

# **Correlation of molecular structure of host materials with lifetime and efficiency of blue phosphorescent organic light-emitting diodes**

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## Experimental

We used Shimadzu, Model UV-2501PC instrument for ultraviolet-visible (UV-vis) measurement. Tetrahydrofuran solution with a sample concentration of  $1 \times 10^{-5}$  M was used for the UV-vis measurement. We used fluorescence of F-7000 instrument of HITACHI for photoluminescence (PL) spectra. The same solution for UV-vis measurement was used in the solution PL measurement and the temperature of low temperature PL measurement was 77K. B09054 cyclic voltammetry of IVIUM Technology was used to measure electron affinity and ionic potential. Ag/AgCl, carbon and platinum wire electrodes were used as reference, working and counter electrodes, respectively. Electrolyte of the electrochemical measurements was 0.1 M tetrabutylammonium perchlorate solution in acetonitrile. Scan rate was 0.1 mV/s.

List of table

Table 1. Summarized photophysical data of the compounds.

Table 1. Summarized photophysical data of the compounds.

	BCzDBT	BCzDBF	BCzBP
Molar concentration (mol/L)	0.00001	0.00001	0.00001
Cell length (cm)	1	1	1
Absorbance	0.887481	0.887256	0.743134
Epsilon (1/cm·M)	$8.87 \times 10^4$	$8.87 \times 10^4$	$7.43 \times 10^4$
Lambda absorption (nm)	240	300	250
Lambda emission (nm)	407	407	406

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Figure S1.  $^1\text{H}$  NMR spectrum of BCzDBT.

Figure S2.  $^1\text{H}$  NMR spectrum of BCzDBF.

Figure S3.  $^1\text{H}$  NMR spectrum of BCzBP.

Figure S4.  $^{13}\text{C}$  NMR spectrum of BCzDBT.

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Figure S6.  $^{13}\text{C}$  NMR spectrum of BCzBP.

Figure S7. Mass spectrum of BCzDBT.

Figure S8. Mass spectrum of BCzDBF.

Figure S9. Mass spectrum of BCzBP.

Figure S10. Solution PL in THF and Toluene of BCzDBT.

Figure S11. Solution PL in THF and Toluene of BCzDBF.

Figure S12. Solution PL in THF and Toluene of BCzBP.

Figure S13. The Cartesian coordinates (x,y,z) of BCzDBT

Figure S14. The Cartesian coordinates (x,y,z) of BCzDBF

Figure S15. The Cartesian coordinates (x,y,z) of BCzBP.

Figure S1

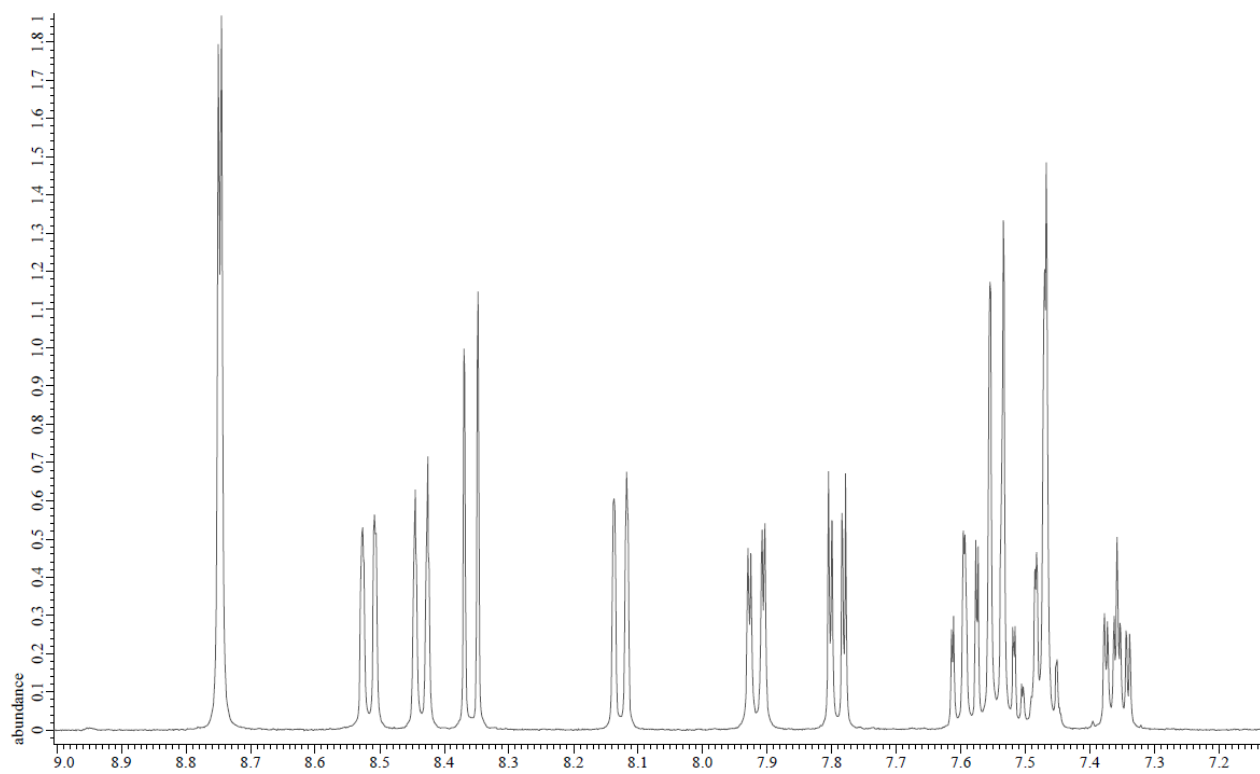
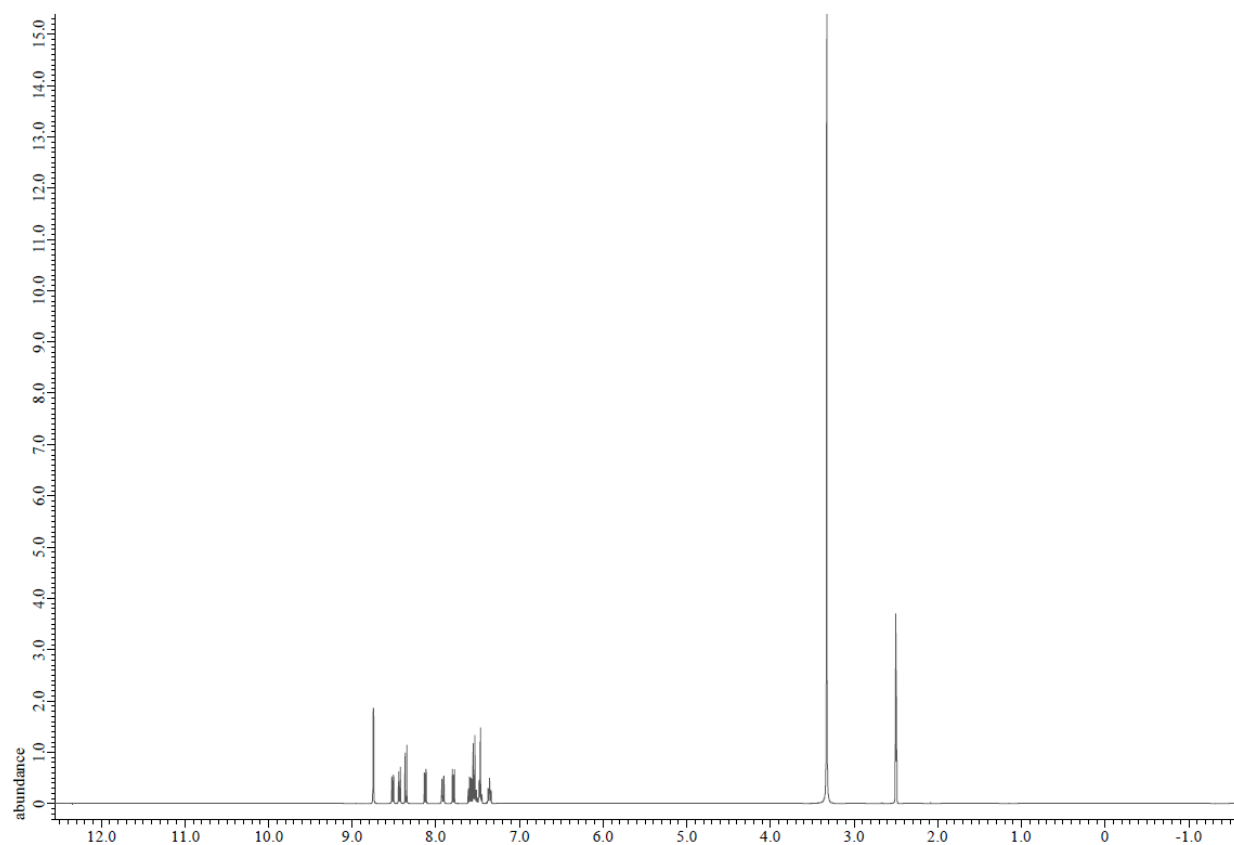


Figure S2

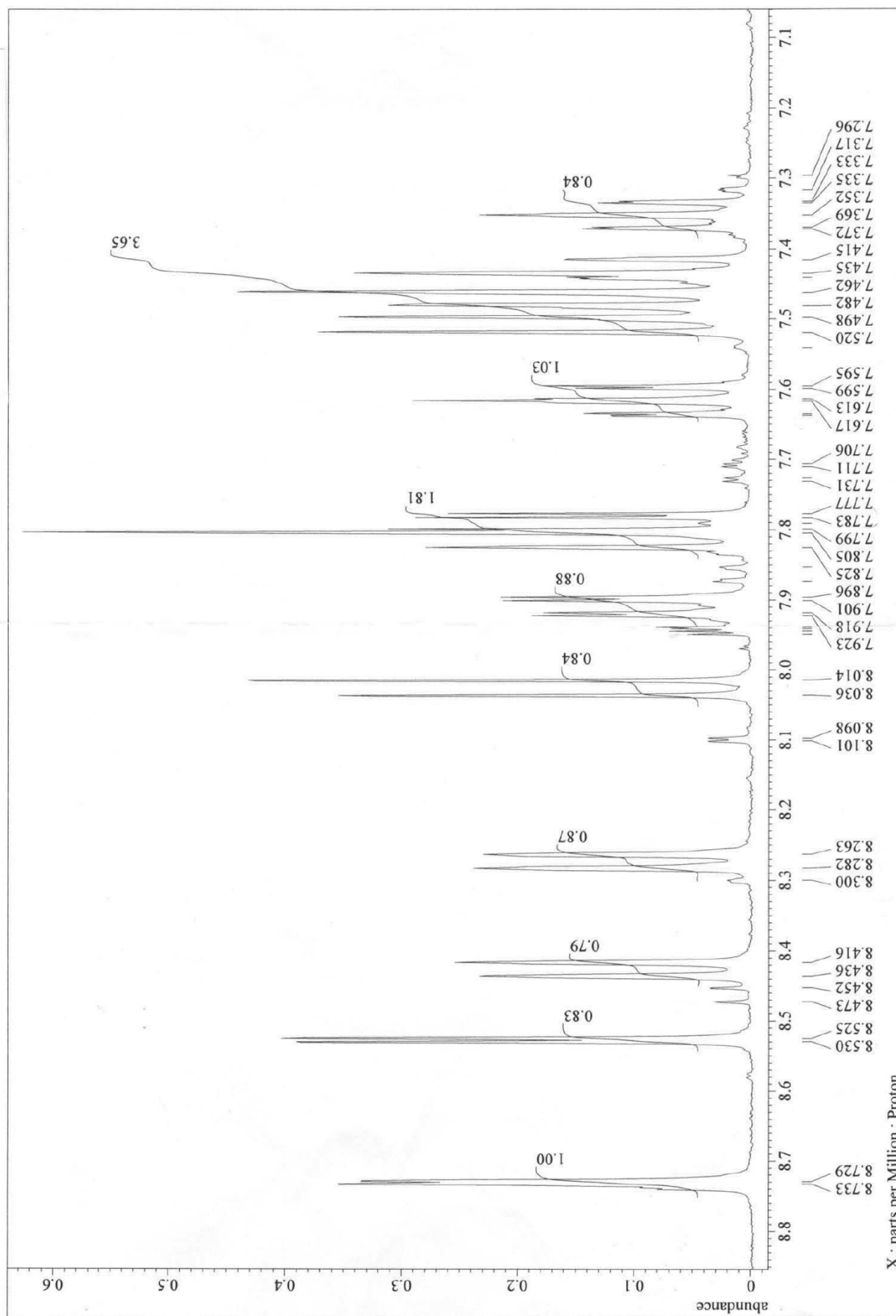


Figure S3

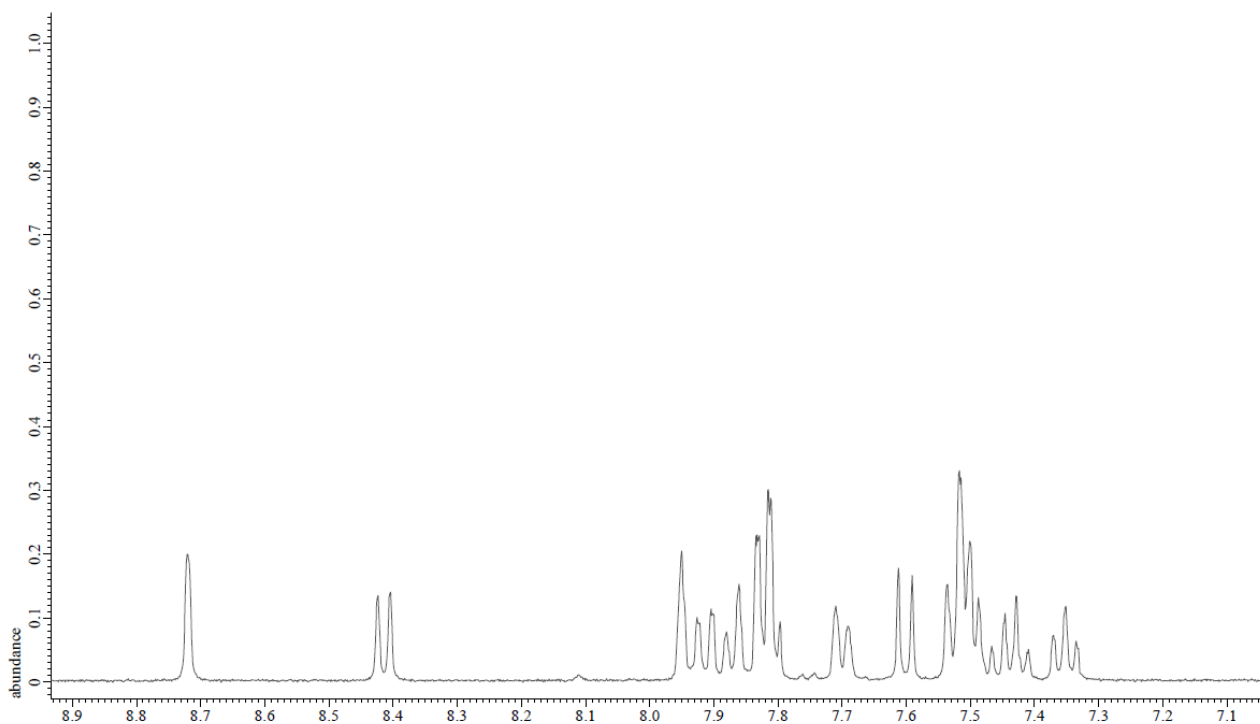
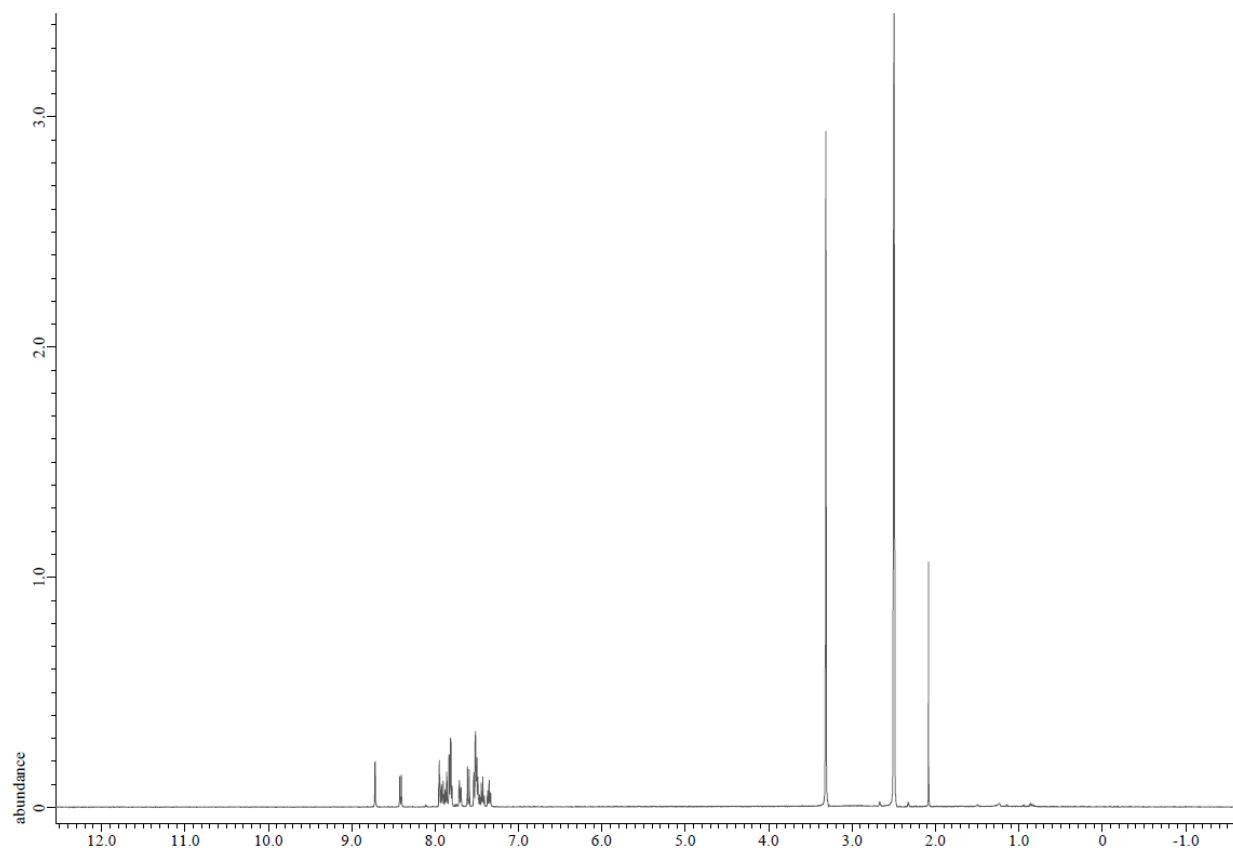




Figure S4

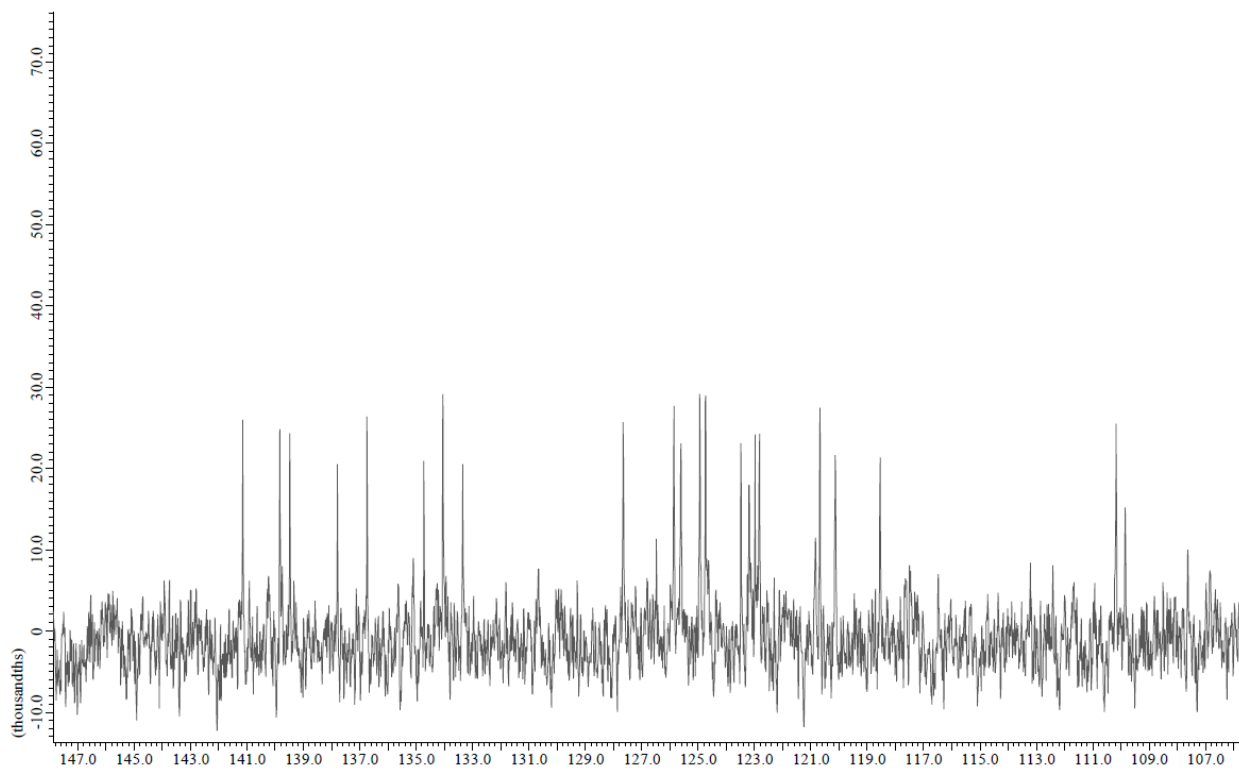
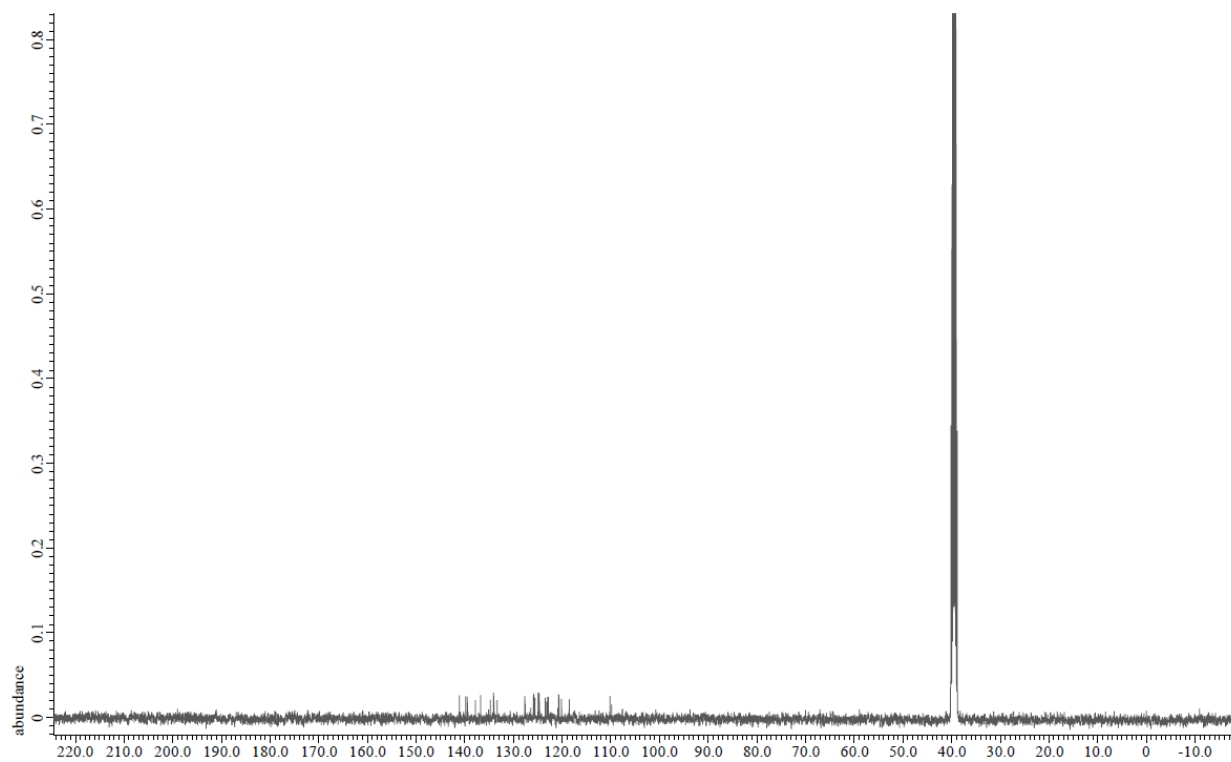


Figure S5

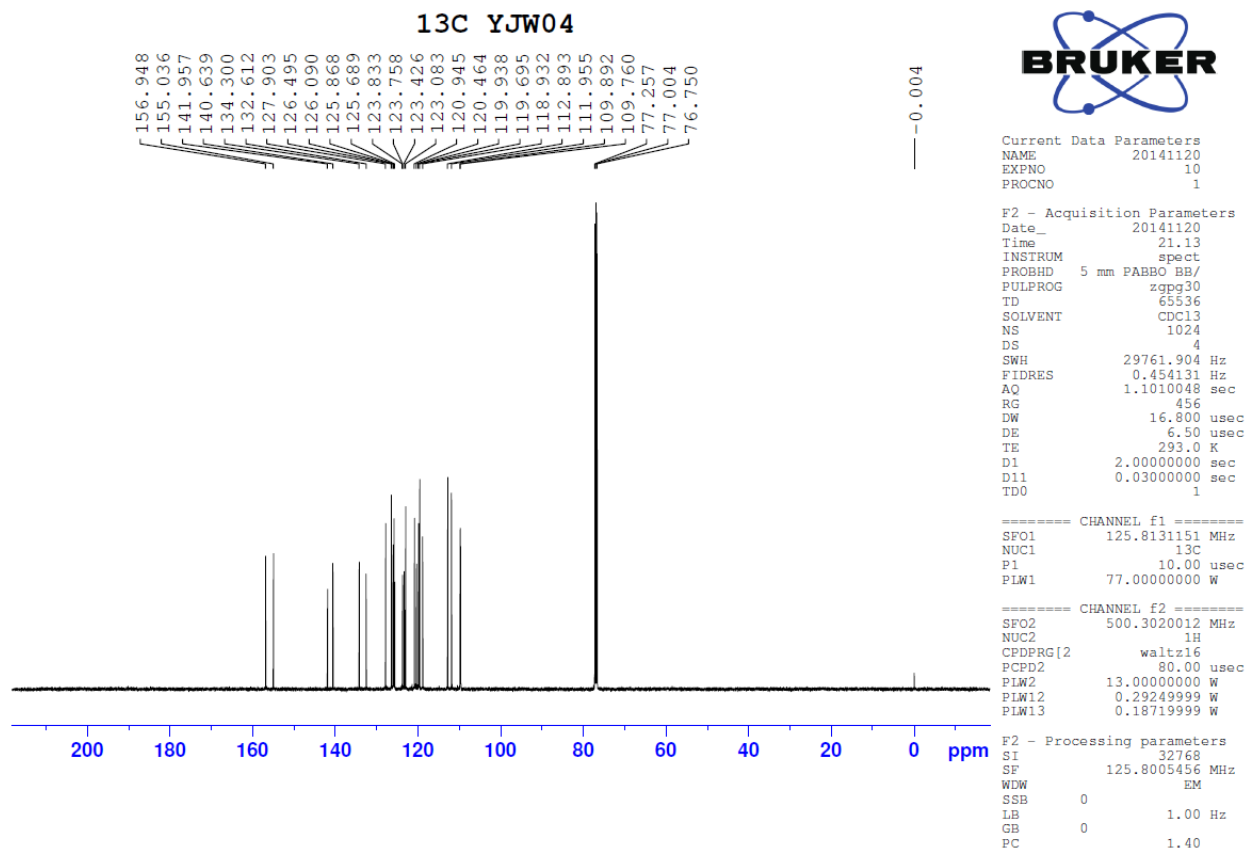


Figure S6

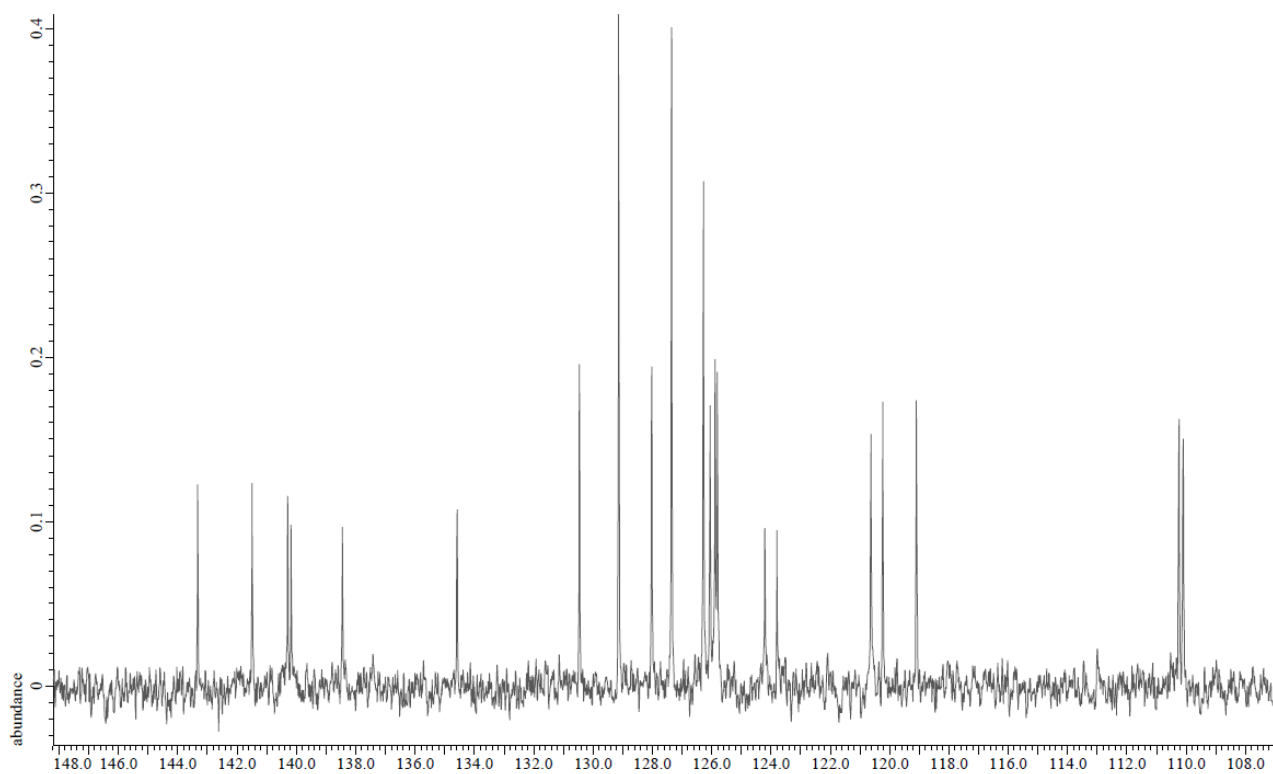
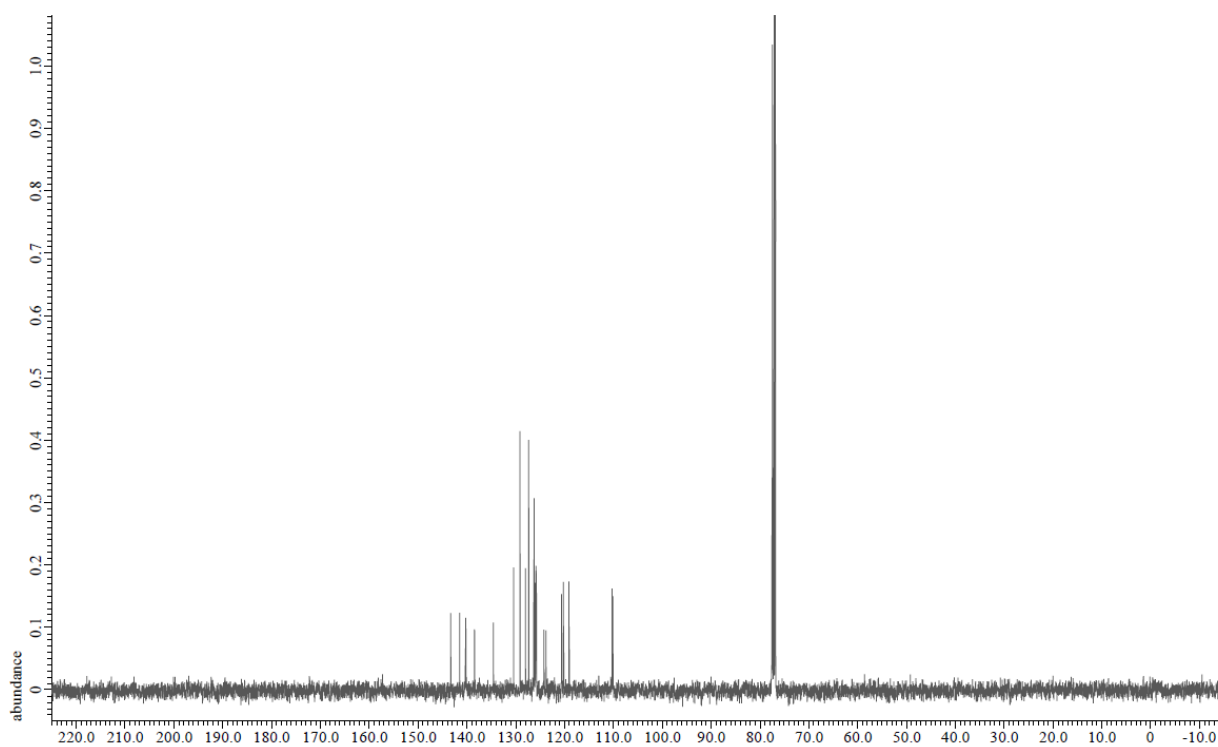


Figure S7

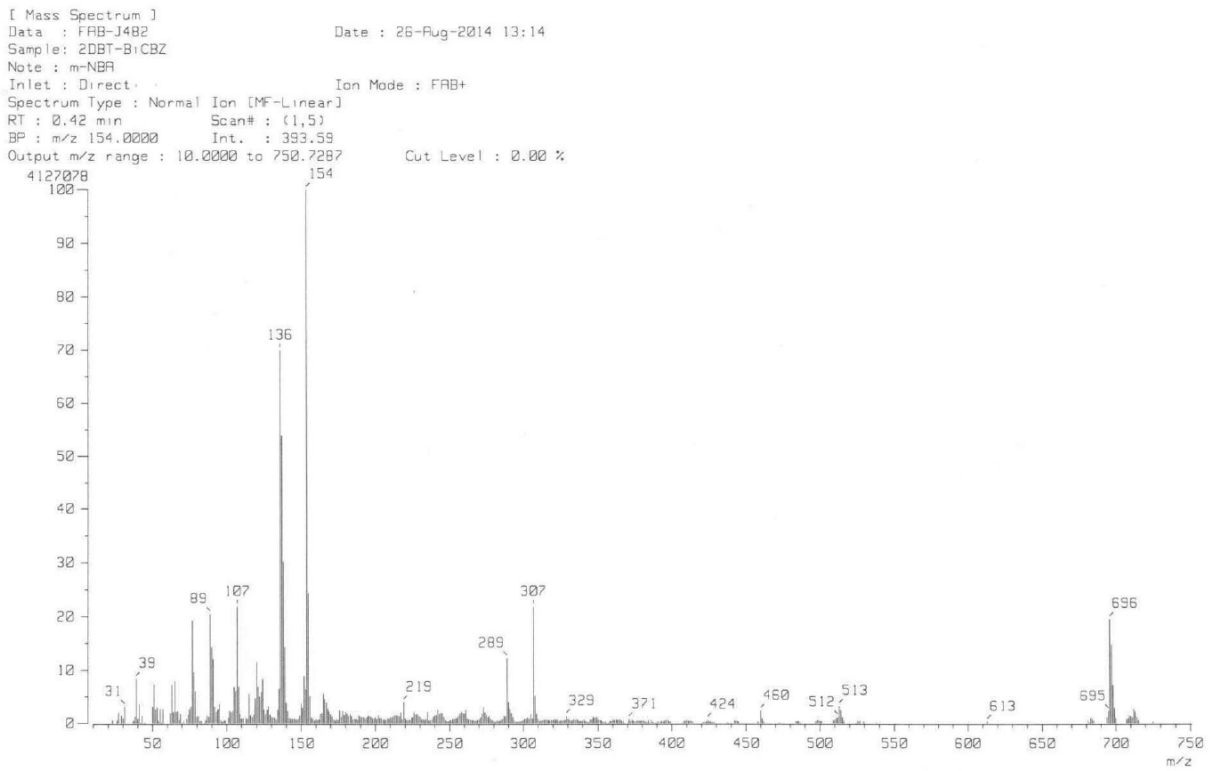


Figure S8

Spectrum RT 7.59 - 7.64 (8 scans) - Background Subtracted 1.72 - 3.29  
yiw04 2015.07.28 15:39:37 ;  
APCI + Max: 6.6E5

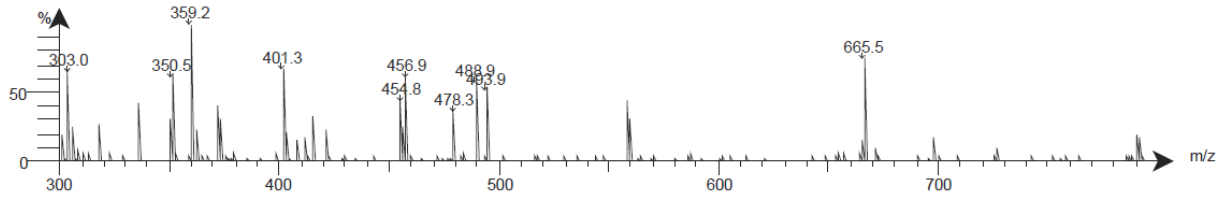


Figure S9

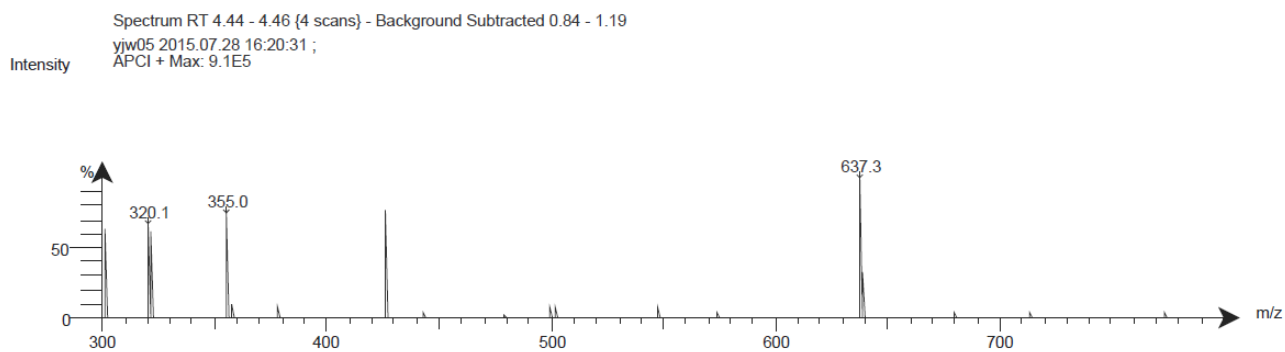


Figure S10

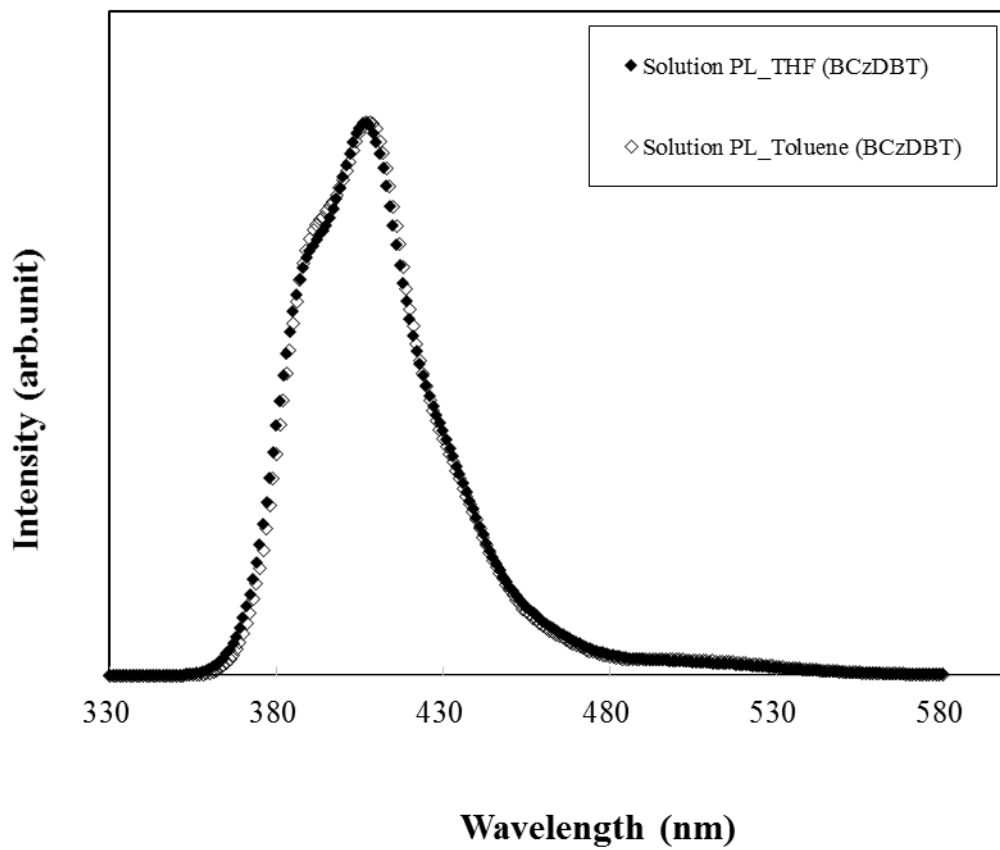


Figure S11

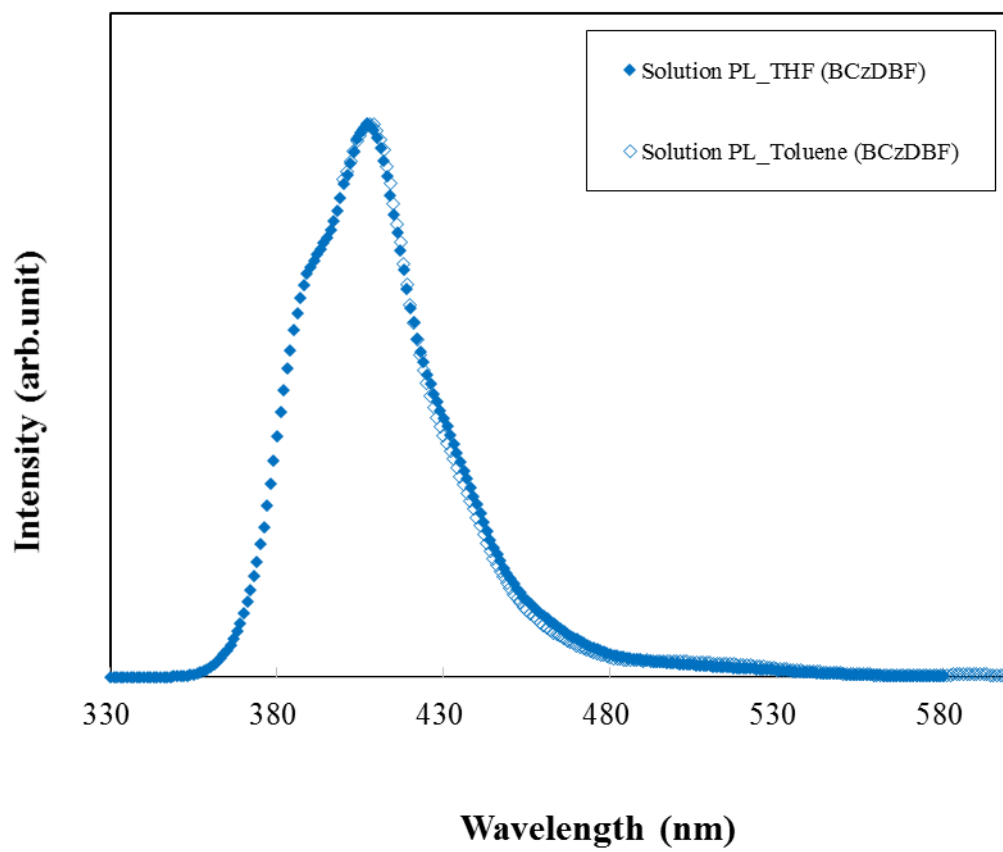




Figure S12

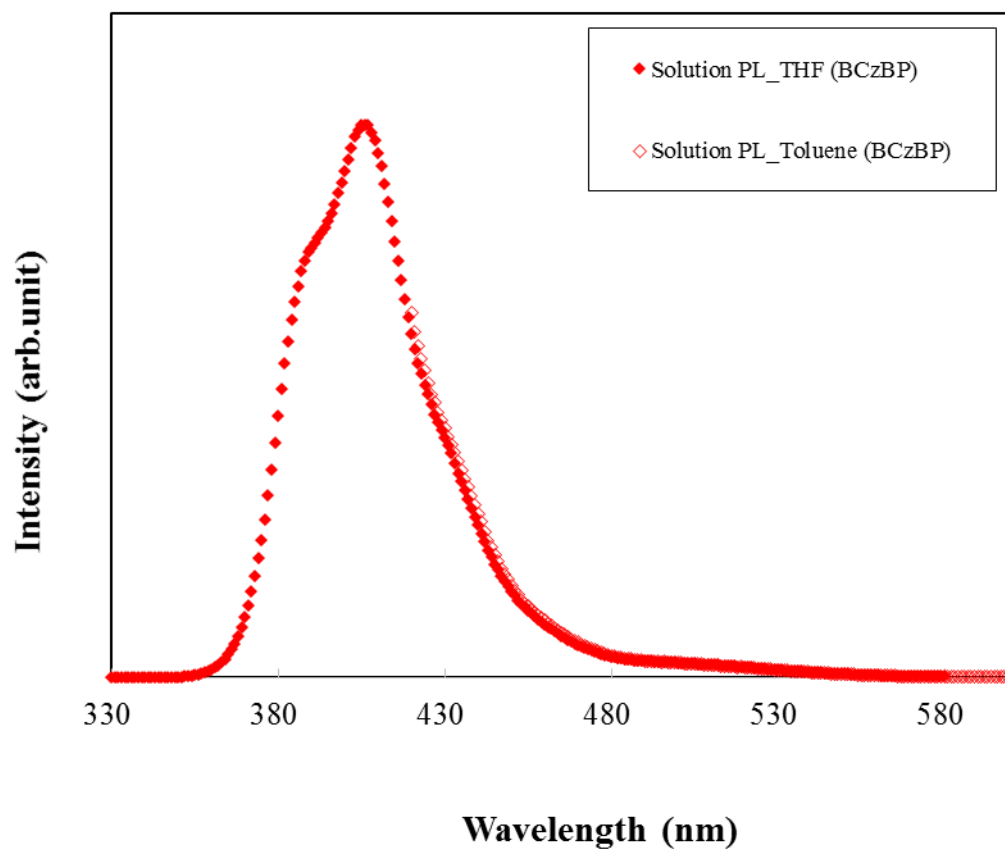


Figure S13

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C	-7.870805000	1.595421000	-1.009903000
C	-7.027531000	1.564838000	0.123757000
C	-7.344730000	2.621411000	1.072264000
C	-6.739474000	2.914894000	2.303704000
C	-7.201778000	3.983711000	3.062932000
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Figure S14

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C	3.822561000	-4.634175000	-0.787837000
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C	7.724365000	0.878311000	-2.007432000
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C	8.570211000	3.362254000	0.376208000
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C	8.926623000	4.910837000	2.132705000
C	7.880209000	4.318525000	2.860003000
C	7.168382000	3.237025000	2.344595000
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H	-1.070447000	0.629043000	-1.452320000		
H		-3.528036000		0.651549000	-1.228831000

Figure S15

C	3.961376000	2.443014000	-0.692728000
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C	7.767405000	-2.720415000	-1.144078000
C	7.846403000	-1.807019000	-0.079217000
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C	9.353493000	-3.173664000	1.399668000
C	10.355212000	-3.278116000	2.363478000
C	10.938459000	-2.128355000	2.898905000
C	10.510540000	-0.873443000	2.461952000
C	9.509415000	-0.769660000	1.497497000
C	6.880366000	-0.792053000	0.000090000
C	3.522844000	0.188287000	-0.821506000
C	2.900630000	1.456521000	-0.711086000
C	1.507524000	1.542136000	-0.642323000
C	0.727919000	0.378972000	-0.670597000
C	-0.753975000	0.452323000	-0.593228000
C	-1.559045000	-0.413984000	-1.370081000
C	-2.949042000	-0.375190000	-1.332832000
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C	-2.779500000	1.439931000	0.303793000
C	-3.710646000	2.243597000	1.069311000
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C	-4.688539000	3.867564000	2.553492000
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N	-4.912443000	0.805448000	-0.253935000
C	-5.999859000	0.120081000	-0.859979000
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C	-8.032194000	-1.208609000	-0.634194000
C	-9.037983000	-1.888653000	0.222626000
C	-9.451140000	-1.322149000	1.440169000
C	-10.395140000	-1.960040000	2.243376000
C	-10.947756000	-3.178891000	1.845905000
C	-10.546723000	-3.754310000	0.638902000
C	-9.601835000	-3.116506000	-0.163298000
C	-8.131930000	-1.242789000	-2.035444000
C	-7.179938000	-0.609917000	-2.832610000
C	-6.116339000	0.081842000	-2.254609000
C	-1.384713000	1.376564000	0.249212000
C	1.382451000	-0.871884000	-0.766526000
C	2.766639000	-0.986228000	-0.841435000
H	3.049403000	4.398364000	-0.545782000
H	5.228566000	5.590014000	-0.581858000
H	7.348795000	4.323840000	-0.773475000
H	7.347211000	1.847339000	-0.916339000
H	5.042448000	-1.487019000	-2.780466000
H	6.719165000	-3.320952000	-2.923727000
H	8.516624000	-3.501001000	-1.236715000
H	8.886858000	-4.074391000	1.010707000
H	10.673757000	-4.260040000	2.703421000
H	11.718765000	-2.209502000	3.650706000
H	10.962360000	0.028281000	2.866761000

H	9.201808000	0.211901000	1.147532000
H	6.883289000	-0.103252000	0.838598000
H	1.024448000	2.513943000	-0.587818000
H	-1.074514000	-1.120483000	-2.037944000
H	-3.538674000	-1.053694000	-1.940529000
H	-2.562727000	3.600131000	2.301760000
H	-4.580738000	4.664675000	3.283568000
H	-6.845698000	3.936925000	2.593617000
H	-7.150705000	2.123713000	0.928324000
H	-6.814554000	-0.525995000	1.016211000
H	-9.046206000	-0.361949000	1.747549000
H	-10.705114000	-1.499432000	3.177645000
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H	-10.963357000	-4.707581000	0.324396000
H	-9.276284000	-3.587315000	-1.086695000
H	-8.974643000	-1.745882000	-2.500084000
H	-7.279265000	-0.635039000	-3.914326000
H	-5.387400000	0.600242000	-2.869235000
H	-0.785661000	2.024613000	0.883035000
H	0.784051000	-1.778274000	-0.752455000
H	3.239429000	-1.961353000	-0.896465000