

Supporting Information

Water-Soluble Trityl Radicals for Fluorescence Imaging

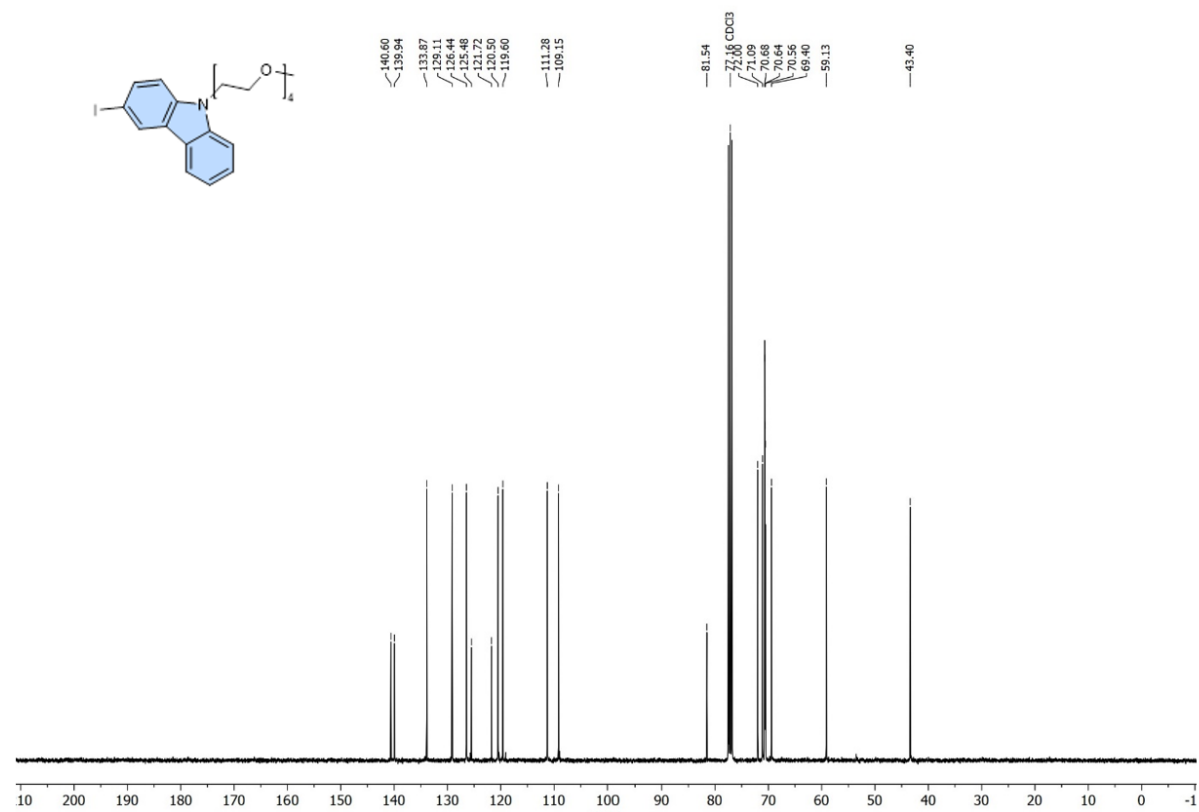
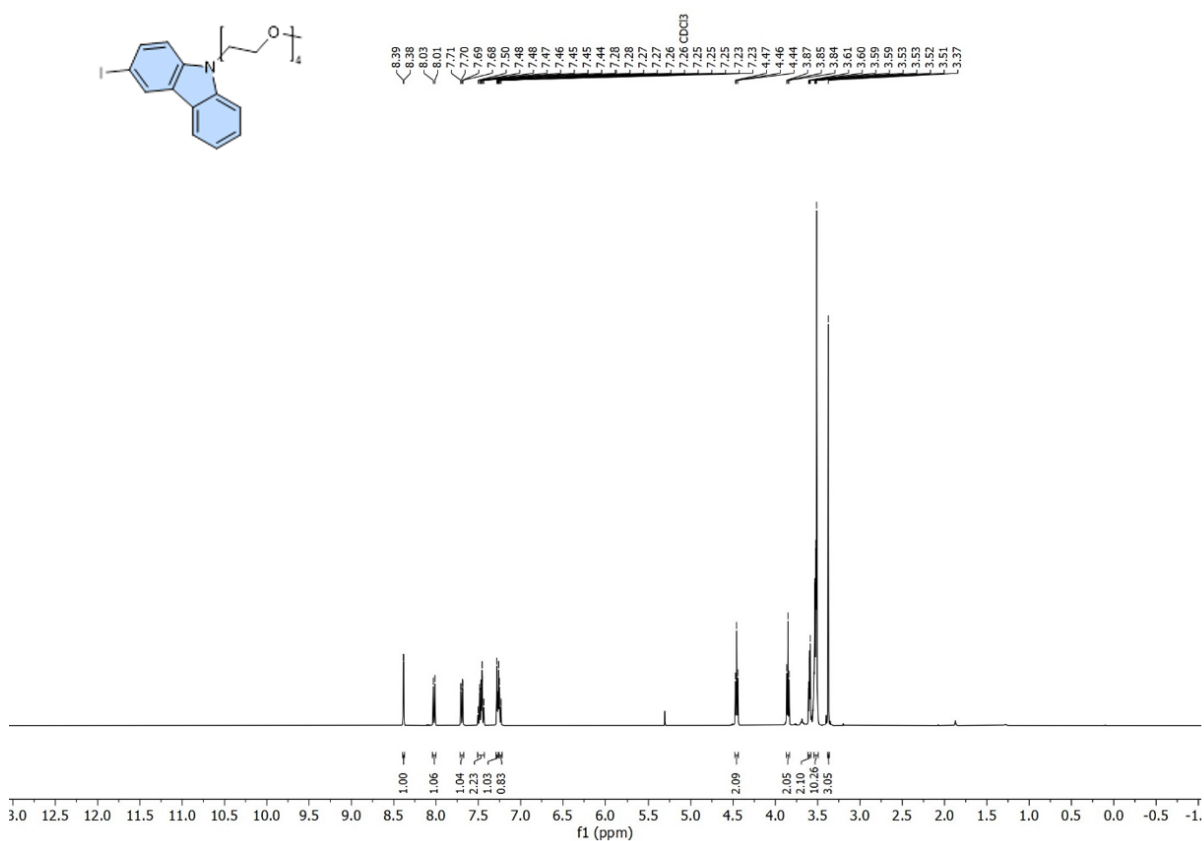
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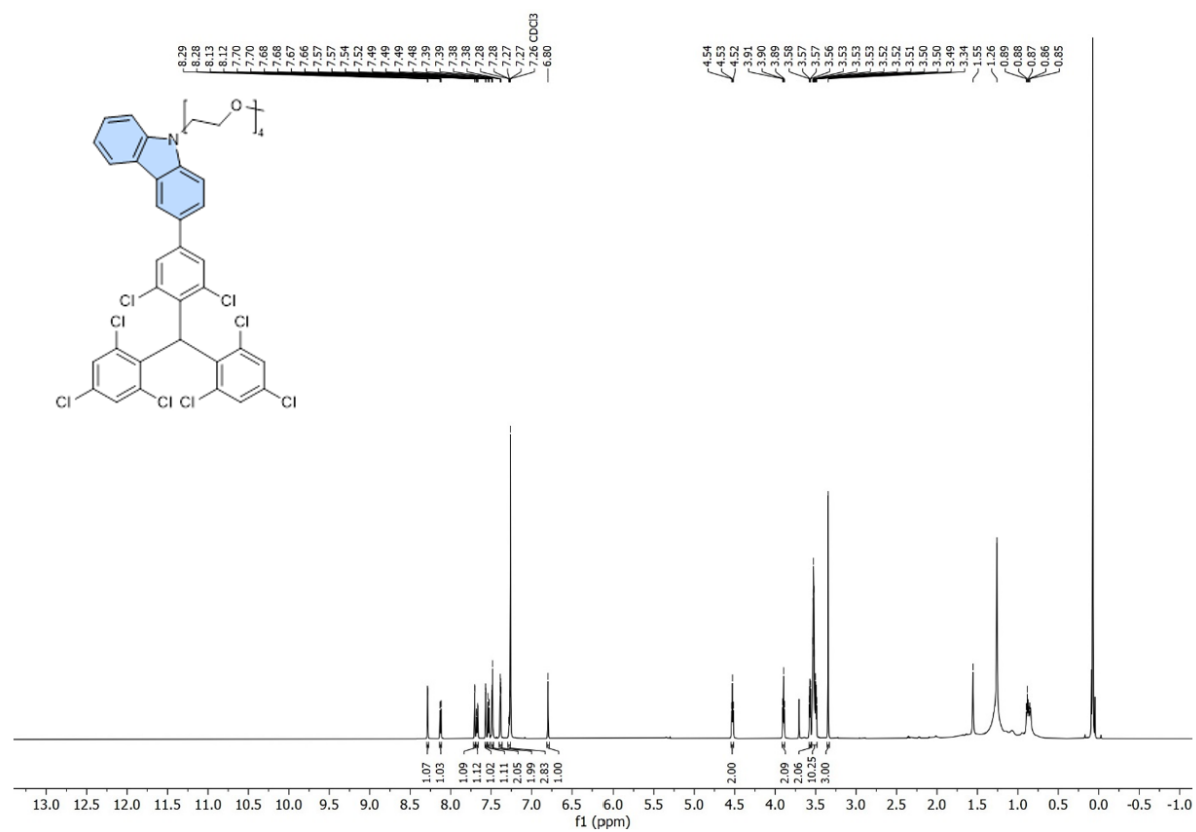
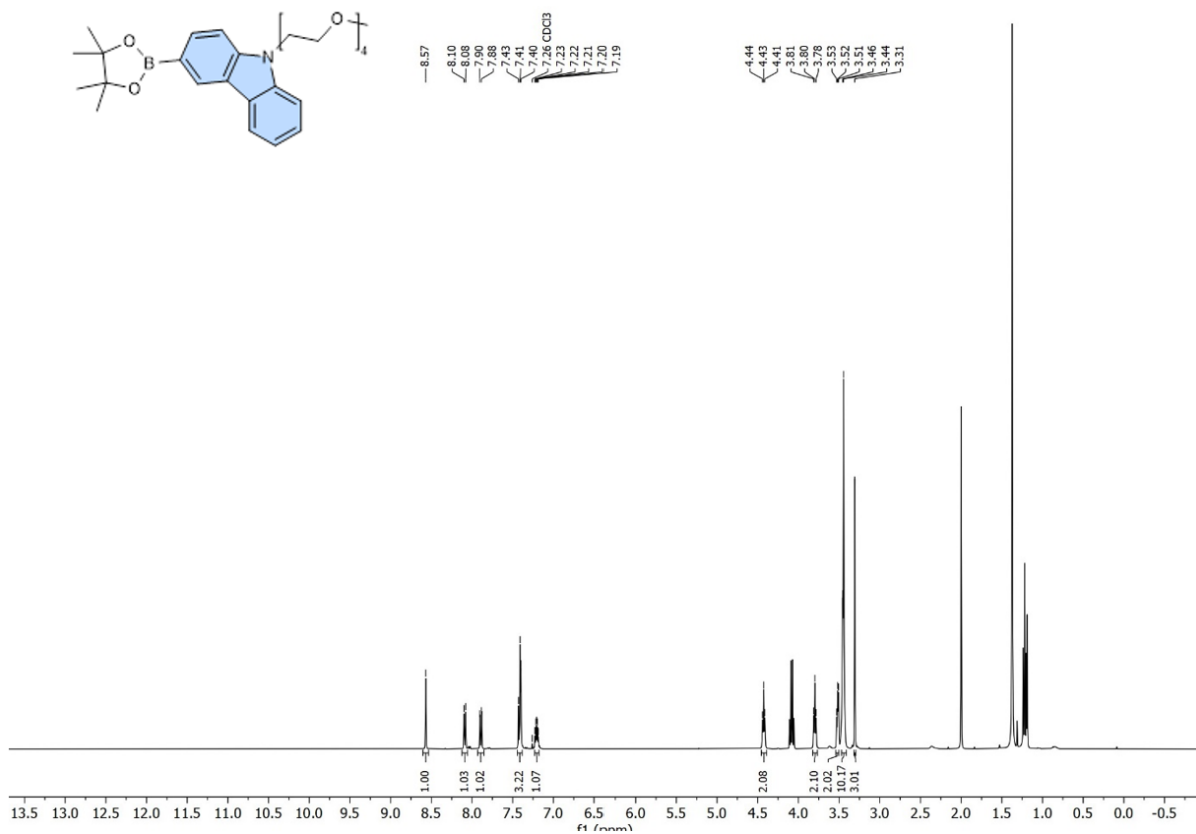
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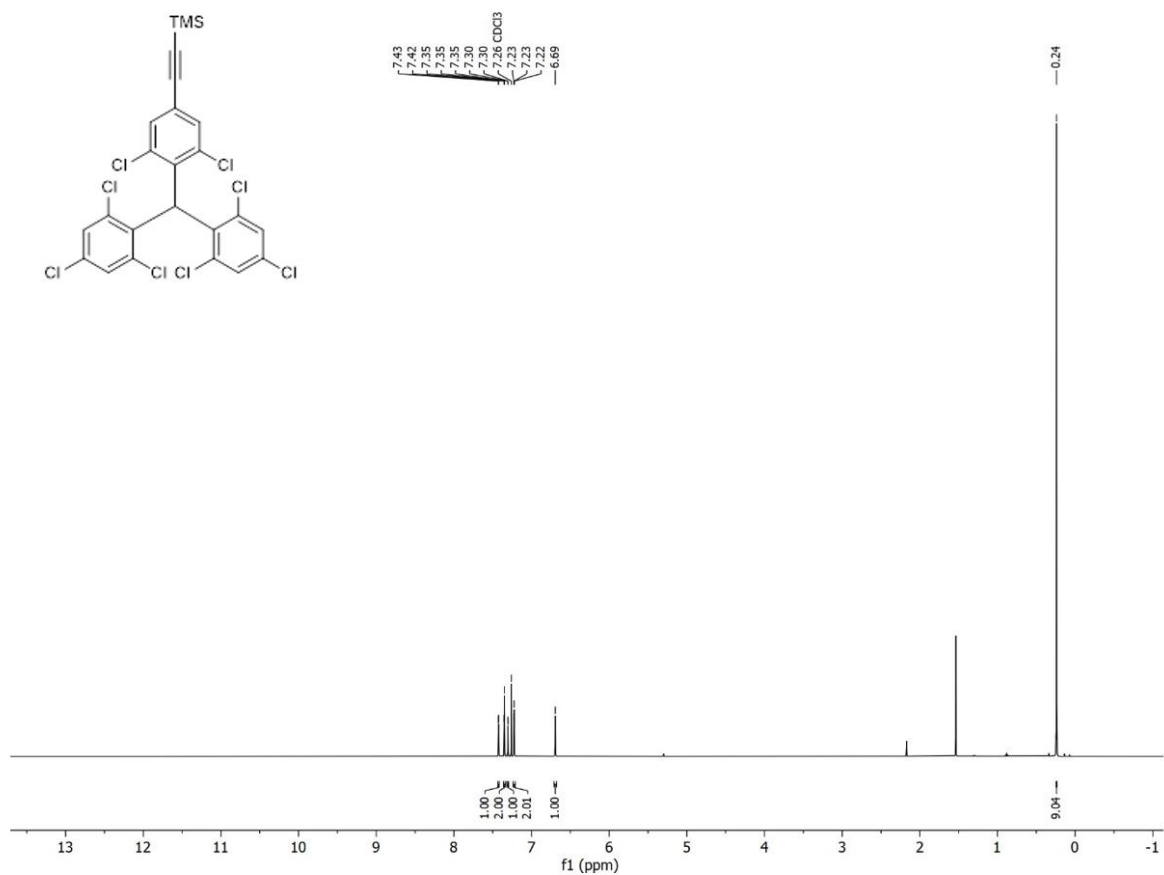
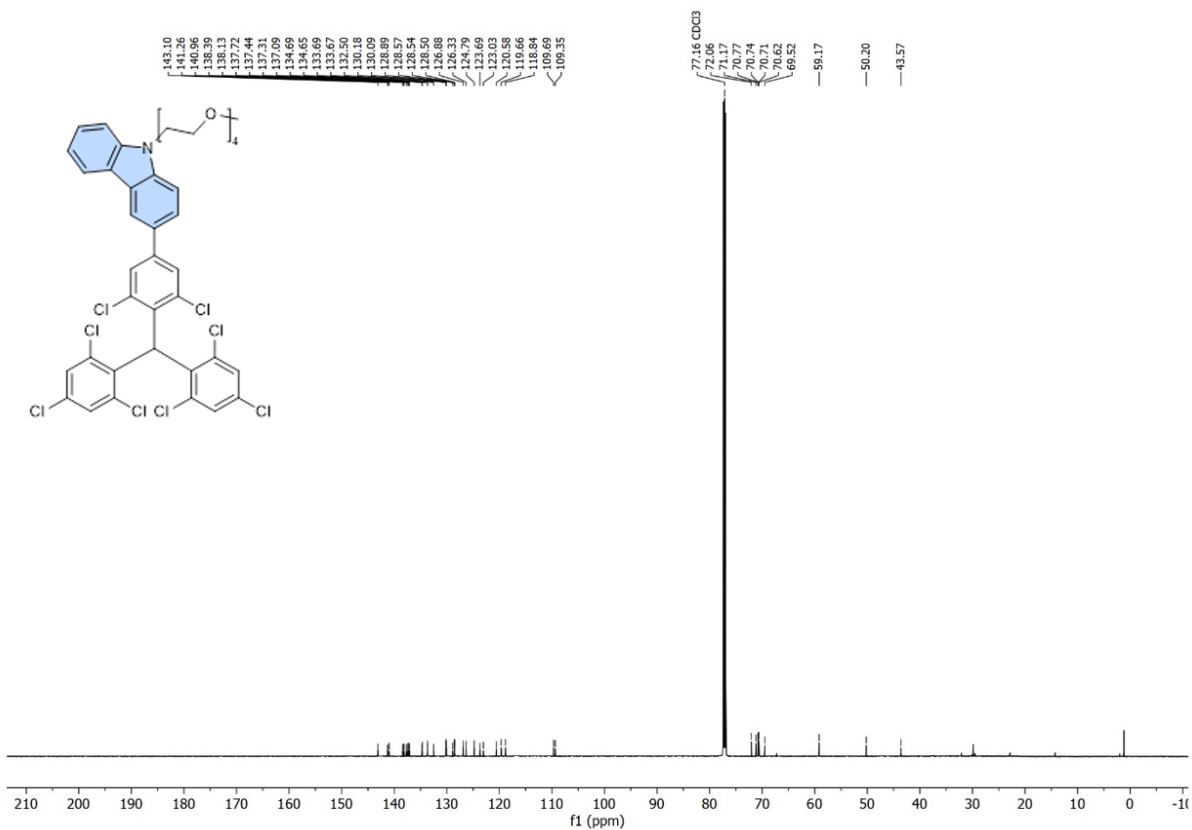
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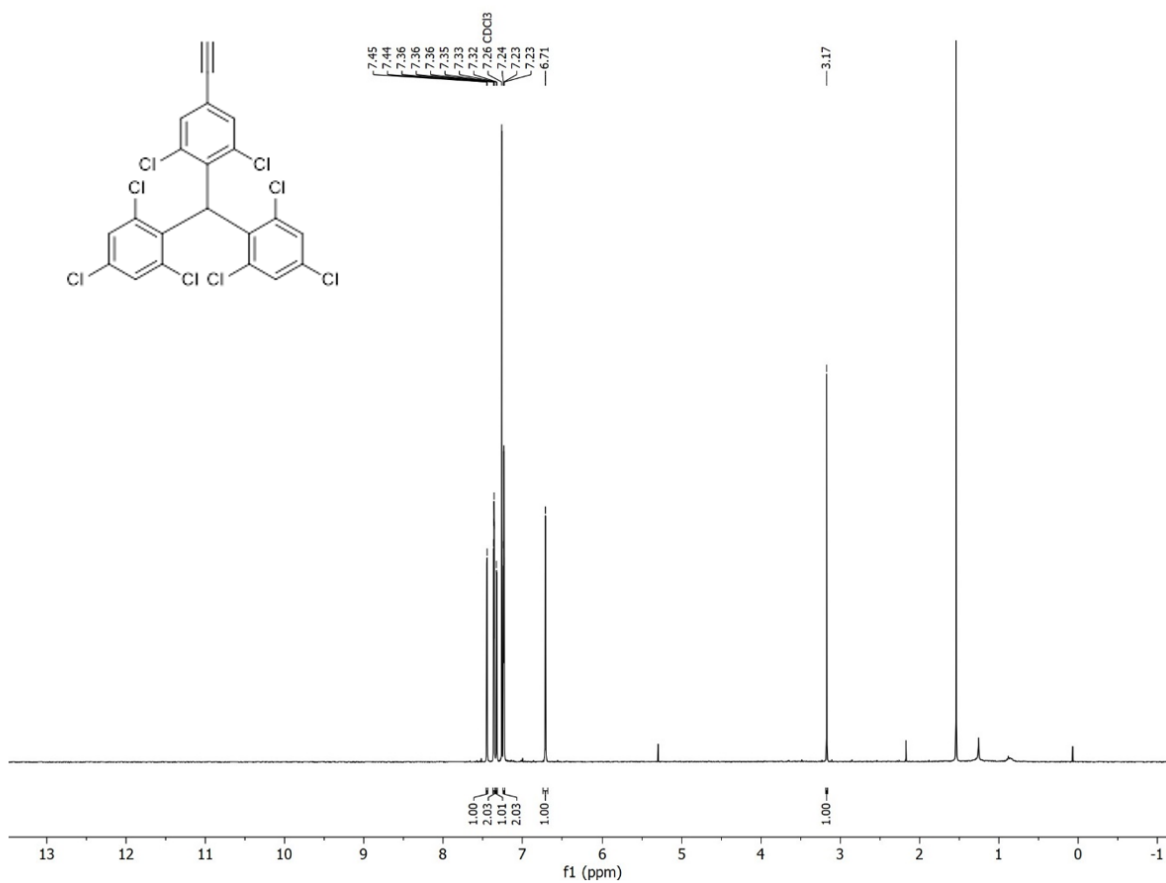
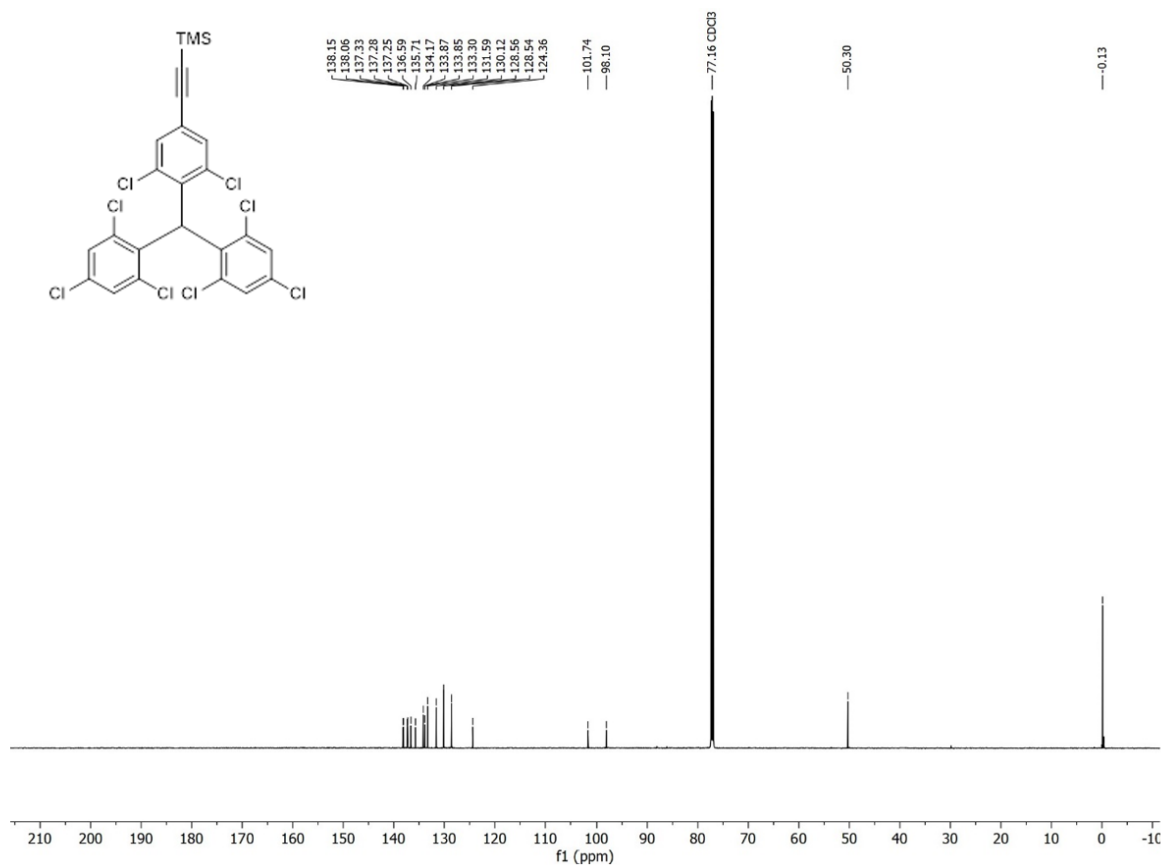
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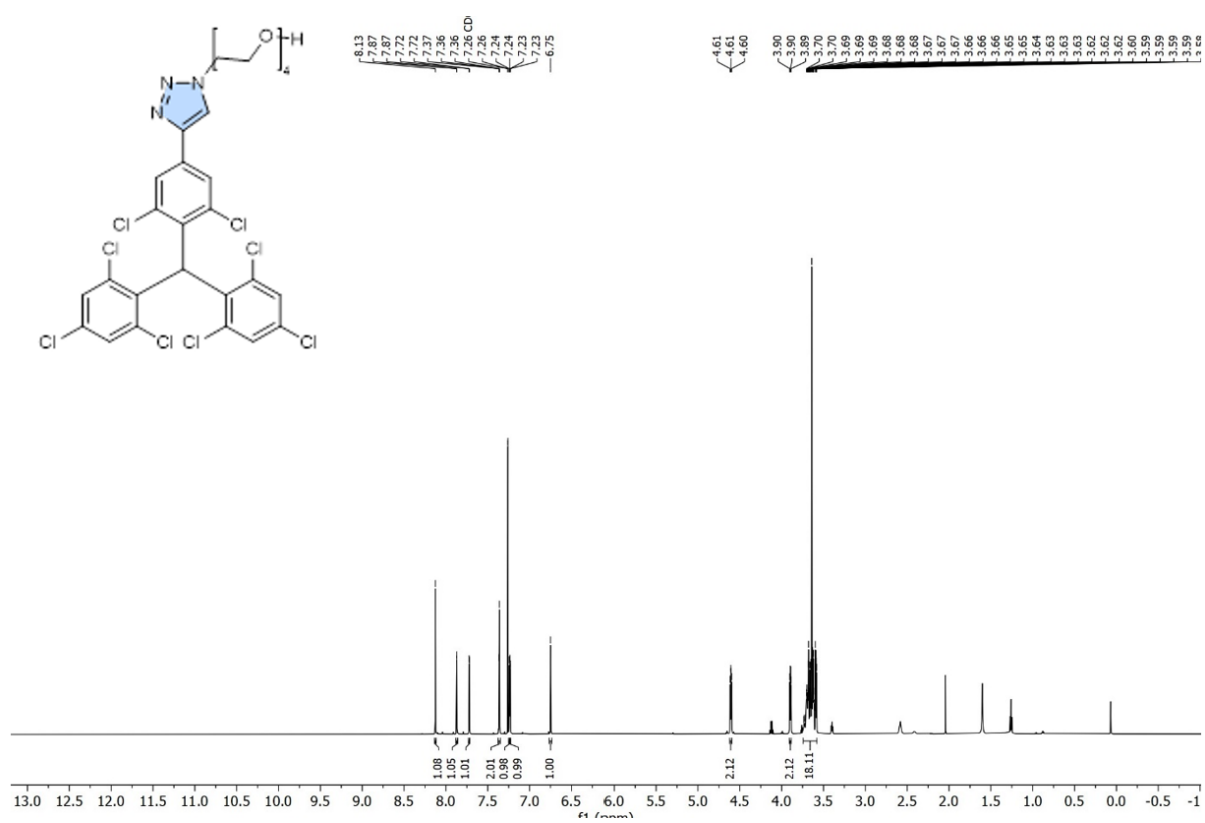
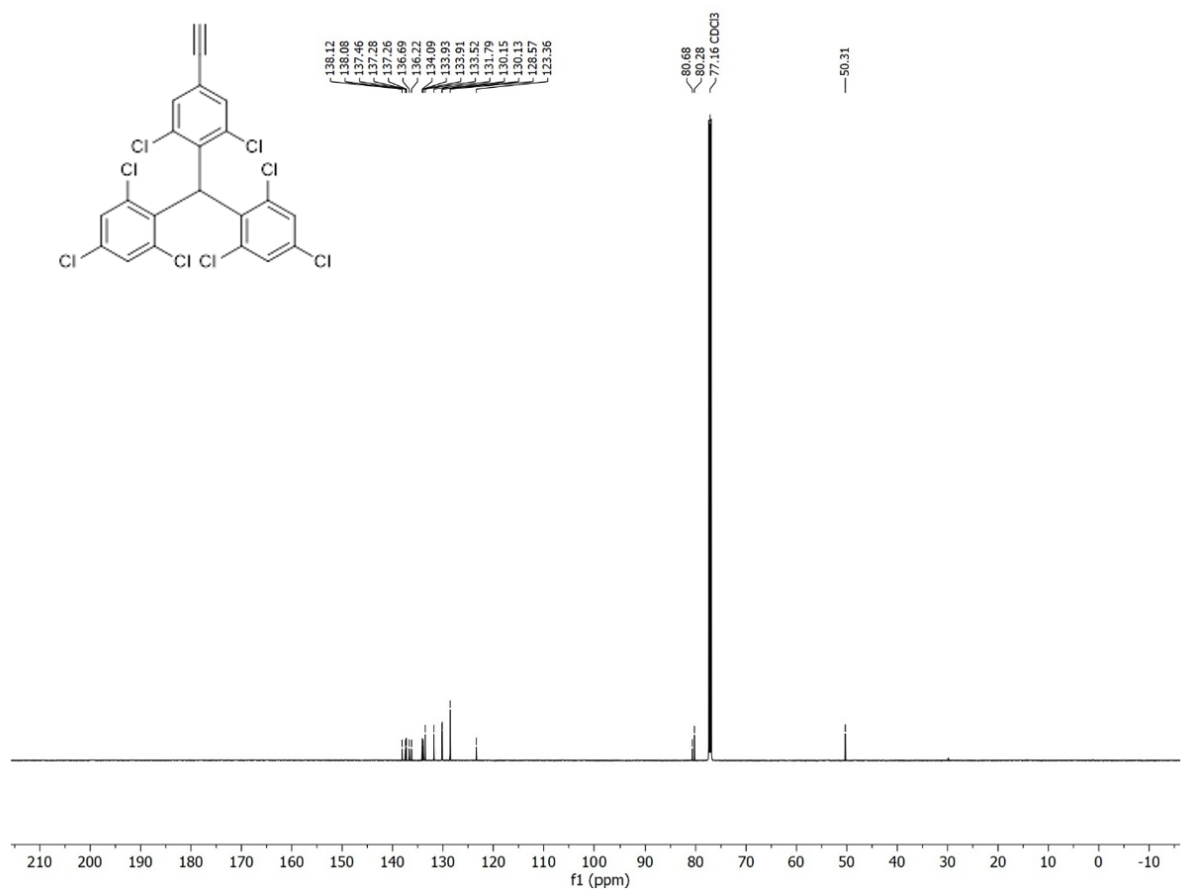
1. NMR Spectra of New Closed-Shell Compounds

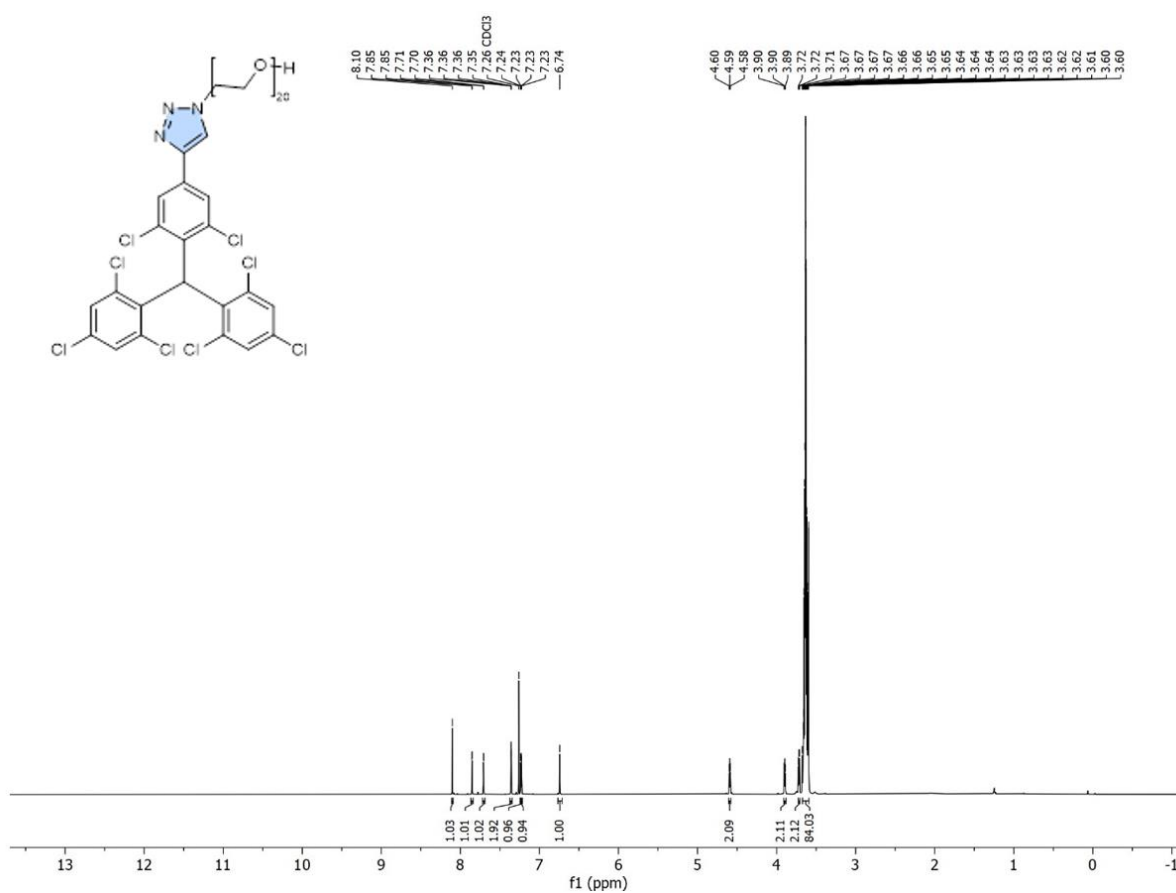
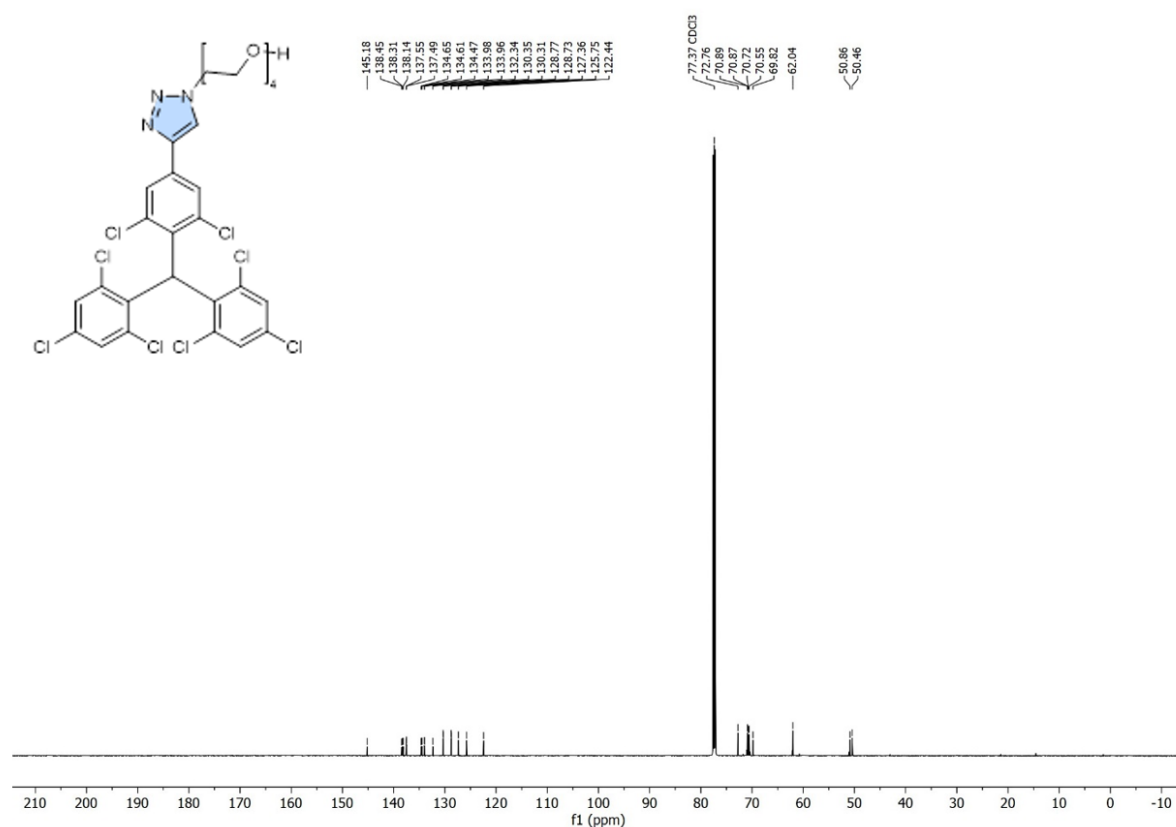












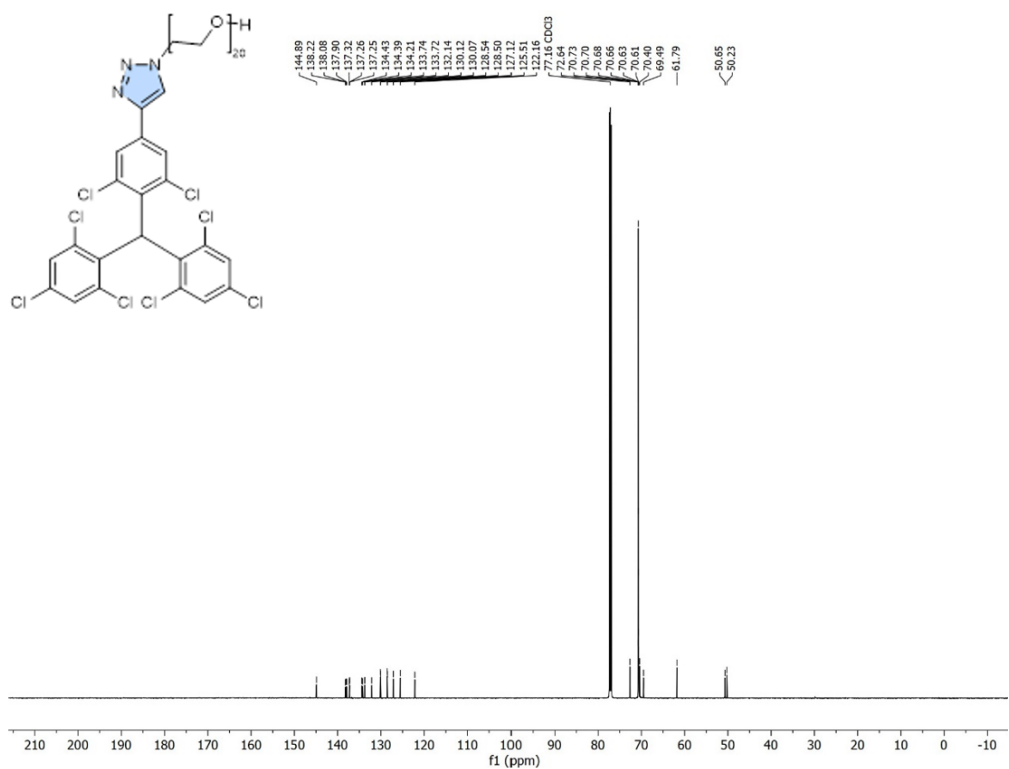


Figure S1: ^1H - and ^{13}C -Spectra of new closed-shell compounds.

2. X-Band EPR Spectra of New Radicals

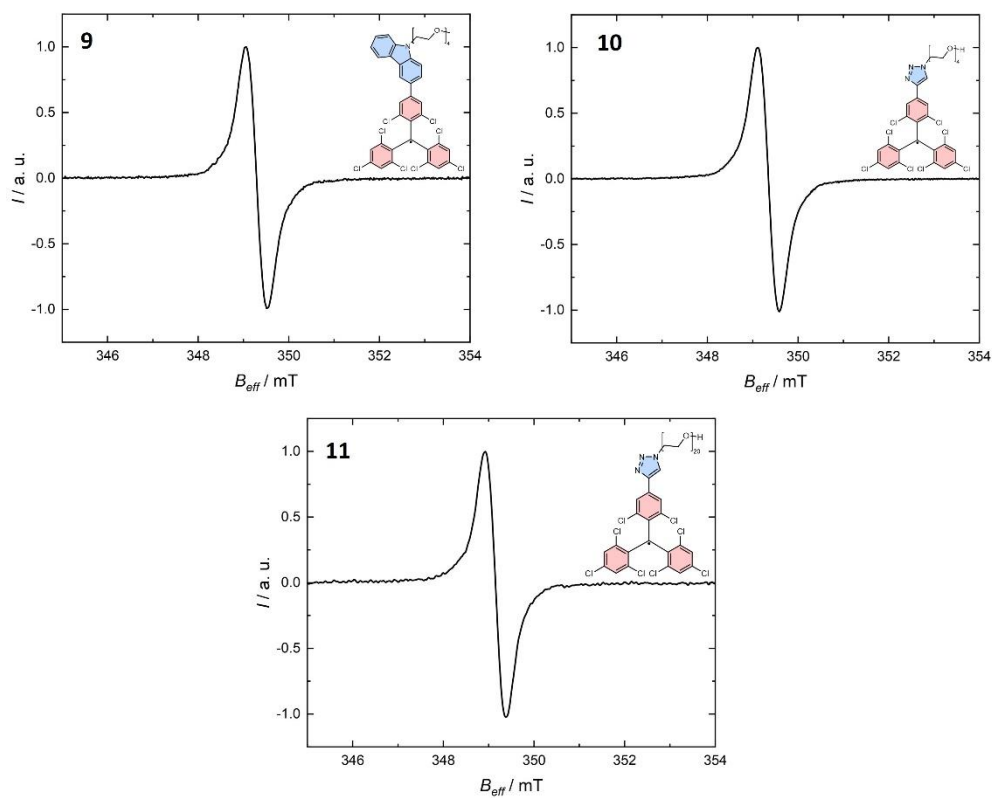


Figure S2: X-Band EPR spectra measured for toluene solutions of the new radicals.

3. Geometries obtained by DFT Calculations

Coordinates D_0 / Å			
	x	y	z
C	-5.14015200	2.93054200	0.31553400
C	-4.68193100	3.73980700	-0.71166400
C	-3.62121600	3.35789900	-1.51720400
C	-3.01889900	2.13506500	-1.27885300
C	-3.43030500	1.26123000	-0.25292000
C	-4.51066200	1.71660200	0.52817000
C	-2.78405600	-0.02749900	-0.02162100
C	-3.59843600	-1.22899900	0.13717700
C	-4.64294600	-1.55804200	-0.74898100
C	-5.42959400	-2.68767300	-0.60642400
C	-5.17401400	-3.53979800	0.45596500
C	-4.16004400	-3.28094000	1.36406400
C	-3.39700100	-2.13928700	1.19367600
Cl	-5.05449000	0.79267900	1.89483000
Cl	-1.76666200	1.66312000	-2.38611200
Cl	-5.45359700	5.26651500	-0.99719200
Cl	-4.93708200	-0.58452200	-2.15722000
Cl	-2.21543600	-1.81272200	2.42420300
Cl	-6.14564400	-4.96261000	0.65523000
C	-1.33400800	-0.11480400	0.05245000
C	-0.55508800	0.77330700	0.82285200
C	0.81982600	0.69455100	0.90628700
C	1.51994900	-0.29233000	0.20503400
C	0.78227400	-1.19024900	-0.57270100
C	-0.59314200	-1.09649900	-0.63742300
Cl	-1.39688700	-2.19013100	-1.72936200
Cl	-1.32820200	1.96616900	1.82947600
C	2.98672100	-0.37828700	0.28184000
C	3.63616800	-1.62213400	0.13226000
C	5.01269700	-1.74839400	0.19819600
C	5.76149900	-0.59343100	0.41880200
C	5.13629900	0.66866400	0.56404500
C	3.75180500	0.76937600	0.49998400
N	7.12531000	-0.44168400	0.53815900
C	7.40793200	0.90242700	0.71110600
C	6.19562100	1.63089400	0.74911100
C	8.64325700	1.53238100	0.84521500
C	8.64411400	2.90890700	1.02749300
C	7.45107100	3.64465200	1.07417800
C	6.22323300	3.01286100	0.93560500
C	8.10569800	-1.47431800	0.29434800
C	8.46607700	-1.55516600	-1.17699700
O	9.43221200	-2.57298200	-1.33377600
C	9.82895000	-2.71285500	-2.68459300
H	-5.95710400	3.24493300	0.95234000
H	-3.28142500	3.98884600	-2.32836100
H	-6.21103900	-2.90621600	-1.32287100
H	-3.97769600	-3.94167000	2.20172900
H	1.34680400	1.38311000	1.55533100
H	1.28478800	-1.94439100	-1.16562900
H	3.04118400	-2.51626000	-0.01894300
H	5.48456800	-2.71811100	0.08586200
H	3.27627700	1.74035600	0.59241900
H	9.57187900	0.97392000	0.80574000
H	9.59229500	3.42593400	1.13437200
H	7.49192400	4.71913200	1.21801600
H	5.29935800	3.58176200	0.96806200
H	7.70245900	-2.42928600	0.63782500
H	8.99624000	-1.26137300	0.88986300
H	8.86865300	-0.59203800	-1.52101100
H	7.57143800	-1.78418400	-1.77313000
H	10.57026300	-3.51221300	-2.72787000
H	10.27619700	-1.78386100	-3.06072900
H	8.97386600	-2.97797000	-3.31950600

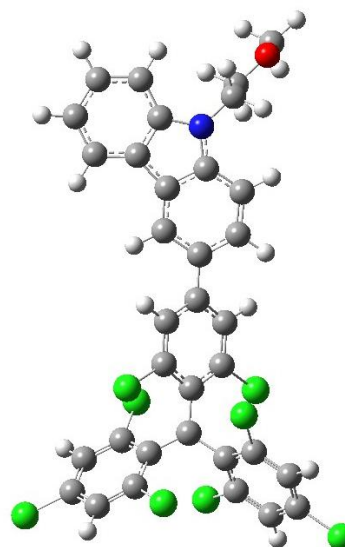


Figure S3: Radical fragment of **9** optimized in its D_0 geometry on the PBE0-GD3(BJ)/6-311++G(d,p), SCRF (SMD, water), level of theory.

Coordinates D ₀ / Å			
	x	y	z
C	2.46611100	3.49407900	-1.05262100
C	3.62210600	3.67245200	-0.30970900
C	4.09540600	2.68767200	0.54230600
C	3.38370300	1.50533400	0.64259600
C	2.20313400	1.25326000	-0.08325600
C	1.78213700	2.29744200	-0.93025000
C	1.46747000	-0.00322300	0.03066200
C	2.18347100	-1.27206800	-0.06620700
C	2.00476600	-2.31042800	0.86923200
C	2.68113000	-3.51566700	0.79929100
C	3.57818700	-3.70961800	-0.23899400
C	3.80313300	-2.73231100	-1.19506400
C	3.10667100	-1.54086500	-1.09567500
Cl	0.40164400	2.08833800	-1.96294800
Cl	3.96251700	0.35215200	1.80490300
Cl	4.49700400	5.16286400	-0.44911600
Cl	0.97231200	-2.08285400	2.24683600
Cl	3.34697500	-0.39632400	-2.37945400
Cl	4.43971200	-5.21049200	-0.34529900
C	0.02724700	0.01165600	0.24135600
C	-0.59138400	0.83611700	1.20420300
C	-1.95581600	0.86508400	1.40829000
C	-2.79389200	0.05103000	0.64522500
C	-2.22550100	-0.78559600	-0.31684500
C	-0.85823500	-0.79497500	-0.50373600
Cl	-0.25761000	-1.78830300	-1.80024400
Cl	0.37608400	1.80392300	2.27939500
C	-4.23427300	0.07816300	0.85203000
C	-5.22812400	-0.65524200	0.23592300
N	-6.36398000	-0.23382900	0.81599400
N	-6.11323700	0.70882500	1.72831500
N	-4.83135400	0.89892200	1.75941100
C	-7.72484800	-0.62200000	0.50156100
C	-8.21834000	0.10216100	-0.73618600
O	-9.54010700	-0.32902700	-0.97295700
C	-10.09770000	0.29882400	-2.11256300
H	2.11306600	4.26188400	-1.72905400
H	4.98862400	2.84254300	1.13389600
H	2.52464600	-4.27766800	1.55217300
H	4.49118400	-2.89944400	-2.01373500
H	-2.37171200	1.50546200	2.17556400
H	-2.84852400	-1.41630400	-0.93925100
H	-5.21785900	-1.41498900	-0.52948100
H	-8.33987000	-0.37377600	1.36679500
H	-7.74566500	-1.70206200	0.34957900
H	-7.57700200	-0.13595000	-1.59623000
H	-8.19086200	1.18860500	-0.57487200
H	-11.11295600	-0.08222700	-2.23051900
H	-9.51614000	0.06506700	-3.01323600
H	-10.13226100	1.38779500	-1.98268200

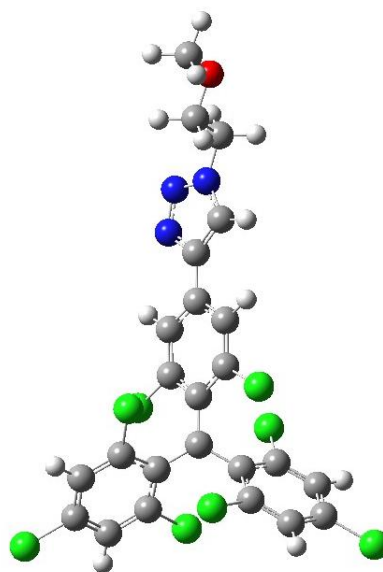


Figure S4: Radical fragment of **10** and **11** optimized in its D₀ geometry on the PBE0-GD3(BJ)/6-311++G(d,p), SCRf (SMD, water), level of theory.

4. Lippert-Mataga Plots

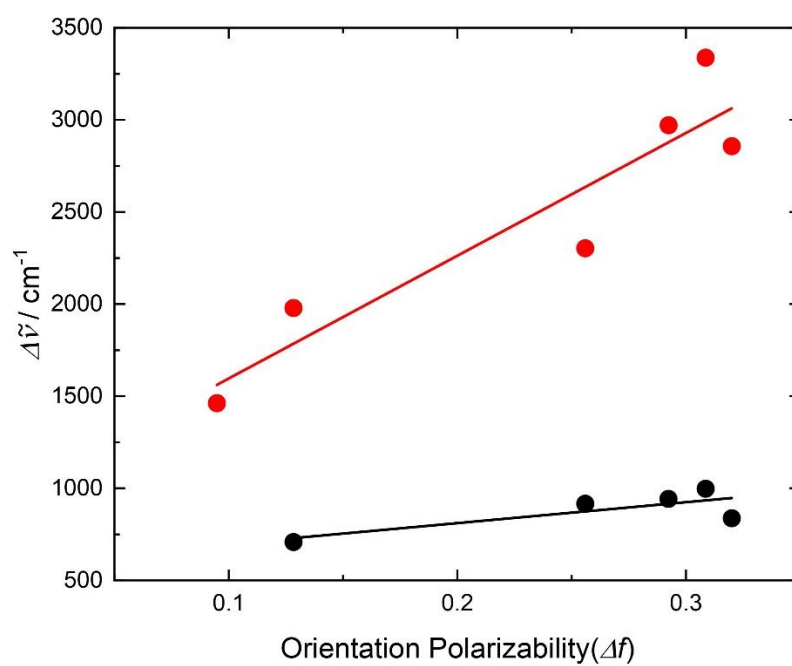


Figure S5: Lippert–Mataga plots of radicals **9** (red) and **10** (black). The Stokes shift is plotted against the orientational polarizability Df of the solvents. While the excited state of **9** has charge transfer character as represented by the slope of the linear fit, the almost horizontal fit indicates LE behavior for **10**.

5. DLS Measurements

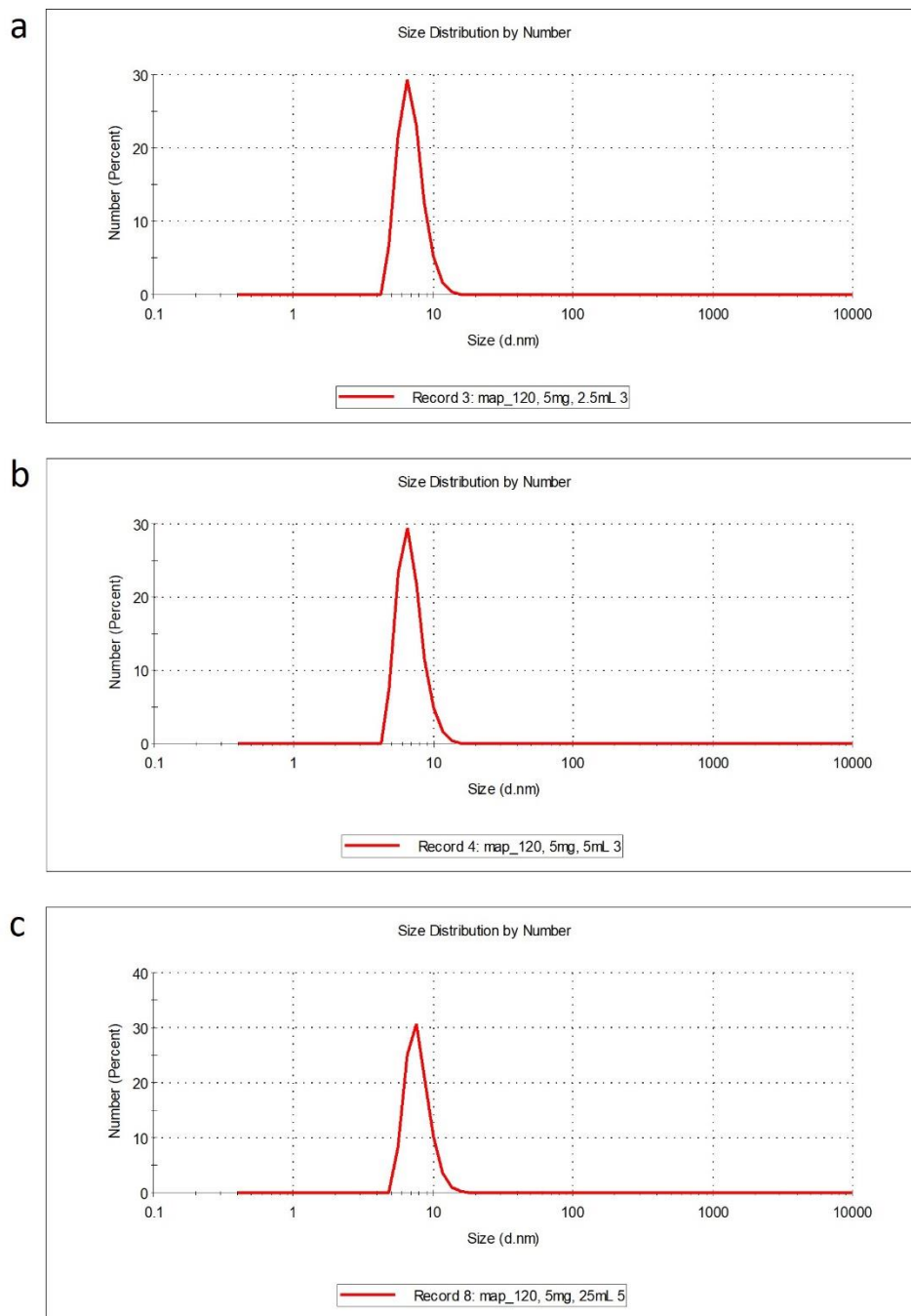


Figure S6: DLS measurements of solutions of 5 mg **8** in 2.5 mL (a), 5 mL (b), and 25 mL (c) water.