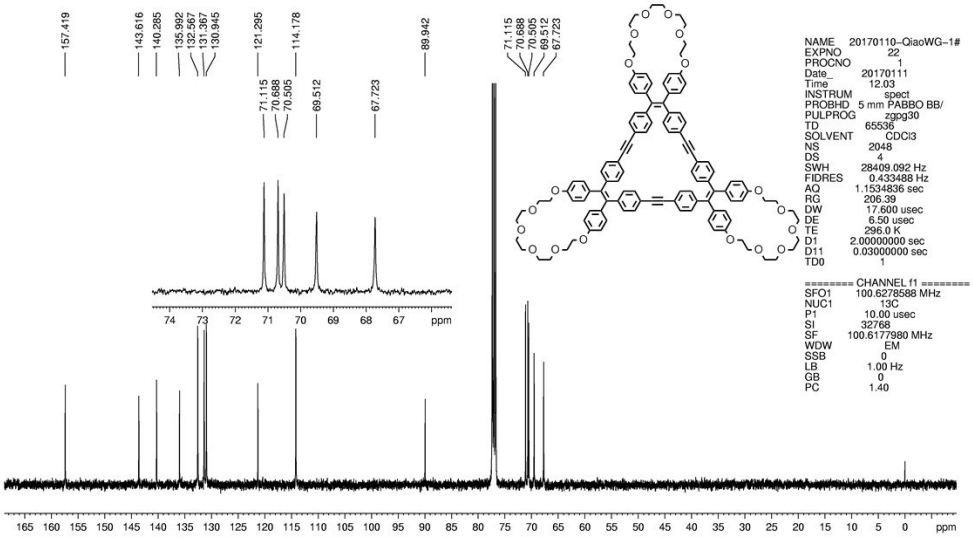


Fig. S14. ^{13}C NMR spectrum of compound **6** in $CDCl_3$.

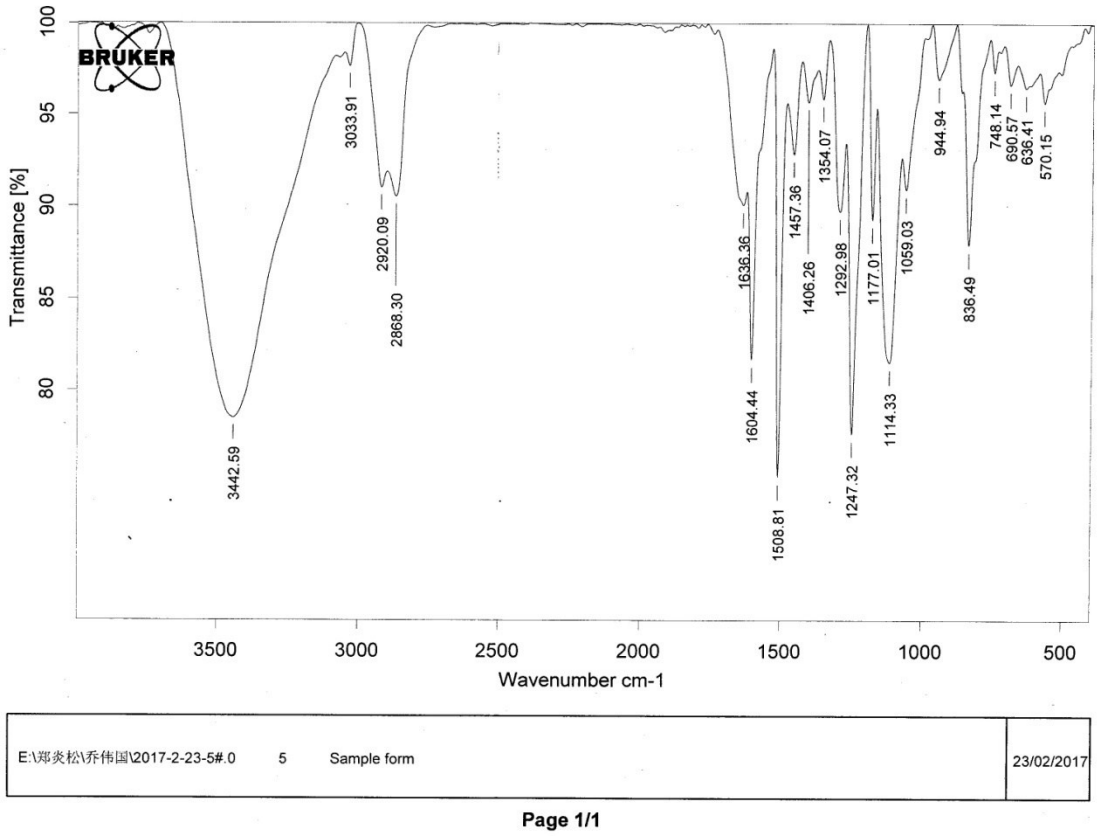


Fig. S15. IR spectrum of compound **6**.

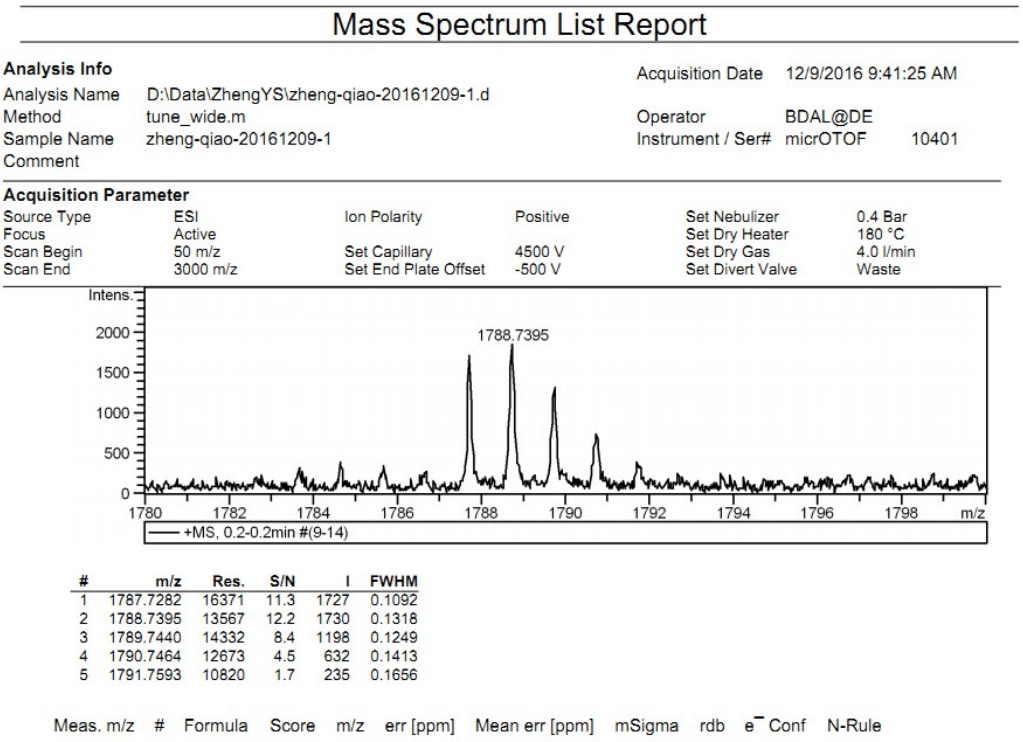


Fig. S16. HRMS spectrum of compound **6**.

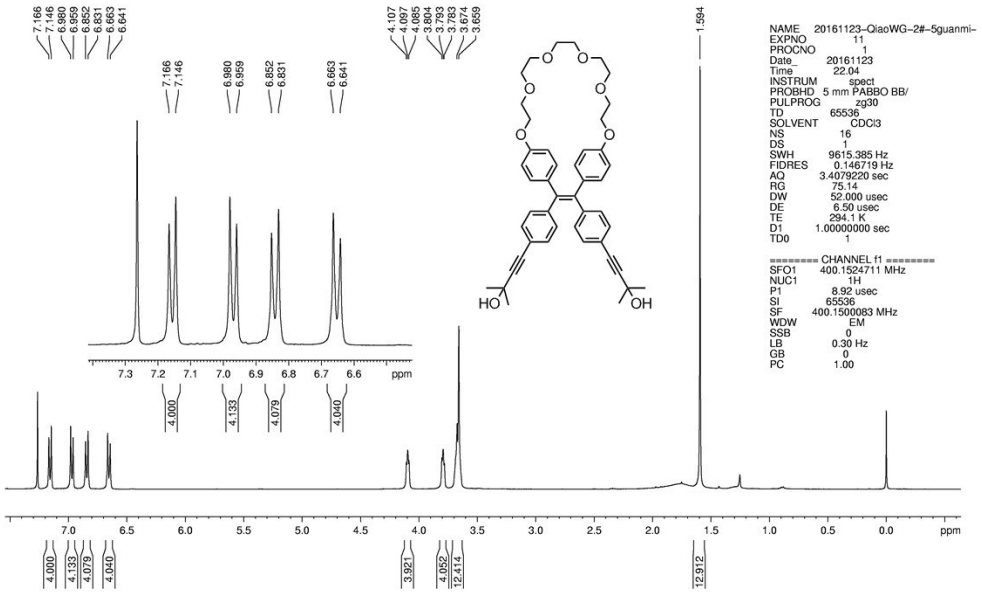


Fig. S17. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

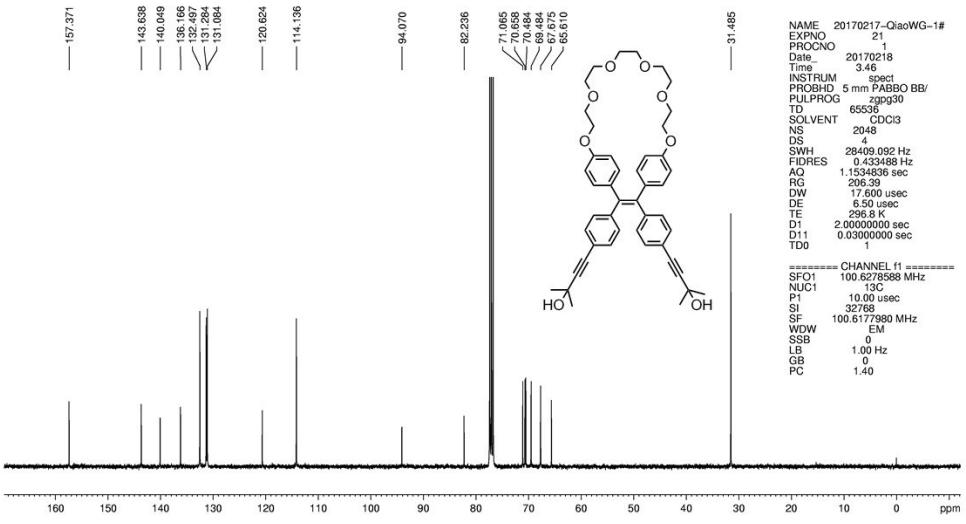


Fig. S18. ^{13}C NMR spectrum of compound **5** in $CDCl_3$.

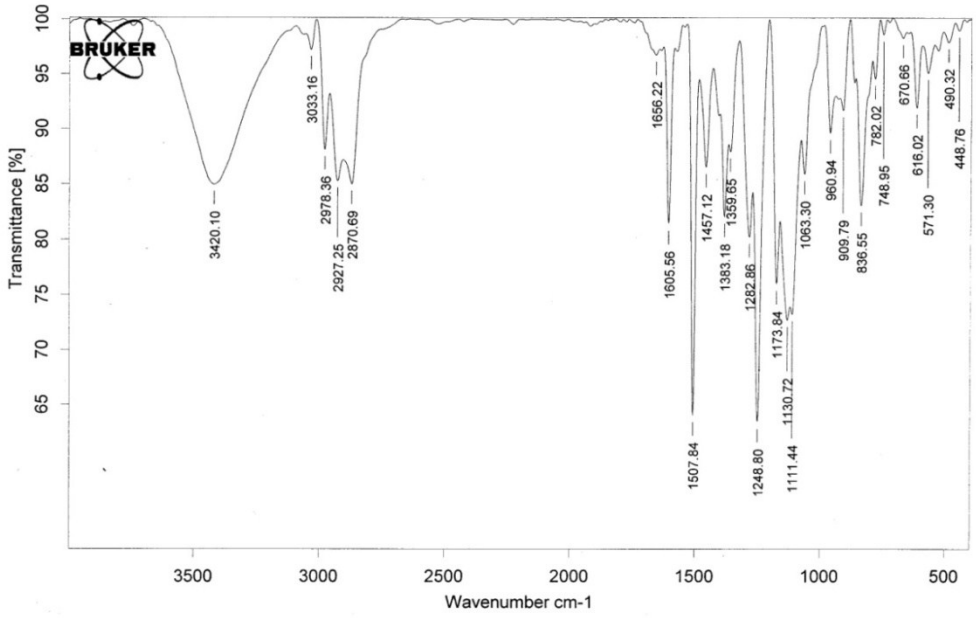


Fig. S19. IR spectrum of compound **5**.

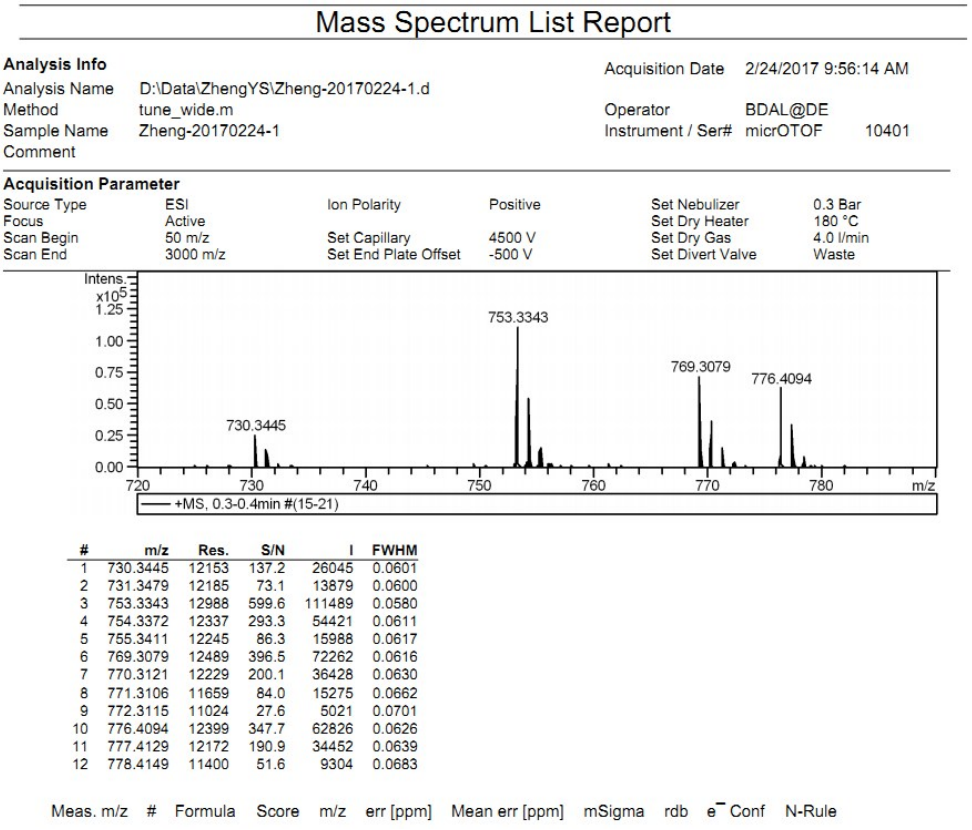


Fig. S20. HRMS spectrum of compound **5**.

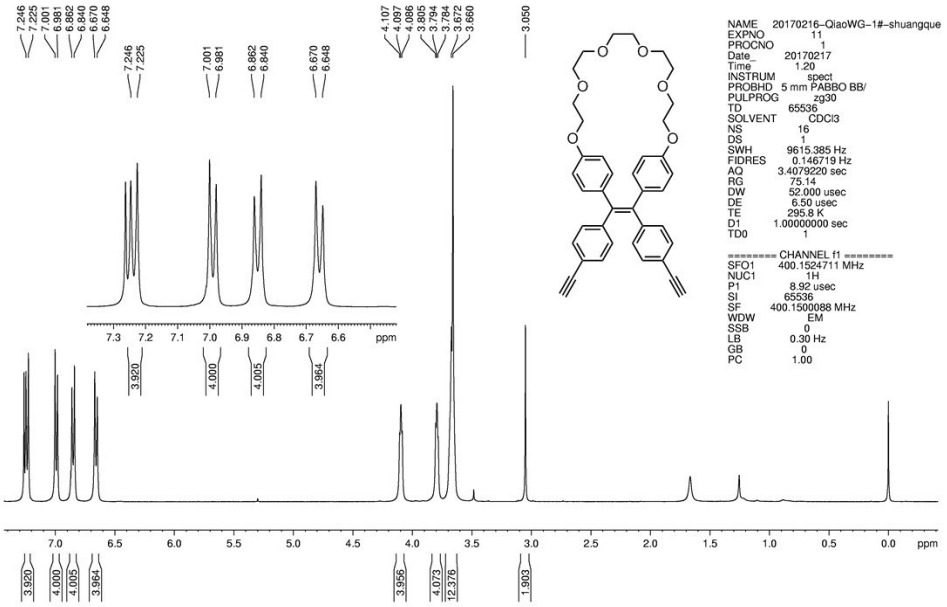


Fig. S21. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

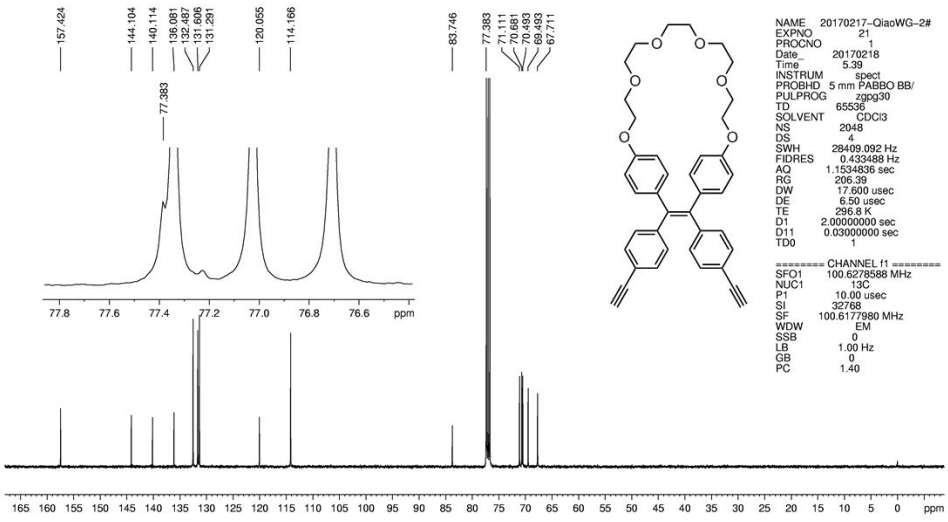


Fig. S22. ^{13}C NMR spectrum of compound **7** in $CDCl_3$.

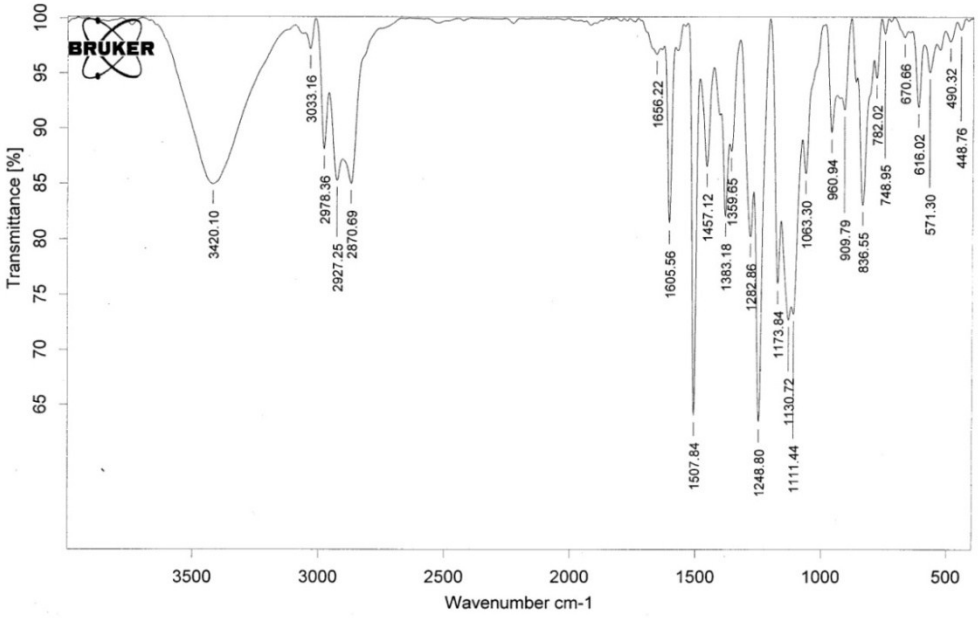
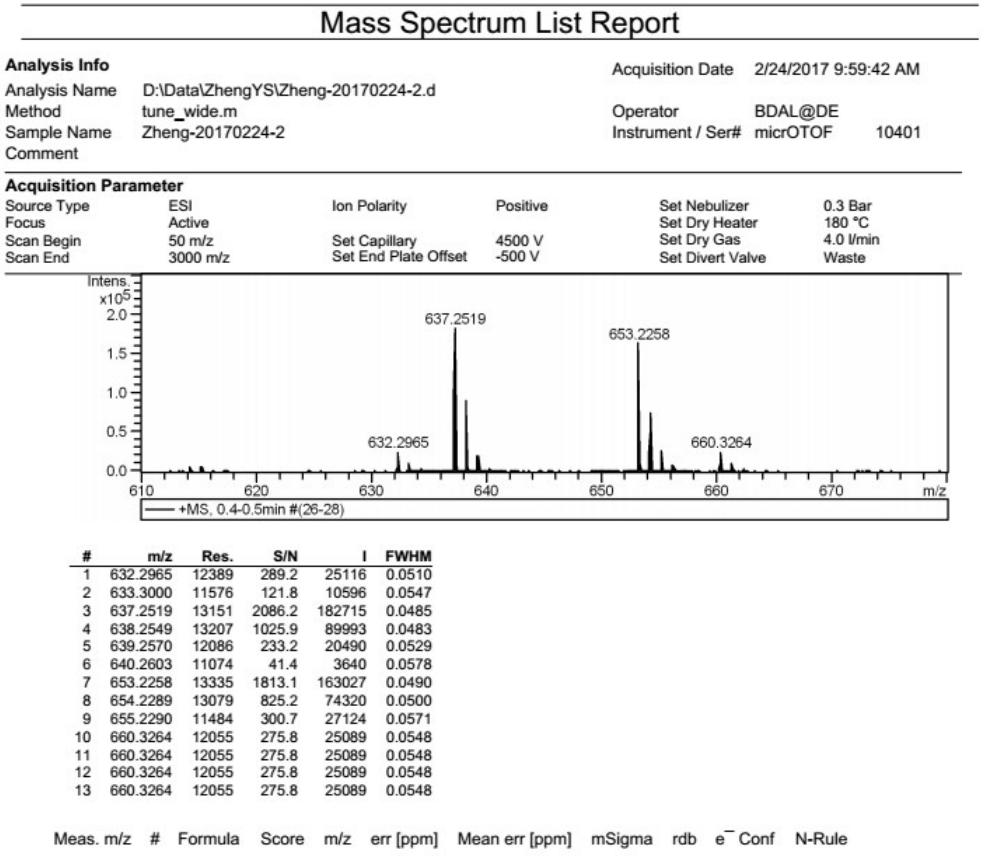


Fig. S23. IR spectrum of compound **7**.



#	m/z	Res.	S/N	I	FWHM
1	632.2965	12389	289.2	25116	0.0510
2	633.3000	11576	121.8	10596	0.0547
3	637.2519	13151	2086.2	182715	0.0485
4	638.2549	13207	1025.9	89993	0.0483
5	639.2570	12086	233.2	20490	0.0529
6	640.2603	11074	41.4	3640	0.0578
7	653.2258	13335	1813.1	163027	0.0490
8	654.2289	13079	825.2	74320	0.0500
9	655.2290	11484	300.7	27124	0.0571
10	660.3264	12055	275.8	25089	0.0548
11	660.3264	12055	275.8	25089	0.0548
12	660.3264	12055	275.8	25089	0.0548
13	660.3264	12055	275.8	25089	0.0548

Meas. m/z # Formula Score m/z err [ppm] Mean err [ppm] mSigma rdb e⁻ Conf N-Rule

Fig. S24. HRMS spectrum of compound **7**.

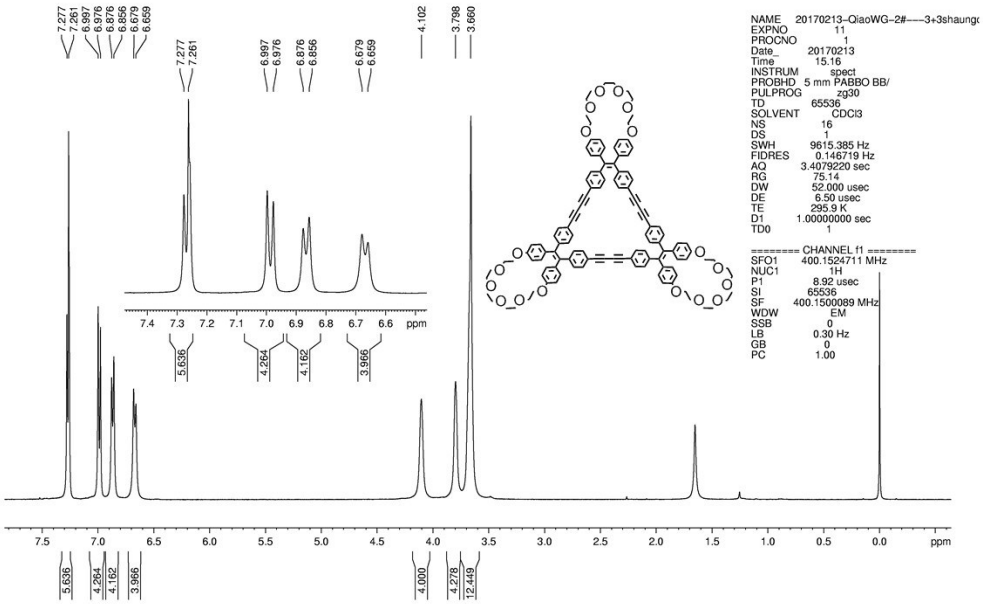


Fig. S25. ^{1}H NMR spectrum of compound **8** in $CDCl_3$.

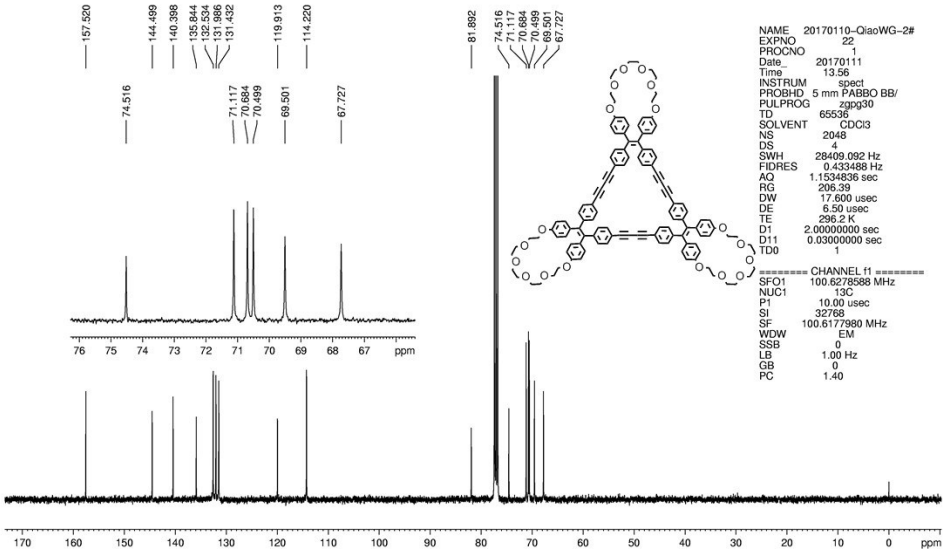


Fig. S26. ^{13}C NMR spectrum of compound **8** in $CDCl_3$.

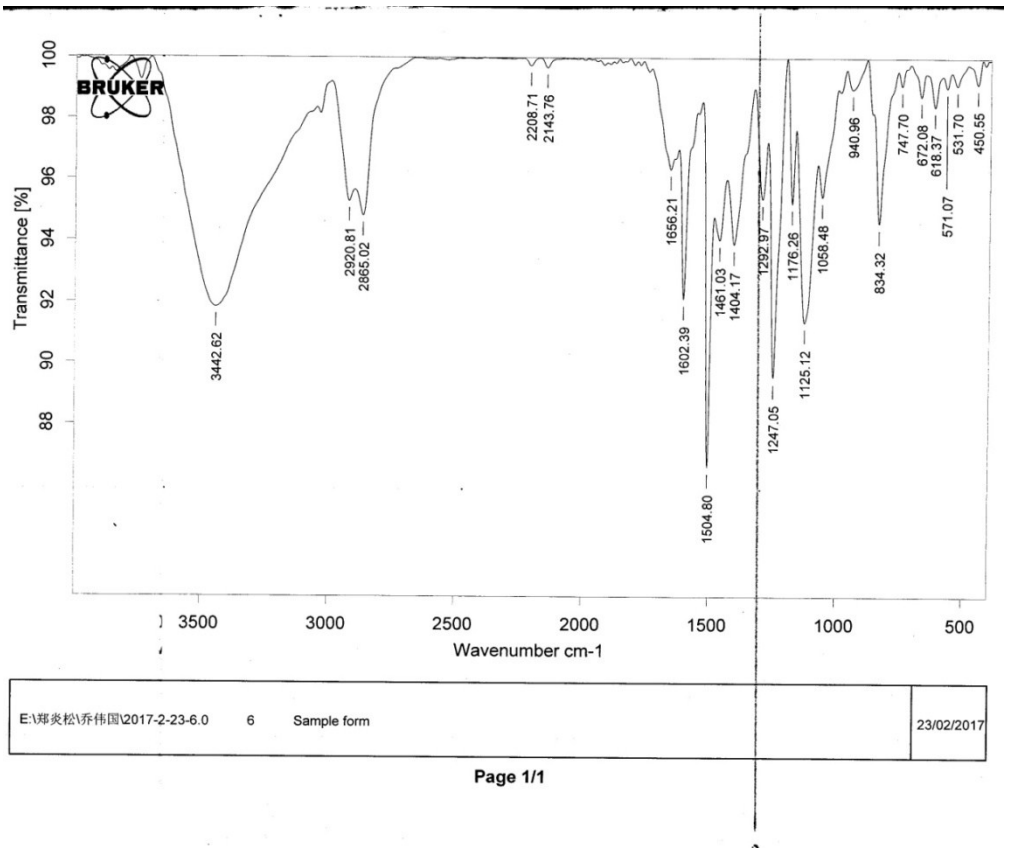


Fig. S27. IR spectrum of compound **8**.

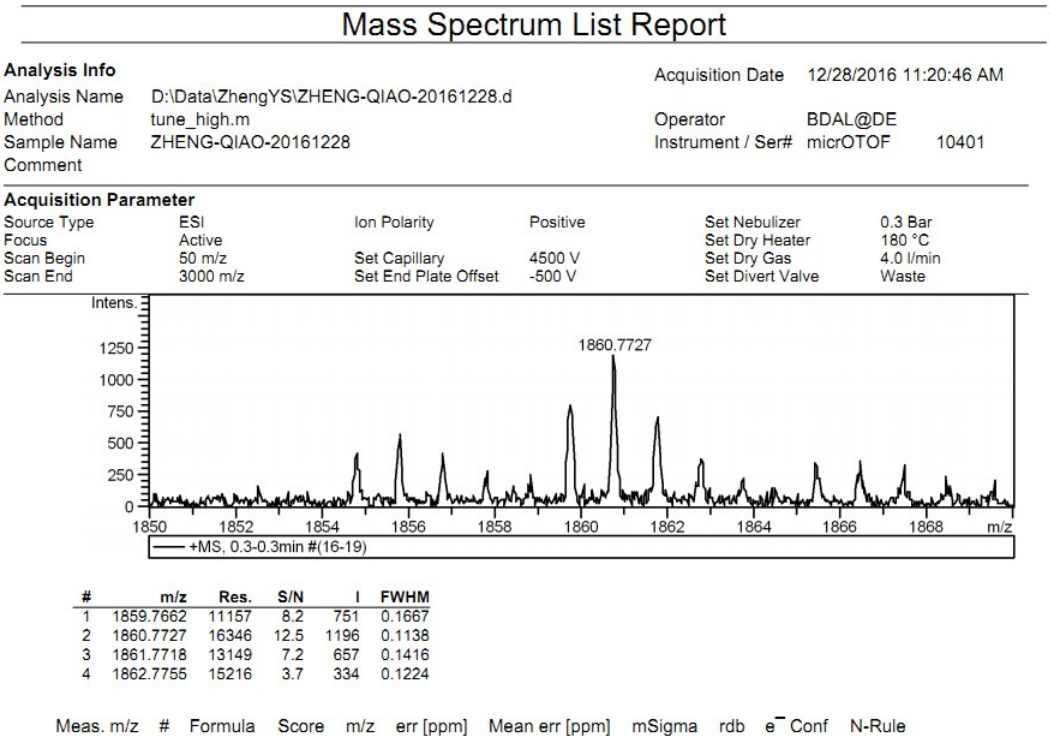


Fig. S28. HRMS spectrum of compound **8**.

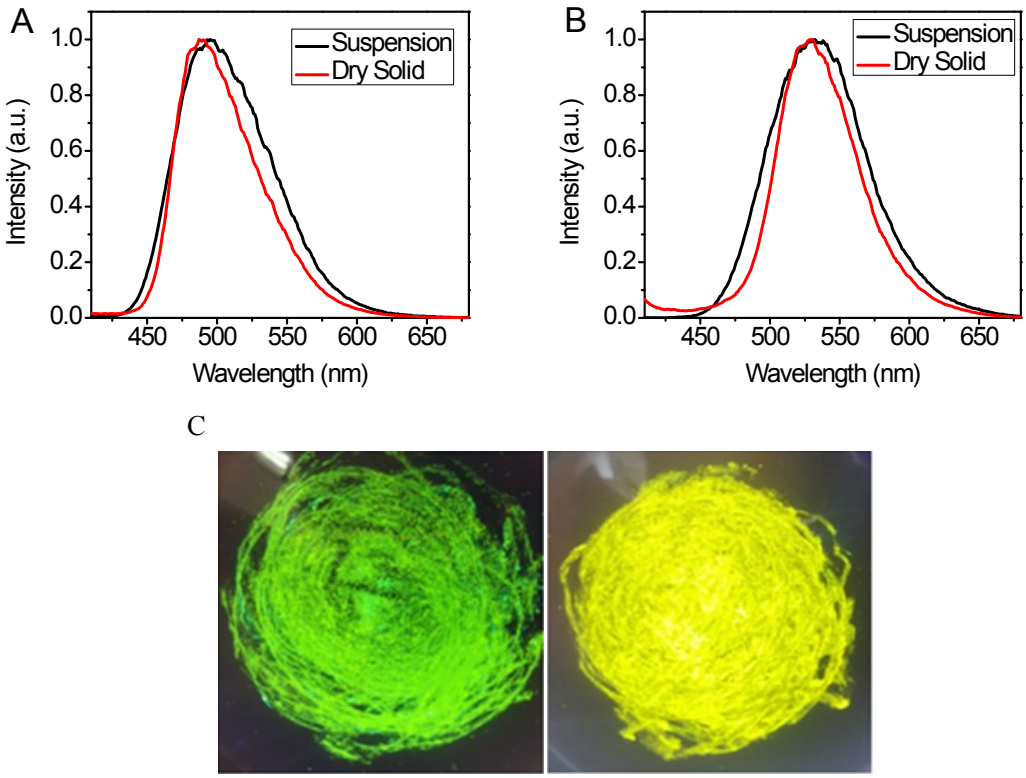


Fig. S29. The normalized fluorescence spectra of **6** (A) and **8** (B) in 90:10 H_2O/THF (V/V) suspension and in dry solid, respectively. (C) Photos of powders of **6** (left) and **8** (right) under a 365 nm portable UV lamp.

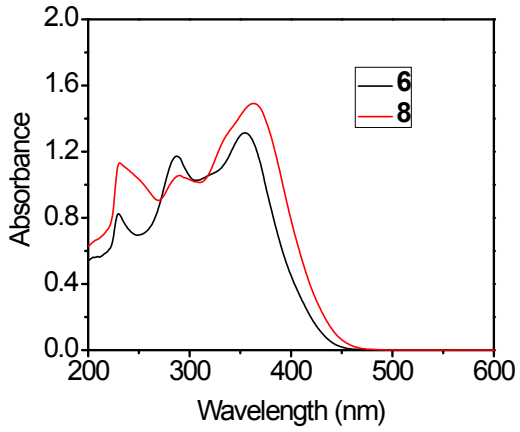
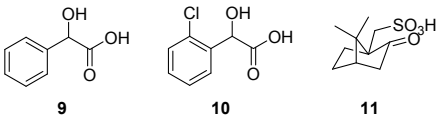


Fig. S30. UV-Vis spectra of compound **6** and **8** in THF. [**6**] = [**8**] = 1.0×10^{-5} M.



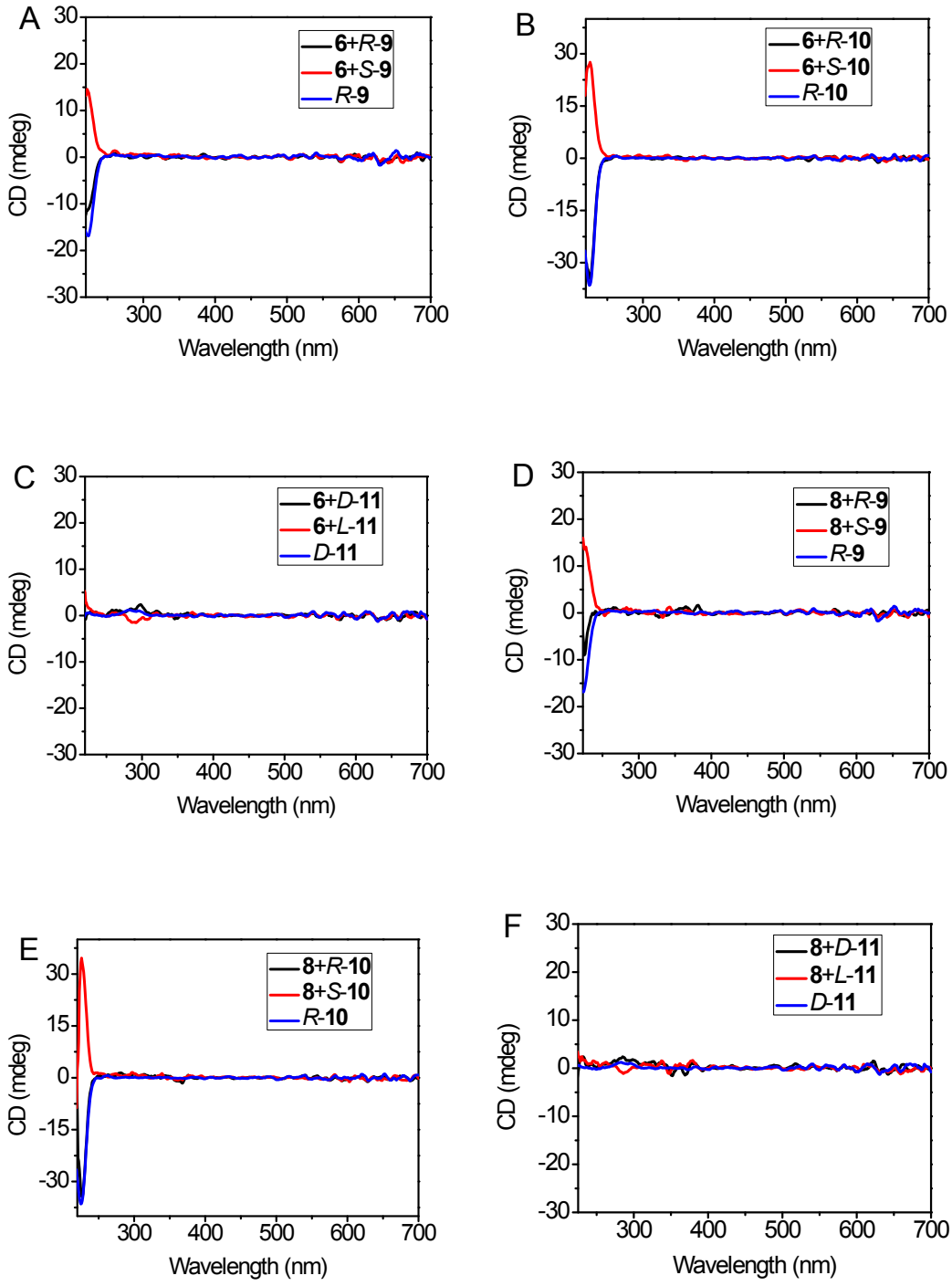


Fig. S31. CD spectra of a solution of macrocycle **6** (A, B and C) and **8** (D, E and F) with enantiomer of chiral acid in 1,2-dichloroethane. [**6**] = [**8**] = 1/3[chiral acid] =2.0×10^{-4} M.

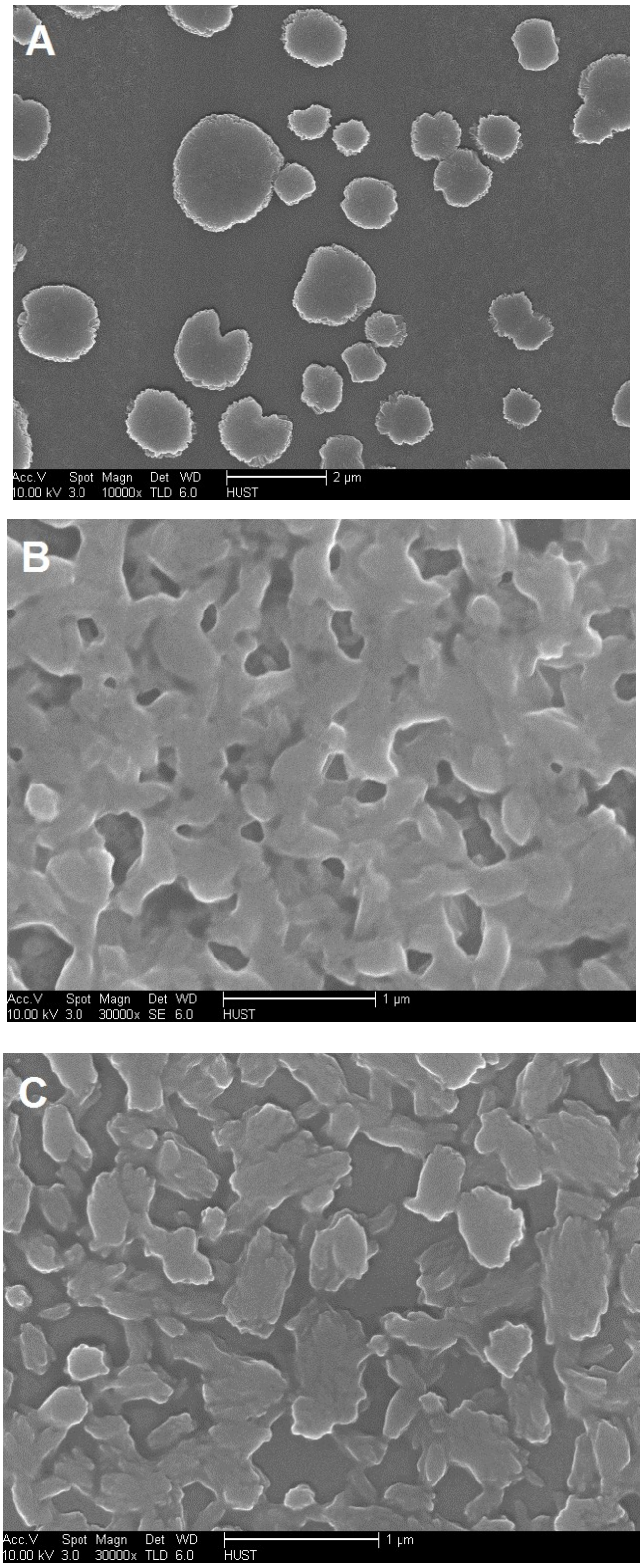


Fig. S32. FE-SEM images of film of **6** (A), **6**-*D*-**10** mixture and **6**-*L*-**10** mixture in 1,2-dichloroethane. The measurement sample was prepared by droping the solution onto one glass slide and air dried.

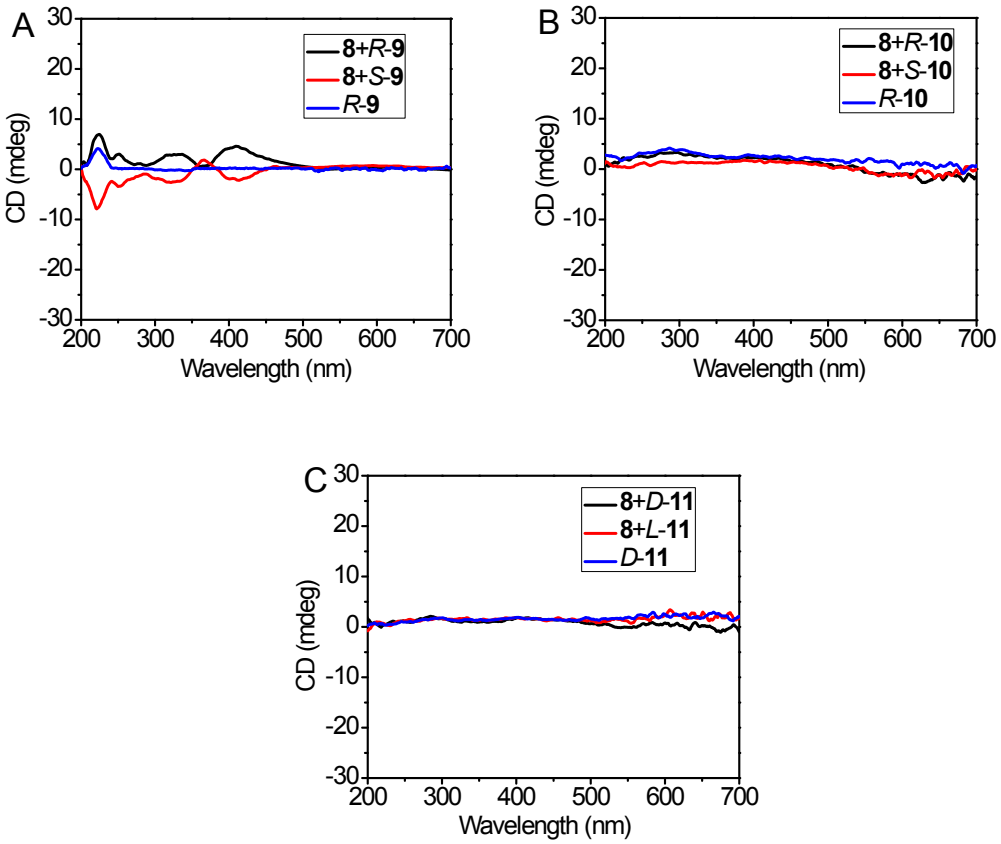


Fig. S33. CD spectra of the films of macrocycle **8** mixed with enantiomer of chiral acid. Preparation: The film was prepared by droping the solution of **8** and 3 equivalents of chiral acid enantiomer in 1,2-dichloroethane onto one glass slide and air dried.

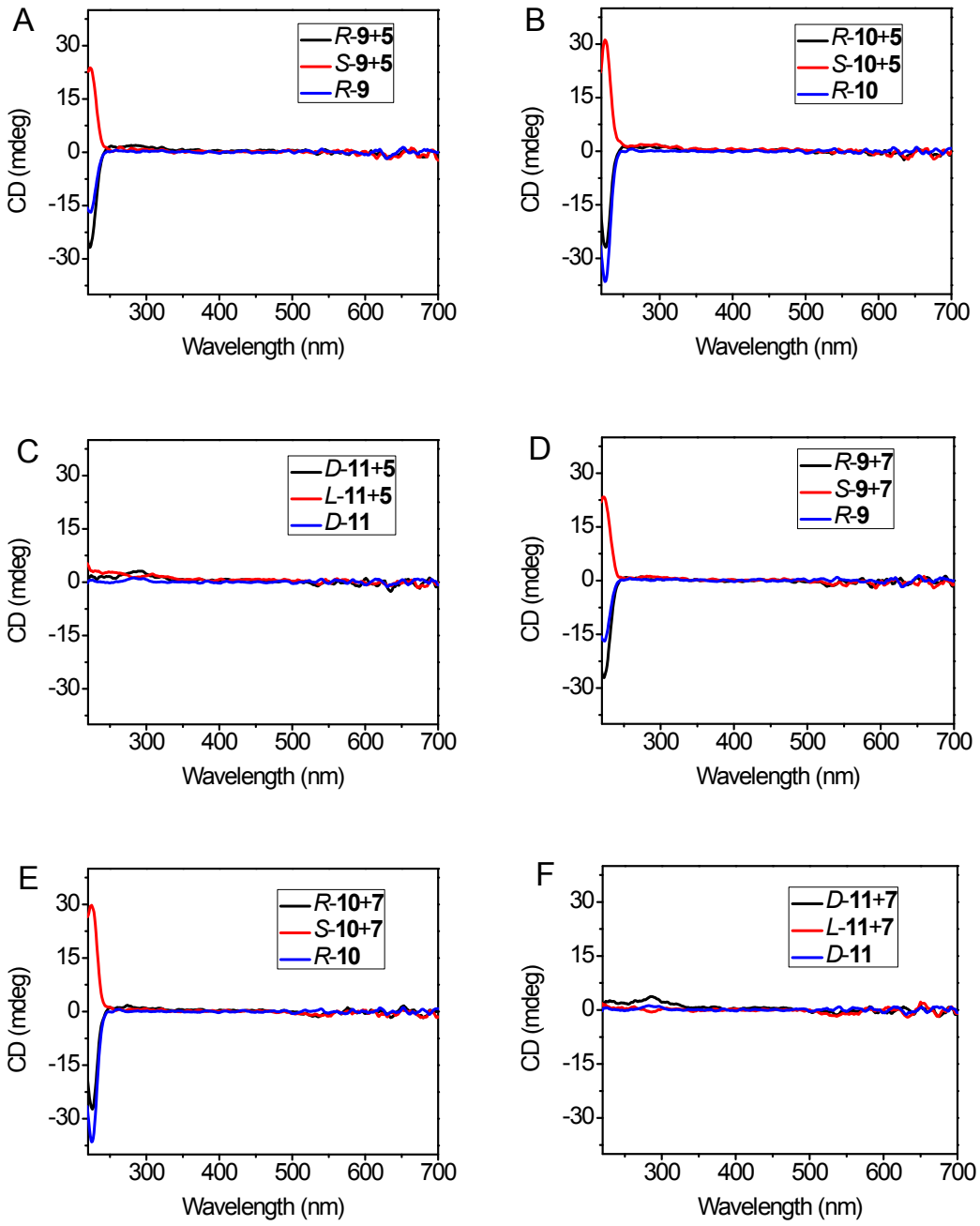


Fig. S34. CD spectra of a solution of intermediate **5** (A, B and C) and **7** (D, E and F) with enantiomer of chiral acid in 1,2-dichloroethane. [**5**] = [**7**] = 1/3[chiral acid] = 2.0×10^{-4} M.

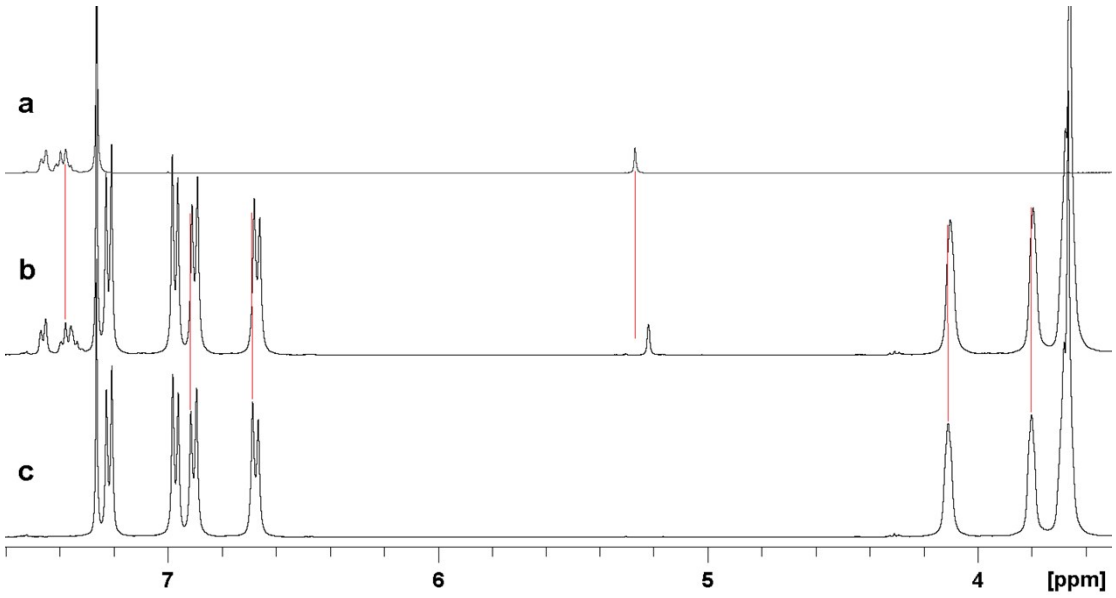


Fig. S35. ^{1}H NMR spectra of (*R*)-mandelic acid **9** (a), a mixture of (*R*)-**9** and macrocycle **6** (b) and macrocycle **6** (c) in $CDCl_3$. [**9**] = [**6**] = 5 mM.