Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information for

Multi-point Interaction Based Recognition of Fluoride Ion by *tert*-Butyldihomooxacalix[4]arenes Bearing Phenolic Hydroxyls and Thiourea

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Table S1 Representative δ and Δδ of **2a** with addition of TBAC ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference) Note a: peak covered fail to confirm the δ; b: Δδ calculated based on three equivalents of TBAC.

	Aromatic							NH		Methylene Bridge				
δ/ppm (0.0 Equiv. TBAC)	7.300	7.172	7.124	7.093	6.997	6.867	6.817	7.543	5.069	4.368	4.259	4.200	4.137	3.997
δ/ppm (5.0 Equiv. TBAC)	7.299	7.179	7.123	7.090	6.996	6.871	6.818	7.627	/[a]	4.371	4.293	4.213	4.140	4.003
Δδ/ppm	-0.001	0.007	-0.001	-0.003	-0.001	0.004	0.001	0.084	0.063[b]	0.003	0.034	0.013	0.003	0.006

Table S2 Representative δ and Δδ of **2a** with addition of TBAB ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference)

	Aromatic						NH		Methylene Bridge					
δ/ppm (0.0 Equiv. TBAB)	7.300	7.172	7.124	7.092	6.997	6.866	7.544	5.070	4.719	4.368	4.259	4.200	4.136	3.997
δ/ppm (5.0 Equiv. TBAB)	7.298	7.180	7.122	7.087	6.993	6.870	7.632	5.029	4.729	4.371	4.294	4.213	4.138	4.002
Δδ/ppm	-0.002	0.008	-0.002	-0.005	-0.004	0.004	0.088	-0.041	0.010	0.003	0.035	0.013	0.002	0.005

Table S3 Representative δ and Δδ of **2a** with addition of TBAI ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference)

	Aromatic						NH	Methylene Bridge						
δ/ppm (0.0 Equiv. TBAI)	7.297	7.175	7.120	7.091	6.865	6.814	7.548	5.058	4.802	4.719	4.270	4.200	3.994	3.955
δ/ppm (5.0 Equiv. TBAI)	7.298	7.179	7.124	7.090	6.867	6.815	7.603	5.037	4.767	4.703	4.280	4.207	3.999	3.961
Δδ/ppm	0.001	0.004	0.004	-0.001	0.002	0.001	0.055	-0.021	-0.035	-0.016	0.010	0.007	0.006	0.006

Table S4 Representative δ and Δδ of **2b** with addition of TBAF ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference)

	Aromatic				NH		Methylene Bridge		
δ/ppm (0.0 Equiv. TBAF)	7.295	7.019	6.994	6.871	7.519	8.146	4.609	4.515	3.964
δ/ppm (5.0 Equiv. TBAF)	7.387	6.996	6.975	6.855	7.983	8.965	4.667	4.544	4.006
Δδ/ppm	0.092	-0.023	-0.019	-0.016	0.464	0.819	0.058	0.029	0.042

Table S5 Representative δ and Δδ of **2b** with addition of TBAC ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference)

	Aromatic					NH		Methylene Bridge						
δ/ppm (0.0 Equiv. TBAC)	7.157	7.111	7.020	6.993	6.905	8.145	7.520	4.605	4.517	4.328	4.111	3.960	3.528	3.474
δ/ppm (5.0 Equiv. TBAC)	7.171	7.112	7.017	7.000	6.914	8.511	7.734	4.647	4.533	4.346	4.129	3.985	3.534	3.471
Δδ/ppm	0.014	0.001	-0.003	0.007	0.008	0.366	0.214	0.042	0.015	0.018	0.018	0.025	0.006	-0.003

Table S6 Representative δ and Δδ of **2b** with addition of TBAB ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference). Note a: peak covered fail to confirm the δ; b: Δδ calculated based on two equivalents of TBAB.

	Aromatic			NH		Methylene Bridge								
δ/ppm (0.0 Equiv. TBAB)	7.157	6.993	6.905	8.145	7.520	4.605	4.517	4.328	4.232	4.199	4.111	3.960	3.528	3.474
δ/ppm (5.0 Equiv. TBAB)	7.172	7.002	6.914	8.506	7.730	4.644	4.530	4.348	/[a]	/[a]	4.128	3.990	3.539	3.472
Δδ/ppm	0.015	0.009	0.009	0.361	0.210	0.039	0.013	0.019	0.011[b]	0.011[b]	0.017	0.030	0.011	-0.002

Table S7 Representative δ and Δδ of **2b** with addition of TBAI ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference).

	Aromatic							NH		Methylene Bridge				
δ/ppm (0.0 Equiv. TBAI)	7.238	7.157	7.122	7.111	6.993	6.905	6.869	8.145	7.517	4.328	4.232	4.199	4.111	3.960
δ/ppm (5.0 Equiv. TBAI)	7.263	7.165	7.125	7.115	7.020	6.908	6.871	8.234	7.588	4.334	4.240	4.206	4.113	3.969
Δδ/ppm	0.025	0.008	0.003	0.004	0.027	0.002	0.002	0.089	0.071	0.006	0.007	0.008	0.002	0.009

Table S8 Representative δ and Δδ of **2c** with addition of TBAF ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference). Note a: peak covered fail to confirm the δ; b: Δδ calculated based on three equivalents of TBAF; c: Δδ calculated based on two equivalents of TBAF.

	Aromatic					NH		Methylene Bridge						
δ/ppm (0.0 Equiv. TBAF)	7.329	7.158	7.020	6.996	6.931	7.401	6.769	4.700	4.524	4.332	4.019	3.605	3.510	3.415
δ/ppm (5.0 Equiv. TBAF)	7.316	□/[a]	7.003	6.985	6.918	7.557	/[a]	4.687	4.502	4.345	4.050	3.590	3.492	3.392
Δδ/ppm	-0.013	-0.005[b]	-0.017	-0.010	-0.013	0.156	0.100[c]	0.013	-0.022	-0.013	0.031	-0.015	-0.018	-0.023

Table S9 Representative δ and Δδ of **2c** with addition of TBAC ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference). Note a: peak covered fail to confirm the δ; b: Δδ calculated based on two equivalents of TBAC; c: Δδ calculated based on one equivalents of TBAC.

	Aromatic			NH		Methylene Bridge								
δ/ppm (0.0 Equiv. TBAC)	7.143	7.110	6.923	7.398	6.748	4.701	4.501	4.298	4.218	4.095	3.997	3.658	3.588	3.489
δ/ppm (5.0 Equiv. TBAC)	7.140	7.101	6.914	/[a]	/[a]	4.693	4.494	/[a]	4.229	4.117	4.020	3.593	3.494	3.398
Δδ/ppm	-0.003	-0.009	-0.010	0.018[b]	0.074[b]	-0.008	-0.007	0.011[c]	0.011	0.022	0.023	-0.065	-0.094	-0.091

Table S10 Representative δ and Δδ of **2c** with addition of TBAB ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference). Note a: peak covered fail to confirm the δ; b: Δδ calculated based on two equivalents of TBAB.

	Aromatic				NH		Methylene Bridge							
δ/ppm (0.0 Equiv. TBAB)	7.327	7.108	6.988	6.923	7.390	6.747	4.890	4.701	4.501	4.105	3.990	3.598	3.481	3.105
δ/ppm (5.0 Equiv. TBAB)	7.318	7.103	6.981	6.911	/[a]	/[a]	4.896	4.692	4.496	4.120	4.004	3.595	3.494	3.091
Δδ/ppm	-0.009	-0.005	-0.007	-0.012	0.072/[b]	0.076/[b]	0.006	-0.009	-0.005	0.015	0.014	-0.003	0.013	-0.014

Table S11 Representative δ and Δδ of **2c** with addition of TBAI ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference).

	Aromatic					NH		Methylene Bridge							
δ/ppm (0.0 Equiv. TBAB)	7.143	7.108	7.012	6.988	6.923	7.390	6.747	4.890	4.701	4.227	4.103	3.990	3.598	3.481
δ/ppm (5.0 Equiv. TBAB)	7.140	7.106	7.011	6.989	6.922	7.544	6.817	4.891	4.698	4.226	4.109	3.994	3.599	3.480
Δδ/ppm	-0.003	-0.002	-0.001	0.001	-0.001	0.154	0.070	0.001	-0.003	-0.002	0.006	0.004	0.001	-0.001

Table S12 NH δ and Δδ of **3** with addition of TBA salts ($CDCl_3$, 400 MHz, 298K, using $CDCl_3$ 7.26 ppm as reference).

	TBAF		TBAC		TBAB		TBAI	
δ/ppm (0.0 Equiv. TBA Salts)	8.999	7.639	9.025	7.650	9.025	7.650	9.000	7.640
δ/ppm (5.0 Equiv. TBA Salts)	9.151	7.711	9.283	7.786	9.177	7.780	9.060	7.710
Δδ/ppm	0.152	0.072	0.258	0.137	0.152	0.130	0.060	0.070

Table S13 The binding constant K (M^{-1}) of **2b** and **2c** with TBAC, TBAB, TBAI in $CDCl_3$.

Compd.	TBAC	TBAB	TBAI
2b	2.070	0.057	0.067
2c	0.575	0.043	0.388

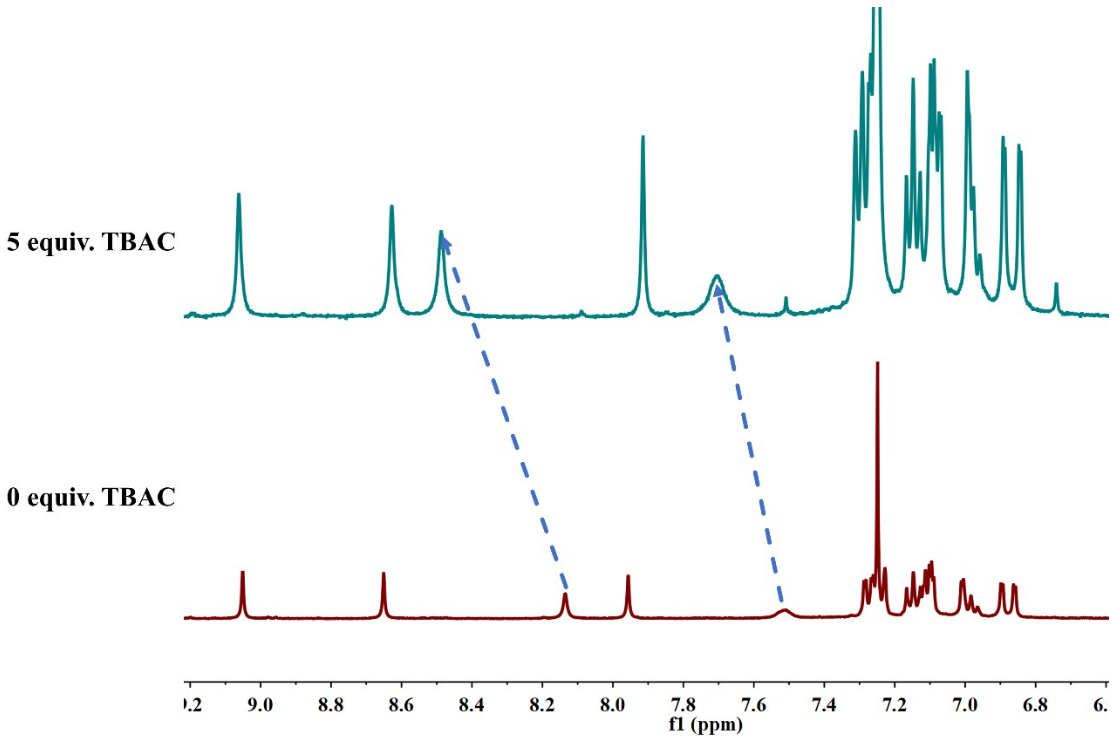

Figure S1. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2a** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAC.

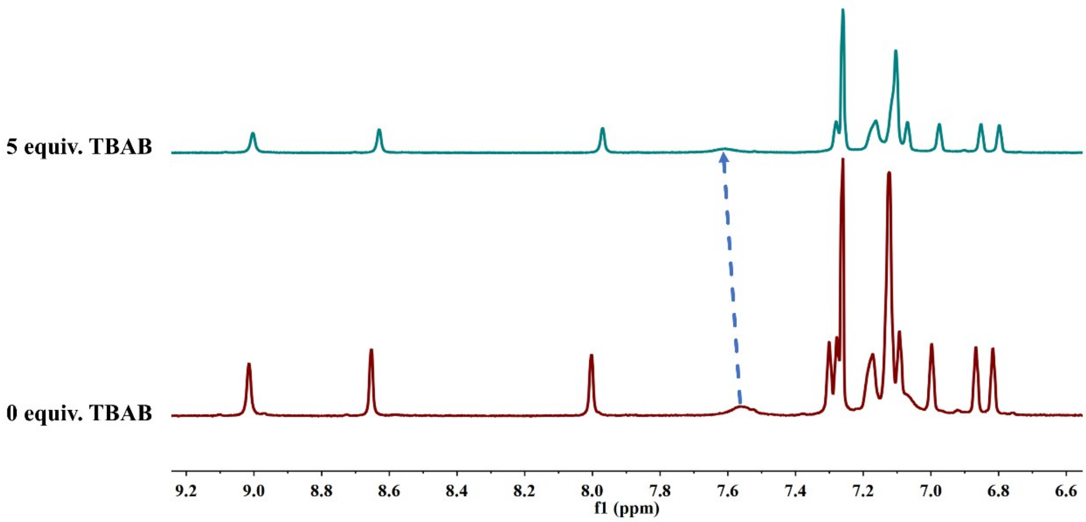

Figure S2. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2a** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAB.

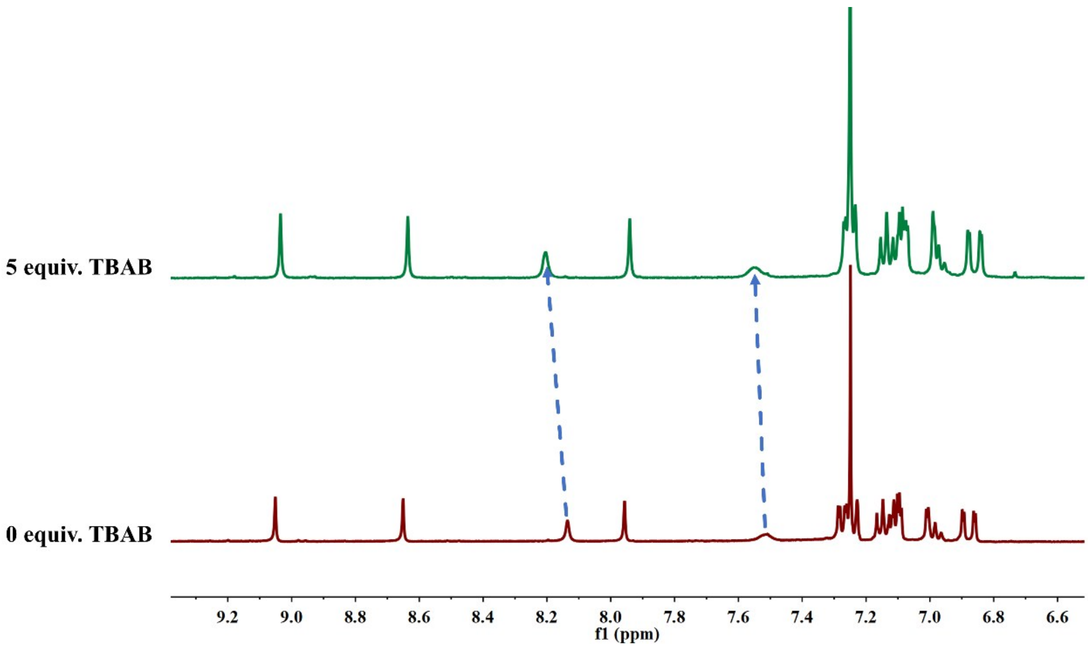

Figure S3. Partial [1]H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2a** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAI.

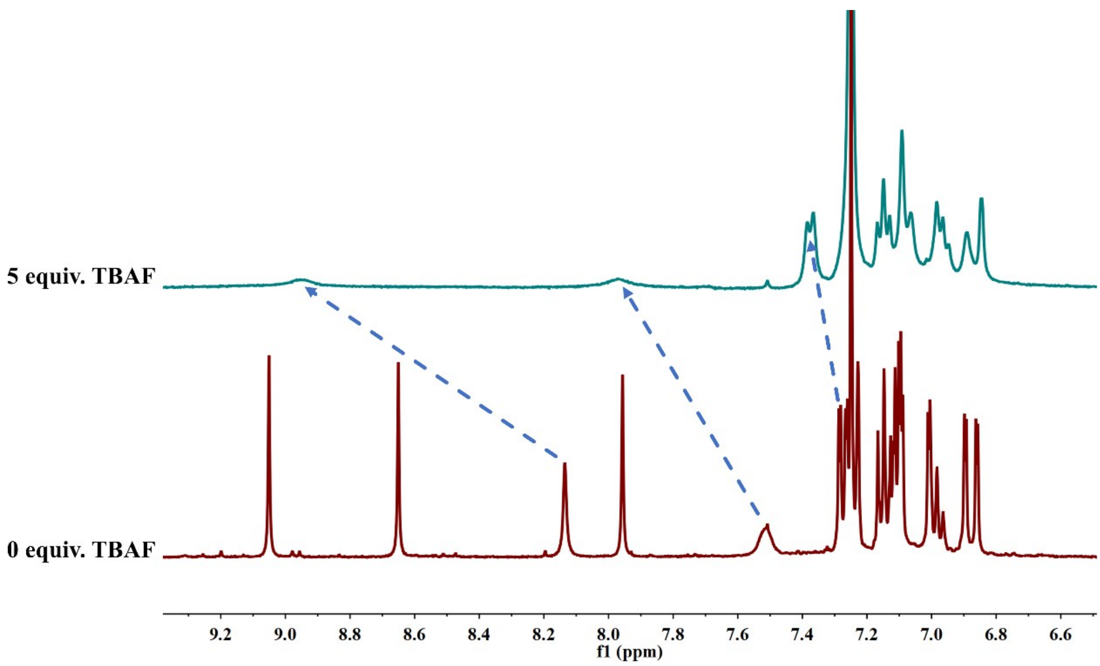

Figure S4. Partial [1]H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2b** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAF.

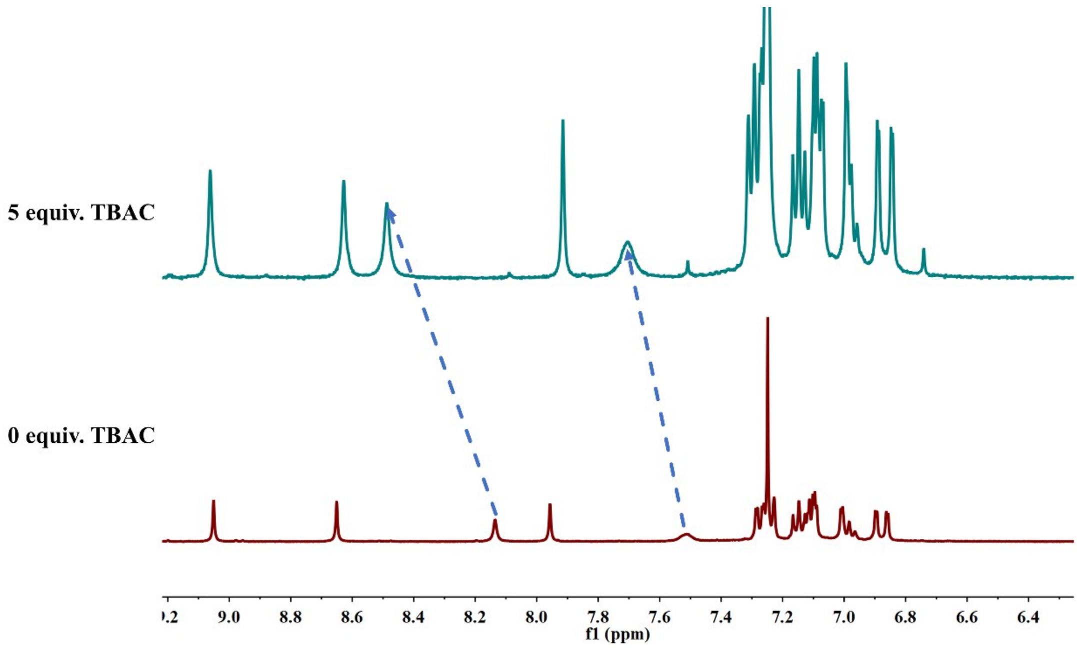

Figure S5. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2b** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAC.

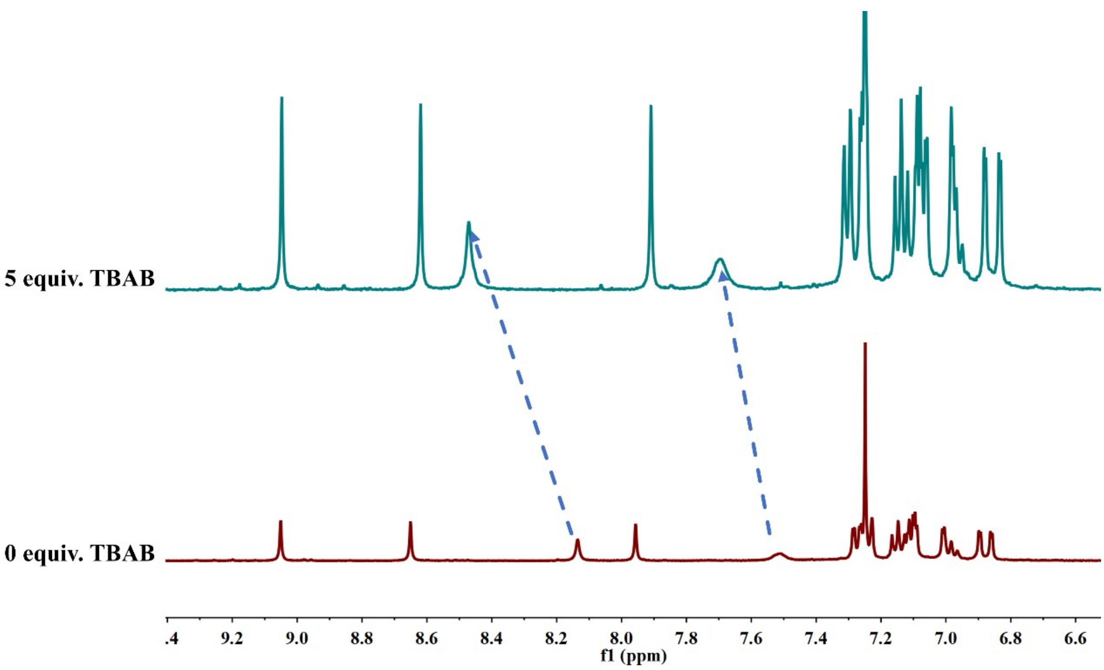

Figure S6. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2b** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAB.

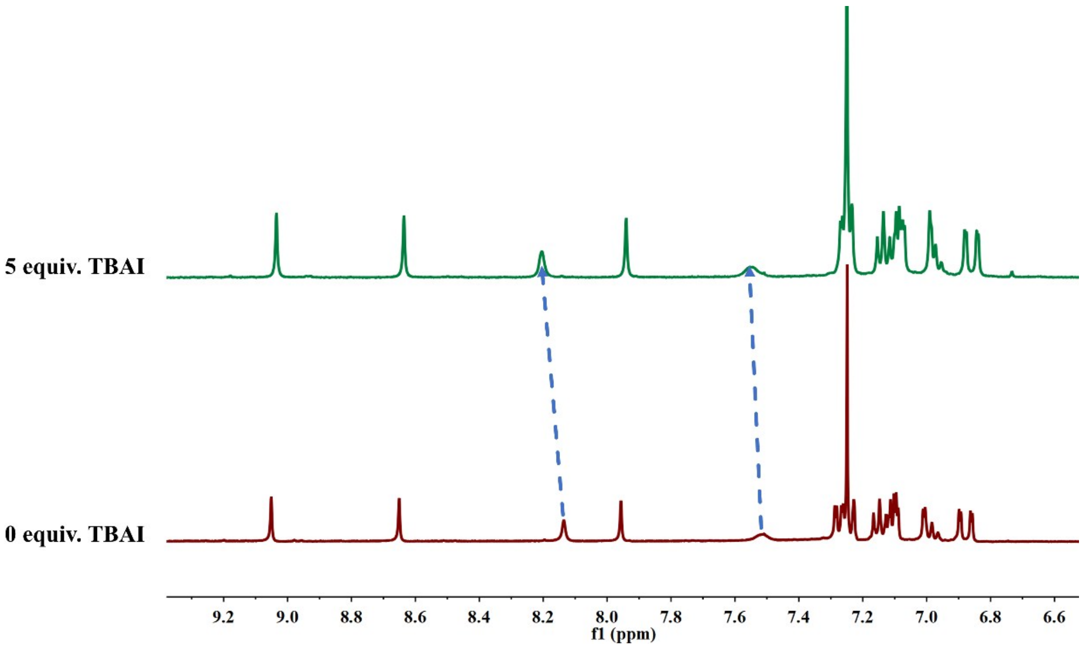

Figure S7. Partial [1]H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2b** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAI.

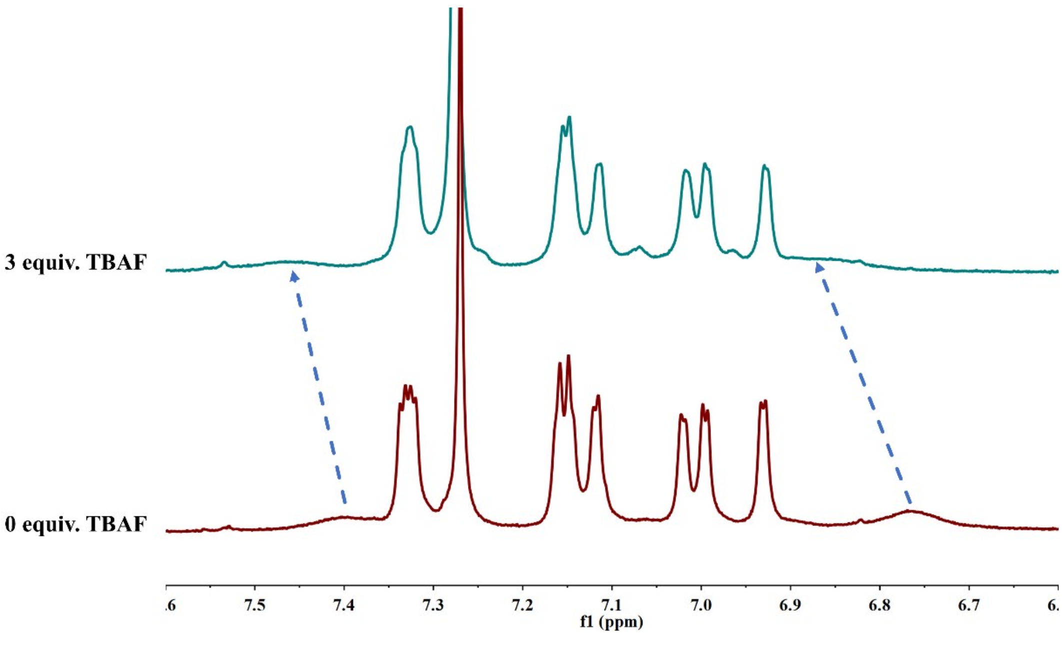

Figure S8. Partial [1]H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2c** after addition of (from bottom to top) 0.0, and 3.0 equivalents of TBAF.

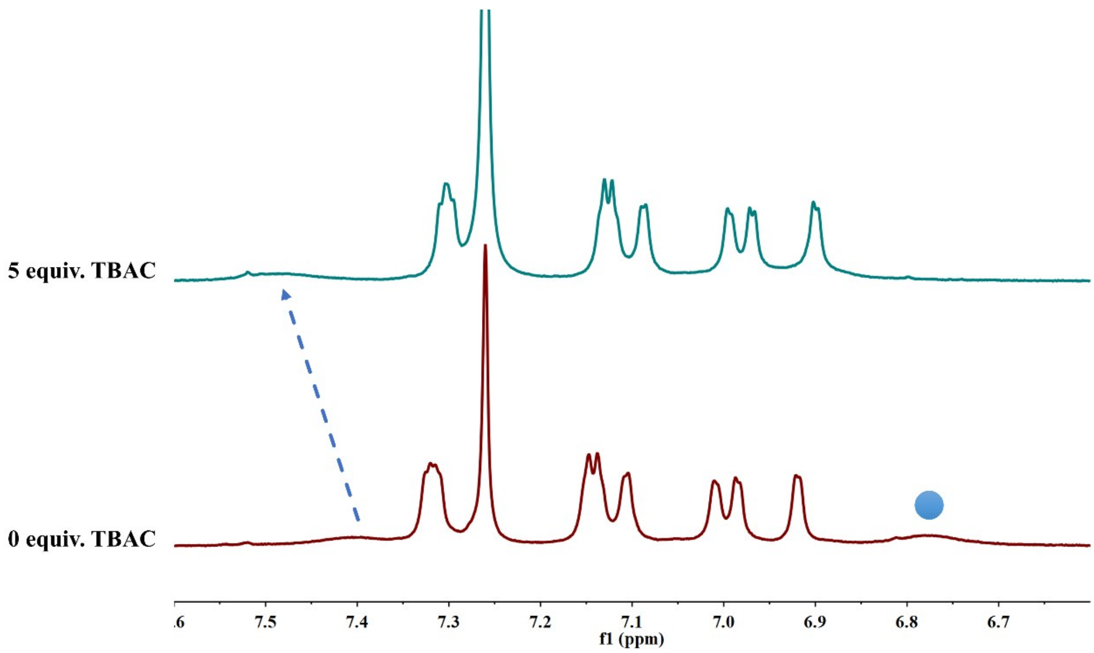

Figure S9. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2c** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAC.

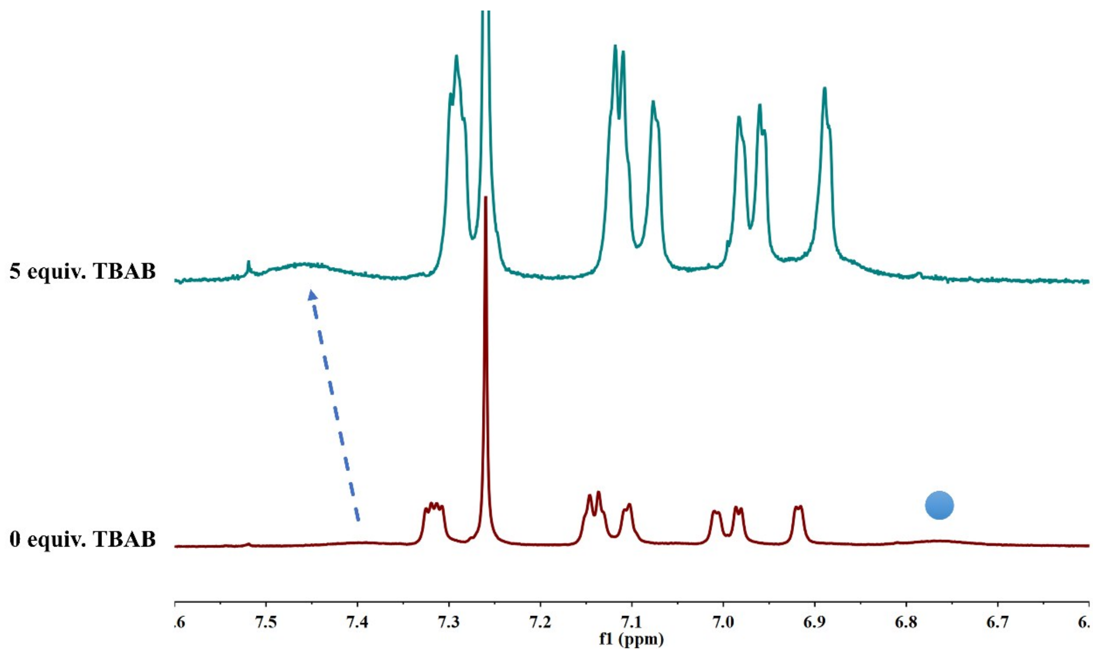

Figure S10. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2c** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAB.

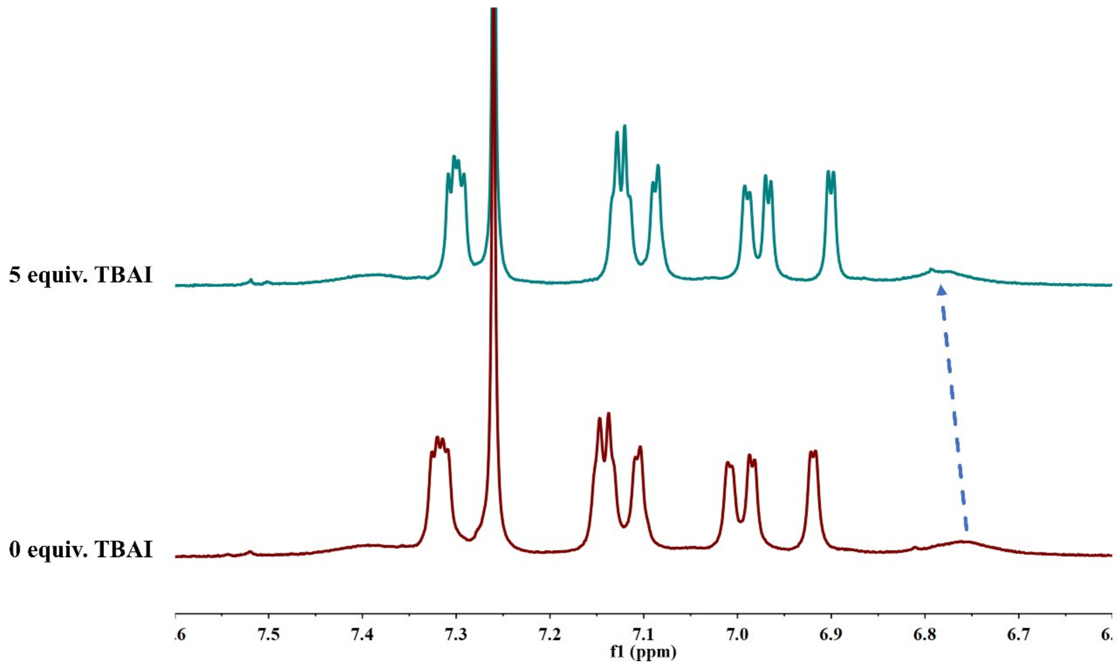

Figure S11. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2c** after addition of (from bottom to top) 0.0, and 5.0 equivalents of TBAI.

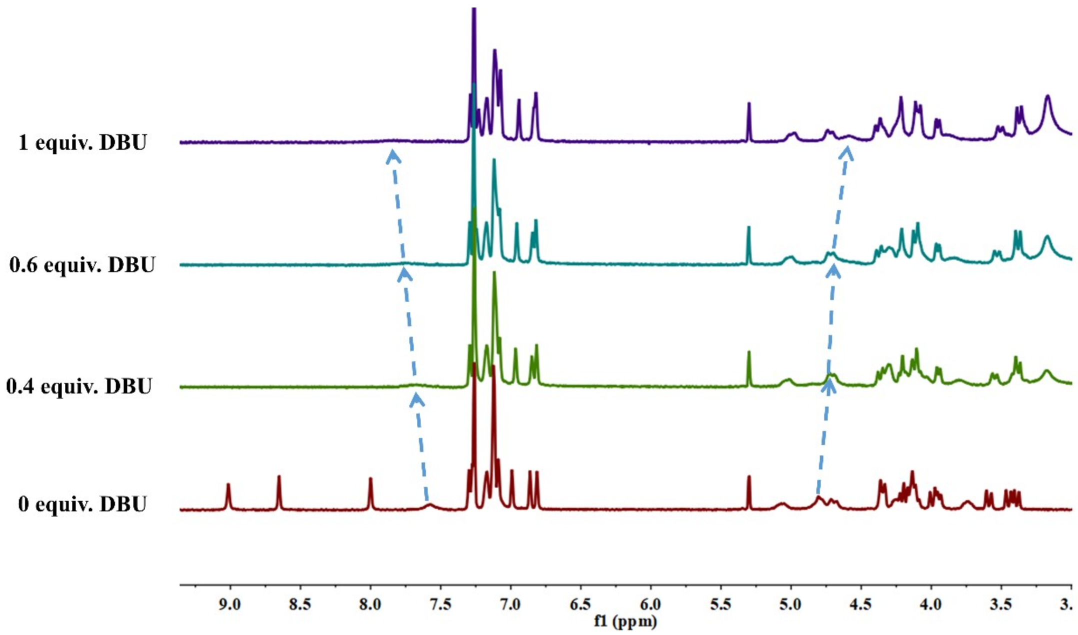

Figure S12. Partial ^{1}H NMR spectra ($CDCl_3$, 400 MHz, 298 K) of **2a** after addition of (from bottom to top) 0.0, and 0.4, 0.6 and 1.0 equivalents of DBU.

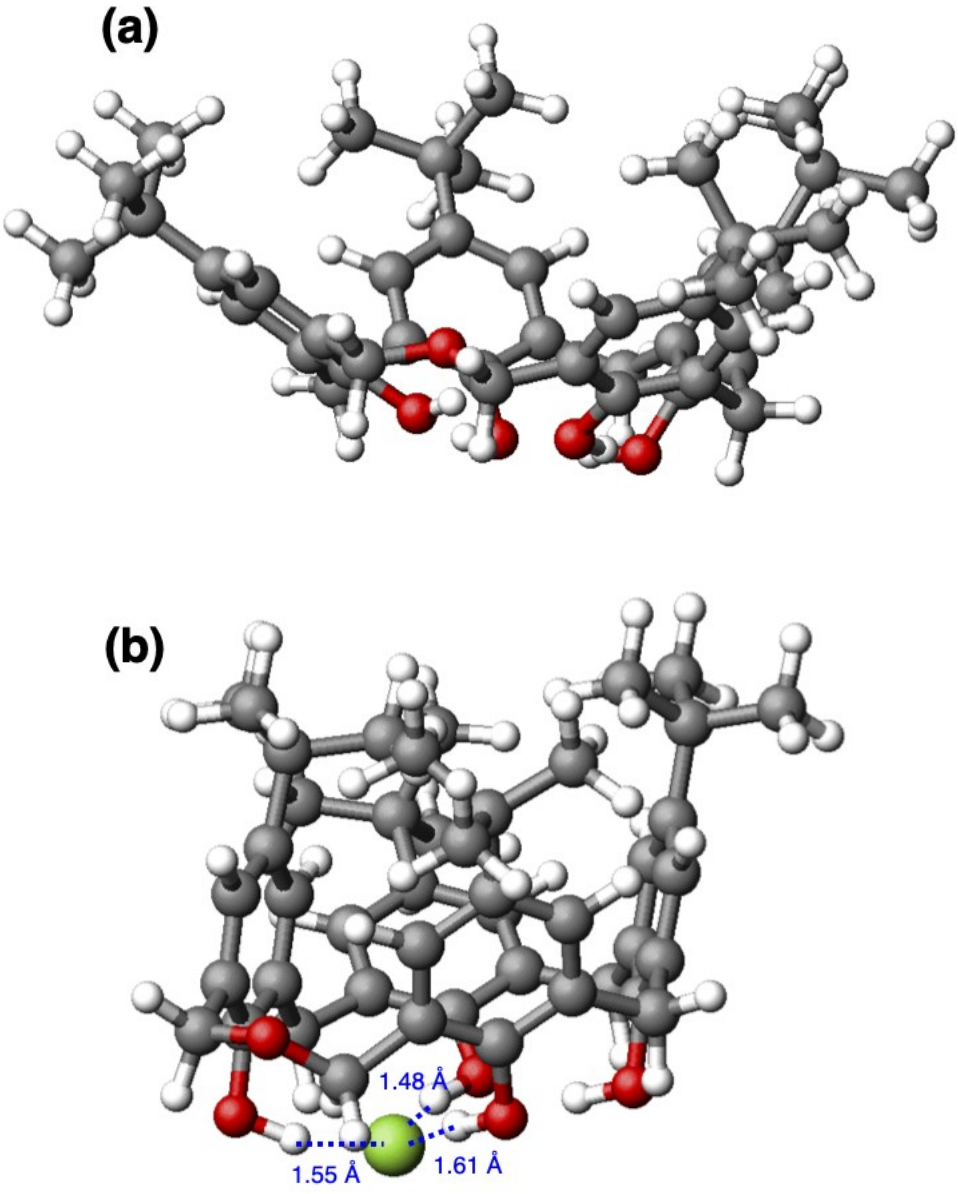

Figure S13. DFT optimized geometry for (a) dihomooxacalix[4]arene precursor 1 and (b) its complex with F-. The O-H···F hydrogen bonds are indicated by blue dash lines.

Cartesian coordinates, number of imaginary frequencies (NIMG) and absolute total energies (ETOT) of all compounds calculated at the CAM-B3LYP-D3/6-31+G* level are presented in the following.

1. The calixarene-F^- complex (monoanion):

NIMG = 0

ETOT = -2224.85790432 a.u.

Coordinates:

F	**0.58016400**	**0.33710200**	**-1.20297100**
O	**0.05338600**	**0.27775000**	**1.21200900**
C	**-0.66546900**	**1.15197600**	**1.95170200**
C	**-1.09231100**	**0.70644200**	**3.21611100**
C	**-1.80729200**	**1.57097500**	**4.03273600**
C	**-2.12831300**	**2.87882200**	**3.65280300**
C	**-1.69621600**	**3.28266600**	**2.39418800**
C	**-0.98330100**	**2.44674000**	**1.52860600**
C	**-2.95092800**	**3.77137900**	**4.58678700**
C	**-0.85202800**	**-0.72701000**	**3.63853000**
O	**0.01087500**	**-2.41274900**	**1.44581500**
C	**-1.30154000**	**-2.44212600**	**1.81643500**
C	**-2.18564600**	**-3.25750300**	**1.09742800**
C	**-3.50307900**	**-3.35239800**	**1.53197200**
C	**-3.99860600**	**-2.62661500**	**2.61878600**
C	**-3.10318400**	**-1.78861400**	**3.27780500**
C	**-1.76280800**	**-1.69074300**	**2.90192400**
C	**-5.47198700**	**-2.76285300**	**3.01779400**
C	**-1.74349500**	**-3.94049300**	**-0.18393800**
O	**-0.24998700**	**-2.07290300**	**-1.71427900**
C	**-1.54464900**	**-2.26066800**	**-2.08018900**
C	**-2.11623800**	**-1.56862400**	**-3.16237200**

C	-3.42490800	-1.84057900	-3.53474000
C	-4.19527400	-2.81500800	-2.89122200
C	-3.59694800	-3.49946400	-1.83789800
C	-2.29638000	-3.22912600	-1.40517200
C	-5.62265000	-3.10147400	-3.37086900
O	-0.04738000	2.33144300	-2.60529600
C	-1.36004700	2.31683700	-2.22884900
C	-1.72104900	2.56382300	-0.89351600
C	-3.06276800	2.48969000	-0.54761200
C	-4.07390900	2.20770200	-1.47362700
C	-3.68440100	1.98466300	-2.78878300
C	-2.34229800	2.02183900	-3.17541500
C	-5.52145200	2.08588900	-0.98908200
C	-1.27488000	-0.59462600	-3.95597200
H	0.39430300	1.59416400	-2.08463600
H	0.21224600	0.46190500	0.22126100
H	0.02267400	-1.12063100	-1.59974700
C	-5.58488800	-3.60961400	-4.82353900
C	-6.32811300	-4.15890500	-2.51271600
C	-6.45949800	-1.81241100	-3.31119100
C	-5.84803000	-1.83824700	4.18226100
C	-6.36945400	-2.40274200	1.82007600
C	-5.75724700	-4.21395200	3.44478800
C	-6.50990800	1.92638600	-2.15051100
C	-5.92885200	3.33850000	-0.19255500
C	-5.63260800	0.84927700	-0.07843800
C	-4.32921900	3.12656500	4.82499400
C	-3.17784300	5.17164500	4.00380600
C	-2.22629200	3.92895900	5.93545200
C	-1.95686900	1.62532100	-4.57876600

O	-2.06899200	0.22046600	-4.81140000
C	-0.65740700	2.92381900	0.13589200
H	-2.13384700	1.19397200	4.99937000
H	-1.92453700	4.27942200	2.03040200
H	-1.04110700	-0.80901800	4.71478000
H	0.19266700	-1.00528200	3.47532400
H	-4.17446500	-3.99540800	0.97022200
H	-3.43261200	-1.17460700	4.11004100
H	-2.10523500	-4.97622000	-0.18278500
H	-0.65491300	-3.95638500	-0.22775700
H	-3.82850200	-1.27323400	-4.36652200
H	-4.14702200	-4.27017300	-1.30882100
H	-3.32601400	2.63684100	0.49408200
H	-4.41547500	1.72847600	-3.54898100
H	-0.57312500	-1.15893400	-4.58626500
H	-0.66733800	0.01921900	-3.29016300
H	0.26457900	-1.47193800	1.33025200
H	-6.90975300	-1.96240100	4.42496600
H	-5.68406000	-0.78534600	3.92942300
H	-5.27158400	-2.06721600	5.08522800
H	-6.18371500	-1.37602400	1.49244200
H	-7.42862300	-2.49348300	2.09264200
H	-6.18686400	-3.05879700	0.96401900
H	-5.13635400	-4.49464900	4.30270600
H	-5.54326600	-4.91789800	2.63464100
H	-6.81109100	-4.33372300	3.72717000
H	-5.12387700	-2.87508800	-5.49060800
H	-6.59976200	-3.81209500	-5.19001200
H	-5.00201600	-4.53456000	-4.89362300
H	-7.34578000	-4.32108900	-2.88685000

H	**-6.40384100**	**-3.84259900**	**-1.46668100**
H	**-5.80573500**	**-5.12115100**	**-2.54247000**
H	**-6.51171900**	**-1.43183500**	**-2.28617200**
H	**-7.48284000**	**-1.99905600**	**-3.66154400**
H	**-6.02855000**	**-1.02596900**	**-3.93726200**
H	**-4.23694700**	**2.13499200**	**5.27865400**
H	**-4.86944500**	**3.00905600**	**3.87938000**
H	**-4.93714400**	**3.74893200**	**5.49386800**
H	**-2.23106600**	**5.69132400**	**3.82120500**
H	**-3.76104700**	**5.77575000**	**4.70826700**
H	**-3.73308100**	**5.13346700**	**3.06069200**
H	**-2.80994700**	**4.56286800**	**6.61491000**
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H	**-5.84954800**	**4.23766600**	**-0.81389300**
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H	**-2.63985200**	**2.07502200**	**-5.30588000**
H	**0.31000500**	**2.53769200**	**-0.18600300**
H	**-0.54879400**	**4.01628000**	**0.15025200**

2. The calixarene molecule:

NIMG = 0

ETOT = -2124.91766189 a.u.

Coordinates:

O	**-0.10798200**	**0.71903300**	**1.01580500**
C	**-0.95917100**	**1.28243300**	**1.94597400**
C	**-1.30557700**	**0.52618300**	**3.06885700**
C	**-2.19187100**	**1.07660400**	**3.98535900**
C	**-2.74962700**	**2.35010100**	**3.82711700**
C	**-2.33418400**	**3.08578600**	**2.72210600**
C	**-1.42859300**	**2.58285600**	**1.78505600**
C	**-3.75804200**	**2.87669300**	**4.85282200**
C	**-0.73552900**	**-0.85959400**	**3.28660600**
O	**-0.19066500**	**-1.92590300**	**0.60958200**
C	**-1.20748000**	**-2.46427700**	**1.36654800**
C	**-1.90174300**	**-3.54735300**	**0.82148400**
C	**-2.95773200**	**-4.09084100**	**1.54089800**
C	**-3.35048400**	**-3.59879000**	**2.78869200**
C	**-2.60369300**	**-2.54723100**	**3.31254600**
C	**-1.52718300**	**-1.97446700**	**2.63198300**
C	**-4.54627900**	**-4.22151100**	**3.51601000**
C	**-1.53000200**	**-4.10636700**	**-0.53672900**
O	**-1.22991500**	**-1.49474400**	**-1.88840500**
C	**-2.21753300**	**-2.36040300**	**-2.25838400**
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C	**-5.49734000**	**-4.88337300**	**-3.62282900**
O	**-1.23817300**	**1.45849500**	**-1.32923600**

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C	-1.91634100	3.58796700	-0.50695400
C	-2.71612100	4.71700000	-0.64632200
C	-3.62366900	4.88512000	-1.69604000
C	-3.67686600	3.86980800	-2.64780200
C	-2.87562500	2.73223400	-2.55984500
C	-4.49528700	6.14330600	-1.75960600
C	-2.78643300	-0.64264200	-3.98700200
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H	-0.38945600	1.01462400	0.11645600
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C	-4.97330500	1.93227200	4.90078000
C	-4.26136300	4.28262600	4.50376800
C	-3.10244100	2.93326100	6.24425900
C	-2.87426900	1.70169800	-3.64947600
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H	**-2.23387300**	**3.60034700**	**6.23913900**
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H	**-4.87478000**	**6.11531600**	**-3.91714500**
H	**-6.03639300**	**7.05386200**	**-2.97390200**
H	**-6.11941500**	**5.28908100**	**-2.95578700**
H	**-2.93393500**	**7.47648800**	**-0.98304800**
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H	**-2.97042000**	**7.35514500**	**-2.74732400**
H	**-6.01105700**	**5.35379300**	**-0.40009500**
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H	**-4.74901200**	**6.28584400**	**0.41628600**
H	**-1.91375500**	**1.72831100**	**-4.19043500**
H	**-3.67442500**	**1.89836000**	**-4.37638000**
H	**0.02076400**	**3.11790500**	**0.29085000**
H	**-0.78078000**	**4.47074600**	**1.05477200**

3. The F- anion:

ETOT = -99.8367667768 a.u.

4. BSSE correction energy (using counterpoise method): 0.004254906506 a.u.

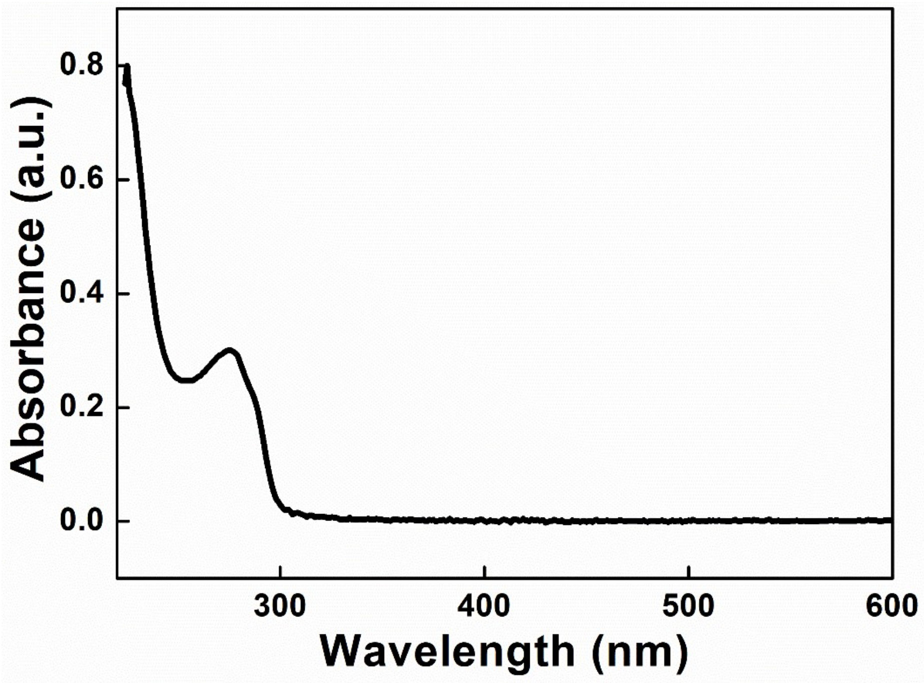

Figure S14 UV/vis absorption of 2b in CH_2Cl_2 (2× 10^{-5} M)

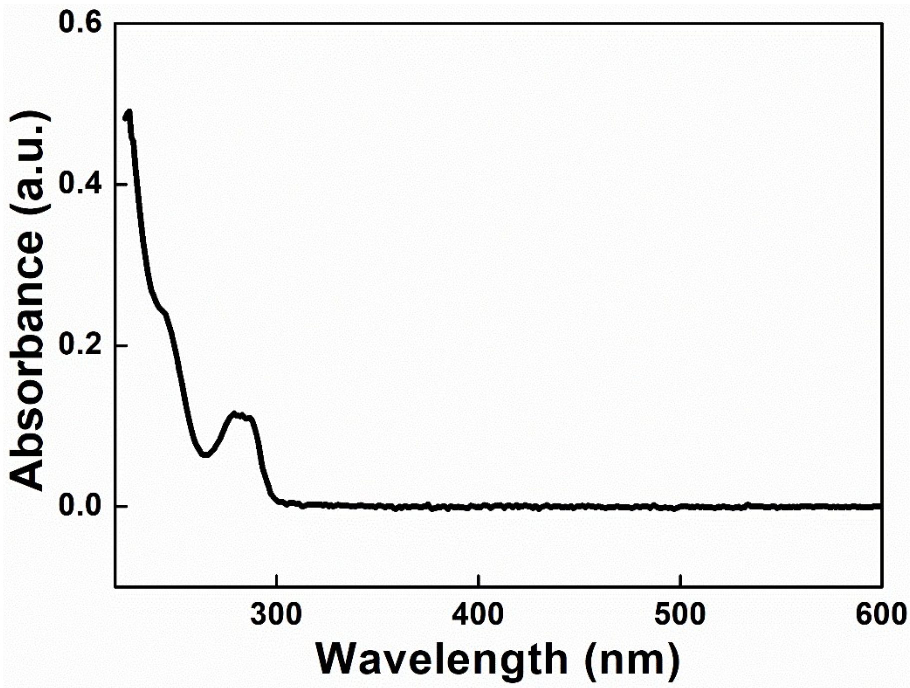

Figure S15 UV/vis absorption of 2c in CH_2Cl_2 (2× 10^{-5} M)

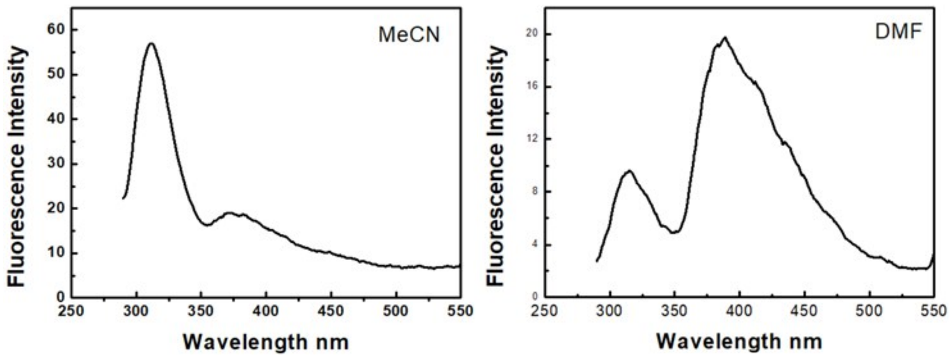

Figure S16 Fluorescent emission of **3** in MeCN and in DMF respectively, (2× 10^{-5} M)

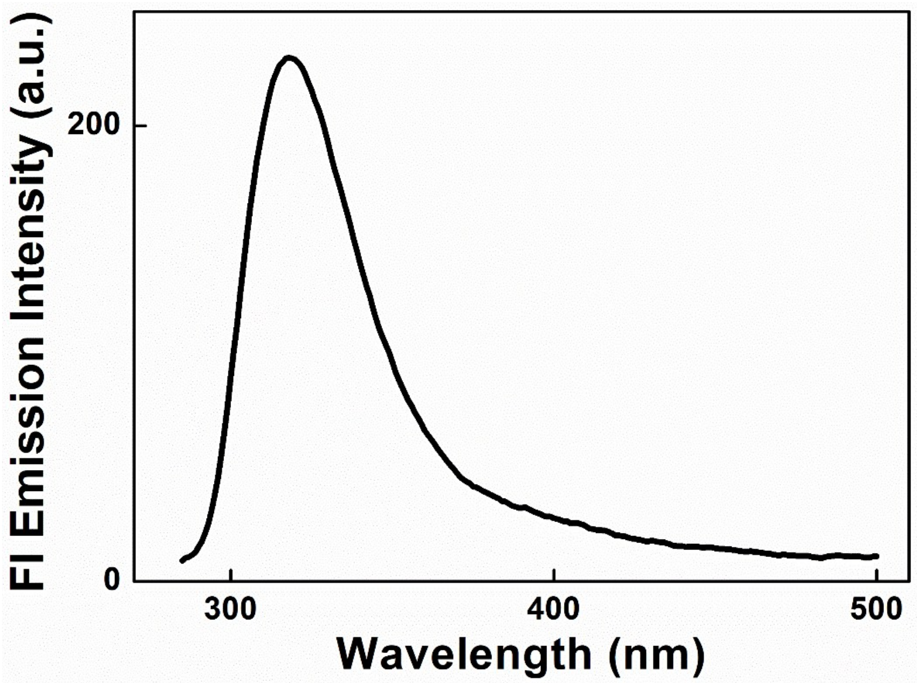

Figure S17 Fluorescent emission of 2b in CH_2Cl_2 (2× 10^{-5} M)

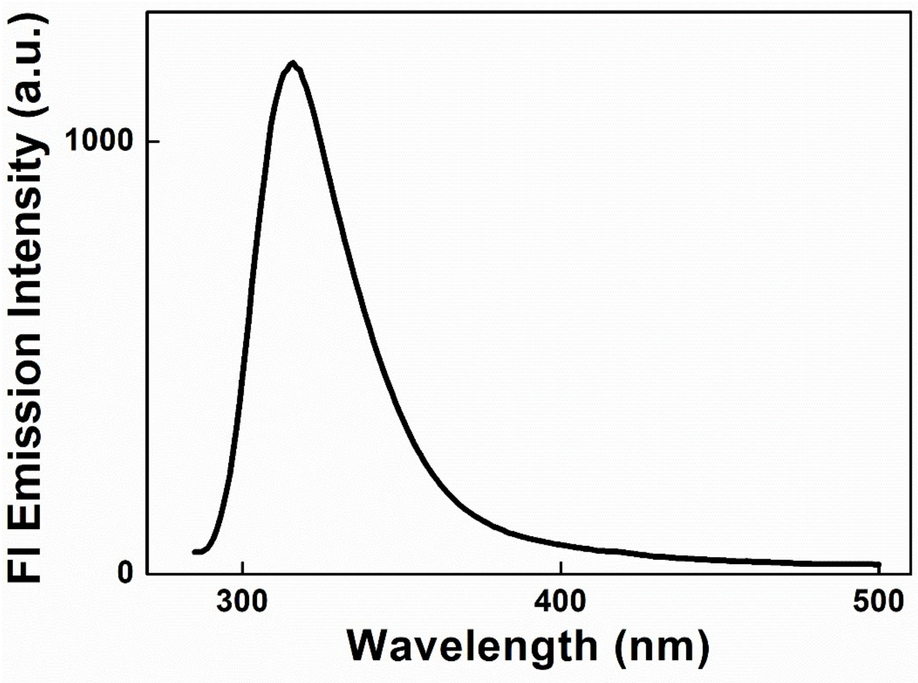

Figure S18 Fluorescent emission of 2c in CH_2Cl_2 (2×10^{-5} M)

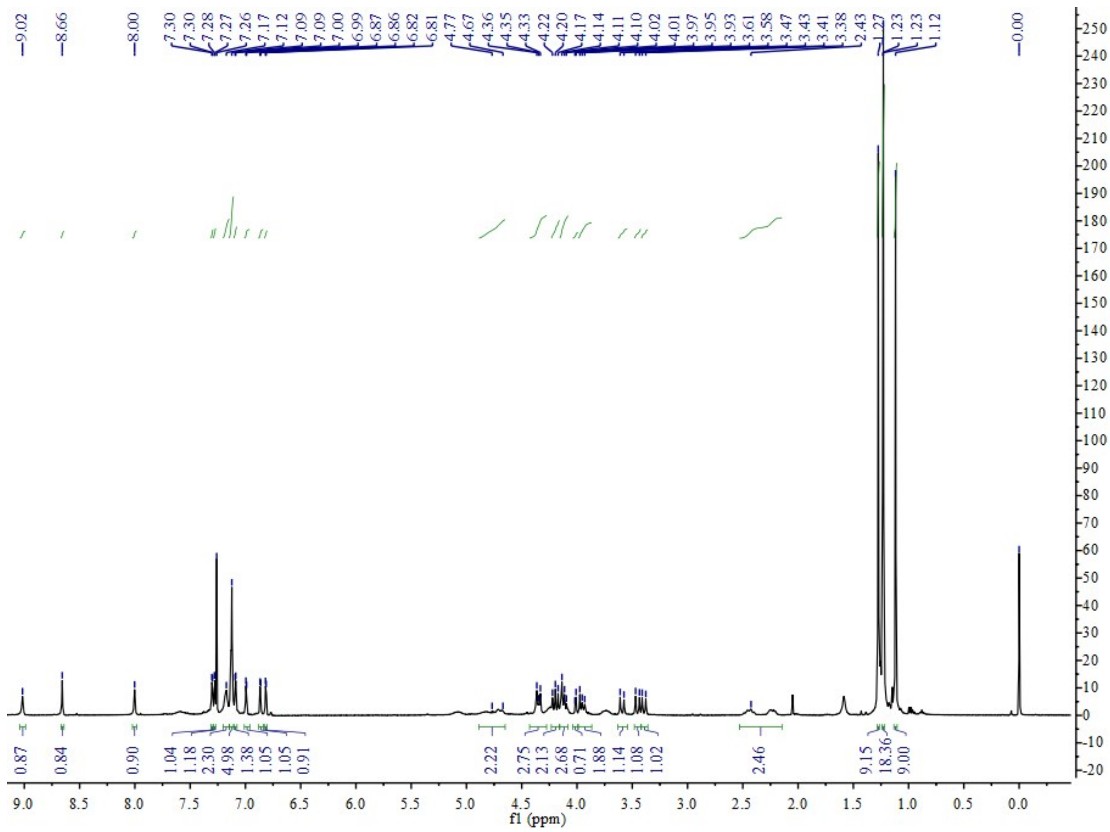

Figure S19. ^{1}H NMR spectrum of 2a ($CDCl_3$, 400 MHz, 298K)

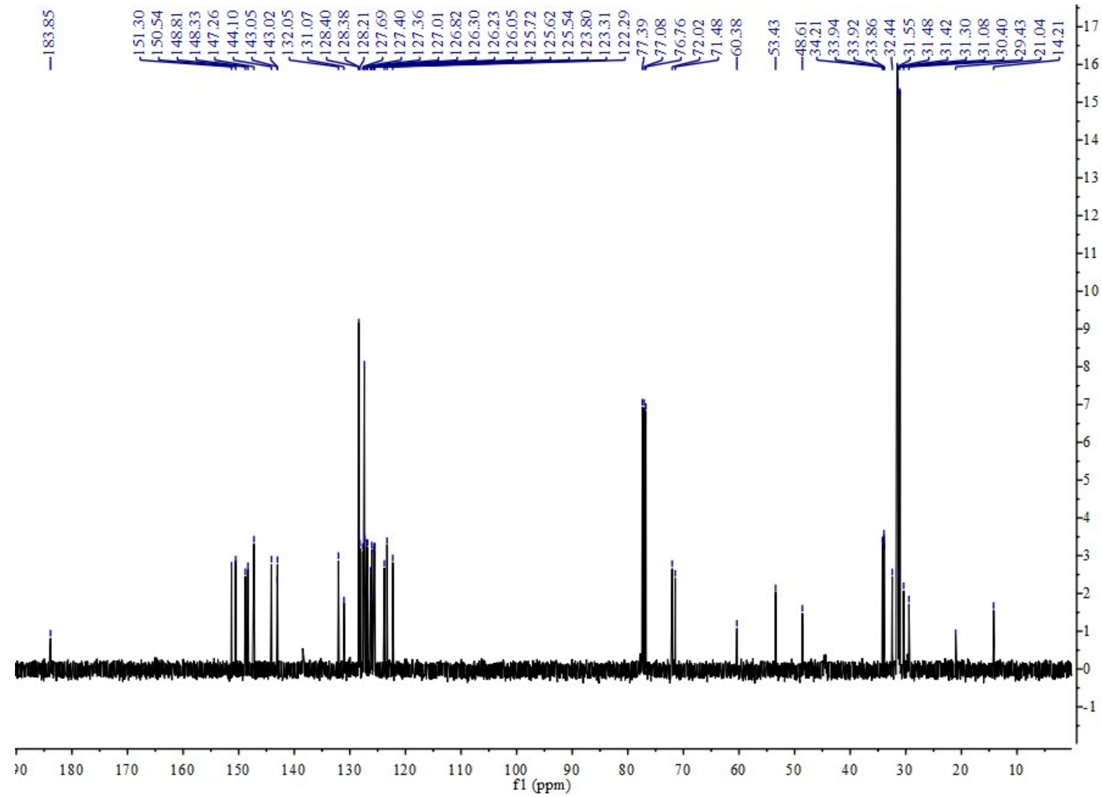

Figure S20. ^{13}C NMR spectrum of 2a ($CDCl_3$, 400 MHz, 298K)

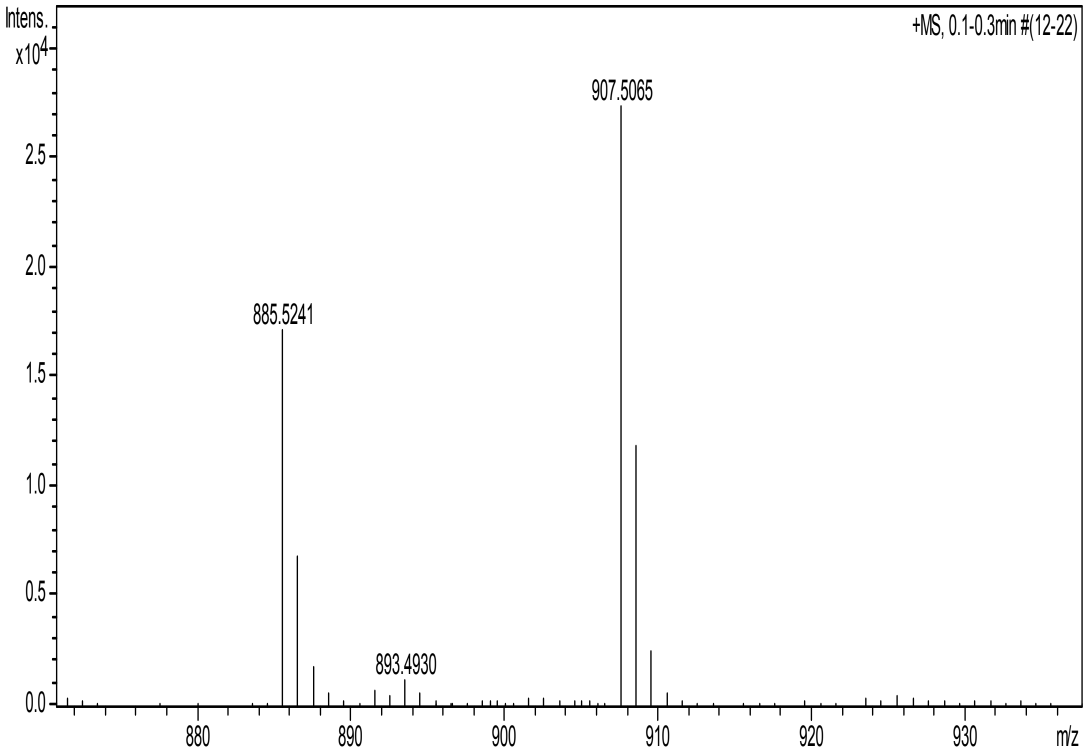

Figure S21. HRMS spectrum of 2a.

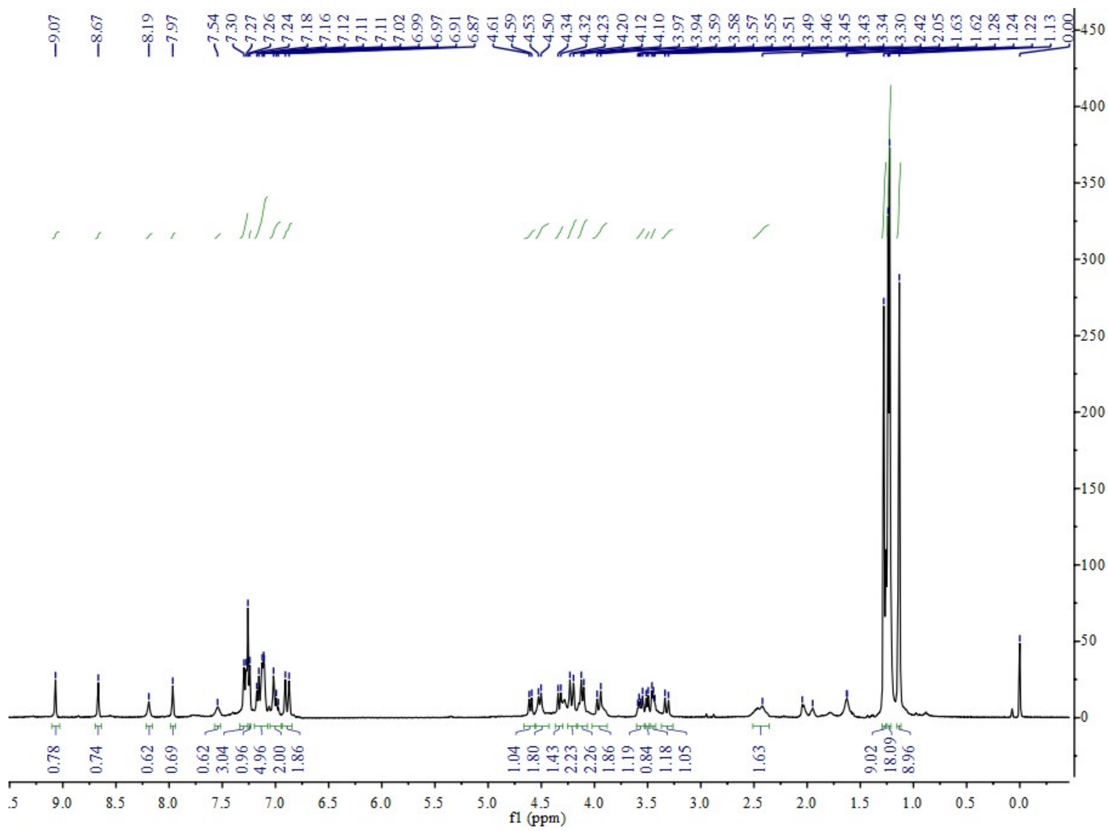

Figure S22. ^{1}H NMR spectrum of 2b ($CDCl_3$, 400 MHz, 298K)

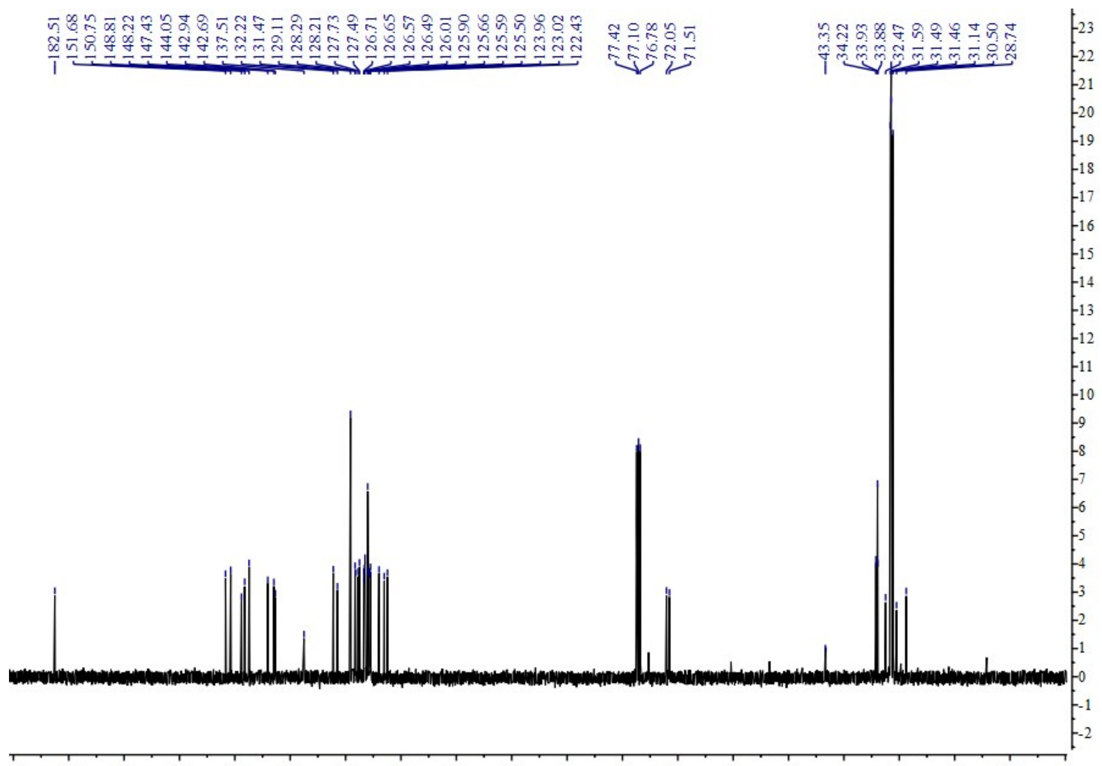

Figure S23. ^{13}C NMR spectrum of 2b ($CDCl_3$, 400 MHz, 298K)

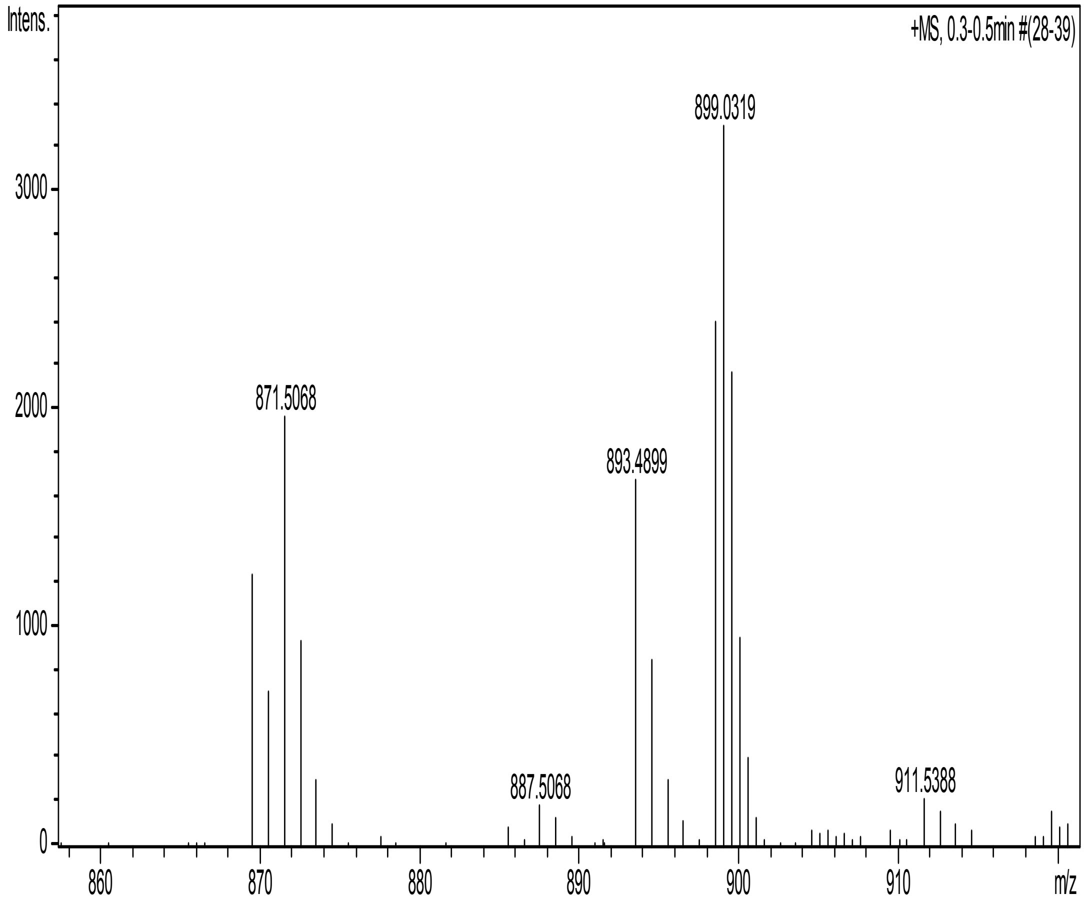

Figure S24. HRMS spectrum of 2b.

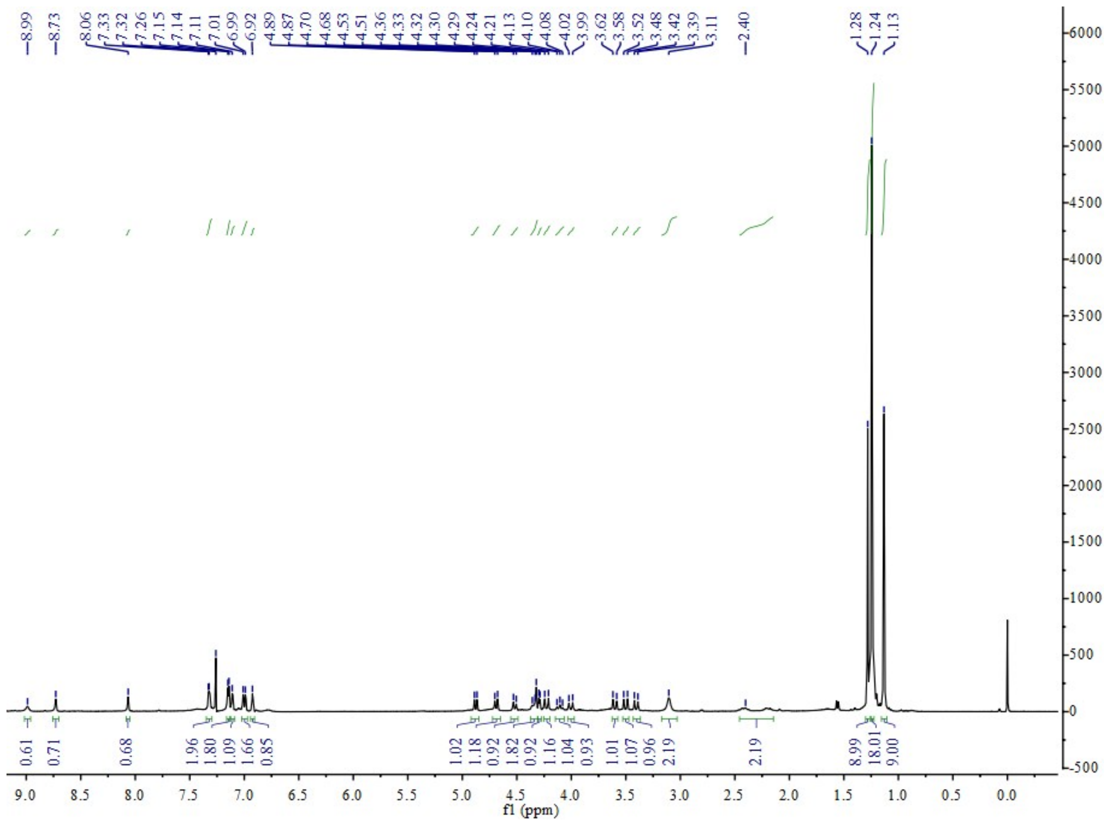

Figure S25. ^{1}H NMR spectrum of 2c ($CDCl_3$, 400 MHz, 298K)

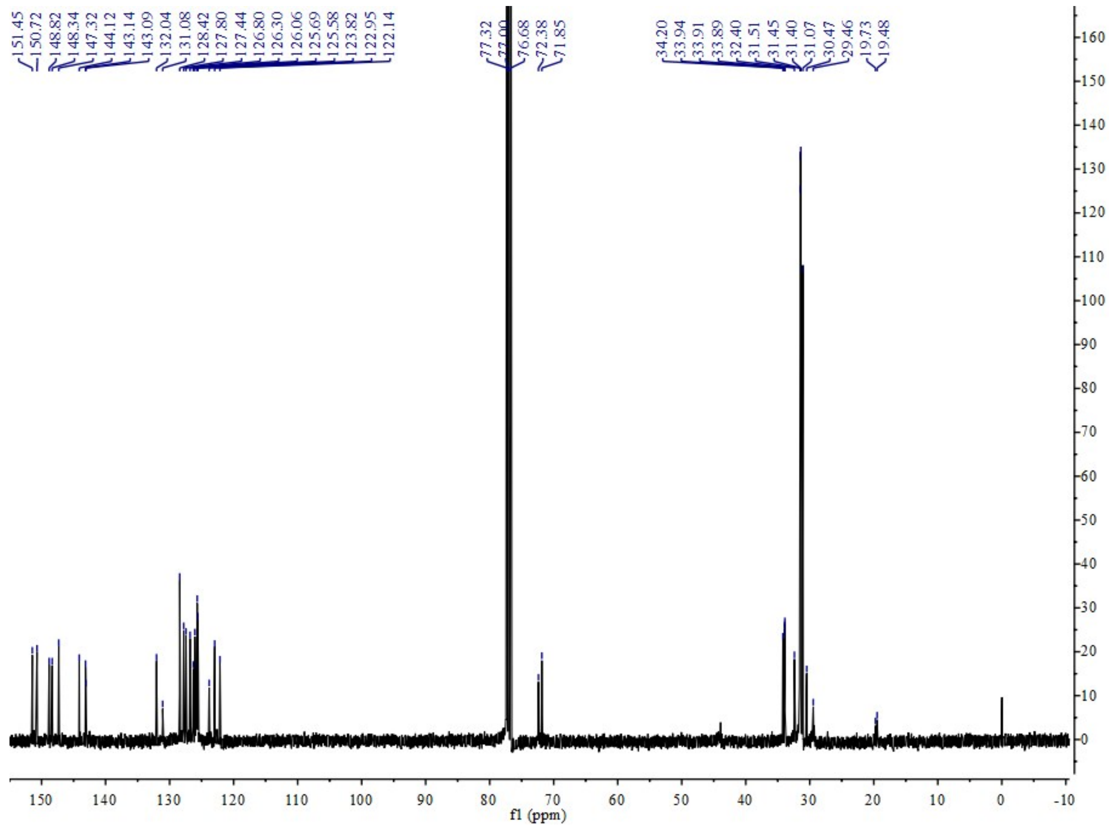

Figure S26. ^{13}C NMR spectrum of 2c ($CDCl_3$, 400 MHz, 298K)

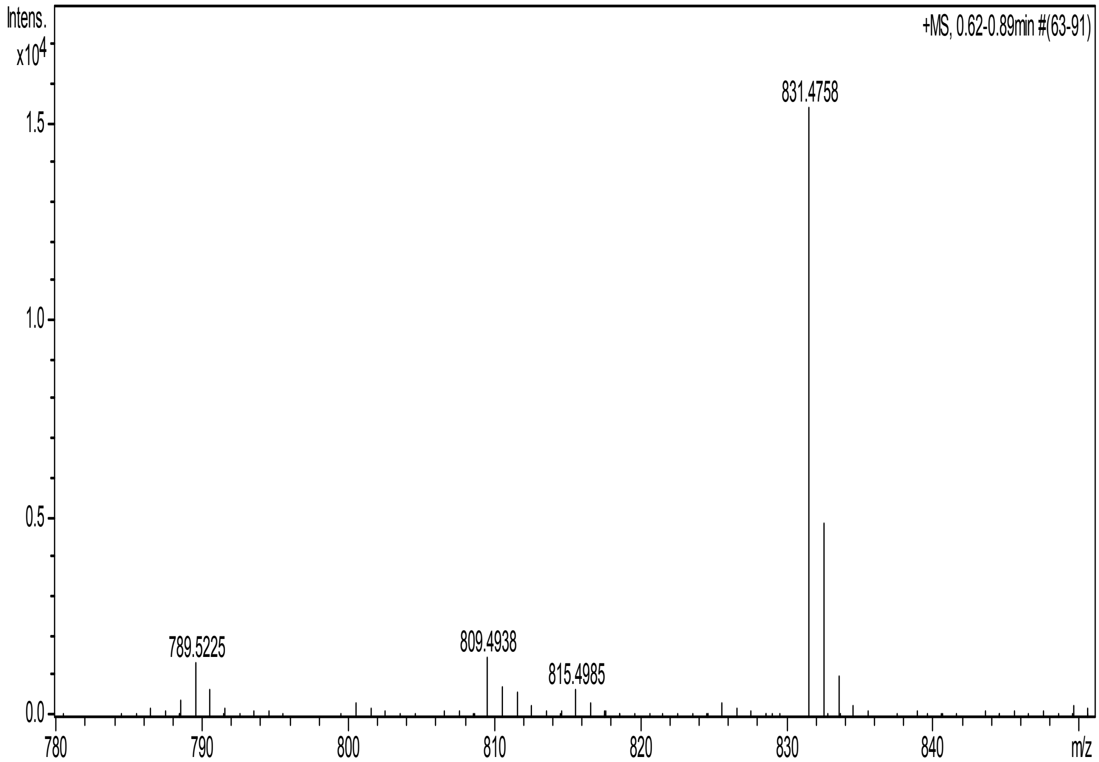

Figure S27. HRMS spectrum of 2c.

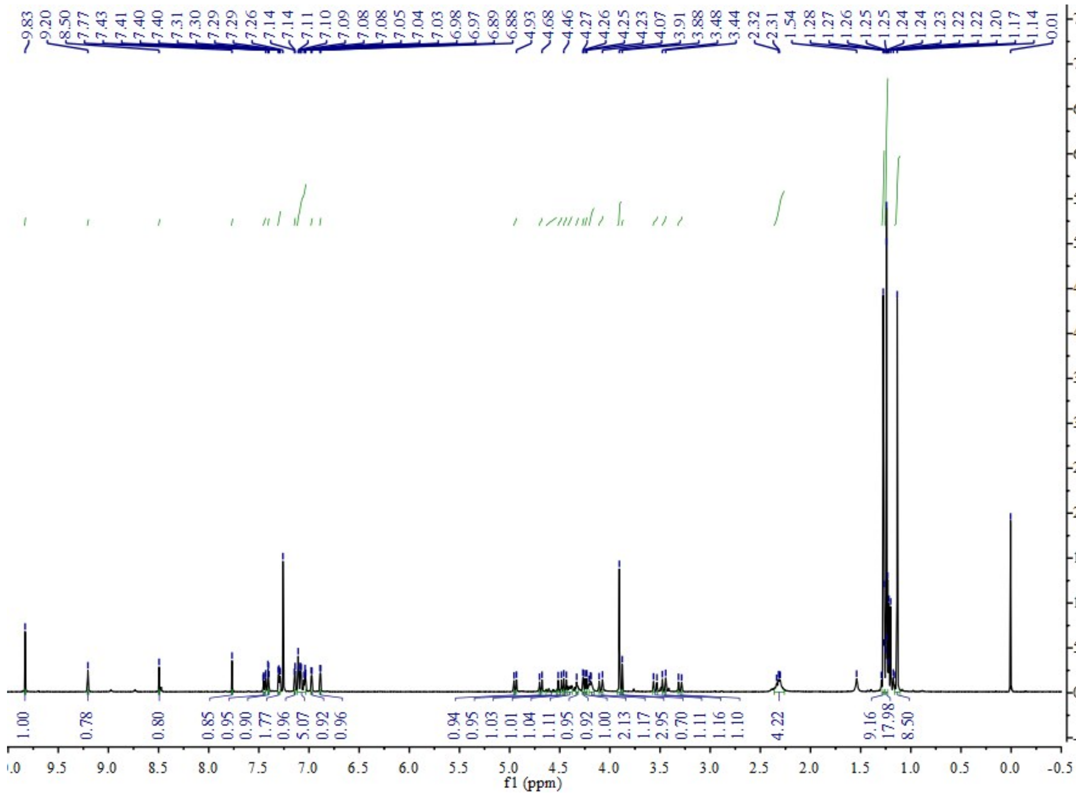

Figure S28. ^{1}H NMR spectrum of 1b ($CDCl_3$, 400 MHz, 298K)

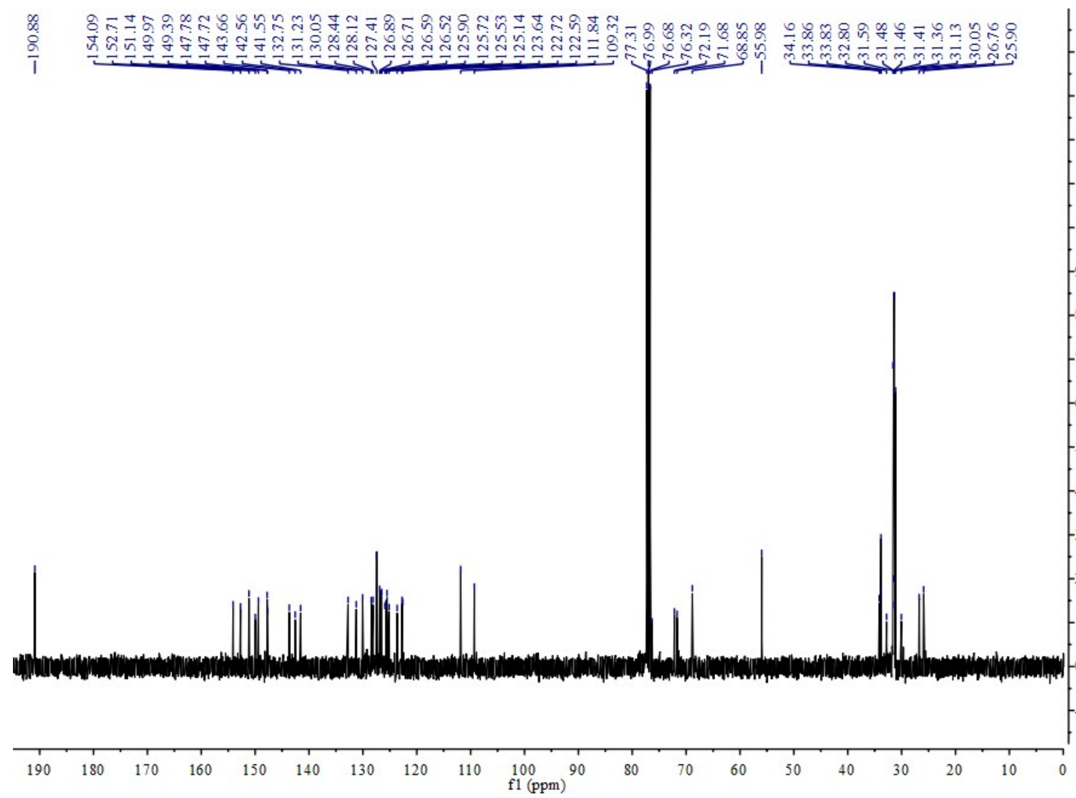

Figure S29. ^{13}C NMR spectrum of 1b ($CDCl_3$, 400 MHz, 298K)

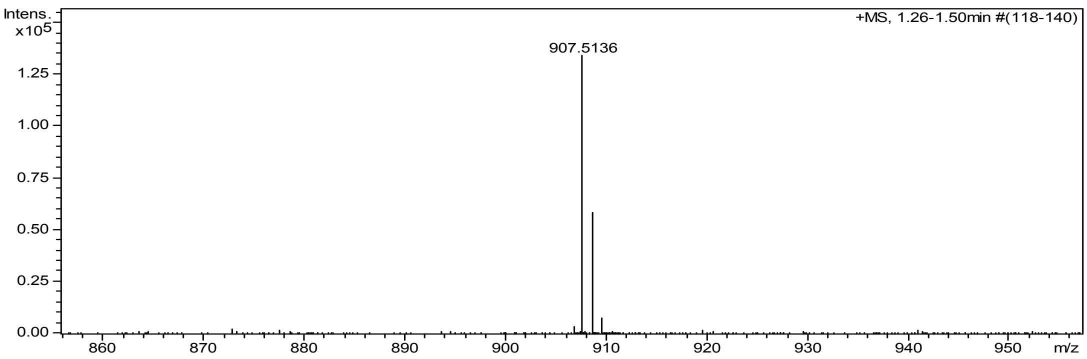

Figure S30. HRMS spectrum of 1b.

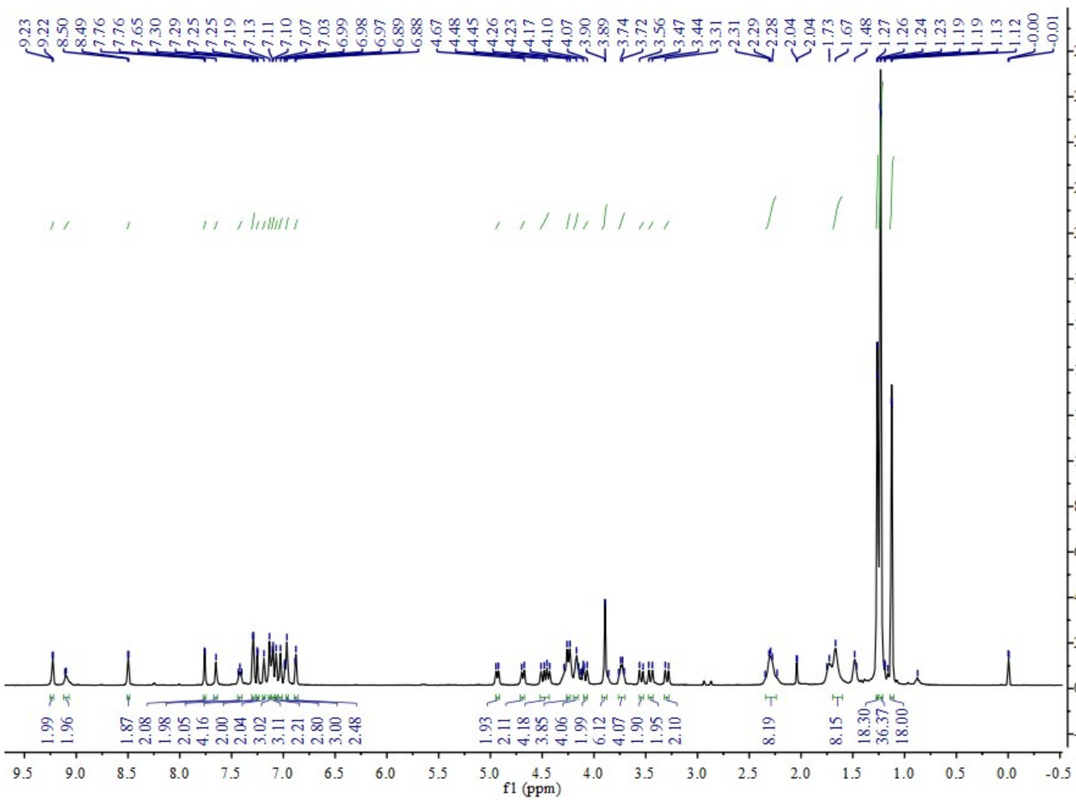

Figure S31. ^{1}H NMR spectrum of 3 ($CDCl_3$, 400 MHz, 298K)

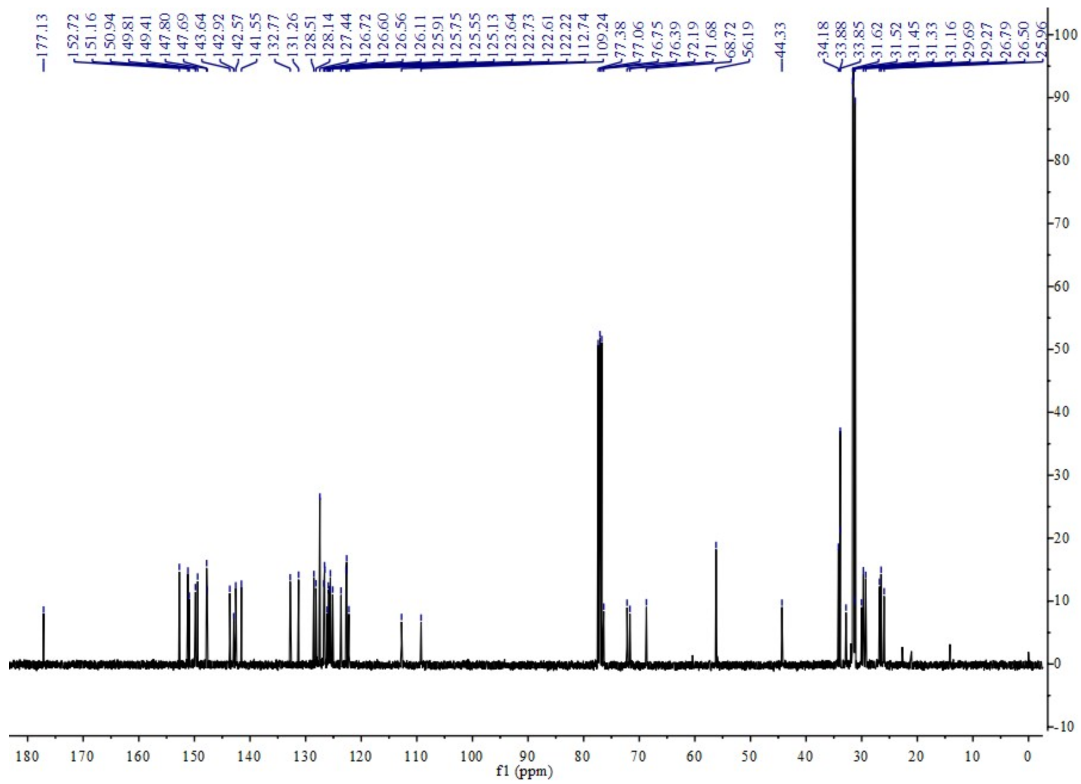

Figure S32. ^{13}C NMR spectrum of 3 ($CDCl_3$, 400 MHz, 298K)

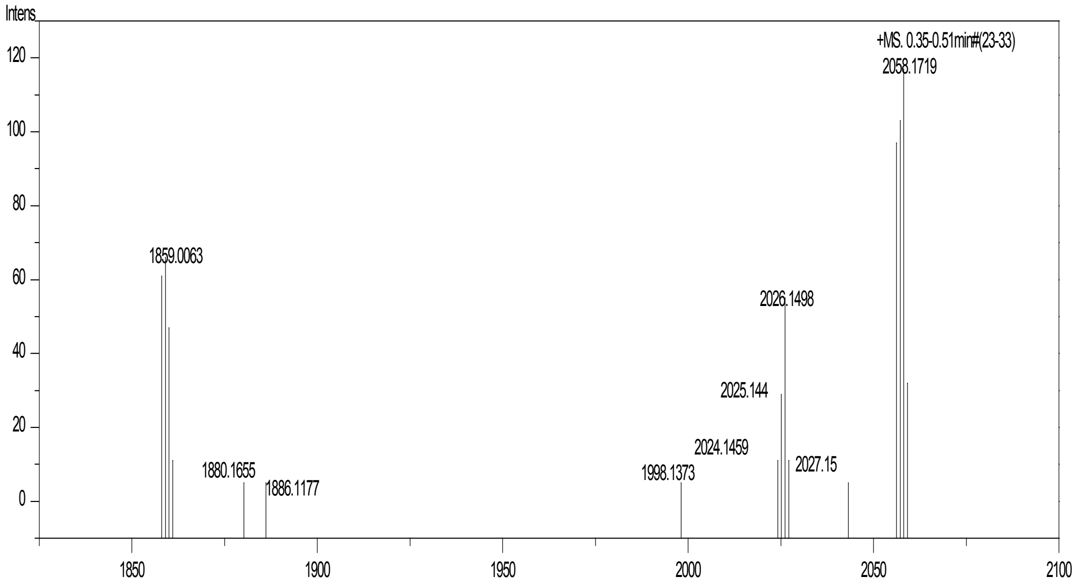

Figure S33. HRMS spectrum of 3.