

Supporting Information

Consecutively Cross-dehydrogenative C-O and C-N Construction for Synthesis of Polyarene with AIE Properties under Electrochemical Condition involving Oxygen Radical Species.

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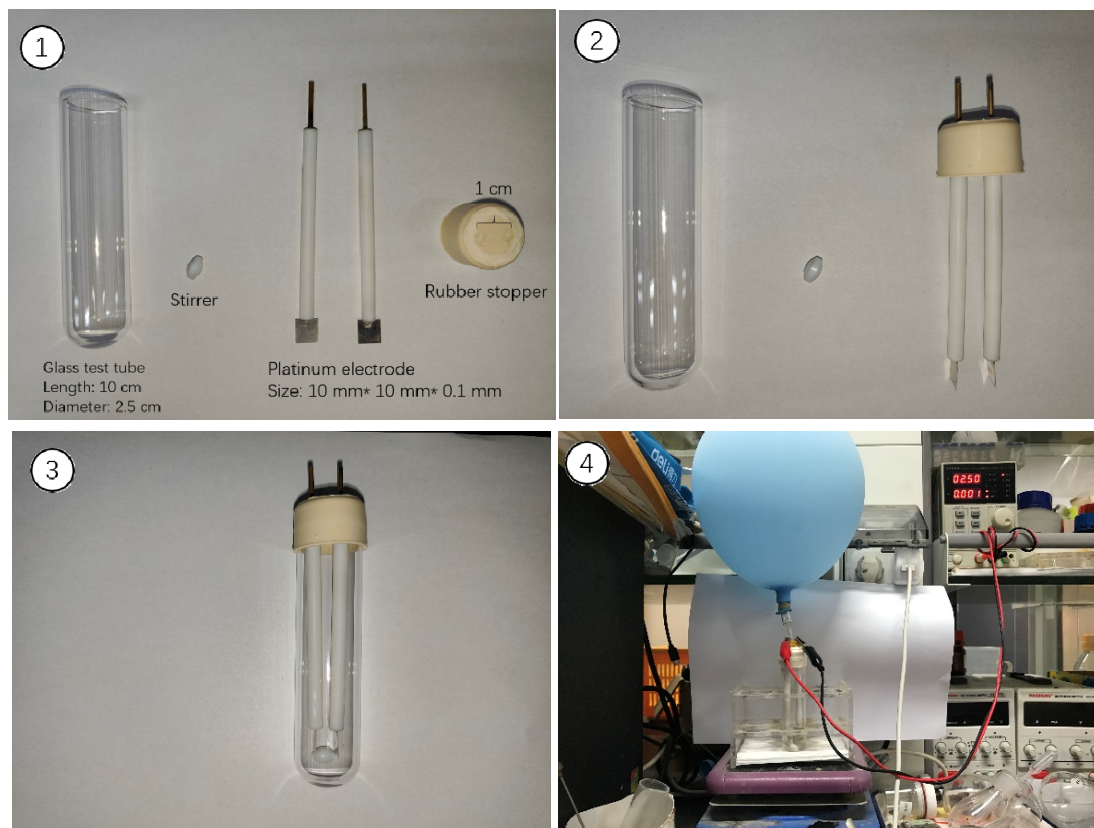
Pengju Feng Email: pfeng@jnu.edu.cn;

1. Materials and Methods:

All commercially available reagents were used without further purification. Analytical grade solvents were bought from Energy Chemical Co., LTD and used without processed. The reactions were carried out under constant cell potential (otherwise noted), an ambient atmosphere, magnetically stirred, and monitored by thin layer chromatography (TLC), visualized by fluorescence quenching under UV light. Flash chromatography was performed on silica gel (200-300 mesh). Cyclic voltammograms were recorded on a CHI 660E potentiostat. The UV spectrum was recorder on a UV-visible absorption instrument (Model: FLA4000, Version: VER 6.0). The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The Both anode electrode and cathode electrode are platinum plate electrodes (10 mm×10 mm×0.1 mm or 30 mm×30 mm×0.1 mm). All deuterated solvents were purchased from Meryer (Shanghai) chemical technology Co., LTD. NMR spectra were recorded on a Bruker Ascend 300 spectrometer operating at 300 MHz for ¹H acquisitions, 75 MHz for ¹³C acquisitions and 282 MHz for ¹⁹F acquisitions. Chemical shifts were referenced to the residual proton solvent peaks (¹H: CDCl₃, δ 7.26; (CD₃)₂SO, δ 2.50; CD₃OD, δ 3.31; CD₃CN, δ 1.94), solvent ¹³C signals (CDCl₃, δ 77.16; (CD₃)₂SO, δ 39.52; CD₃OD, δ 49.00), dissolved or external neat PhCF₃ (¹⁹F, δ -63.3 relative to CFCF₃). Signals are listed in ppm, and multiplicity identified as s = singlet, br = broad, d = doublet, t = triplet, q = quartet, m = multiplet; coupling constants in Hz; integration. High-resolution mass spectra were obtained using Agilent LC-UV-TOF mass spectrometer. Yields refer to purified and spectroscopically pure compounds. All the calculations in this study were performed with Gaussian09 D.01.¹ The structures were optimized by the density functional theory (DFT) with (U)B3LYP²-D3^{3,4} functional with basis set def2-SVP⁵ using SMD⁶ continuum solvent model (solvent =HFIP, using the parameters of 2-propanol, except for ϵ set at the HFIP value of 16.7⁷) . Frequency analyses (at 298.15 K and 1 atm) were carried out to confirm that each structure is a local minimum (no imaginary frequency) or a transition state (only one imaginary frequency). All transition states were confirmed by intrinsic reaction coordinate (IRC) calculations were performed to confirm the connection between two correct minima for a transition state. In order to get more accurate electronic energies, the single point energy were calculated at the M06-2x⁸-D3 /def2-TZVP level of theory. The solvation effect of HFIP (using the parameters of 2-propanol, except for ϵ set at the HFIP value of 16.7) was simulated by SMD continuum solvent model at the M06-2x-D3 /def2-TZVP level of theory.

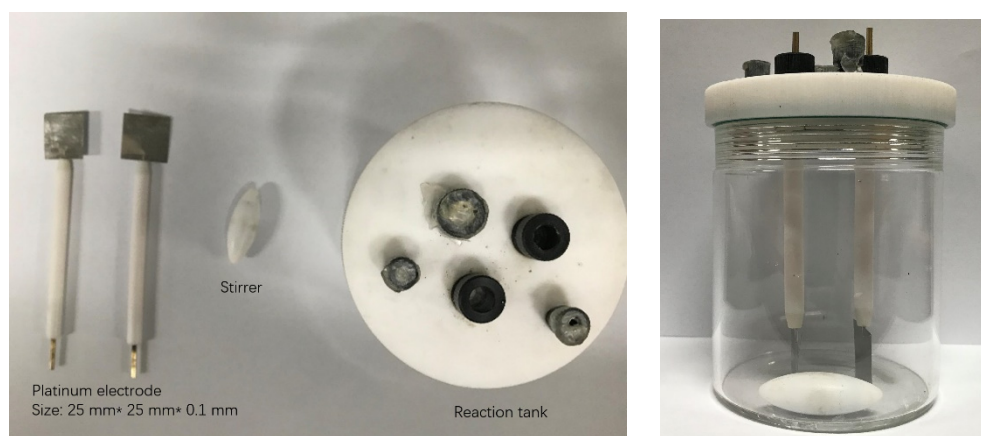
2. Information for reaction set up:

2.1. Small scale reaction:



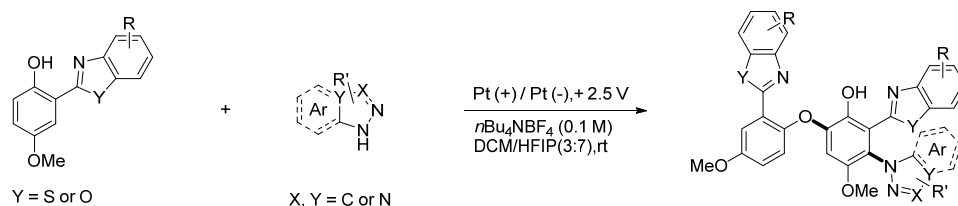
The detail process for home-made electrolysis equipment: 1) Prepare the materials in picture 1 according to the specific information displayed. 2) push the electrode to pass through the rubber stopper and set the distance between the two platinum sheet in 1.2 cm as shown in picture 2. 3) using the rubber stopper to cap on the glass test tube as in picture 3. 4) the reaction set-up was shown in picture 4.

2.2. Large scale reaction:



The large scale reaction setup was using the commercially available equipment bought in Stony-lab (stonyLab.com).

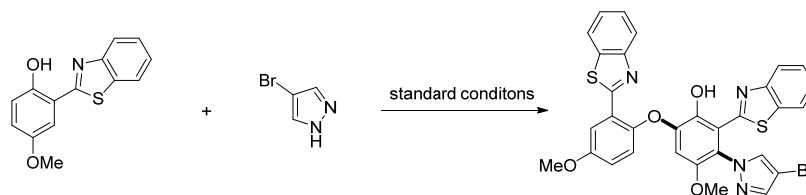
3. General Procedure for Electro-oxidative Azolation



A solution of *phenols* (**1**) (0.25 mmol), *azoles* (**2**) (0.25 mmol) and $n\text{Bu}_4\text{NBF}_4$ (0.5 mmol) in HFIP/DCM = 7/3 (5 mL) was stirred at room temperature in a test tube which was equipped with platinum plate electrodes (1.0 cm×1.0 cm×0.1 mm) as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant cell potential of 2.5 V until the disappearance of **1** (detected by TLC plate under UV lamp) about 7 hours. The electricity was firstly disconnected and the electrode was removed from the test tube before rinsing twice with EtOAc. The reaction mixture was transformed to round bottom flask and was directly concentrated *in vacuo*. The residue was purified by chromatography on silica gel, eluting with Petroleum ether (PE):EtOAc (EA), to afford pure product.

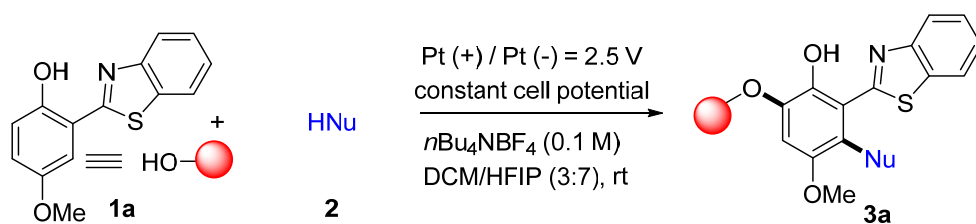
4. Further investigation about this electrochemical transformation.

Table S1 Optimization of Reaction Conditions

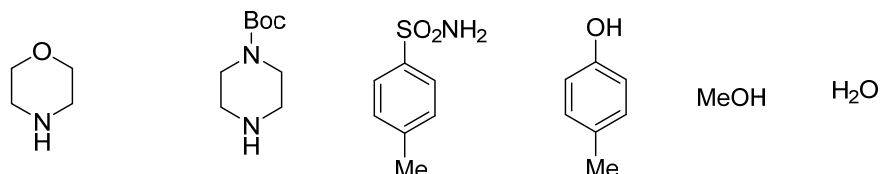


Entry	Variation from standard conditions	Yield(%)
1	RVC(+)/Pt(-)	86
2	Ni(+)/Pt(-)	0
3	Pt(+)/Fe(-)	77
4	Pt(+)/C Cloth(-)	0

Replacing the anode or cathode materials was found crucial for achieving a sufficient consecutive coupling transformation.



HNu:



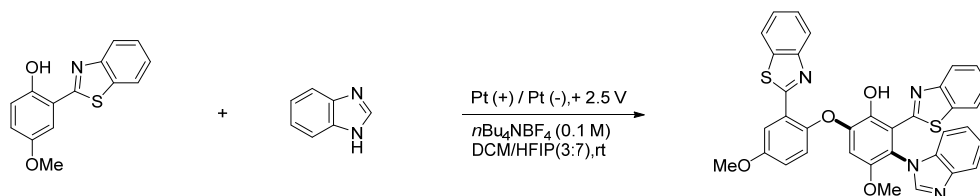
Scheme S1 Tested other Nucleophile for this electrochemical transformation.

We also explored the reaction with sulfonamide, morpholine and other nucleophiles. Unfortunately, no desired product was obtained.

5. Procedure for synthesis of compound 4

A solution of 2-(benzo[d]thiazol-2-yl)-4-methoxyphenol (**1a**) (0.25 mmol), and $n\text{Bu}_4\text{NBF}_4$ (0.5 mmol) in HFIP/DCM = 7/3 (5 mL) was stirred at room temperature in a test tube which was equipped with platinum plate electrodes (1.0 cm×1.0 cm×0.1 mm) as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant cell potential of 2.5 V about 2.5 h. Compound **1a** was still left a lot in the mixed solvent (detected by TLC plate under UV lamp). We found that compound **4** will be over-oxidized if electrolysis is not stopped. The electricity was firstly disconnected and the electrode was removed from the test tube before rinsing twice with EtOAc. The reaction mixture was transferred to round bottom flask and was directly concentrated *in vacuo*. The residue was purified by chromatography on silica gel, eluting with Petroleum ether (PE):EtOAc (EA), to afford pure product **4** as a yellow solid in 45% yield.

6. Procedure for Gram Scale Synthesis



A solution of 2-(benzo[d]thiazol-2-yl)-4-methoxyphenol (1.03g, 4.0 mmol), 1H-benzo[d]imidazole (0.47g, 4.0 mmol) and $n\text{Bu}_4\text{NBF}_4$ (1.0 g, 3.04 mmol) in HFIP/DCM = 7/3 (20 mL) was stirred at room temperature in a test tube which was equipped with platinum plate electrodes (30 mm×30 mm×0.1 mm) as both the anode and cathode. A balloon was connected to the electrolytic cell for collecting H_2 . The

reaction mixture was stirred and electrolyzed at a constant cell potential of 2.5 V until the disappearance of 2-(benzo[d]thiazol-2-yl)-4-methoxyphenol (detected by TLC plate under UV lamp). The reaction mixture was directly concentrated *in vacuo*. The residue was purified by chromatography on silica gel, eluting with Petroleum ether: EtOAc, to afford pure the title product as yellow solid (1.27 g, 99%).

7. Cyclic voltammetry studies

Cyclic voltammograms were recorded on a CHI 660E potentiostat. The cyclic voltammograms of compounds **1a** (SM1), **2j** (SM2), **3j** and **4** were recorded in an electrolyte of *n*Bu₄NBF₄ (0.1 M) in HFIP/DCM (7:3) using a Pt working electrode (diameter, 2 mm), a Pt wire auxiliary electrode and a SCE reference electrode. The scan rate is 100 mV/s (T = 20 °C, c = 0.01M).

The structure of **1a**, **2j**, **3j** and **4**

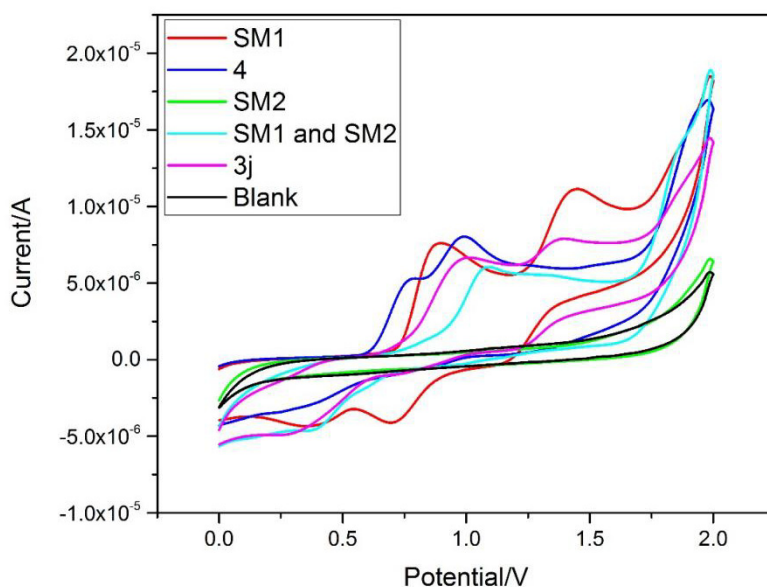
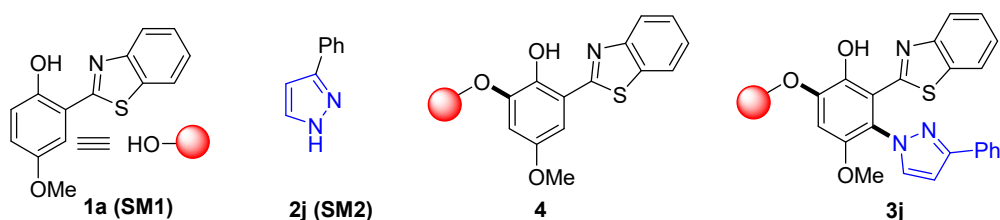


Figure S1 Cyclic voltammetry studies of selected compounds

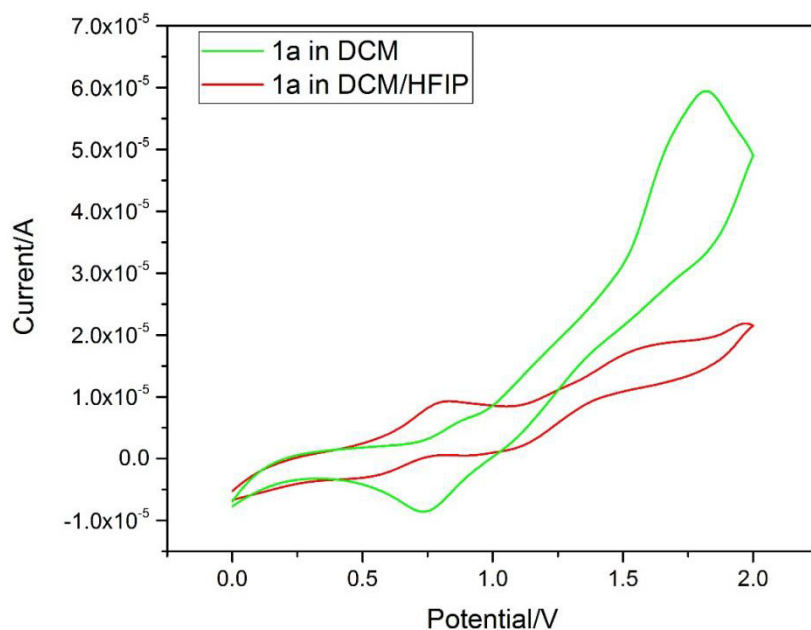
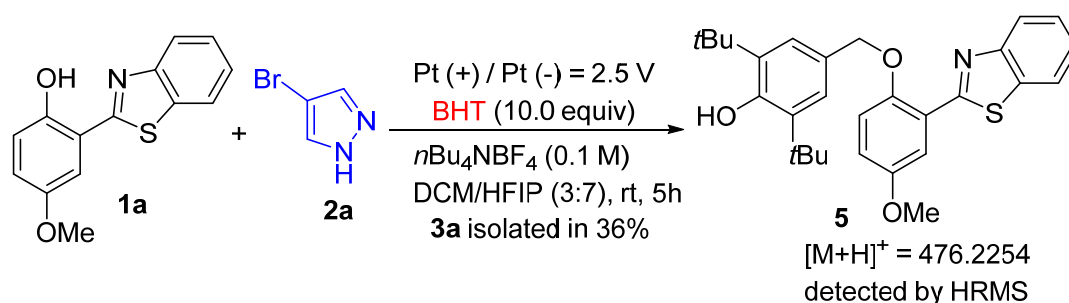


Figure S2 Cyclic voltammetry studies of effect of HFIP

8. Radical capture experiment



A solution of 2-(benzo[d]thiazol-2-yl)-4-methoxyphenol (64.3 mg, 0.25 mmol), 2,6-di-tert-butyl-4-methylphenol **1a** (275.2 mg, 1.25 mmol), bromopyrrole **2a** (36.7 mg, 0.25 mmol) and $n\text{Bu}_4\text{NBF}_4$ (165 mg, 0.5 mmol) in HFIP/DCM = 7/3 (5 mL) was stirred at room temperature in a test tube which was equipped with platinum plate electrodes (10 mm×10 mm×0.1 mm) as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant cell potential of 2.5 V for about 5 hours. The reaction solution was directly draw with a syringe and dilute with methanol. The diluted solution was injected to High resolution liquid chromatography mass spectrometry. Compound **5** was detected by HRMS. We also did CV study about BHT and we found it show higher oxidation potential than the starting materials.

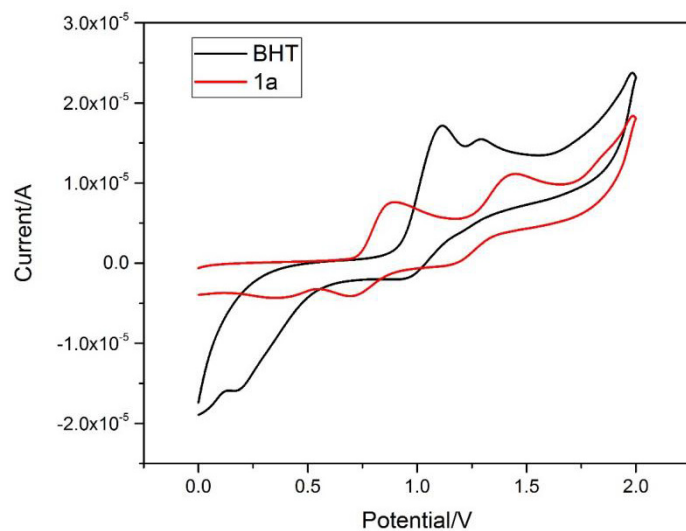


Figure S3 Cyclic voltametry studies of BHT and **1a**

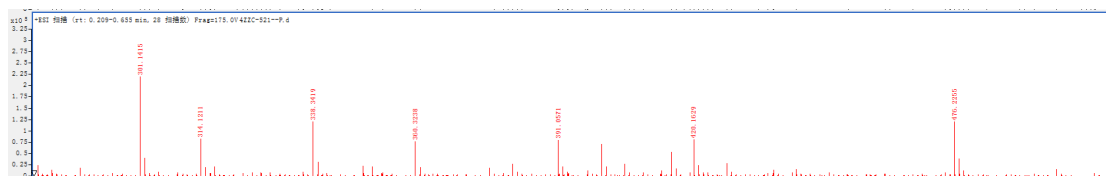
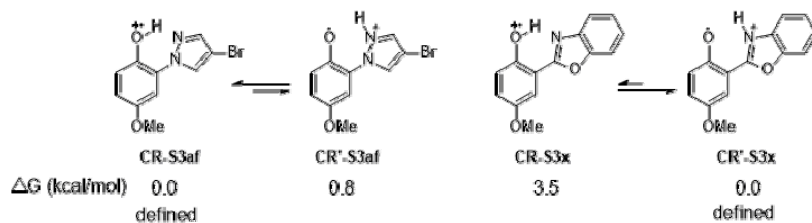


Figure S4 HRMS of compound **5**

9. Computational details



Scheme S2 the corresponding structures for calculation.

Table S2. Calculated energy data and imaginary frequencies for all structure.

	Energy (au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)	Imaginary frequency (cm ⁻¹)
	(U)M06-2x-D3 /def2-TZVP/SMD	(U)B3LYP-D3 /def2-SVP/SMD	(U)B3LYP-D3 /def2-SVP/SMD	(U)B3LYP-D3 /def2-SVP/SMD
CR-S3x	-820.334926	0.238786	0.182779	None
CR'-S3x	-820.340569	0.239364	0.182800	None
CR-S3af	-3220.393027	0.191947	0.138885	None
CR'-S3af	-3220.391695	0.191916	0.138789	None
Pyrazol	-226.204388	0.075993	0.045155	None

S3x	-820.544937	0.238621	0.181923	None
TS-S3x-pyr	-1046.527126	0.315933	0.248059	-329.30
TS'-S3x-pyr	-1046.526359	0.315708	0.247607	-283.04
TS-S3af-pyr	-3446.581868	0.269773	0.20298	-323.97
TS-S3x-OC	-1640.68117	0.480476	0.393385	-273.15
TS-S3x-CC	-1640.673057	0.480735	0.389531	-245.79
TS-S3x-CR-Sub	-1640.858689	0.478238	0.386149	-375.32
TS-S3af-OC	-6440.780306	0.388632	0.304183	-339.75
TS'-S3af-OC	-6440.772798	0.387282	0.301272	-423.24
TS-S3af-CC	-6440.774223	0.388866	0.301426	-325.89

Table S3. Calculated spin populations

	O1	C2	C3	C5	O8
CR-S3x	0.160028	0.227554	0.065545	0.247669	0.164111
CR'-S3x	0.254375	-0.012449	0.223829	0.304585	0.132333
CR-S3af	0.178901	0.258505	0.035044	0.239552	0.140669
CR'-S3af	0.277759	0.059546	0.172797	0.296995	0.120983

Figure S5 The optimized structures and calculated Mulliken spin population for the radical cations.

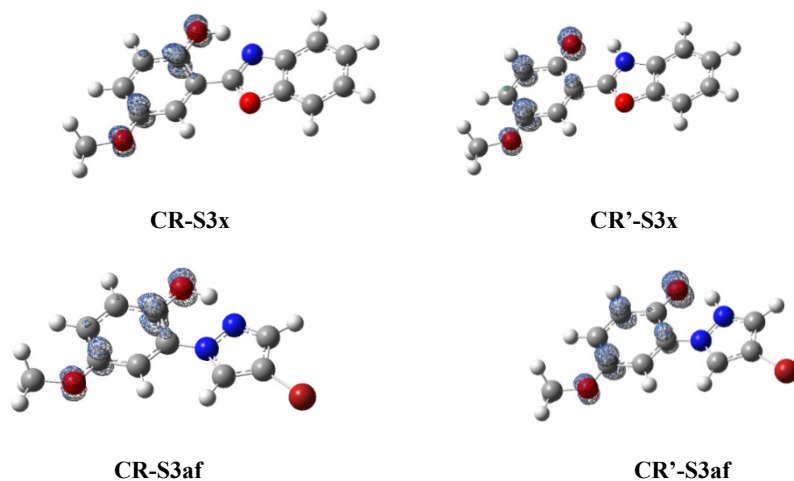
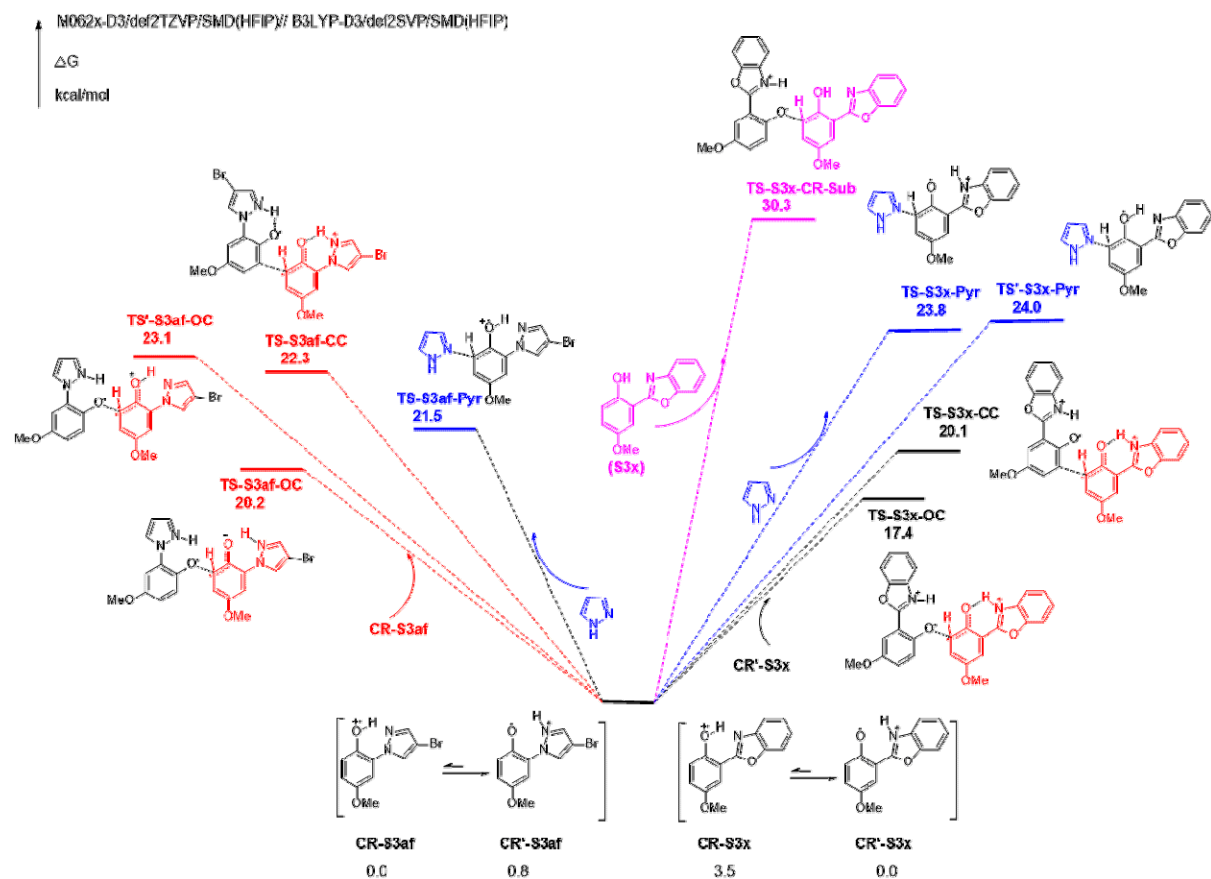
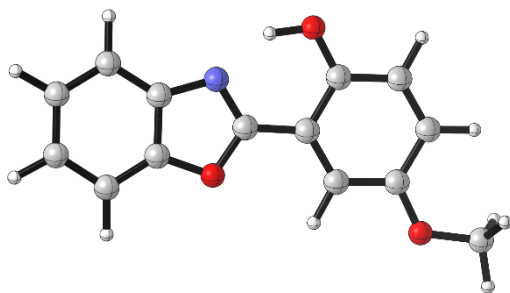


Figure S6 Structure and Relative Free Energies of Cationic Radicals and Transition states.



Cartesian coordinates for all calculated structure

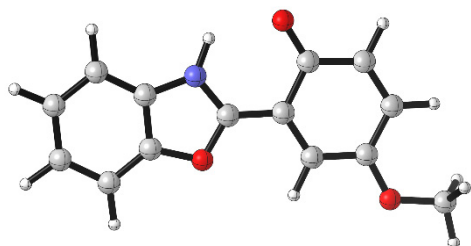
CR-S3x



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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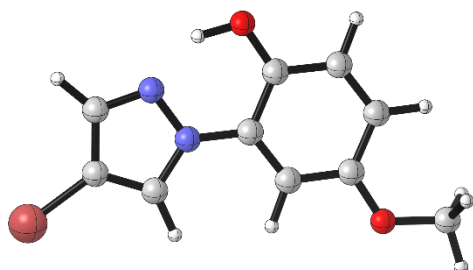
1	6	0	3.672728	0.776040	0.000039
2	6	0	2.804286	1.836194	0.000019
3	6	0	1.392190	1.625248	-0.000022
4	6	0	0.875247	0.268910	-0.000023
5	6	0	1.755435	-0.792513	-0.000015
6	6	0	3.159813	-0.560350	0.000016
7	1	0	4.747741	0.954397	0.000066
8	1	0	3.162583	2.867076	0.000023
9	1	0	1.399161	-1.823567	-0.000020
10	8	0	0.607460	2.664189	-0.000085
11	1	0	-0.367483	2.356372	-0.000163
12	8	0	3.910826	-1.638590	0.000028
13	6	0	5.348344	-1.566569	0.000061
14	1	0	5.702443	-1.049273	0.904682
15	1	0	5.693872	-2.606627	0.000067
16	1	0	5.702483	-1.049271	-0.904544
17	6	0	-0.563366	0.099562	-0.000018
18	6	0	-2.477685	-0.901183	-0.000028
19	6	0	-2.673035	0.493473	0.000026
20	6	0	-3.512264	-1.826532	-0.000054
21	6	0	-3.969777	1.025723	0.000061
22	6	0	-4.800580	-1.282883	-0.000021
23	1	0	-3.327084	-2.901619	-0.000098
24	6	0	-5.023506	0.112779	0.000035
25	1	0	-4.137613	2.104169	0.000104
26	1	0	-5.659890	-1.957801	-0.000040
27	1	0	-6.051532	0.482755	0.000060
28	7	0	-1.421364	1.087526	0.000035
29	8	0	-1.123550	-1.130187	-0.000048

CR²-S3x



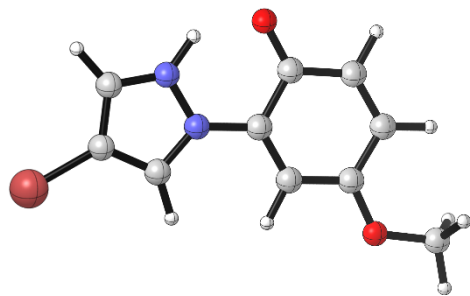
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5	6	0	1.743887	-0.755249	-0.000034
6	6	0	3.149773	-0.571835	-0.000021
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8	1	0	3.274571	2.850871	0.000148
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12	8	0	3.869154	-1.683858	-0.000042
13	6	0	5.302989	-1.640390	-0.000019
14	1	0	5.674541	-1.131766	0.903472
15	1	0	5.632505	-2.686337	-0.000042
16	1	0	5.674569	-1.131717	-0.903470
17	6	0	-0.530444	0.152015	-0.000019
18	6	0	-2.462428	-0.873399	-0.000002
19	6	0	-2.717969	0.503396	-0.000039
20	6	0	-3.459485	-1.836469	0.000025
21	6	0	-4.022080	0.999733	-0.000056
22	6	0	-4.767110	-1.340217	0.000013
23	1	0	-3.231151	-2.902951	0.000055
24	6	0	-5.040252	0.044295	-0.000027
25	1	0	-4.226320	2.071206	-0.000087
26	1	0	-5.600444	-2.046490	0.000034
27	1	0	-6.080263	0.378267	-0.000037
28	7	0	-1.462566	1.099131	-0.000054
29	8	0	-1.092564	-1.054360	0.000001

CR-S3af



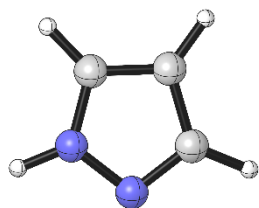
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4	6	0	1.121551	0.441177	0.000064
5	6	0	1.794763	-0.760554	0.000272
6	6	0	3.213736	-0.793167	0.000225
7	1	0	5.061134	0.395090	0.000016
8	1	0	3.846419	2.567113	-0.000445
9	1	0	1.274020	-1.717798	0.000544
10	8	0	1.323656	2.858052	-0.000605
11	8	0	3.748793	-1.994729	0.000408
12	6	0	5.174088	-2.190052	0.000373
13	1	0	5.620816	-1.751047	0.905223
14	1	0	5.320888	-3.276435	0.000464
15	1	0	5.620752	-1.751204	-0.904584
16	6	0	-2.434728	0.056915	0.000074
17	6	0	-2.208601	1.459347	0.000947
18	7	0	-0.911541	1.702585	0.001094
19	7	0	-0.282438	0.496130	0.000185
20	6	0	-1.186876	-0.531015	-0.000368
21	1	0	-2.935342	2.271262	0.001505
22	1	0	-0.892968	-1.576400	-0.001103
23	35	0	-4.093541	-0.816966	-0.000434
24	1	0	0.304908	2.731245	-0.000443

CR²-S3af



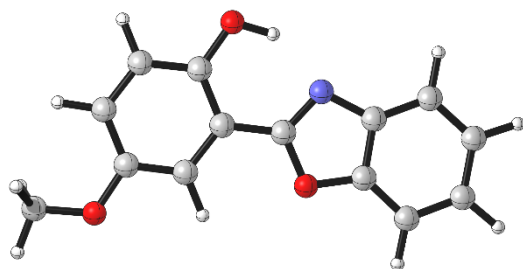
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4	6	0	-1.148500	0.458291	0.000044
5	6	0	-1.809801	-0.746759	-0.000018
6	6	0	-3.229257	-0.783808	0.000006
7	1	0	-5.073357	0.395735	0.000033
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10	8	0	-1.308072	2.850845	0.000101
11	8	0	-3.759444	-1.997463	-0.000038
12	6	0	-5.181121	-2.184225	0.000011
13	1	0	-5.631605	-1.744748	-0.903643
14	1	0	-5.337874	-3.269813	0.000004
15	1	0	-5.631539	-1.744768	0.903708
16	6	0	2.442924	0.069342	-0.000041
17	6	0	2.245345	1.459467	-0.000036
18	7	0	0.932738	1.672861	-0.000025
19	7	0	0.270152	0.495707	0.000010
20	6	0	1.178928	-0.511200	0.000002
21	1	0	2.953811	2.286482	-0.000038
22	1	0	0.883241	-1.556346	0.000029
23	35	0	4.085423	-0.828968	-0.000064
24	1	0	0.308781	2.524379	0.000059

Pyrazol



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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3	6	0	-1.099261	-0.386825	-0.000162
4	7	0	1.017505	-0.383337	-0.000048
5	1	0	1.956838	-0.772972	-0.000098
6	1	0	1.435222	1.714008	-0.000101
7	1	0	-1.340093	1.859048	0.000272
8	1	0	-2.109477	-0.798975	-0.000211
9	7	0	-0.044397	-1.202659	0.000139

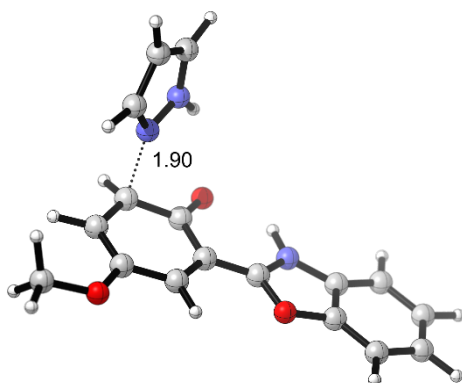
S3x



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.657236	0.718010	-0.000085
2	6	0	2.805061	1.822351	-0.000054

3	6	0	1.412280	1.669890	0.000075
4	6	0	0.879425	0.349887	0.000108
5	6	0	1.743891	-0.759082	0.000100
6	6	0	3.129320	-0.587761	0.000006
7	1	0	4.734626	0.885442	-0.000159
8	1	0	3.213450	2.835513	-0.000075
9	1	0	1.336276	-1.771178	0.000126
10	8	0	0.636449	2.771242	0.000318
11	1	0	-0.315063	2.490643	0.000585
12	8	0	3.880261	-1.724158	-0.000016
13	6	0	5.293943	-1.615613	-0.000113
14	1	0	5.665357	-1.092709	0.899527
15	1	0	5.684192	-2.642913	-0.000111
16	1	0	5.665238	-1.092758	-0.899830
17	6	0	-0.559499	0.176949	0.000088
18	6	0	-2.450056	-0.891020	0.000063
19	6	0	-2.684843	0.495247	-0.000131
20	6	0	-3.456542	-1.846845	0.000116
21	6	0	-3.997719	0.982139	-0.000288
22	6	0	-4.765064	-1.347717	-0.000035
23	1	0	-3.237148	-2.915937	0.000263
24	6	0	-5.028118	0.037631	-0.000233
25	1	0	-4.200236	2.055110	-0.000444
26	1	0	-5.601757	-2.050803	-0.000005
27	1	0	-6.066275	0.379531	-0.000351
28	7	0	-1.451631	1.135112	-0.000128
29	8	0	-1.090852	-1.078349	0.000158

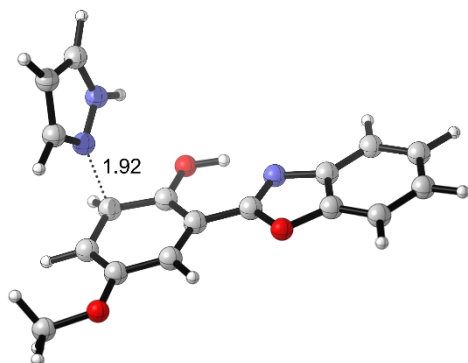
TS-S3x-pyr



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.798121	1.167388	0.850380
2	6	0	-2.272288	-0.093884	1.246455
3	6	0	-0.803808	-0.350569	1.168327
4	6	0	-0.029625	0.615855	0.416372
5	6	0	-0.628795	1.774612	-0.110723
6	6	0	-2.001274	2.052236	0.125720
7	1	0	-3.835352	1.398801	1.089340
8	1	0	-2.757505	-0.611122	2.077430
9	1	0	-0.044635	2.499230	-0.679463
10	8	0	-0.332461	-1.392522	1.678753
11	8	0	-2.420146	3.231753	-0.363975
12	6	0	-3.780448	3.619584	-0.201001
13	1	0	-4.030982	3.756865	0.864544
14	1	0	-3.890328	4.578335	-0.724875
15	1	0	-4.466064	2.879430	-0.647326
16	6	0	1.356455	0.360744	0.231335
17	6	0	3.425914	0.635168	-0.445116
18	6	0	3.380165	-0.557376	0.286283
19	6	0	4.581512	1.129081	-1.027728
20	6	0	4.523458	-1.331904	0.476474
21	6	0	5.731475	0.351510	-0.839065
22	1	0	4.586877	2.062091	-1.592836
23	6	0	5.701140	-0.849385	-0.104079
24	1	0	4.495101	-2.261410	1.046832
25	1	0	6.675643	0.688046	-1.273283
26	1	0	6.624290	-1.420774	0.017514
27	7	0	2.054771	-0.682913	0.688398
28	8	0	2.155037	1.181305	-0.460970
29	1	0	1.586940	-1.410009	1.243067
30	6	0	-3.005818	-3.411766	-0.924789
31	6	0	-3.817663	-2.549641	-1.655399
32	6	0	-3.668454	-1.291434	-1.039469
33	7	0	-2.432920	-2.680913	0.054283

34	1	0	-1.748723	-2.955845	0.761280
35	1	0	-2.795385	-4.474819	-1.030556
36	1	0	-4.432637	-2.796556	-2.518005
37	1	0	-4.118121	-0.327735	-1.277339
38	7	0	-2.826350	-1.406192	-0.015632

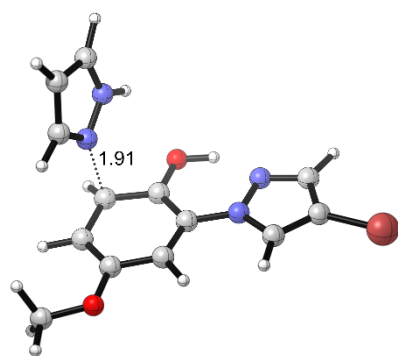
TS'-S3x-pyr



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.811577	1.122062	0.869141
2	6	0	-2.233938	-0.116735	1.285800
3	6	0	-0.790960	-0.289554	1.166158
4	6	0	-0.037003	0.637509	0.403149
5	6	0	-0.665741	1.763617	-0.124574
6	6	0	-2.053325	2.014599	0.129447
7	1	0	-3.856187	1.313156	1.109139
8	1	0	-2.691992	-0.640379	2.127870
9	1	0	-0.106824	2.490869	-0.714771
10	8	0	-0.277756	-1.376356	1.712613
11	8	0	-2.495435	3.174573	-0.371386
12	6	0	-3.860106	3.545778	-0.189556
13	1	0	-4.093593	3.680390	0.879946
14	1	0	-3.989088	4.501243	-0.714245
15	1	0	-4.539247	2.793192	-0.624156
16	6	0	1.378757	0.374829	0.222332
17	6	0	3.410615	0.672330	-0.460454
18	6	0	3.333262	-0.509703	0.297177

19	6	0	4.579629	1.143744	-1.041764
20	6	0	4.478591	-1.287858	0.504427
21	6	0	5.717482	0.357328	-0.828296
22	1	0	4.604325	2.066162	-1.624175
23	6	0	5.666582	-0.832443	-0.071521
24	1	0	4.436790	-2.208011	1.090409
25	1	0	6.670240	0.674597	-1.259181
26	1	0	6.583459	-1.410682	0.066923
27	7	0	2.014937	-0.657001	0.712402
28	8	0	2.151728	1.223613	-0.496631
29	6	0	-2.926062	-3.417732	-0.971266
30	6	0	-3.596139	-2.502474	-1.776668
31	6	0	-3.484776	-1.269261	-1.106347
32	7	0	-2.465097	-2.739367	0.100432
33	1	0	-1.905882	-3.078913	0.882424
34	1	0	-2.746634	-4.486196	-1.079962
35	1	0	-4.098413	-2.699617	-2.721140
36	1	0	-3.853947	-0.280426	-1.376384
37	7	0	-2.804548	-1.448472	0.023888
38	1	0	0.709909	-1.412373	1.500389

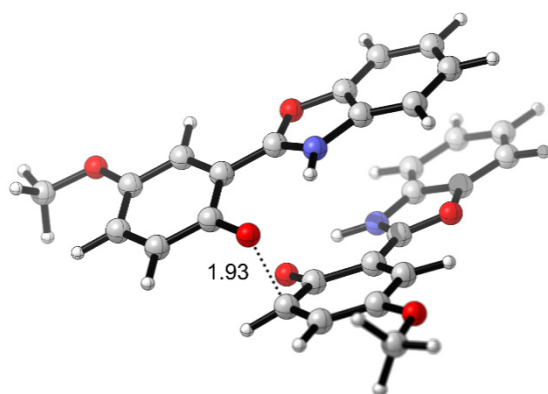
TS-S3af-pyr



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.941051	1.349764	0.776690
2	6	0	-2.580019	0.042796	1.226092

3	6	0	-1.171819	-0.342259	1.241940
4	6	0	-0.229800	0.455210	0.541628
5	6	0	-0.639332	1.656043	-0.017948
6	6	0	-1.993142	2.111608	0.120782
7	1	0	-3.963446	1.692296	0.923876
8	1	0	-3.173048	-0.406217	2.026298
9	1	0	0.050839	2.305395	-0.555235
10	8	0	-0.893566	-1.496021	1.827752
11	8	0	-2.204582	3.324726	-0.405006
12	6	0	-3.511010	3.893046	-0.347383
13	1	0	-3.824053	4.061474	0.696577
14	1	0	-3.449414	4.856448	-0.869538
15	1	0	-4.247600	3.246782	-0.853586
16	6	0	3.264643	-0.198235	0.032392
17	6	0	2.784260	-1.298729	0.779545
18	7	0	1.490201	-1.146619	1.018645
19	6	0	-3.531572	-3.146547	-1.071812
20	6	0	-4.074358	-2.167040	-1.897102
21	6	0	-3.847417	-0.950367	-1.225780
22	7	0	-3.028566	-2.518373	0.011200
23	1	0	-2.526710	-2.910482	0.807942
24	1	0	-3.467380	-4.228545	-1.174760
25	1	0	-4.568759	-2.312230	-2.855049
26	1	0	-4.100791	0.071218	-1.506708
27	7	0	-3.219183	-1.197846	-0.078377
28	1	0	0.095151	-1.677677	1.686677
29	1	0	2.091659	1.582411	-0.686557
30	6	0	2.175290	0.632896	-0.165583
31	7	0	1.119354	0.025653	0.446795
32	1	0	3.324832	-2.171950	1.142480
33	35	0	5.022378	0.082647	-0.568943

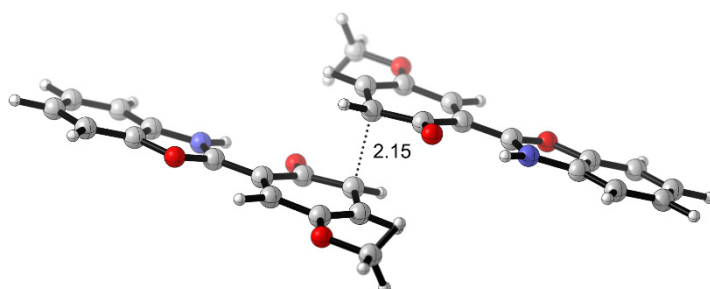
TS-S3x-OC



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.305279	-1.605293	-1.924888
2	6	0	-1.813352	-0.556841	-1.169265
3	6	0	-0.458596	-0.148837	-1.253288
4	6	0	0.399694	-0.895336	-2.139085
5	6	0	-0.100681	-1.951898	-2.906943
6	6	0	-1.449911	-2.319000	-2.804477
7	1	0	-3.357257	-1.876502	-1.835982
8	1	0	-2.468390	-0.011499	-0.486793
9	1	0	0.544153	-2.499034	-3.595957
10	8	0	0.003535	0.852916	-0.547676
11	8	0	-1.843531	-3.344777	-3.569508
12	6	0	-3.200638	-3.786054	-3.537381
13	1	0	-3.887287	-2.986266	-3.861032
14	1	0	-3.263279	-4.624798	-4.242591
15	1	0	-3.484062	-4.133729	-2.529890
16	6	0	1.785875	-0.532978	-2.243201
17	6	0	3.914655	-0.701509	-2.738066
18	6	0	3.741154	0.499500	-2.040764
19	6	0	5.148252	-1.159458	-3.173999
20	6	0	4.820255	1.329899	-1.738372
21	6	0	6.232037	-0.328926	-2.870651
22	1	0	5.259339	-2.105437	-3.704582
23	6	0	6.071100	0.885944	-2.171608
24	1	0	4.687453	2.263294	-1.190391
25	1	0	7.233972	-0.635424	-3.178123
26	1	0	6.953266	1.492789	-1.956671
27	7	0	2.379836	0.554405	-1.757371
28	8	0	2.678030	-1.311363	-2.851812
29	6	0	0.530152	1.724590	1.947522

30	6	0	0.221100	0.482889	1.337943
31	6	0	1.280590	-0.524285	1.088193
32	6	0	2.676155	-0.063702	1.274419
33	6	0	2.926762	1.181829	1.785451
34	6	0	1.852778	2.087236	2.131834
35	1	0	-0.287204	2.385344	2.232991
36	1	0	-0.784756	0.077698	1.453960
37	1	0	3.948857	1.529023	1.951391
38	8	0	0.997832	-1.648636	0.669063
39	8	0	2.280671	3.231137	2.652986
40	6	0	1.335886	4.223289	3.066540
41	1	0	0.686024	3.831256	3.865658
42	1	0	1.927730	5.063725	3.449265
43	1	0	0.722834	4.556412	2.213126
44	6	0	3.756800	-0.944065	0.910458
45	6	0	5.797616	-1.585463	0.456397
46	6	0	4.942807	-2.642774	0.124584
47	6	0	7.169804	-1.621697	0.266962
48	6	0	5.429756	-3.825265	-0.432620
49	6	0	7.660042	-2.805359	-0.292261
50	1	0	7.810492	-0.778661	0.526753
51	6	0	6.809947	-3.879353	-0.634167
52	1	0	4.766488	-4.649755	-0.696816
53	1	0	8.732852	-2.899380	-0.474505
54	1	0	7.246511	-4.780040	-1.071296
55	7	0	3.668754	-2.185618	0.445482
56	8	0	5.024161	-0.550921	0.948425
57	1	0	2.763376	-2.652971	0.325109
58	1	0	1.851252	1.266880	-1.241065

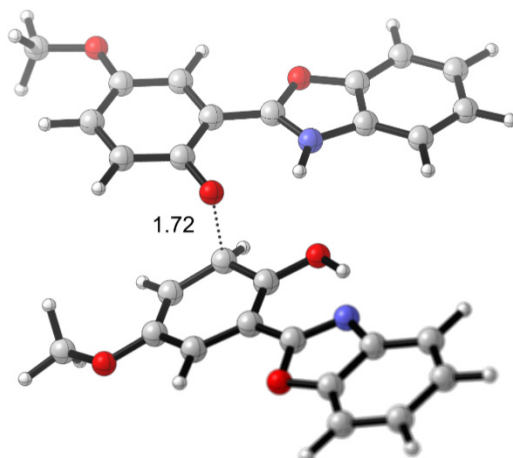
TS-S3x-CC



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.269622	1.423727	0.971235
2	6	0	-0.600925	0.043161	1.019406
3	6	0	-2.014512	-0.384770	0.992520
4	6	0	-2.973758	0.634039	0.507457
5	6	0	-2.571860	1.934619	0.320777
6	6	0	-1.217808	2.349318	0.570996
7	1	0	0.757153	1.721526	1.175495
8	1	0	0.067086	-0.641270	1.547426
9	1	0	-3.279534	2.698471	-0.009628
10	8	0	-2.358677	-1.524535	1.317387
11	8	0	-1.005145	3.654082	0.387002
12	6	0	0.317830	4.172004	0.528831
13	1	0	1.010944	3.661652	-0.161356
14	1	0	0.258108	5.237825	0.275189
15	1	0	0.676127	4.060277	1.565773
16	6	0	-4.336643	0.240069	0.276532
17	6	0	-6.433670	0.377345	-0.328250
18	6	0	-6.212588	-0.928561	0.125070
19	6	0	-7.659349	0.828260	-0.792671
20	6	0	-7.235675	-1.876945	0.137572
21	6	0	-8.686036	-0.121598	-0.781632
22	1	0	-7.804033	1.852074	-1.139561
23	6	0	-8.478051	-1.441219	-0.327228
24	1	0	-7.068543	-2.895518	0.490190
25	1	0	-9.678204	0.168405	-1.134710
26	1	0	-9.314607	-2.143526	-0.340077
27	7	0	-4.872477	-0.955560	0.495456
28	8	0	-5.244339	1.074594	-0.219286
29	6	0	-0.521492	-2.107636	-0.896119
30	6	0	-0.190160	-0.727075	-0.944264

31	6	0	1.223437	-0.299175	-0.917423
32	6	0	2.182689	-1.318023	-0.432471
33	6	0	1.780775	-2.618599	-0.245806
34	6	0	0.426698	-3.033260	-0.495967
35	1	0	-1.548279	-2.405409	-1.100359
36	1	0	-0.858153	-0.042614	-1.472266
37	1	0	2.488455	-3.382478	0.084530
38	8	0	1.567612	0.840594	-1.242267
39	8	0	0.214026	-4.338031	-0.312031
40	6	0	-1.108968	-4.855927	-0.453796
41	1	0	-1.467316	-4.744182	-1.490718
42	1	0	-1.049252	-5.921753	-0.200168
43	1	0	-1.802036	-4.345572	0.236435
44	6	0	3.545600	-0.924091	-0.201653
45	6	0	5.642685	-1.061439	0.402900
46	6	0	5.421567	0.244511	-0.050277
47	6	0	6.868405	-1.512410	0.867157
48	6	0	6.444661	1.192888	-0.062791
49	6	0	7.895099	-0.562558	0.856105
50	1	0	7.013113	-2.536256	1.213938
51	6	0	7.687079	0.757107	0.401847
52	1	0	6.277503	2.211496	-0.415294
53	1	0	8.887299	-0.852603	1.209057
54	1	0	8.523642	1.459406	0.414681
55	7	0	4.081419	0.271553	-0.420529
56	8	0	4.453335	-1.758667	0.293993
57	1	0	-4.313972	-1.721707	0.890631
58	1	0	3.522894	1.037740	-0.815588

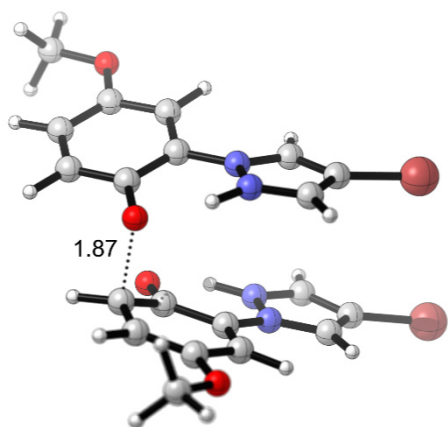
TS-S3x-CR-Sub



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.269622	1.423727	0.971235
2	6	0	-0.600925	0.043161	1.019406
3	6	0	-2.014512	-0.384770	0.992520
4	6	0	-2.973758	0.634039	0.507457
5	6	0	-2.571860	1.934619	0.320777
6	6	0	-1.217808	2.349318	0.570996
7	1	0	0.757153	1.721526	1.175495
8	1	0	0.067086	-0.641270	1.547426
9	1	0	-3.279534	2.698471	-0.009628
10	8	0	-2.358677	-1.524535	1.317387
11	8	0	-1.005145	3.654082	0.387002
12	6	0	0.317830	4.172004	0.528831
13	1	0	1.010944	3.661652	-0.161356
14	1	0	0.258108	5.237825	0.275189
15	1	0	0.676127	4.060277	1.565773
16	6	0	-4.336643	0.240069	0.276532
17	6	0	-6.433670	0.377345	-0.328250
18	6	0	-6.212588	-0.928561	0.125070
19	6	0	-7.659349	0.828260	-0.792671
20	6	0	-7.235675	-1.876945	0.137572
21	6	0	-8.686036	-0.121598	-0.781632
22	1	0	-7.804033	1.852074	-1.139561
23	6	0	-8.478051	-1.441219	-0.327228
24	1	0	-7.068543	-2.895518	0.490190
25	1	0	-9.678204	0.168405	-1.134710
26	1	0	-9.314607	-2.143526	-0.340077
27	7	0	-4.872477	-0.955560	0.495456
28	8	0	-5.244339	1.074594	-0.219286
29	6	0	-0.521492	-2.107636	-0.896119
30	6	0	-0.190160	-0.727075	-0.944264

31	6	0	1.223437	-0.299175	-0.917423
32	6	0	2.182689	-1.318023	-0.432471
33	6	0	1.780775	-2.618599	-0.245806
34	6	0	0.426698	-3.033260	-0.495967
35	1	0	-1.548279	-2.405409	-1.100359
36	1	0	-0.858153	-0.042614	-1.472266
37	1	0	2.488455	-3.382478	0.084530
38	8	0	1.567612	0.840594	-1.242267
39	8	0	0.214026	-4.338031	-0.312031
40	6	0	-1.108968	-4.855927	-0.453796
41	1	0	-1.467316	-4.744182	-1.490718
42	1	0	-1.049252	-5.921753	-0.200168
43	1	0	-1.802036	-4.345572	0.236435
44	6	0	3.545600	-0.924091	-0.201653
45	6	0	5.642685	-1.061439	0.402900
46	6	0	5.421567	0.244511	-0.050277
47	6	0	6.868405	-1.512410	0.867157
48	6	0	6.444661	1.192888	-0.062791
49	6	0	7.895099	-0.562558	0.856105
50	1	0	7.013113	-2.536256	1.213938
51	6	0	7.687079	0.757107	0.401847
52	1	0	6.277503	2.211496	-0.415294
53	1	0	8.887299	-0.852603	1.209057
54	1	0	8.523642	1.459406	0.414681
55	7	0	4.081419	0.271553	-0.420529
56	8	0	4.453335	-1.758667	0.293993
57	1	0	-4.313972	-1.721707	0.890631
58	1	0	3.522894	1.037740	-0.815588

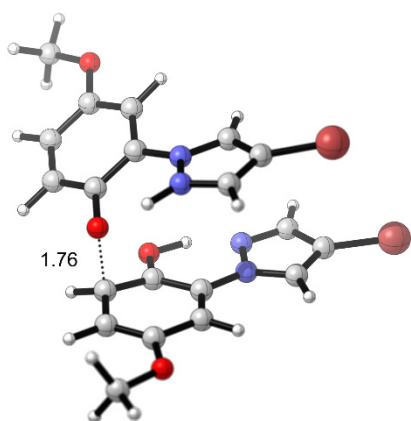
TS-S3af-OC



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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2	6	0	-1.708328	-0.790087	-1.029508
3	6	0	-0.425192	-0.208903	-1.145110
4	6	0	0.477764	-0.803559	-2.084445
5	6	0	0.082690	-1.859642	-2.893432
6	6	0	-1.205677	-2.408722	-2.754219
7	1	0	-3.104784	-2.275378	-1.683147
8	1	0	-2.391839	-0.356393	-0.296601
9	1	0	0.740950	-2.280373	-3.653360
10	8	0	-0.070507	0.843010	-0.423650
11	8	0	-1.488703	-3.433371	-3.567919
12	6	0	-2.771835	-4.056856	-3.514924
13	1	0	-3.575434	-3.338254	-3.745595
14	1	0	-2.757665	-4.843113	-4.280837
15	1	0	-2.951368	-4.512250	-2.526725
16	6	0	3.961895	0.042234	-2.595615
17	6	0	3.423471	1.187275	-1.992832
18	7	0	2.127356	0.952808	-1.789163
19	6	0	0.602177	1.849043	1.925887
20	6	0	0.179809	0.590665	1.412187
21	6	0	1.147808	-0.511598	1.214321
22	6	0	2.575972	-0.141555	1.266073
23	6	0	2.941095	1.104954	1.665492
24	6	0	1.951157	2.110207	2.013018
25	1	0	-0.149927	2.586535	2.200723
26	1	0	-0.837838	0.256128	1.619527
27	1	0	3.984682	1.411781	1.743831
28	8	0	0.743028	-1.638706	0.900695
29	8	0	2.504747	3.246361	2.426980
30	6	0	1.668479	4.349462	2.787322

31	1	0	1.032683	4.091557	3.649878
32	1	0	2.346177	5.168200	3.058711
33	1	0	1.037769	4.654489	1.936160
34	6	0	5.366451	-2.222476	0.288107
35	6	0	4.247618	-3.054328	0.129310
36	7	0	3.178884	-2.356549	0.506027
37	1	0	2.159088	-2.569092	0.532132
38	1	0	1.405452	1.466108	-1.249155
39	7	0	3.545499	-1.116549	0.901488
40	6	0	4.891391	-1.007338	0.773363
41	1	0	5.426877	-0.095856	1.026029
42	1	0	4.155790	-4.082226	-0.217968
43	35	0	7.148243	-2.661227	-0.078181
44	7	0	1.802168	-0.288944	-2.211965
45	6	0	2.916126	-0.871178	-2.718986
46	1	0	3.878584	2.130871	-1.696858
47	1	0	2.907914	-1.883366	-3.115191
48	35	0	5.741498	-0.220239	-3.113311

TS'-S3af-OC

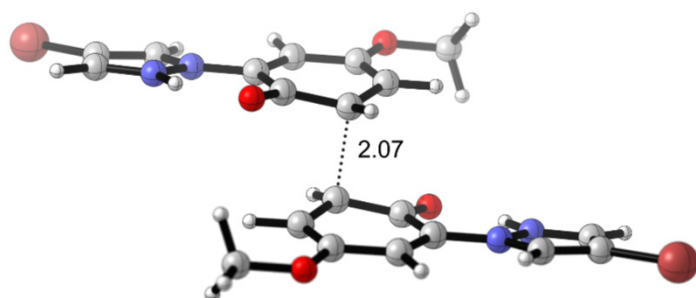


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4	6	0	0.467151	-0.807020	-2.064023
5	6	0	0.058100	-1.823322	-2.910379
6	6	0	-1.230266	-2.381248	-2.767812
7	1	0	-3.109957	-2.299495	-1.655288
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9	1	0	0.702092	-2.206581	-3.701779
10	8	0	-0.039422	0.759325	-0.326261
11	8	0	-1.528172	-3.362774	-3.618474
12	6	0	-2.812249	-3.991094	-3.577415
13	1	0	-3.615499	-3.262712	-3.775064
14	1	0	-2.801684	-4.748820	-4.371128
15	1	0	-2.980410	-4.481510	-2.604671
16	6	0	3.959158	-0.005088	-2.568811
17	6	0	3.426793	1.175648	-2.032832
18	7	0	2.125765	0.967768	-1.832774
19	6	0	0.601702	1.826854	1.916828
20	6	0	0.206730	0.542589	1.406849
21	6	0	1.221521	-0.501541	1.240915
22	6	0	2.617322	-0.134022	1.265987
23	6	0	2.947390	1.138782	1.643675
24	6	0	1.939667	2.123183	1.990734
25	1	0	-0.175199	2.541232	2.181722
26	1	0	-0.781652	0.167666	1.683423
27	1	0	3.986501	1.465499	1.700132
28	8	0	0.802611	-1.670303	0.918596
29	8	0	2.472195	3.278667	2.389145
30	6	0	1.609369	4.358975	2.750012
31	1	0	0.986678	4.089154	3.618933
32	1	0	2.265143	5.198462	3.012440
33	1	0	0.962859	4.642772	1.902928
34	6	0	5.371353	-2.229853	0.319316
35	6	0	4.214263	-3.029926	0.157435
36	7	0	3.144312	-2.335860	0.513799
37	1	0	1.426851	1.553993	-1.359153
38	7	0	3.576556	-1.107572	0.905479

39	6	0	4.931703	-1.006753	0.795149
40	1	0	5.478803	-0.103391	1.052189
41	1	0	4.129242	-4.057991	-0.192668
42	35	0	7.144661	-2.726446	-0.033490
43	7	0	1.790503	-0.291357	-2.192857
44	6	0	2.903920	-0.910385	-2.656360
45	1	0	3.887786	2.130276	-1.785152
46	1	0	2.880733	-1.942147	-2.998193
47	35	0	5.740251	-0.308315	-3.051808
48	1	0	1.658206	-2.256629	0.669342

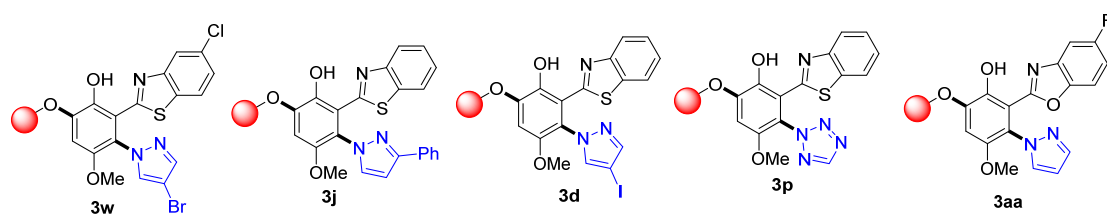
TS-S3af-CC



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.170144	1.339918	0.874927
2	6	0	-0.565534	-0.032335	0.885547
3	6	0	-2.000234	-0.388748	0.871808
4	6	0	-2.911407	0.673200	0.397796
5	6	0	-2.462292	1.950247	0.251747
6	6	0	-1.083601	2.301546	0.507523
7	1	0	0.868793	1.589449	1.081181
8	1	0	0.047365	-0.744441	1.444135
9	1	0	-3.122710	2.766809	-0.044340
10	8	0	-2.388882	-1.516957	1.203056
11	8	0	-0.835638	3.605698	0.358215

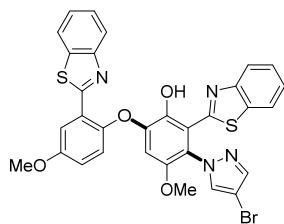
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13	1	0	1.172207	3.564183	-0.215138
14	1	0	0.475699	5.150880	0.273840
15	1	0	0.871082	3.925224	1.526499
16	6	0	-6.411640	0.292069	-0.423456
17	6	0	-6.056265	-0.943873	0.136300
18	7	0	-4.769015	-0.871384	0.468867
19	6	0	-0.547987	-2.196706	-0.957645
20	6	0	-0.195319	-0.813126	-0.999876
21	6	0	1.226074	-0.412882	-1.010736
22	6	0	2.173712	-1.433113	-0.520384
23	6	0	1.767154	-2.720986	-0.342312
24	6	0	0.399287	-3.121769	-0.580771
25	1	0	-1.580305	-2.481932	-1.148576
26	1	0	-0.834439	-0.129243	-1.564470
27	1	0	2.456465	-3.507785	-0.031515
28	8	0	1.574813	0.719993	-1.370875
29	8	0	0.194358	-4.430850	-0.406055
30	6	0	-1.129316	-4.948148	-0.537020
31	1	0	-1.501749	-4.823489	-1.567578
32	1	0	-1.065950	-6.017328	-0.298220
33	1	0	-1.814356	-4.448398	0.168733
34	6	0	5.656855	-0.902143	0.290271
35	6	0	5.262092	0.297003	-0.320681
36	7	0	3.979504	0.167542	-0.654061
37	1	0	-4.093283	-1.548149	0.885478
38	1	0	3.278880	0.806287	-1.090816
39	7	0	-4.272813	0.344084	0.151787
40	6	0	-5.265060	1.081888	-0.402822
41	1	0	-6.633928	-1.849847	0.312688
42	1	0	-5.102076	2.099761	-0.748356
43	35	0	-8.097018	0.783770	-1.073372
44	7	0	3.523970	-1.050960	-0.290160
45	6	0	4.538224	-1.731348	0.295960
46	1	0	4.408497	-2.739739	0.680033
47	1	0	5.810659	1.213124	-0.533283
48	35	0	7.353462	-1.307722	0.970601

10. Fluorescence properties of the selected products



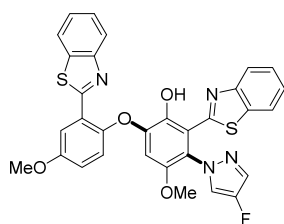
11. Characterization of Products

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(4-bromo-1H-pyrazol-1-yl)-4-methoxyphenol (3a)



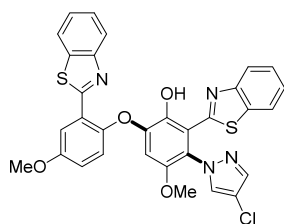
Yellow solid (72 mg, 88 % yield, electrolysis time: 6.5 h, $R_f = 0.17$ (petroleum ether/ethyl acetate = 10 : 1 (v/v))); M.P. 292.5-295.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.95 (s, 1H), 8.18 – 8.17 (m, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 7.97 (d, $J = 7.8$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.86 (s, 1H), 7.81 (d, $J = 8.1$ Hz, 1H), 7.63 (s, 1H), 7.53 - 7.47 (m, 2H), 7.43 - 7.34 (m, 2H), 7.07 - 7.00 (m, 2H), 6.82 (s, 1H), 3.97 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.3, 162.4, 156.2, 152.3, 149.1, 149.1, 148.5, 146.8, 145.2, 142.7, 136.5, 133.9, 133.8, 126.9, 126.2, 125.3, 125.2, 123.1, 122.3, 121.9, 121.6, 121.4, 119.9, 119.3, 116.4, 112.7, 106.9, 95.5, 57.1, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{22}\text{BrN}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 657.0260, found, 657.0248.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(4-fluoro-1H-pyrazol-1-yl)-4-methoxyphenol (3b)



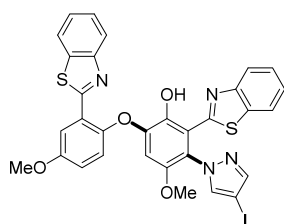
Yellow solid (17 mg, 23 % yield, electrolysis time: 6.8 h, $R_f = 0.25$ (petroleum ether/ethyl acetate = 10 : 1 (v/v))); M.P. 287.3-288.5 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.95 (s, 1H), 8.17 (d, $J = 0.9$ Hz, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 7.97 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.81 (d, $J = 7.8$ Hz, 1H), 7.77 (d, $J = 3.9$ Hz, 1H), 7.52 - 7.47 (m, 3H), 7.43 - 7.34 (m, 2H), 7.07 - 7.00 (m, 2H), 6.82 (s, 1H), 3.96 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.5, 162.4, 156.2, 152.8, 152.3, 149.3, 149.2, 148.5, 146.7, 145.2, 136.5, 133.9, 129.9 (d, $J = 13.5$ Hz, 1C), 126.9, 126.2, 125.3, 125.2, 123.1, 122.6, 122.3, 121.6, 121.3, 119.9, 119.5, 119.3, 116.6, 112.7, 107.1, 57.2, 56.1. ^{19}F NMR (282 MHz, CDCl_3 , 25 °C, δ): -174.8 (s). Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{22}\text{FN}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 597.1061, found, 597.1070.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(4-chloro-1H-pyrazol-1-yl)-4-methoxyphenol (3c)



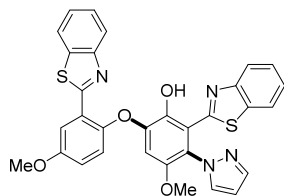
Yellow solid (32 mg, 42 % yield, electrolysis time: 7.5 h, $R_f = 0.20$ (petroleum ether/ethyl acetate = 10 : 1 (v/v))); M.P. 265.6-268.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.86 (s, 1H), 8.16 (d, $J = 1.5$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.96 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.84 (s, 1H), 7.80 (d, $J = 7.8$ Hz, 1H), 7.62 (s, 1H), 7.51 - 7.46 (m, 3H), 7.42 - 7.34 (m, 2H), 7.07 - 7.03 (m, 2H), 6.83 (s, 1H), 3.95 (s, 3H), 3.60 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.3, 162.4, 156.2, 152.3, 149.1, 148.5, 146.8, 145.1, 140.7, 136.5, 133.9, 131.7, 126.9, 126.2, 125.3, 125.2, 123.1, 122.3, 122.0, 121.6, 121.4, 119.9, 119.3, 116.5, 112.7, 112.4, 106.9, 57.1, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{22}\text{ClN}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 613.0766, found, 613.0775.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(4-iodo-1H-pyrazol-1-yl)-4-methoxyphenol (3d)



Yellow solid (38 mg, 43 % yield, electrolysis time: 7.3 h, $R_f = 0.35$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 283.3-285.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.96 (s, 1H), 8.17 (d, $J = 1.8$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.95 (d, $J = 7.8$ Hz, 1H), 7.91 - 7.87 (m, 2H), 7.79 (d, $J = 8.1$ Hz, 1H), 7.66 (s, 1H), 7.52 - 7.45 (m, 2H), 7.41 - 7.33 (m, 2H), 7.06 - 6.99 (m, 2H), 6.84 (s, 1H), 3.95 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.4, 162.4, 156.2, 152.3, 149.1, 149.0, 148.5, 147.1, 146.7, 145.2, 138.0, 136.5, 133.9, 126.9, 126.2, 125.3, 125.2, 123.1, 122.3, 121.9, 121.6, 121.4, 119.9, 119.3, 116.4, 112.7, 107.0, 57.1, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{22}\text{IN}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 705.0122, found, 705.0131.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(1H-pyrazol-1-yl)phenol (3e)



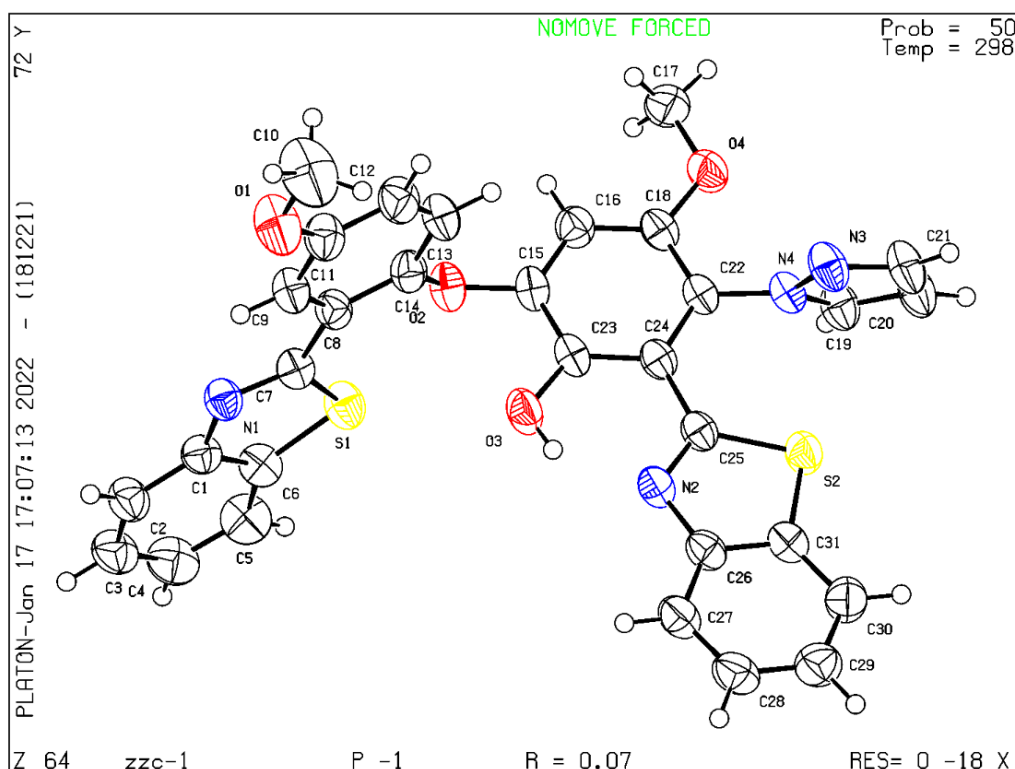
Yellow solid (51 mg, 70 % yield, electrolysis time: 7.0 h, $R_f = 0.3$ (petroleum ether/ethyl acetate = 5 : 1 (v/v))); M.P. 280.3-281.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.01 (s, 1H), 8.17 (d, $J = 1.8$ Hz, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 7.97 - 7.88 (m, 3H), 7.75 (d, $J = 7.5$ Hz, 1H), 7.60 (d, $J = 2.4$ Hz, 1H), 7.53 - 7.44 (m, 2H), 7.37 (t, $J = 7.8$ Hz, 2H), 7.07 - 7.00 (m, 2H), 6.86 (s, 1H), 6.86 (t, $J = 2.1$ Hz, 1H), 3.96 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.9, 162.5, 156.1, 152.3, 149.3, 149.1, 148.7, 146.3, 145.3, 142.1, 136.5, 134.1, 133.8,

126.8 126.2, 126.0, 125.2, 125.1, 123.1, 122.9, 122.2, 121.6, 121.3, 119.8, 119.3, 116.7, 112.7, 108.1, 107.5, 57.3, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for C₃₁H₂₃N₄O₄S₂⁺ ([M + H]⁺), 579.1155, found, 579.1170.

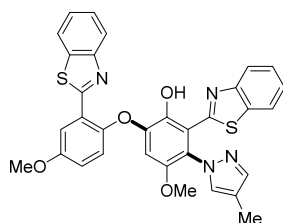
Crystal structure determination of **3e**: C₃₁H₂₂N₄O₄S₂, light yellow block crystal, CCDC number: 2142731.

Datablock: zzc-1

Bond precision:	C-C = 0.0040 Å	Wavelength=1.54184
Cell:	a=10.3322(2) b=10.7423(2) c=14.3583(2)	
	alpha=97.245(2) beta=100.734(2) gamma=116.704(2)	
Temperature:	298 K	
	Calculated	Reported
Volume	1358.21(5)	1358.21(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H22 N4 O4 S2	0.33(C31 H22 N4 O4 S2)
Sum formula	C31 H22 N4 O4 S2	C10.33 H7.33 N1.33 O1.33 S0.67
Mr	578.65	192.88
Dx, g cm ⁻³	1.415	1.415
Z	2	6
Mu (mm ⁻¹)	2.157	2.157
F000	600.0	600.0
F000'	603.00	
h, k, lmax	12, 13, 17	12, 13, 17
Nref	5506	5313
Tmin, Tmax		0.736, 1.000
Tmin'		
Correction method= # Reported T Limits:	Tmin=0.736 Tmax=1.000 AbsCorr =	
MULTI-SCAN		
Data completeness= 0.965	Theta(max)= 74.179	
R(reflections)= 0.0683(4260)	wR2(reflections)= 0.2069(5313)	
S = 1.049	Npar= 373	

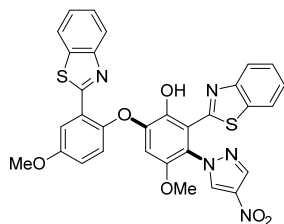


2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(4-methyl-1H-pyrazol-1-yl)phenol (3f)



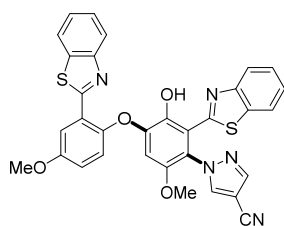
Yellow solid (49 mg, 67 % yield, electrolysis time: 7.5 h, $R_f = 0.21$ (petroleum ether/ethyl acetate = 5 : 1 (v/v))); M.P. 272.4-274.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.96 (s, 1H), 8.18 – 8.17 (m, 1H), 8.13 (d, $J = 7.8$ Hz, 1H), 7.94 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 7.5$ Hz, 1H), 7.77 (d, $J = 7.5$ Hz, 1H), 7.73 (s, 1H), 7.52 - 7.43 (m, 2H), 7.39 - 7.34 (m, 3H), 7.06 - 7.00 (m, 2H), 6.86 (s, 1H), 3.96 (s, 3H), 3.60 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.9, 162.5, 155.9, 152.3, 149.3, 149.1, 148.8, 145.9, 145.2, 142.9, 136.5, 134.2, 132.0, 126.7, 126.1, 125.9, 125.1, 123.3, 123.1, 122.1, 121.6, 121.3, 119.6, 119.2, 118.6, 116.8, 112.6, 107.6, 57.3, 56.1, 9.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{32}\text{H}_{26}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 593.1312, found, 593.1327.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(4-nitro-1H-pyrazol-1-yl)phenol (3g)



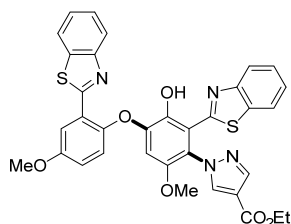
Yellow solid (50 mg, 64 % yield, electrolysis time: 6.3 h, $R_f = 0.16$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 286.5-289.6 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.80 (s, 1H), 8.42 (d, $J = 3.3$ Hz, 2H), 8.14 (d, $J = 2.7$ Hz, 1H), 8.11 (d, $J = 8.1$ Hz, 1H), 7.96 (d, $J = 7.8$ Hz, 1H), 7.87 (d, $J = 7.8$ Hz, 1H), 7.79 (d, $J = 7.8$ Hz, 1H), 7.52 - 7.41 (m, 3H), 7.39 - 7.31 (m, 1H), 7.07 - 6.98 (m, 2H), 6.84 (s, 1H), 3.93 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 163.4, 162.2, 156.3, 152.2, 149.1, 148.6, 147.9, 147.1, 145.0, 137.7, 136.3, 133.8, 133.3, 127.2, 126.5, 126.2, 125.5, 125.2, 123.1, 122.4, 121.5, 121.4, 120.2, 119.2, 115.8, 112.7, 106.3, 56.9, 56.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{22}\text{N}_5\text{O}_6\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 624.1006, found, 624.1005.

1-(2-(benzo[d]thiazol-2-yl)-4-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-hydroxy-6-methoxyphenyl)-1H-pyrazole-4-carbonitrile (3h)



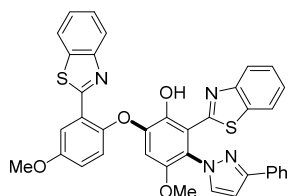
Yellow solid (52 mg, 68 % yield, electrolysis time: 7.1 h, $R_f = 0.10$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 267.2-271.4 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.86 (s, 1H), 8.15 (s, 2H), 8.12 (d, $J = 8.1$ Hz, 1H), 8.08 (s, 1H), 7.98 (d, $J = 8.1$ Hz, 1H), 7.88 (d, $J = 7.8$ Hz, 1H), 7.81 (d, $J = 7.5$ Hz, 1H), 7.79 (d, $J = 7.8$ Hz, 1H), 7.54 - 7.46 (m, 2H), 7.45 - 7.40 (m, 1H), 7.38 - 7.33 (m, 1H), 7.07 - 6.99 (m, 2H), 6.80 (s, 1H), 3.95 (s, 3H), 3.58 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 163.6, 162.3, 156.4, 152.3, 149.2, 148.8, 148.0, 147.6, 145.1, 144.1, 139.6, 136.4, 133.4, 127.2, 126.5, 126.3, 125.5, 125.2, 123.2, 122.4, 121.6, 121.4, 120.3, 120.2, 119.3, 116.1, 113.2, 112.8, 106.4, 94.9, 57.0, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{32}\text{H}_{22}\text{N}_5\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 604.1108, found, 604.1120.

Ethyl 1-(2-(benzo[d]thiazol-2-yl)-4-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-hydroxy-6-methoxyphenyl)-1H-pyrazole-4-carboxylate (3i)



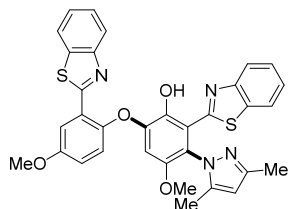
Yellow solid (37 mg, 46 % yield, electrolysis time: 6.4 h, $R_f = 0.32$ (petroleum ether/ethyl acetate = 5 : 1 (v/v)); M.P. 265.1-269.8 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.93 (s, 1H), 8.29 (s, 1H), 8.16 (d, $J = 2.1$ Hz, 1H), 8.12 (d, $J = 8.4$ Hz, 2H), 7.95 (d, $J = 8.1$ Hz, 1H), 7.95 (d, $J = 7.5$ Hz, 1H), 7.88 (d, $J = 7.5$ Hz, 1H), 7.77 (d, $J = 7.8$ Hz, 1H), 7.51 - 7.45 (m, 2H), 7.41 - 7.33 (m, 2H), 7.07 - 6.99 (m, 2H), 6.84 (s, 1H), 4.41 - 4.34 (q, $J = 9$ Hz, 2H), 3.95 (s, 3H), 3.59 (s, 3H), 1.39 (t, $J = 9$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.2, 162.9, 162.3, 156.2, 152.3, 149.1, 148.9, 148.4, 146.9, 145.1, 143.1, 137.6, 136.4, 133.7, 126.9, 126.2, 126.1, 125.3, 125.1, 123.1, 122.2, 121.6, 121.5, 121.3, 119.9, 117.5, 116.2, 112.6, 106.9, 60.7, 57.1, 56.0, 14.5. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{34}\text{H}_{27}\text{N}_4\text{O}_6\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 651.1367, found, 651.1351.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(3-phenyl-1H-pyrazol-1-yl)phenol (3j)



Yellow solid (63 mg, 76 % yield, electrolysis time: 7.5 h, $R_f = 0.29$ (petroleum ether/ethyl acetate = 5 : 1 (v/v)); M.P. 276.4-279.1 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.12 (s, 1H), 8.18 (d, $J = 2.4$ Hz, 1H), 8.14 (d, $J = 8.1$ Hz, 1H), 7.98 - 7.89 (m, 4H), 7.72 (d, $J = 7.8$ Hz, 1H), 7.62 (d, $J = 2.4$ Hz, 1H), 7.53 - 7.48 (m, 1H), 7.47 - 7.43 (m, 2H), 7.40 - 7.32 (m, 4H), 7.09 - 7.01 (m, 2H), 6.95 (d, $J = 2.4$ Hz, 1H), 6.87 (s, 1H), 3.97 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.9, 162.5, 156.1, 154.0, 152.4, 149.4, 149.1, 148.7, 146.4, 145.4, 136.6, 135.1, 134.2, 133.1, 128.8, 128.3, 126.8, 126.2, 125.9, 125.3, 125.1, 123.1, 122.9, 122.2, 121.7, 121.4, 119.9, 119.3, 116.8, 112.6, 107.6, 105.4, 57.4, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{37}\text{H}_{27}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 655.1468, found, 655.1478.

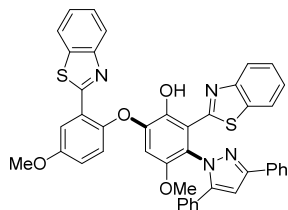
2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(3,5-dimethyl-1H-pyrazol-1-yl)-4-methoxyphenol (3k)



Yellow solid (62 mg, 81 % yield, electrolysis time: 6.8 h, $R_f = 0.27$ (petroleum ether/ethyl acetate = 3 : 1 (v/v)); M.P. 252.6-255.3 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.16 (s, 1H), 7.18 (t, $J = 1.5$ Hz, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 7.94 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 7.8$ Hz, 1H), 7.79 (d, $J = 7.8$ Hz, 1H),

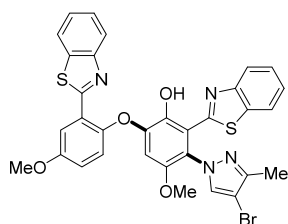
7.52 - 7.43 (m, 2H), 7.39 - 7.34 (m, 2H), 7.02 (d, $J = 1.5$ Hz, 2H), 6.88 (s, 1H), 6.18 (s, 1H), 3.95 (s, 3H), 3.62 (s, 3H), 2.37 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 165.1, 162.5, 155.9, 152.3, 151.3, 149.2, 149.1, 148.9, 145.8, 145.5, 143.0, 136.5, 134.2, 126.7, 126.1, 125.9, 125.0, 124.8, 123.0, 122.1, 121.6, 121.3, 119.4, 119.1, 117.0, 112.6, 107.7, 107.0, 57.0, 56.0, 14.0, 11.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{33}\text{H}_{27}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 607.1468, found, 607.1477.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(3,5-di phenyl-1H-pyrazol-1-yl)-4-methoxyphenol (3l)



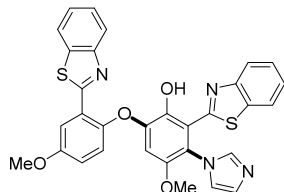
Yellow solid (82 mg, 90 % yield, electrolysis time: 7.6 h, $R_f = 0.23$ (petroleum ether/ethyl acetate = 5 : 1 (v/v))); M.P. 255.3-258.8 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.25 (s, 1H), 8.16 - 8.12 (m, 2H), 7.98 - 7.91 (m, 4H), 7.75 (d, $J = 7.8$ Hz, 1H), 7.51 - 7.44 (m, 3H), 7.41 - 7.36 (m, 3H), 7.33 - 7.29 (m, 2H), 7.26 - 7.22 (m, 4H), 7.09 (s, 1H), 7.01 (s, 2H), 6.77 (s, 1H), 3.96 (s, 3H), 3.42 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 165.1, 162.6, 156.0, 154.0, 152.4, 149.2, 149.0, 148.9, 147.8, 146.1, 145.8, 136.6, 134.2, 133.1, 129.9, 128.8, 128.7, 128.6, 128.4, 127.6, 126.9, 126.2, 126.0, 125.1, 124.9, 123.2, 122.7, 122.2, 121.7, 121.5, 119.5, 119.2, 117.1, 112.8, 108.1, 104.9, 57.0, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{43}\text{H}_{31}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 731.1781, found, 731.1791.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(4-bromo-3-methyl-1H-pyrazol-1-yl)-4-methoxyphenol (3m)



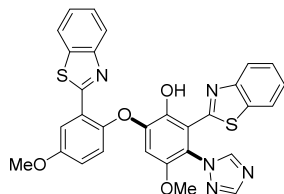
Yellow solid (51 mg, 61 % yield, electrolysis time: 6.8 h, $R_f = 0.18$ (petroleum ether/ethyl acetate = 5 : 1 (v/v))); M.P. 271.6-273.8 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.98 (s, 1H), 8.17 (s, 1H), 8.12 (d, $J = 8.4$ Hz, 1H), 7.96 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.83 (d, $J = 8.4$ Hz, 1H), 7.57 (s, 1H), 7.52 - 7.46 (m, 2H), 7.42 - 7.34 (m, 2H), 7.04 - 7.02 (m, 2H), 6.82 (s, 1H), 3.96 (s, 3H), 3.60 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.5, 162.4, 156.0, 152.2, 150.3, 149.1, 149.0, 148.5, 146.4, 145.1, 136.4, 134.0, 133.9, 126.8, 126.1, 126.0, 125.1, 125.0, 123.0, 122.1, 121.5, 121.3, 119.8, 116.5, 112.6, 106.9, 96.2, 56.9, 55.9, 12.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{32}\text{H}_{24}\text{BrN}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 671.0417, found, 671.0410.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(1*H*-imidazol-1-yl)-4-methoxyphenol (3n)



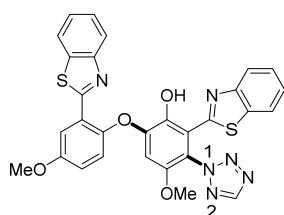
Yellow solid (48 mg, 66 % yield, electrolysis time: 7.9 h, $R_f = 0.14$ (petroleum ether/ethyl acetate = 1 : 1 (v/v))); M.P. 290.0-292.9 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.00 (s, 1H), 8.16 (d, $J = 2.4$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.96 (d, $J = 8.1$ Hz, 1H), 7.88 (d, $J = 7.8$ Hz, 1H), 7.77 (d, $J = 7.8$ Hz, 1H), 7.56 (s, 1H), 7.49 (t, $J = 7.2$ Hz, 2H), 7.42 - 7.33 (m, 3H), 7.08 - 7.00 (m, 2H), 6.96 (s, 1H), 6.84 (s, 1H), 3.96 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.3, 162.3, 156.1, 152.2, 148.9, 148.6, 148.4, 146.2, 145.0, 138.7, 136.4, 133.7, 130.4, 126.9, 126.2, 126.1, 125.2, 125.1, 123.1, 122.1, 121.5, 121.4, 119.8, 119.2, 118.9, 116.2, 112.6, 106.8, 56.8, 55.9. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{23}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 579.1155, found, 579.1157.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(1*H*-1,2,4-triazol-1-yl)phenol (3o)



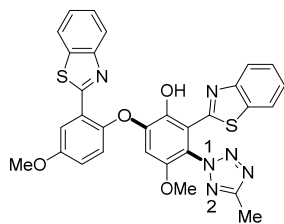
Yellow solid (40 mg, 56 % yield, electrolysis time: 8.0 h, $R_f = 0.45$ (petroleum ether/ethyl acetate = 1 : 1 (v/v))); M.P. 282.4-288.3 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.93 (s, 1H), 8.32 (d, $J = 9$ Hz, 2H), 8.15 (d, $J = 2.1$ Hz, 1H), 8.11 (d, $J = 6$ Hz, 1H), 7.96 (d, $J = 6.3$ Hz, 1H), 7.88 (d, $J = 6$ Hz, 1H), 7.75 (d, $J = 6$ Hz, 1H), 7.51 - 7.46 (m, 2H), 7.41 - 7.33 (m, 2H), 7.07 - 7.01 (m, 2H), 6.82 (s, 1H), 3.95 (s, 3H), 3.57 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 163.9, 162.3, 156.3, 153.5, 152.3, 149.1, 148.9, 148.2, 147.6, 147.1, 145.2, 136.4, 133.4, 127.2, 126.4, 126.2, 125.5, 125.2, 123.2, 122.4, 121.6, 121.4, 120.2, 119.3, 118.2, 116.2, 112.8, 106.5, 57.0, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{30}\text{H}_{22}\text{N}_5\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 580.1108, found, 580.1108.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(1*H*-tetrazol-1-yl)phenol (3p)



isomer 1, Yellow solid (10 mg, 14 % yield, electrolysis time: 6.0 h, $R_f = 0.35$ (petroleum ether/ethyl acetate = 3 : 1 (v/v)); M.P. 297.6-301.2 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.75 (s, 1H), 8.93 (s, 1H), 8.17 (d, $J = 2.7$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.99 (d, $J = 8.1$ Hz, 1H), 7.90 (d, $J = 7.5$ Hz, 1H), 7.74 (d, $J = 7.5$ Hz, 1H), 7.54 - 7.48 (m, 2H), 7.43 - 7.35 (m, 2H), 7.12 - 7.04 (m, 2H), 6.84 (s, 1H), 3.98 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 163.2, 162.2, 156.6, 153.9, 152.3, 149.3, 149.1, 148.8, 147.9, 145.1, 136.4, 133.2, 127.3, 126.6, 126.3, 125.8, 125.3, 123.2, 122.5, 121.7, 121.4, 120.6, 119.3, 118.0, 115.8, 112.9, 106.2, 57.2, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{29}\text{H}_{20}\text{N}_6\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 581.1060, found, 581.1072. isomer 2, Yellow solid (24 mg, 32 % yield, electrolysis time: 6.0 h, $R_f = 0.25$ (petroleum ether/ethyl acetate = 3 : 1 (v/v)); M.P. 295.4-296.9 °C; NMR Spectroscopy: ^1H NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$, 25 °C, δ): 11.7 (s, 1H), 9.8 (s, 1H), (s, 1H), 8.18 - 8.11 (m, 3H), 8.07 - 8.06 (m, 1H), 7.85 - 7.82 (m, 1H), 7.60 - 7.53 (m, 1H), 7.52 - 7.44 (m, 3H), 7.22 (d, $J = 1.1$ Hz, 2H), 7.18 (s, 1H), 3.91 (s, 3H), 3.63 (s, 3H). ^{13}C NMR (75 MHz, $(\text{CD}_3)_2\text{SO}$, 25 °C, δ): 161.6, 160.1, 155.7, 151.6, 150.5, 148.3, 147.9, 147.3, 146.6, 142.5, 135.5, 134.3, 126.6, 126.5, 126.0, 125.4, 124.7, 122.7, 122.1, 121.9, 120.4, 119.2, 118.8, 115.7, 112.2, 106.6, 57.2, 55.8. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{29}\text{H}_{21}\text{N}_6\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 581.1060, found, 581.1072.

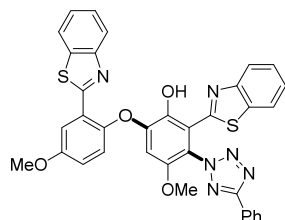
2-(Benzo[*d*]thiazol-2-yl)-6-(2-(benzo[*d*]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(5-methyl-1*H*-tetrazol-1-yl)phenol (3q)



isomer 1, Yellow solid (23 mg, 31 % yield, electrolysis time: 6.3 h, $R_f = 0.32$ (petroleum ether/ethyl acetate = 3 : 1 (v/v)); M.P. 271.1-276.7 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 13.84 (s, 1H), 8.17 (d, $J = 2.1$ Hz, 1H), 8.13 (d, $J = 7.8$ Hz, 1H), 7.99 (d, $J = 8.1$ Hz, 1H), 7.89 (d, $J = 7.5$ Hz, 1H), 7.76 (d, $J = 7.5$ Hz, 1H), 7.54 - 7.48 (m, 2H), 7.43 - 7.35 (m, 2H), 7.10 - 7.03 (m, 2H), 6.83 (s, 1H), 3.97 (s, 3H), 3.60 (s, 3H), 2.77 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.2, 163.4, 162.3, 156.5, 152.3, 149.3, 149.1, 148.5, 147.9, 145.0, 136.4, 133.3, 127.3, 126.5, 126.3, 125.7, 125.3, 123.2, 122.5, 121.7, 121.4, 120.5, 119.3, 118.4, 115.9, 112.9, 106.3, 57.1, 56.1, 11.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{30}\text{H}_{22}\text{N}_6\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 595.1217, found, 595.1230. isomer 2, Yellow solid (19 mg, 26 % yield, electrolysis time: 6.3 h, $R_f = 0.23$ (petroleum ether/ethyl acetate = 3 : 1 (v/v)); M.P. 275.3-278.1 °C; NMR Spectroscopy: ^1H NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$, 25 °C, δ): 11.90 (s, 1H), 8.18 - 8.11 (m, 3H), 8.07 (d, $J = 3$ Hz, 1H), 7.88 - 7.85 (m, 1H), 7.59 - 7.44 (m, 4H), 7.28 - 7.18 (m, 3H), 3.91 (s, 3H), 3.67 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (75 MHz, $(\text{CD}_3)_2\text{SO}$, 25 °C, δ): 161.7, 160.3, 155.6, 154.8, 151.6, 150.4, 148.3, 148.1, 147.3, 142.9, 135.6, 134.2, 126.7, 126.5, 126.1, 125.4, 124.4, 122.7,

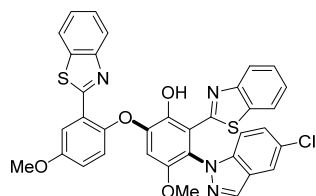
122.6, 122.1, 121.9, 120.2, 119.1, 118.7, 114.7, 112.2, 107.1, 57.1, 55.8, 8.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $C_{30}H_{23}N_6O_4S_2^+$ ($[M + H]^+$), 595.1217, found, 595.1228.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(5-phenyl-2H-tetrazol-2-yl)phenol (3r)



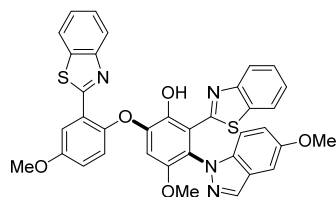
Yellow solid (39 mg, 48 % yield, electrolysis time: 7.7 h, $R_f = 0.41$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 272.9-275.7 °C; NMR Spectroscopy: 1H NMR (300 MHz, $CDCl_3$, 25 °C, δ): 13.85 (s, 1H), 8.33 (d, $J = 4.2$ Hz, 2H), 8.18 (d, $J = 1.5$ Hz, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 8.00 (d, $J = 8.1$ Hz, 1H), 7.92 (d, $J = 7.8$ Hz, 1H), 7.72 (d, $J = 8.4$ Hz, 1H), 7.55 - 7.49 (m, 5H), 7.41 - 7.36 (m, 2H), 7.12 - 7.09 (m, 2H), 6.85 (s, 1H), 3.99 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C, δ): 166.2, 163.4, 162.3, 156.6, 152.4, 149.3, 149.2, 148.8, 147.9, 145.1, 136.5, 133.3, 139.0, 129.2, 127.4, 127.3, 127.2, 126.5, 126.3, 125.9, 125.3, 123.2, 122.5, 121.7, 121.5, 120.6, 119.4, 118.3, 115.9, 112.9, 106.3, 57.2, 56.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $C_{35}H_{25}N_6O_4S_2^+$ ($[M + H]^+$), 657.1373, found, 657.1383.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-3-(5-chloro-1H-indazol-1-yl)-4-methoxyphenol (3s)



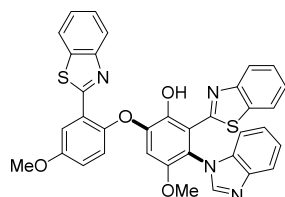
Yellow solid (46 mg, 56 % yield, electrolysis time: 7.8 h, $R_f = 0.31$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 284.8-287.7 °C; NMR Spectroscopy: 1H NMR (300 MHz, $CDCl_3$, 25 °C, δ): 14.02 (s, 1H), 8.18 (d, $J = 2.7$ Hz, 1H), 8.14 - 8.12 (m, 2H), 7.96 - 7.89 (m, 2H), 7.79 - 7.75 (m, 2H), 7.62 (d, $J = 8.1$ Hz, 1H), 7.53 - 7.42 (m, 2H), 7.39 - 7.29 (m, 3H), 7.09 - 7.02 (m, 2H), 6.87 (s, 1H), 3.96 (s, 3H), 3.55 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C, δ): 164.3, 162.4, 156.2, 152.3, 149.0, 148.6, 148.5, 147.0, 145.2, 136.5, 133.8, 128.6, 128.4, 127.5, 126.9, 126.2, 126.1, 125.4, 125.2, 123.3, 123.2, 122.5, 122.2, 121.6, 121.4, 120.1, 120.0, 119.5, 119.3, 116.2, 112.7, 106.9, 57.1, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $C_{35}H_{24}ClN_4O_4S_2^+$ ($[M + H]^+$), 663.0922, found, 663.0932.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(5-methoxy-1H-indazol-1-yl)phenol (3t)



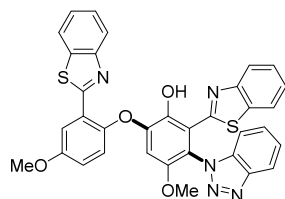
Yellow solid (45 mg, 55 % yield, electrolysis time: 6.4 h, $R_f = 0.40$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 280.4-285.8 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.06 (s, 1H), 8.18 (d, $J = 2.4$ Hz, 1H), 8.13 (d, $J = 8.1$ Hz, 1H), 8.01 (s, 1H), 7.92 (t, $J = 9.3$ Hz, 2H), 7.72 (d, $J = 9.3$ Hz, 1H), 7.61 (d, $J = 7.8$ Hz, 1H), 7.53 - 7.28 (m, 5H), 7.13 - 7.09 (m, 1H), 7.06 - 7.04 (m, 2H), 6.99 (d, $J = 2.1$ Hz, 1H), 6.88 (s, 1H), 3.96 (s, 3H), 3.89 (s, 3H), 3.55 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.7, 162.5, 156.1, 155.7, 152.3, 149.0, 148.8, 148.7, 147.3, 146.6, 145.2, 136.5, 134.0, 126.8, 126.5, 126.2, 125.9, 125.2, 125.1, 123.2, 123.1, 122.9, 122.4, 122.2, 121.6, 119.9, 119.3, 116.4, 112.7, 107.2, 96.5, 57.2, 56.1, 55.5. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{36}\text{H}_{27}\text{N}_4\text{O}_5\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 659.1417, found, 659.1419.

3-(1H-benzo[d]imidazol-1-yl)-2-(benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxyphenol (3u)



Yellow solid (77 mg, 98 % yield, electrolysis time: 6.6 h, $R_f = 0.19$ (petroleum ether/ethyl acetate = 5 : 1 (v/v))); M.P. 276.8-280.7 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.07 (s, 1H), 8.19 (d, $J = 3$ Hz, 1H), 8.14 (d, $J = 8.1$ Hz, 1H), 7.97 - 7.89 (m, 4H), 7.57 (d, $J = 6$ Hz, 1H), 7.52 - 7.49 (m, 1H), 7.46 (d, $J = 9$ Hz, 1H), 7.42 - 7.33 (m, 3H), 7.29 (d, $J = 9$ Hz, 1H), 7.24 (d, $J = 9$ Hz, 1H), 7.13 - 7.03 (m, 3H), 6.91 (s, 1H), 3.96 (s, 3H), 3.49 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.2, 162.4, 156.2, 152.3, 149.2, 148.9, 148.5, 146.6, 145.4, 144.3, 143.9, 136.5, 134.9, 133.4, 127.0, 126.2, 125.3, 125.2, 124.2, 123.2, 123.1, 122.1, 121.6, 121.5, 120.6, 119.9, 119.3, 116.9, 116.8, 112.7, 110.4, 107.1, 56.8, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{35}\text{H}_{25}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 629.1312, found, 629.1329.

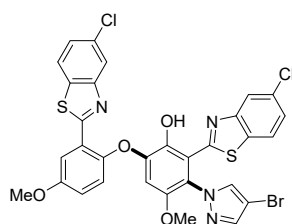
3-(1H-benzo[d][1,2,3]triazol-1-yl)-2-(benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxyphenol (3v)



Yellow solid (74 mg, 94 % yield, electrolysis time: 7.8 h, $R_f = 0.49$ (petroleum

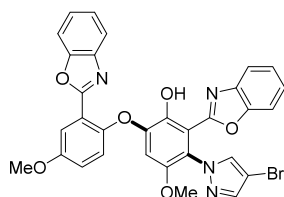
ether/ethyl acetate = 3 : 1 (v/v)); M.P. 296.8-299.6 °C; NMR Spectroscopy: ¹H NMR (300 MHz, CDCl₃, 25 °C, δ): 14.01 (s, 1H), 8.26 - 8.23 (m, 1H), 8.19 (d, *J* = 3 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 6 Hz, 1H), 7.54 - 7.45 (m, 4H), 7.42 - 7.38 (m, 1H), 7.36 - 7.28 (m, 2H), 7.15 - 7.05 (m, 2H), 6.91 (s, 1H), 3.97 (s, 3H), 3.49 (s, 3H). ¹³C NMR (75 MHz, CDCl₃, 25 °C, δ): 163.9, 162.5, 156.3, 152.3, 149.2, 148.9, 148.2, 147.7, 146.2, 145.4, 136.4, 135.4, 128.8, 127.1, 126.3, 125.4, 125.3, 124.6, 123.1, 122.2, 121.6, 121.3, 120.3, 120.2, 119.3, 116.8, 116.7, 112.8, 110.0, 106.9, 56.9, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (*m/z*): calcd for C₃₄H₂₄N₅O₄S₂⁺ ([M + H]⁺), 630.1264, found, 630.1275.

3-(4-Bromo-1*H*-pyrazol-1-yl)-2-(5-chlorobenzo[*d*]thiazol-2-yl)-6-(2-(5-chlorobenzo[*d*]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxyphenol (3w)



Yellow solid (57 mg, 63 % yield, electrolysis time: 7.8 h, *R_f* = 0.11 (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 285.9-289.4 °C; NMR Spectroscopy: ¹H NMR (300 MHz, CDCl₃, 25 °C, δ): 13.61 (s, 1H), 8.13 - 8.12 (m, 1H), 7.92 (d, *J* = 1.8 Hz, 1H), 7.85 (s, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 8.7 Hz, 1H), 7.64 (s, 1H), 7.38 - 7.30 (m, 2H), 7.02 (s, 2H), 6.85 (s, 1H), 3.95 (s, 3H), 3.61 (s, 3H). ¹³C NMR (75 MHz, CDCl₃, 25 °C, δ): 166.0, 164.0, 156.1, 153.1, 149.9, 149.1, 148.4, 146.6, 145.1, 142.8, 134.6, 133.7, 133.0, 132.1, 126.7, 125.5, 124.8, 122.8, 122.2, 122.1, 121.9, 121.8, 119.7, 119.5, 116.1, 112.6, 107.3, 95.6, 57.1, 55.9. Mass Spectrometry: HRMS (ESI-TOF) (*m/z*): calcd for C₃₁H₂₀BrCl₂N₄O₄S₂⁺ ([M + H]⁺), 724.9481, found, 724.9474.

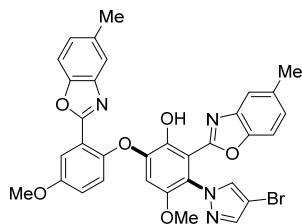
2-(Benzo[*d*]oxazol-2-yl)-6-(2-(benzo[*d*]oxazol-2-yl)-4-methoxyphenoxy)-3-(4-bromo-1*H*-pyrazol-1-yl)-4-methoxyphenol (3x)



Light yellow solid (50 mg, 64 % yield, electrolysis time: 7.3 h, *R_f* = 0.15 (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 270.2-272.1 °C; NMR Spectroscopy: ¹H NMR (300 MHz, CDCl₃, 25 °C, δ): 12.18 (s, 1H), 7.82 (d, *J* = 2.7 Hz, 1H), 7.79 - 7.76 (m, 1H), 7.70 - 7.66 (m, 3H), 7.55 - 7.52 (m, 1H), 7.36 - 7.28 (m, 5H), 7.12 - 7.04 (m, 2H), 6.88 (s, 1H), 3.92 (s, 3H), 3.64 (s, 3H). ¹³C NMR (75 MHz, CDCl₃, 25 °C, δ): 160.8, 160.5, 156.0, 150.8, 149.2, 148.8, 147.7, 145.1, 141.7, 140.9, 138.4, 132.9, 126.1, 125.4, 125.3, 124.6, 121.5, 121.4, 120.3, 119.6, 119.4, 119.3, 114.6, 110.9, 110.8, 110.6, 107.8, 93.8, 57.1, 56.0. Mass Spectrometry: HRMS (ESI-TOF) (*m/z*): calcd for

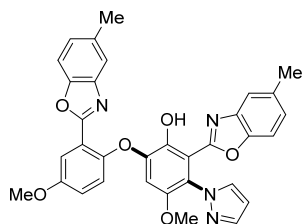
C₃₁H₂₂BrN₄O₆⁺ ([M + H]⁺), 625.0717, found, 625.0710.

3-(4-Bromo-1*H*-pyrazol-1-yl)-4-methoxy-6-(4-methoxy-2-(5-methylbenzo[*d*]oxazol-2-yl)phenoxy)-2-(5-methylbenzo[*d*]oxazol-2-yl)phenol (3y)



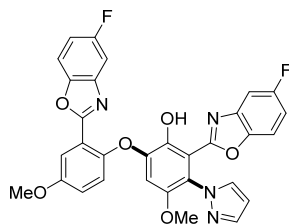
Light yellow solid (47 mg, 58 % yield, electrolysis time: 7.4 h, $R_f = 0.19$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 294.4-295.8 °C; NMR Spectroscopy: ¹H NMR (300 MHz, CDCl₃, 25 °C, δ): 12.26 (s, 1H), 7.80 (d, $J = 2.7$ Hz, 1H), 7.69 (s, 1H), 7.63 (s, 1H), 7.55 (s, 1H), 7.48 (s, 1H), 7.40 (d, $J = 8.1$ Hz, 1H), 7.18 - 7.04 (m, 5H), 6.84 (s, 1H), 3.92 (s, 3H), 3.63 (s, 3H), 2.45 (s, 6H). ¹³C NMR (75 MHz, CDCl₃, 25 °C, δ): 160.9, 160.6, 156.1, 149.1, 148.8, 148.6, 147.8, 147.5, 145.0, 141.9, 141.0, 138.6, 135.4, 134.4, 133.0, 127.3, 126.6, 121.5, 121.3, 120.1, 119.5, 119.3, 114.5, 110.7, 110.3, 107.4, 93.8, 57.2, 56.1, 21.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for C₃₃H₂₆BrN₄O₆⁺ ([M + H]⁺), 653.1030, found, 653.1034.

4-Methoxy-6-(4-methoxy-2-(5-methylbenzo[*d*]oxazol-2-yl)phenoxy)-2-(5-methylbenzo[*d*]oxazol-2-yl)-3-(1*H*-pyrazol-1-yl)phenol (3z)



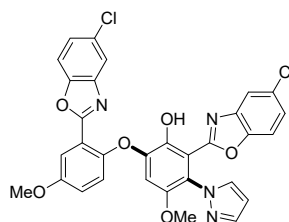
Light yellow solid (40 mg, 55 % yield, electrolysis time: 6.9 h, $R_f = 0.21$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 274.4-276.1 °C; NMR Spectroscopy: ¹H NMR (300 MHz, CDCl₃, 25 °C, δ): 12.31 (s, 1H), 7.81 (d, $J = 2.7$ Hz, 1H), 7.75 (d, $J = 1.5$ Hz, 1H), 7.60 (d, $J = 2.1$ Hz, 1H), 7.56 (s, 1H), 7.46 (s, 1H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.13 - 7.03 (m, 5H), 6.88 (s, 1H), 6.51 (t, $J = 2.1$ Hz, 1H), 3.92 (s, 3H), 3.62 (s, 3H), 2.44 (d, $J = 3.5$ Hz, 6H). ¹³C NMR (75 MHz, CDCl₃, 25 °C, δ): 160.9, 160.8, 155.8, 149.0, 148.8, 148.8, 147.4, 147.1, 145.0, 141.8, 140.4, 138.6, 135.1, 134.3, 132.7, 127.0, 126.4, 122.3, 121.2, 120.1, 119.4, 119.3, 119.1, 114.4, 110.9, 110.2, 110.1, 107.9, 106.1, 57.2, 55.9, 21.5, 21.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for C₃₃H₂₇N₄O₆⁺ ([M + H]⁺), 575.1925, found, 575.1935.

2-(5-Fluorobenzo[*d*]oxazol-2-yl)-6-(2-(5-fluorobenzo[*d*]oxazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(1*H*-pyrazol-1-yl)phenol (3aa)



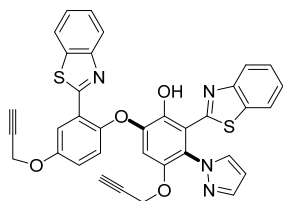
Light yellow solid (35 mg, 49 % yield, electrolysis time: 7.0 h, $R_f = 0.23$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 299.1-301.5 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 11.95 (s, 1H), 7.79 (s, 1H), 7.74 (d, $J = 1.5$ Hz, 1H), 7.63 (d, $J = 2.1$ Hz, 1H), 7.49 - 7.44 (m, 2H), 7.37 - 7.34 (m, 1H), 7.19 - 7.14 (m, 1H), 7.09 - 7.00 (m, 4H), 6.92 (s, 1H), 6.52 (t, $J = 2.1$ Hz, 1H), 3.92 (s, 3H), 3.64 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 162.7, 162.5, 161.9 (d, $J = 18.4$ Hz, 1C), 158.7 (d, $J = 16.5$ Hz, 1C), 155.9, 149.1, 148.9, 147.2, 147.0, 145.6, 145.2, 142.5 (d, $J = 13.3$ Hz, 1C), 140.6, 139.3 (d, $J = 13.4$ Hz, 1C), 132.9, 122.6, 121.1, 119.9, 118.9, 114.6, 113.9 - 112.9 (m, 2C), 111.4 - 111.2 (m, 1C), 110.7, 108.6, 106.8 - 105.6 (m, 2C), 106.4, 57.3, 56.1. ^{19}F NMR (282 MHz, CDCl_3 , 25 °C, δ): -116.3, -117.7. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{21}\text{F}_2\text{N}_4\text{O}_6^+$ ($[\text{M} + \text{H}]^+$), 583.1424, found, 583.1434.

2-(5-Chlorobenzo[d]oxazol-2-yl)-6-(2-(5-chlorobenzo[d]oxazol-2-yl)-4-methoxyphenoxy)-4-methoxy-3-(1H-pyrazol-1-yl)phenol (3ab)



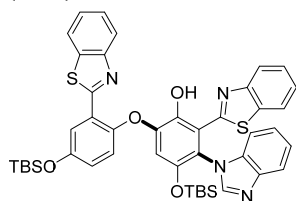
Light yellow solid (42 mg, 54 % yield, electrolysis time: 8.0 h, $R_f = 0.12$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 292.5-294.0 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 11.89 (s, 1H), 7.80 (t, $J = 1.5$ Hz, 1H), 7.76 (d, $J = 2.1$ Hz, 1H), 7.74 (d, $J = 1.5$ Hz, 1H), 7.67 (d, $J = 2.1$ Hz, 1H), 7.62 (d, $J = 2.1$ Hz, 1H), 7.47 (d, $J = 8.7$ Hz, 1H), 7.32 - 7.27 (m, 2H), 7.16 (d, $J = 8.7$ Hz, 1H), 7.09 (d, $J = 1.8$ Hz, 2H), 6.92 (s, 1H), 6.52 (t, $J = 2.1$ Hz, 1H), 3.93 (s, 3H), 3.65 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 162.2, 162.1, 156.0, 149.4, 149.1, 148.9, 147.9, 146.9, 145.2, 142.9, 140.6, 139.7, 132.9, 130.8, 130.1, 126.3, 125.7, 121.1, 120.2, 119.9, 119.3, 118.7, 114.7, 111.7, 110.7, 108.7, 106.4, 57.3, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{31}\text{H}_{21}\text{Cl}_2\text{N}_4\text{O}_6^+$ ($[\text{M} + \text{H}]^+$), 615.0833, found, 615.0831.

2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-(prop-2-yn-1-yloxy)phenoxy)-4-(prop-2-yn-1-yloxy)-3-(1H-pyrazol-1-yl)phenol (3ac)



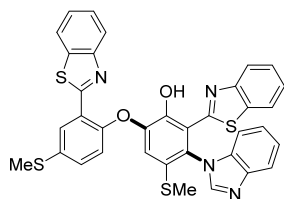
Light yellow solid (27 mg, 35 % yield, electrolysis time: 7.4 h, $R_f = 0.23$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 283.9-287.8 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.17 (s, 1H), 7.25 (d, $J = 2.4$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.96 (d, $J = 8.1$ Hz, 1H), 7.92 - 7.88 (m, 2H), 7.76 (d, $J = 7.8$ Hz, 1H), 7.64 (d, $J = 2.4$ Hz, 1H), 7.52 - 7.45 (m, 2H), 7.41 - 7.34 (m, 2H), 7.10 - 7.05 (m, 3H), 6.64 (t, $J = 2.1$ Hz, 1H), 4.84 (d, $J = 2.4$ Hz, 2H), 4.40 (d, $J = 2.4$ Hz, 2H), 2.57 (t, $J = 2.4$ Hz, 1H), 2.37 (t, $J = 2.4$ Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.8, 162.2, 154.1, 152.3, 149.2, 149.1, 146.9, 146.6, 146.0, 142.2, 136.5, 134.1, 133.8, 126.9, 126.2, 126.1, 125.5, 125.2, 124.6, 123.2, 122.2, 121.6, 121.3, 120.1, 119.9, 116.6, 114.4, 110.8, 108.2, 78.5, 77.9, 77.4, 75.9, 58.6, 56.8. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{35}\text{H}_{23}\text{N}_4\text{O}_4\text{S}_2^+$ ($[\text{M} + \text{H}]^+$), 627.1155, found, 627.1154.

3-(1H-Benzo[d]imidazol-1-yl)-2-(benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-((*tert*-butyldimethylsilyl)oxy)phenoxy)-4-((*tert*-butyldimethylsilyl)oxy)phenol (3ad)



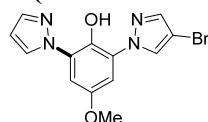
Yellow solid (42 mg, 41 % yield, electrolysis time: 7.7 h, $R_f = 0.17$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 287.4-289.5 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.18 (s, 1H), 8.14 - 8.12 (m, 2H), 7.98 - 7.89 (m, 4H), 7.59 (d, $J = 7.8$ Hz, 1H), 7.52 - 7.43 (m, 2H), 7.39 - 7.28 (m, 3H), 7.22 (d, $J = 7.2$ Hz, 1H), 7.11 - 7.07 (m, 2H), 7.02 - 6.98 (m, 1H), 6.70 (s, 1H), 1.05 (d, $J = 3$ Hz, 9H), 0.43 (s, 9H), 0.29 (s, 6H), -0.13 (s, 3H), -0.3 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.6, 162.1, 152.6, 152.5, 149.1, 148.2, 147.2, 145.7, 145.2, 144.1, 144.0, 136.5, 134.9, 133.4, 127.0, 126.3, 126.2, 126.1, 125.2, 124.1, 123.5, 123.3, 123.1, 122.1, 121.6, 121.5, 120.8, 120.7, 120.6, 118.5, 116.4, 112.2, 110.6, 25.9, 24.9, 18.4, 17.5, -4.2, -4.4, -4.8. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{45}\text{H}_{49}\text{N}_4\text{O}_4\text{S}_2\text{Si}_2^+$ ($[\text{M} + \text{H}]^+$), 829.2728, found, 829.2739.

3-(1H-benzo[d]imidazol-1-yl)-2-(benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-(methylthio)phenoxy)-4-(methylthio)phenol (3ae)



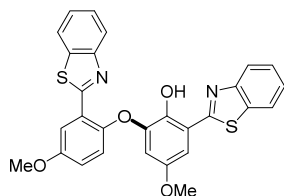
Yellow solid (39 mg, 47 % yield, electrolysis time: 7.2 h, $R_f = 0.27$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 279.3-283.0 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 14.59 (s, 1H), 8.15 (d, $J = 8.1$ Hz, 1H), 8.00 (d, $J = 8.0$ Hz, 2H), 7.91 (d, $J = 8.1$ Hz, 2H), 7.59 (d, $J = 7.9$ Hz, 1H), 7.54 - 7.45 (m, 2H), 7.43 - 7.38 (m, 2H), 7.37 - 7.35 (m, 1H), 7.32 - 7.28 (m, 1H), 2.61 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 164.1, 162.0, 152.9, 152.4, 150.3, 148.7, 145.8, 143.9, 143.3, 136.4, 134.1, 133.2, 130.7, 130.4, 128.8, 128.2, 127.2, 126.4, 126.3, 125.2, 124.6, 123.5, 123.3, 122.1, 121.5, 121.4, 120.9, 117.9, 117.8, 110.3, 16.9, 16.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{35}\text{H}_{25}\text{N}_4\text{O}_2\text{S}_4^+$ ($[\text{M} + \text{H}]^+$), 661.0855, found, 661.0855.

2-(4-Bromo-1H-pyrazol-1-yl)-4-methoxy-6-(1H-pyrazol-1-yl)phenol (3af)



White solid (14 mg, 21 % yield, electrolysis time: 5.0 h, $R_f = 0.27$ (petroleum ether/ethyl acetate = 3 : 1 (v/v))); M.P. 280.5-284.5 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 11.74 (s, 1H), 8.38 (d, $J = 0.3$ Hz, 1H), 8.08 (d, $J = 2.7$ Hz, 1H), 7.76 (d, $J = 1.8$ Hz, 1H), 7.68 (s, 1H), 7.26 (d, $J = 2.7$ Hz, 1H), 7.02 (d, $J = 3$ Hz, 1H), 6.54 (t, $J = 2.4$ Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 152.3, 140.5, 139.5, 135.4, 131.3, 129.2, 128.3, 126.8, 107.2, 105.7, 104.5, 94.8, 56.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): calcd for $\text{C}_{13}\text{H}_{12}\text{BrN}_4\text{O}_2^+$ ($[\text{M} + \text{H}]^+$), 335.0138, found, 335.0138.

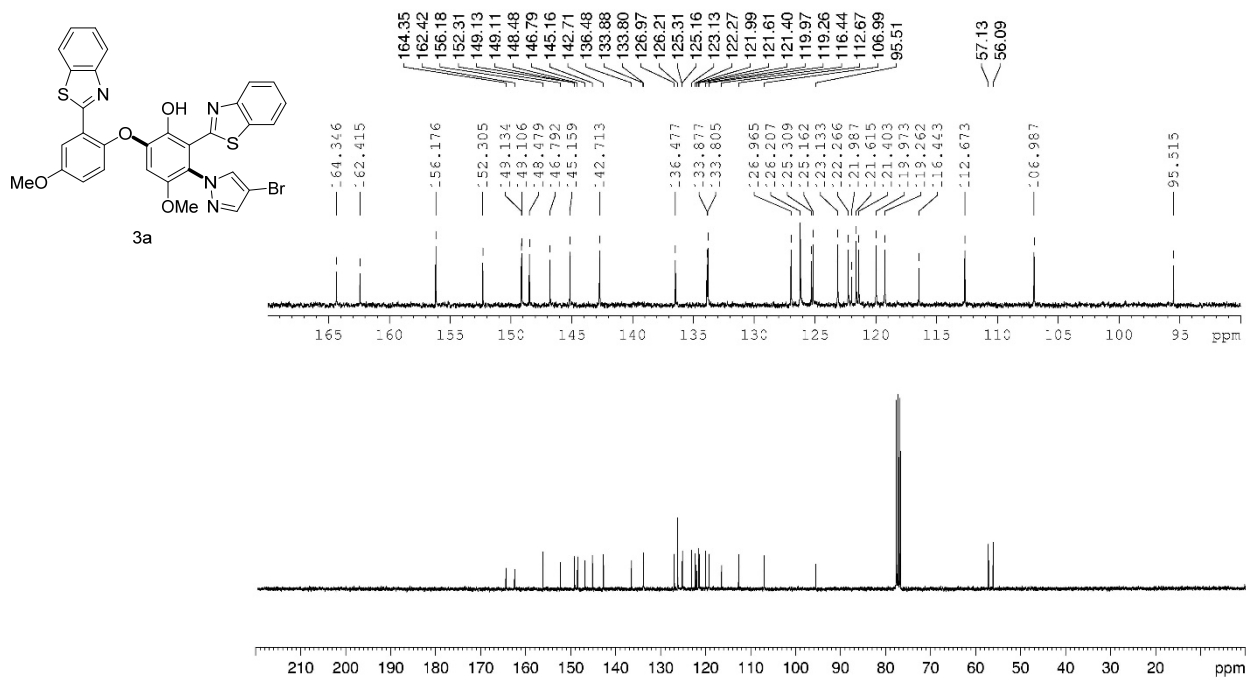
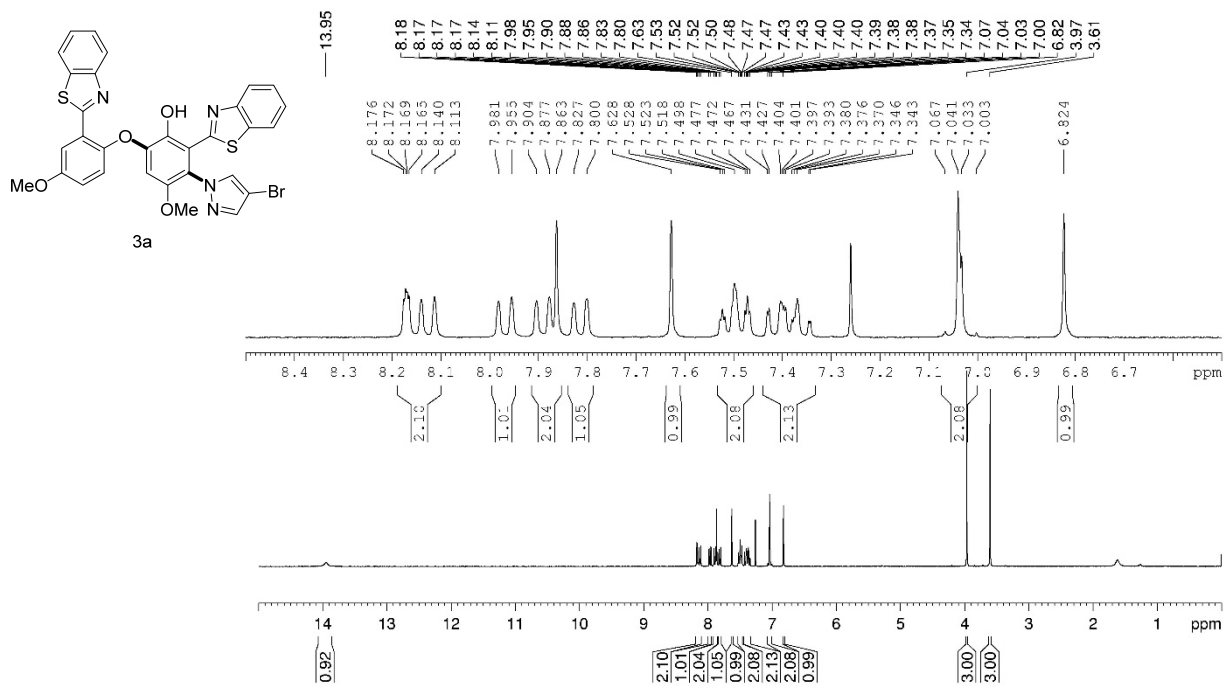
2-(Benzo[d]thiazol-2-yl)-6-(2-(benzo[d]thiazol-2-yl)-4-methoxyphenoxy)-4-methoxyphenol (4)

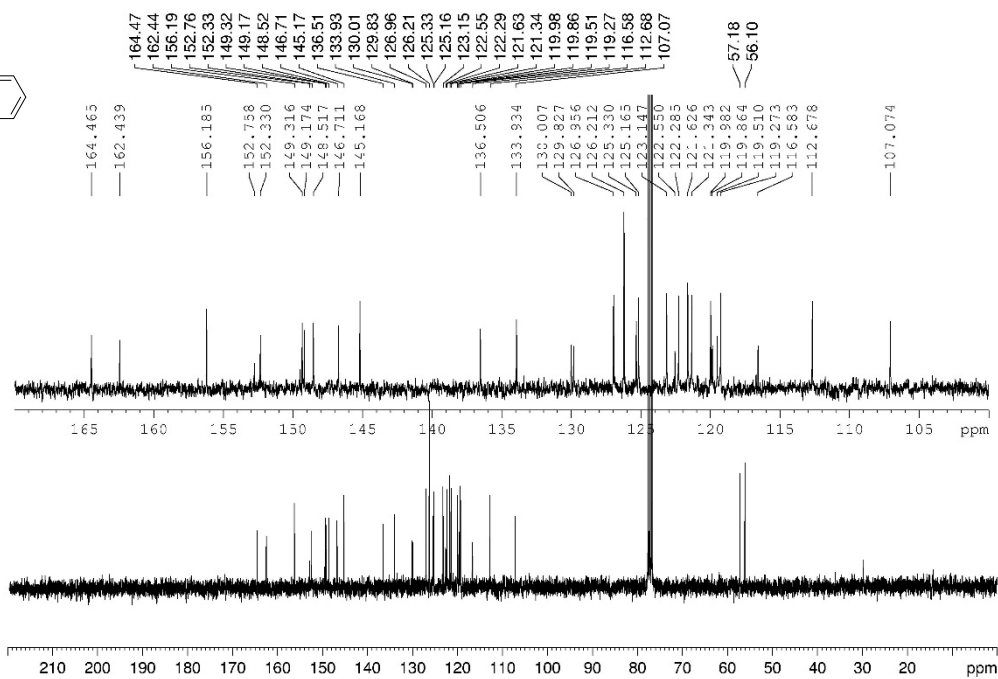
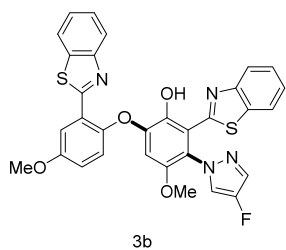
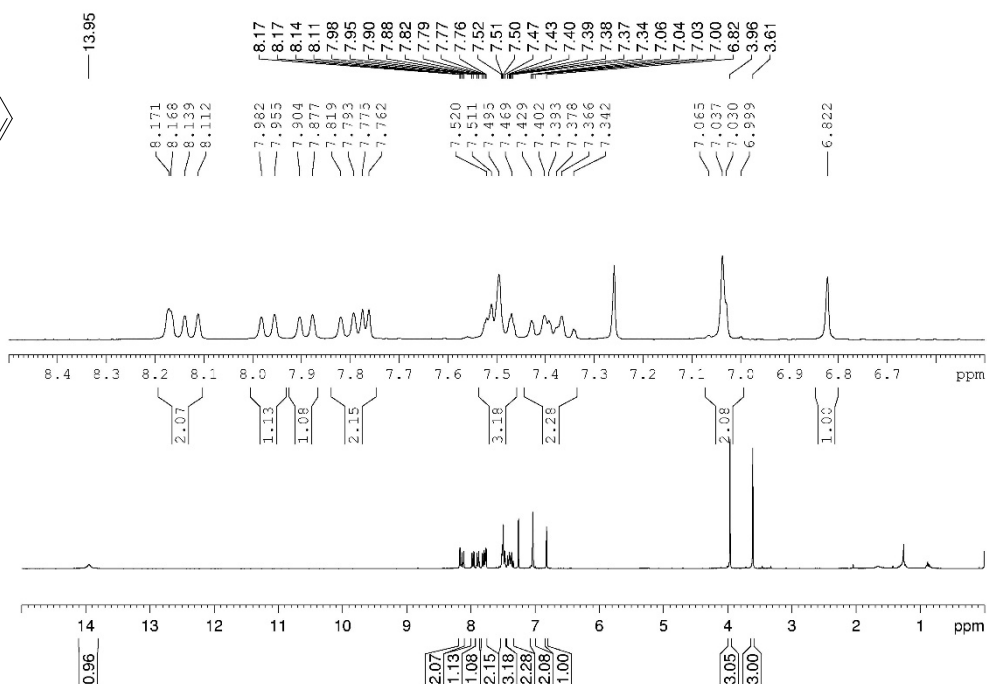
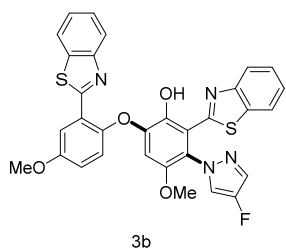


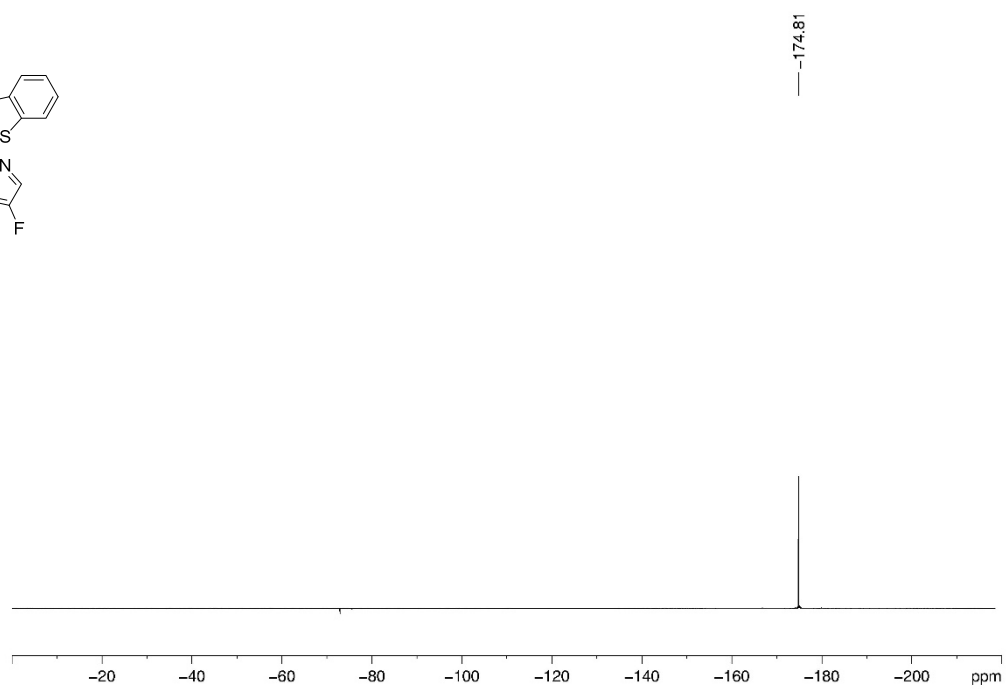
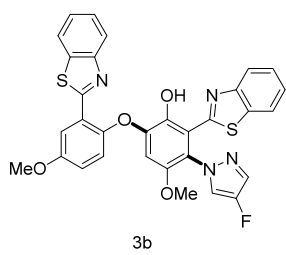
Yellow solid (29 mg, 45 % yield, electrolysis time: 2.5 h, $R_f = 0.45$ (petroleum ether/ethyl acetate = 10 : 1 (v/v))); M.P. 277.8-279.9 °C; NMR Spectroscopy: ^1H NMR (300 MHz, CDCl_3 , 25 °C, δ): 12.50 (s, 1H), 8.16 - 8.15 (m, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.95 (d, $J = 8.1$ Hz, 1H), 7.92 - 7.86 (m, 2H), 7.53 - 7.48 (m, 2H), 7.46 - 7.42 (m, 1H), 7.39 - 7.32 (m, 1H), 7.04 - 6.97 (m, 3H), 6.72 (d, $J = 2.7$ Hz, 1H), 3.95 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, δ): 168.7, 162.7, 155.9, 152.3, 151.9, 148.9, 145.8, 144.5, 136.5, 132.9, 127.0, 126.1, 125.9, 125.2, 125.0, 123.1, 122.4,

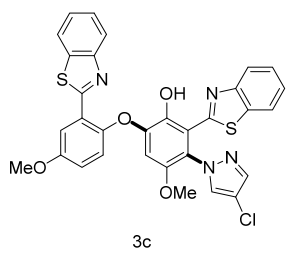
121.7, 121.6, 119.9, 119.3, 117.8, 112.5, 110.3, 107.0, 56.1. Mass Spectrometry:
HRMS (ESI-TOF) (m/z): calcd for $C_{28}H_{21}N_2O_4S_2^+$ ($[M + H]^+$), 513.0937,
found, 513.0946.

12. NMR Spectrum

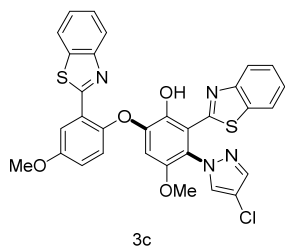
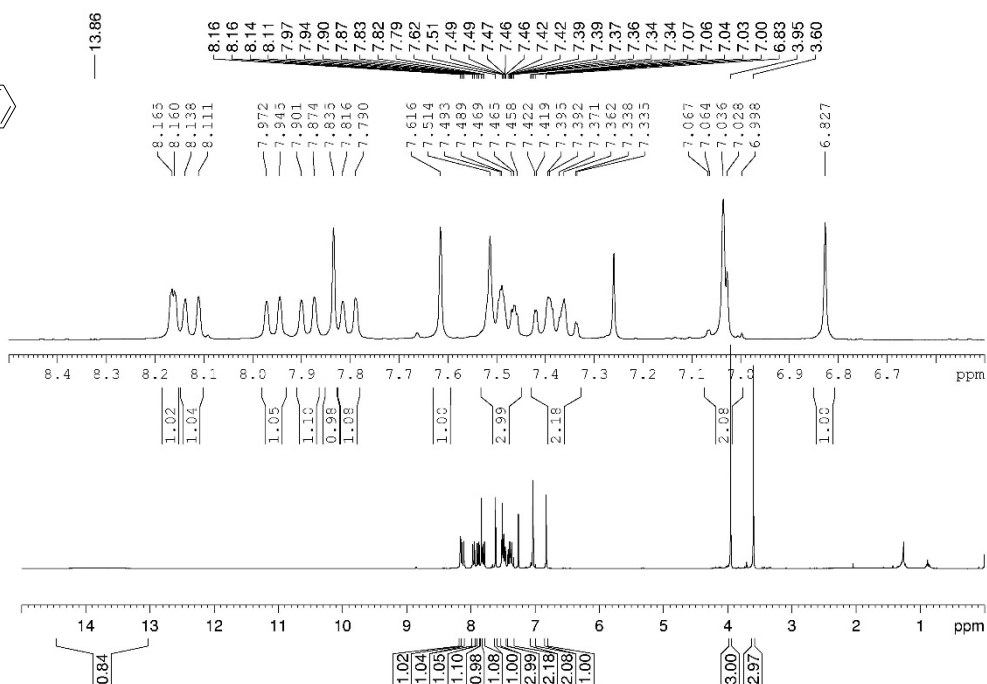




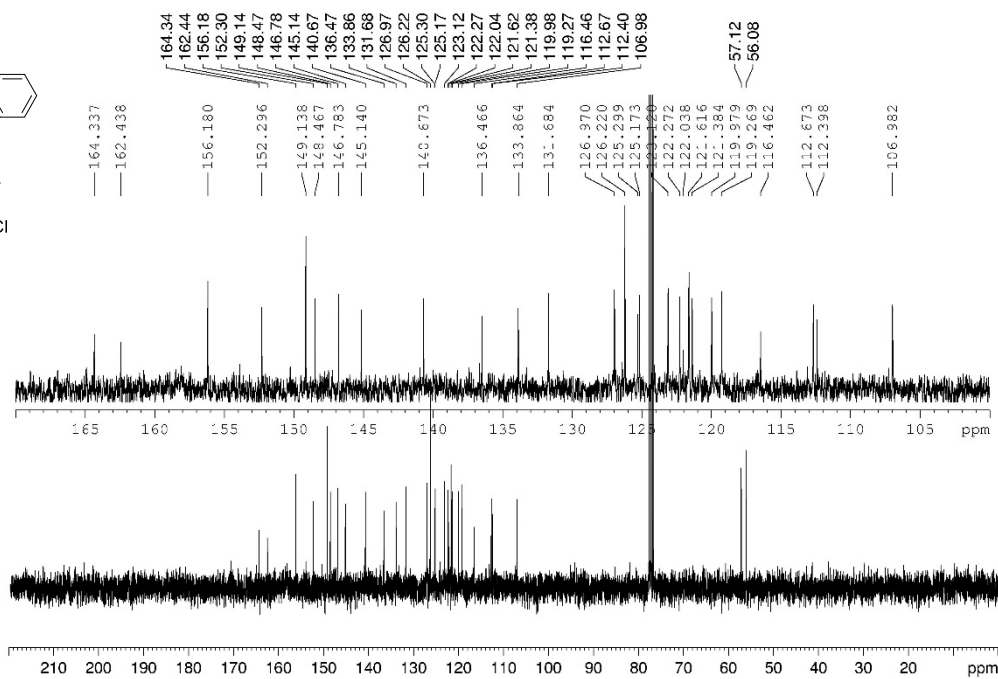


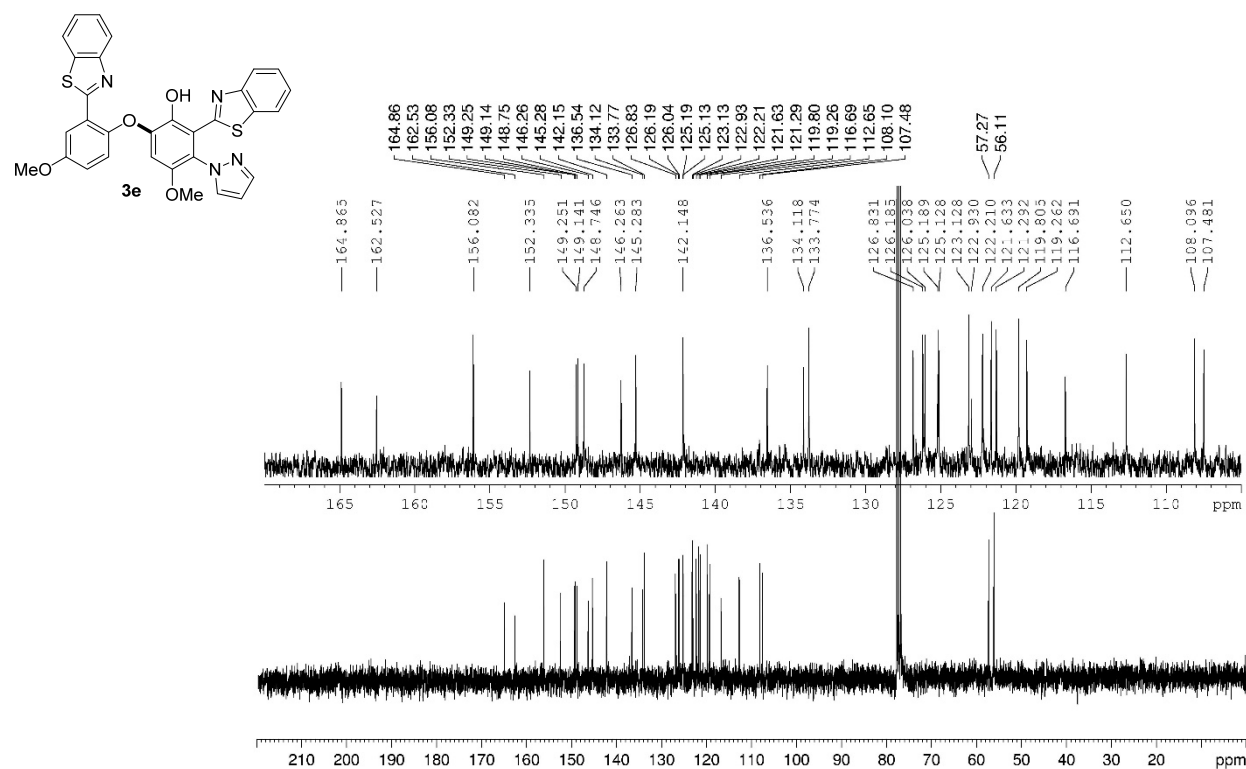
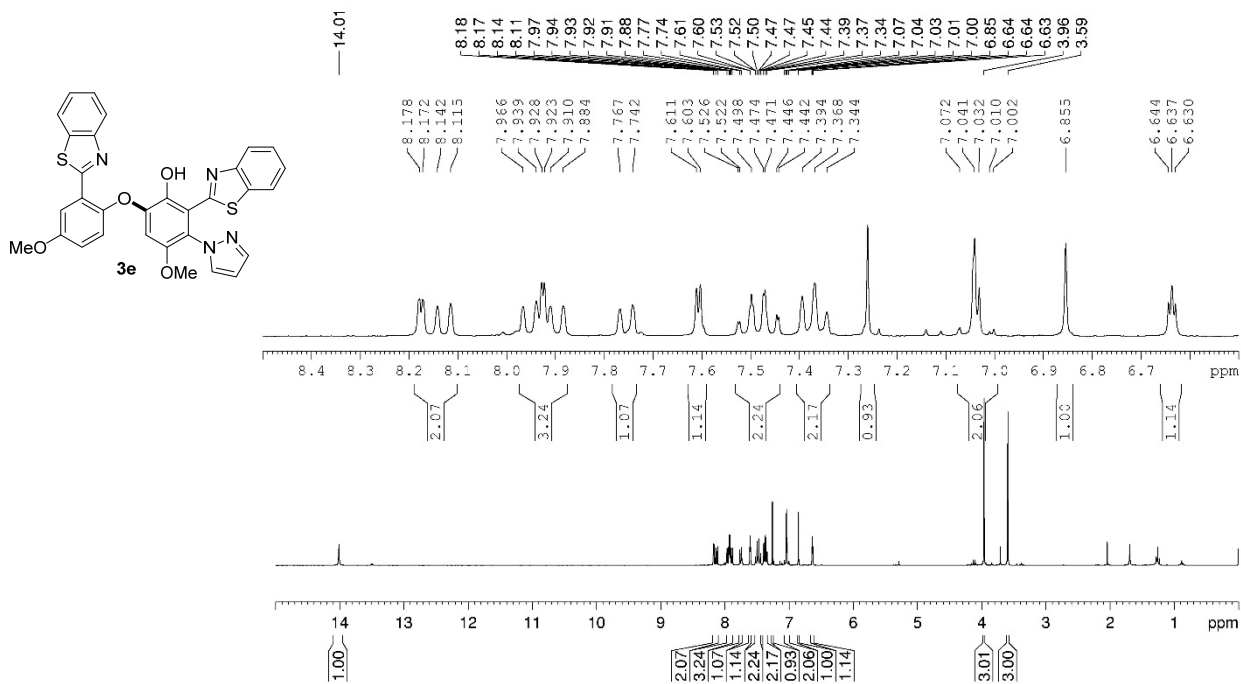


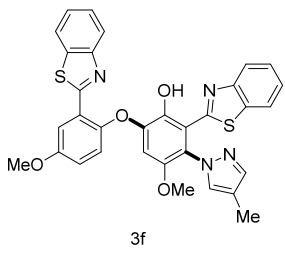
3c



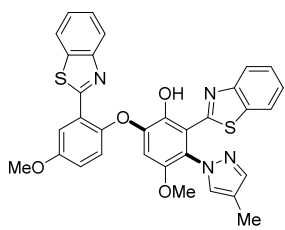
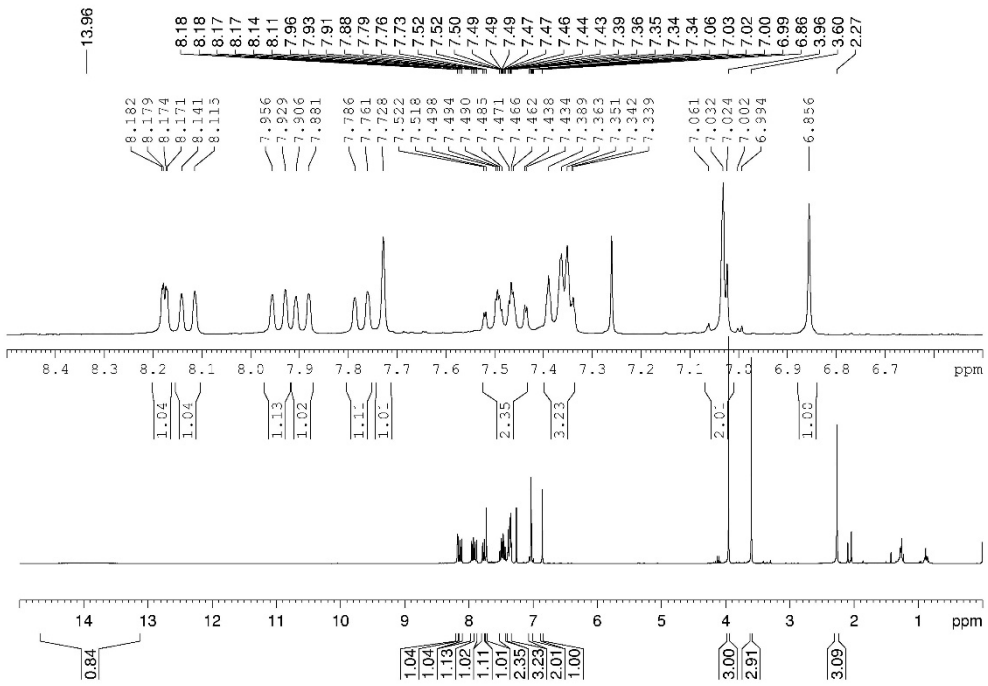
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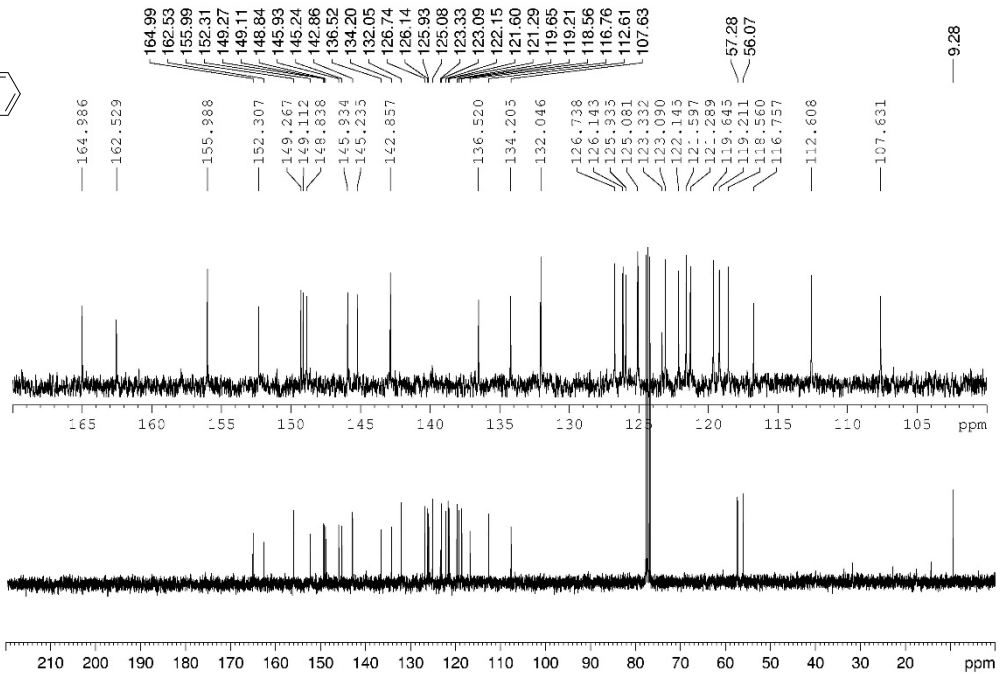


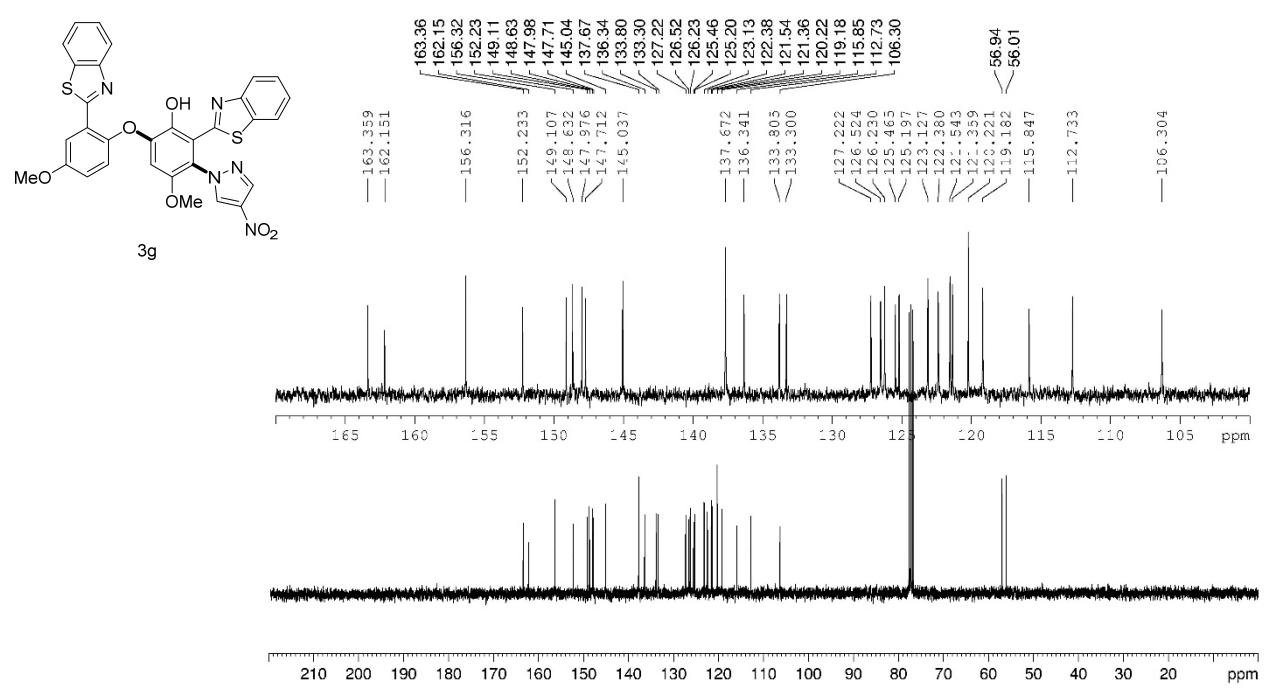
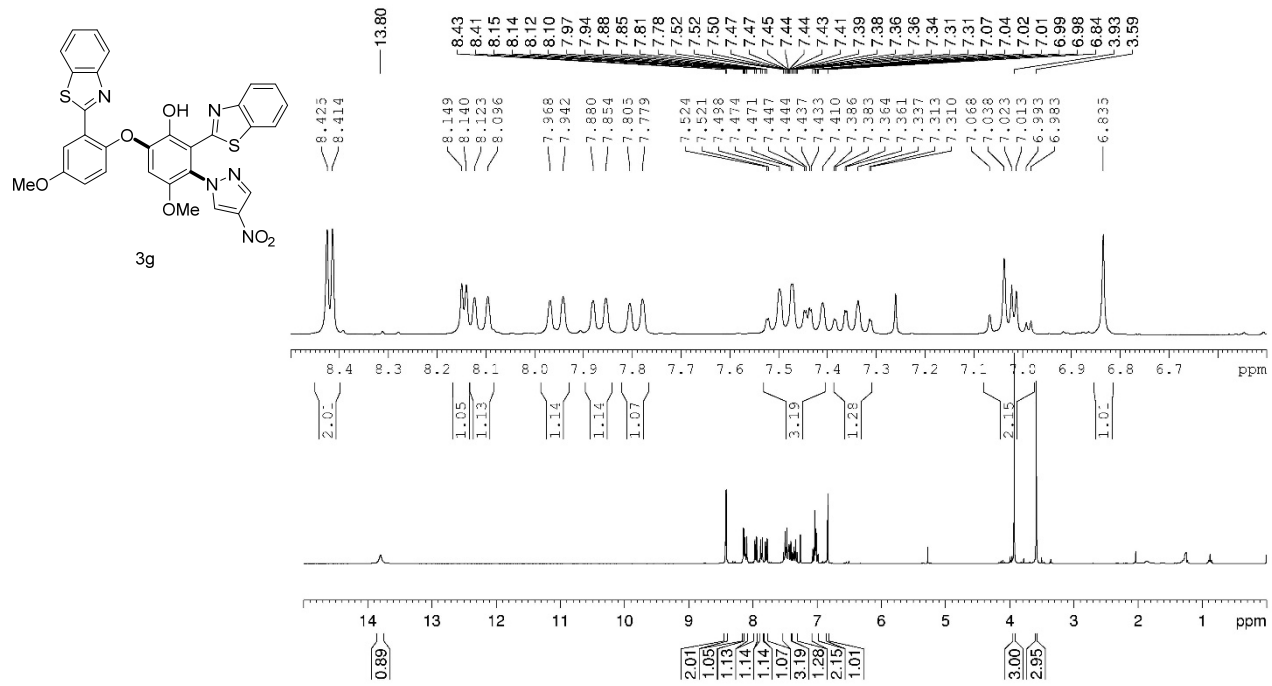


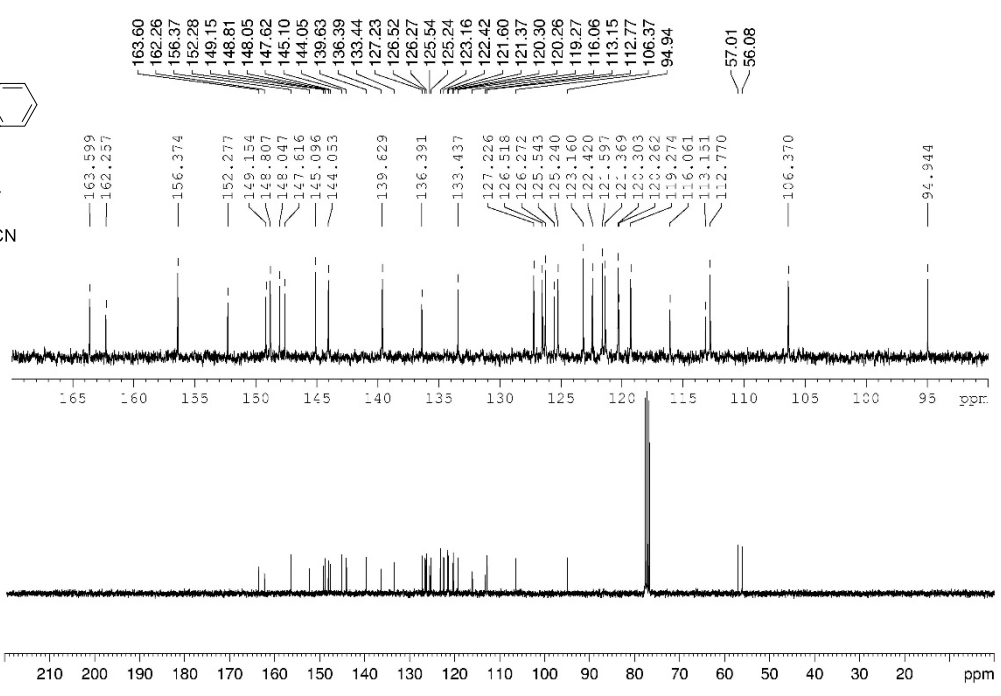
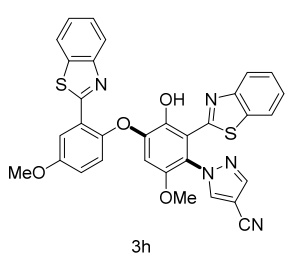
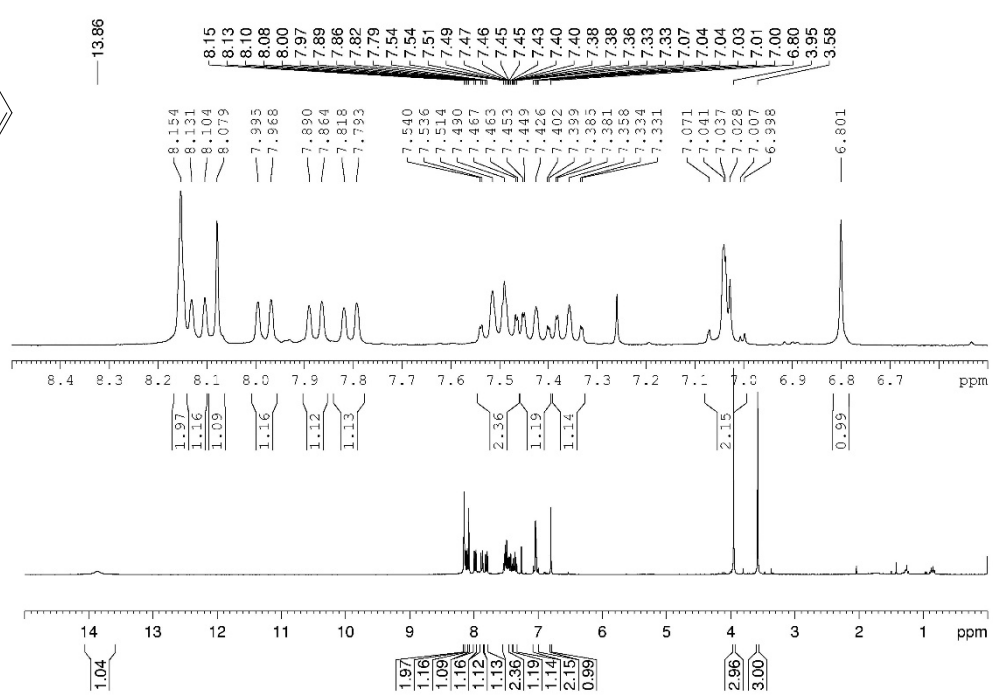
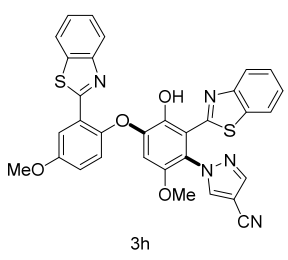
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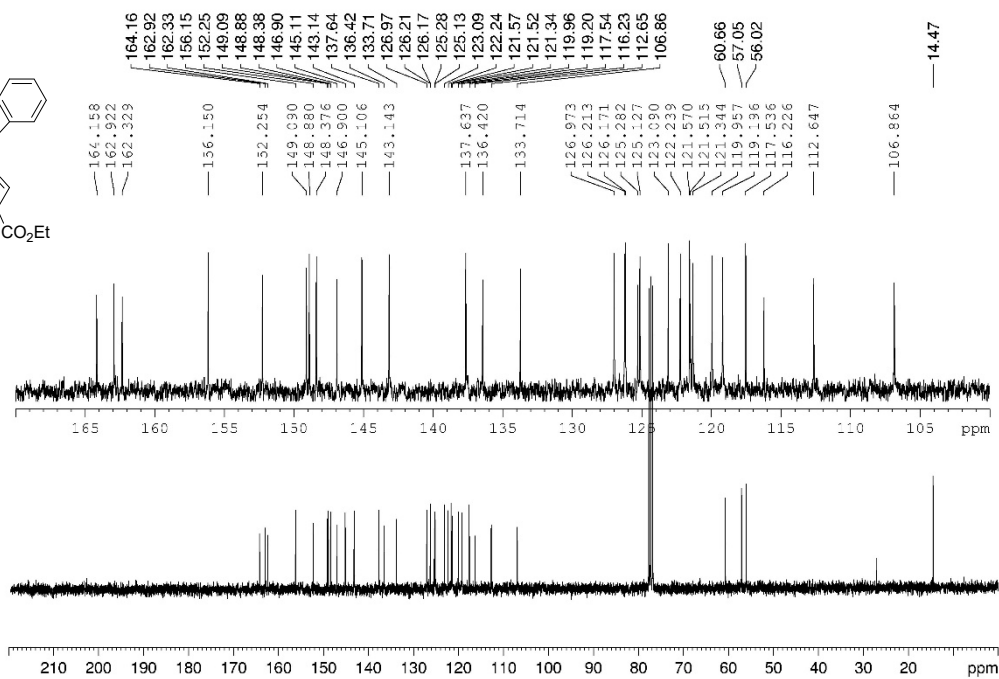
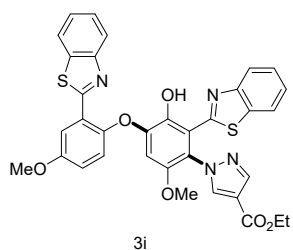
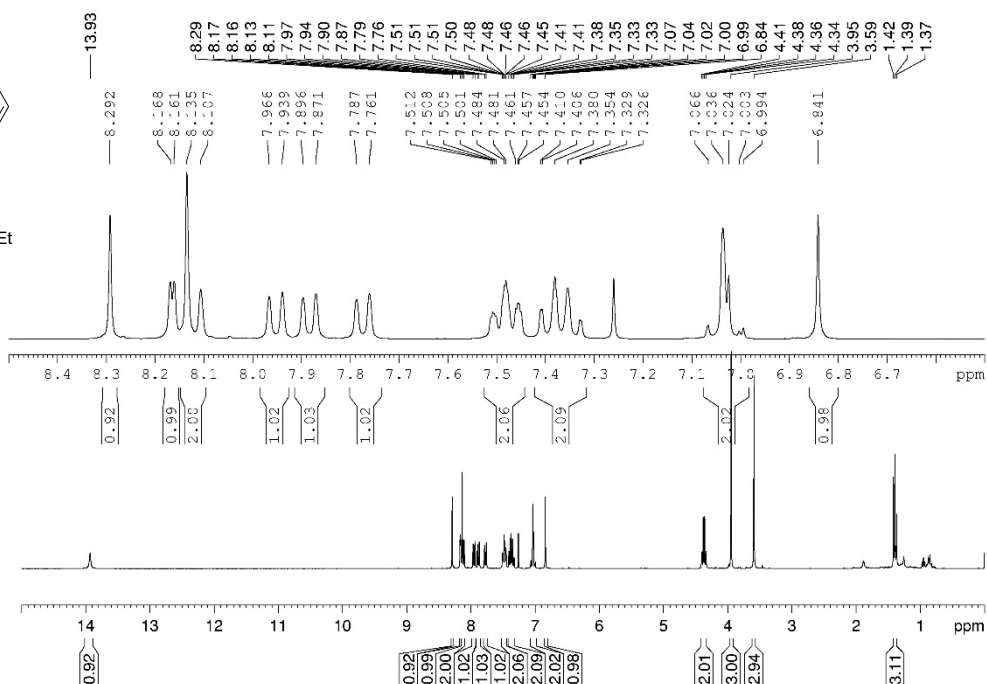
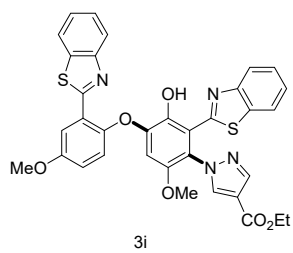


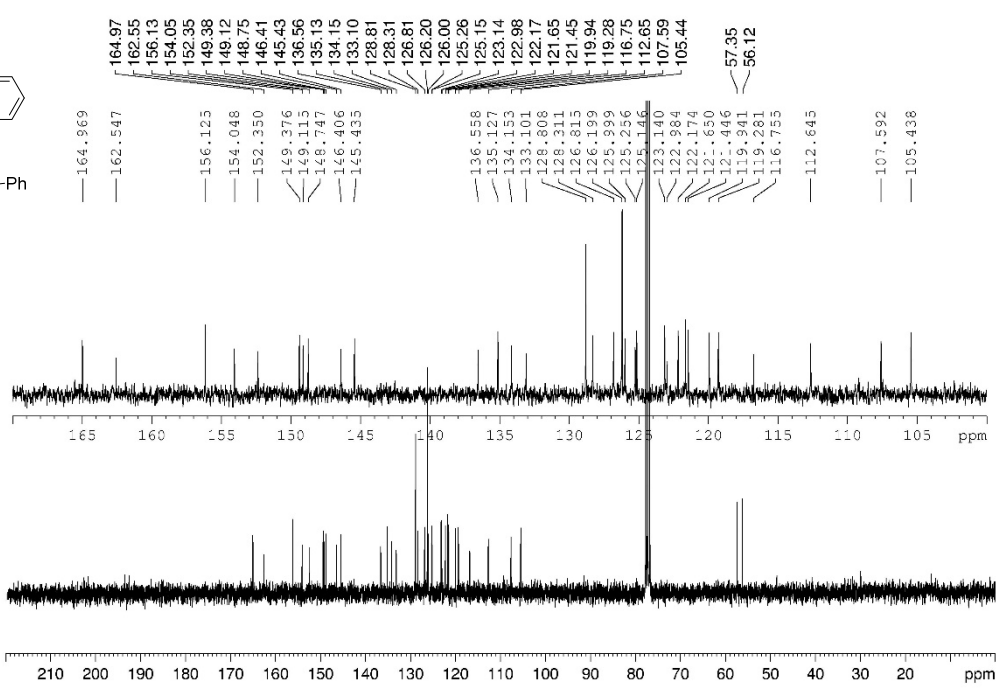
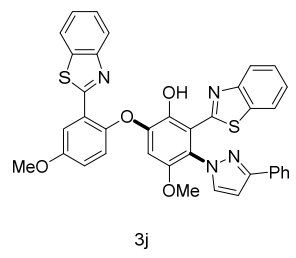
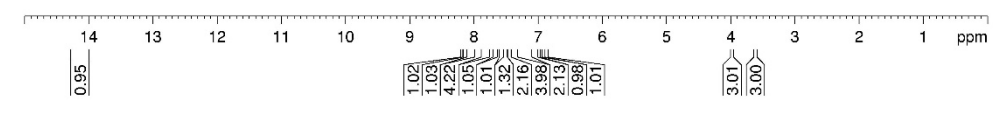
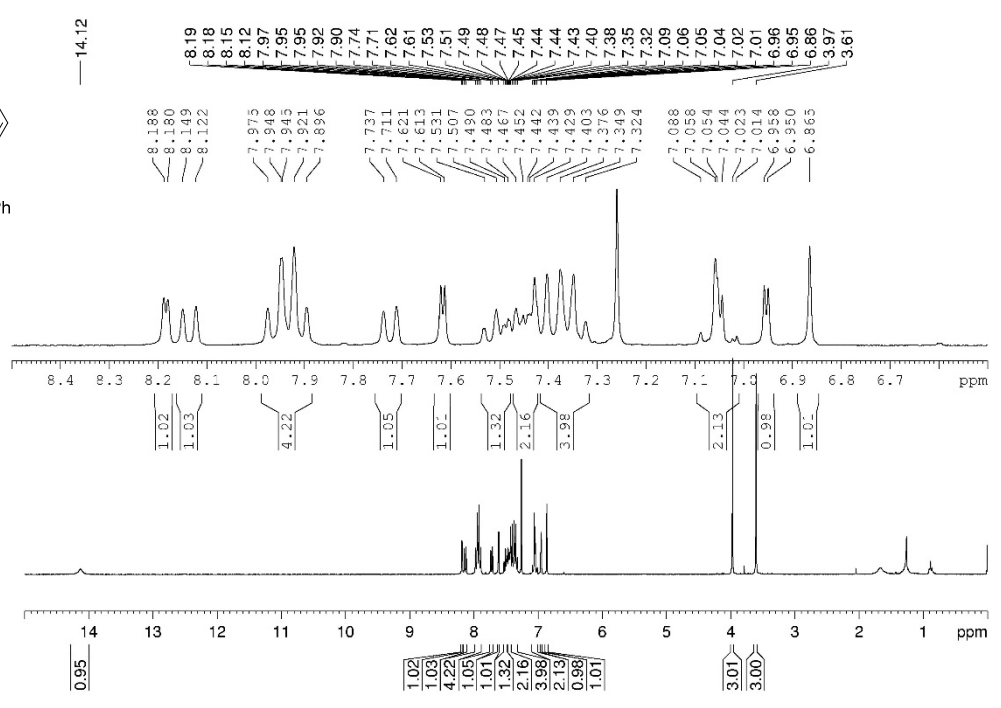
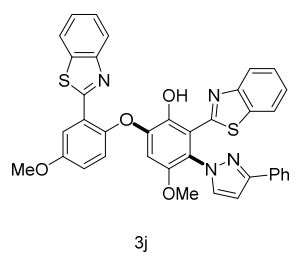
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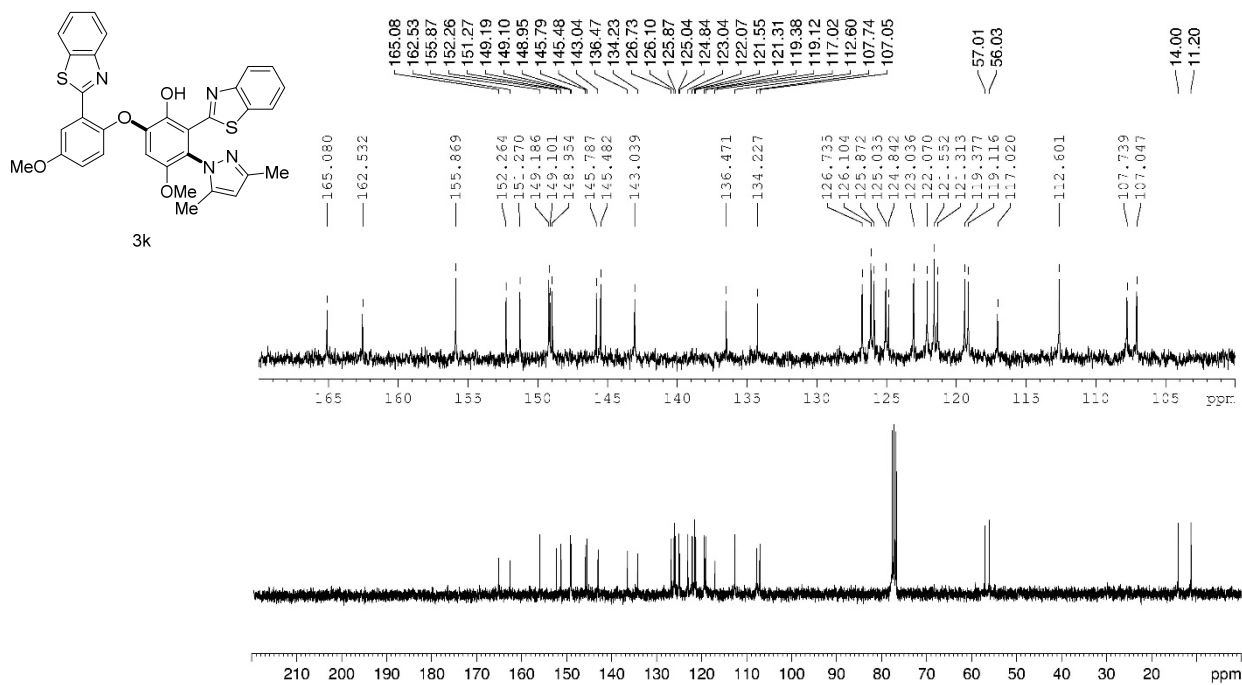
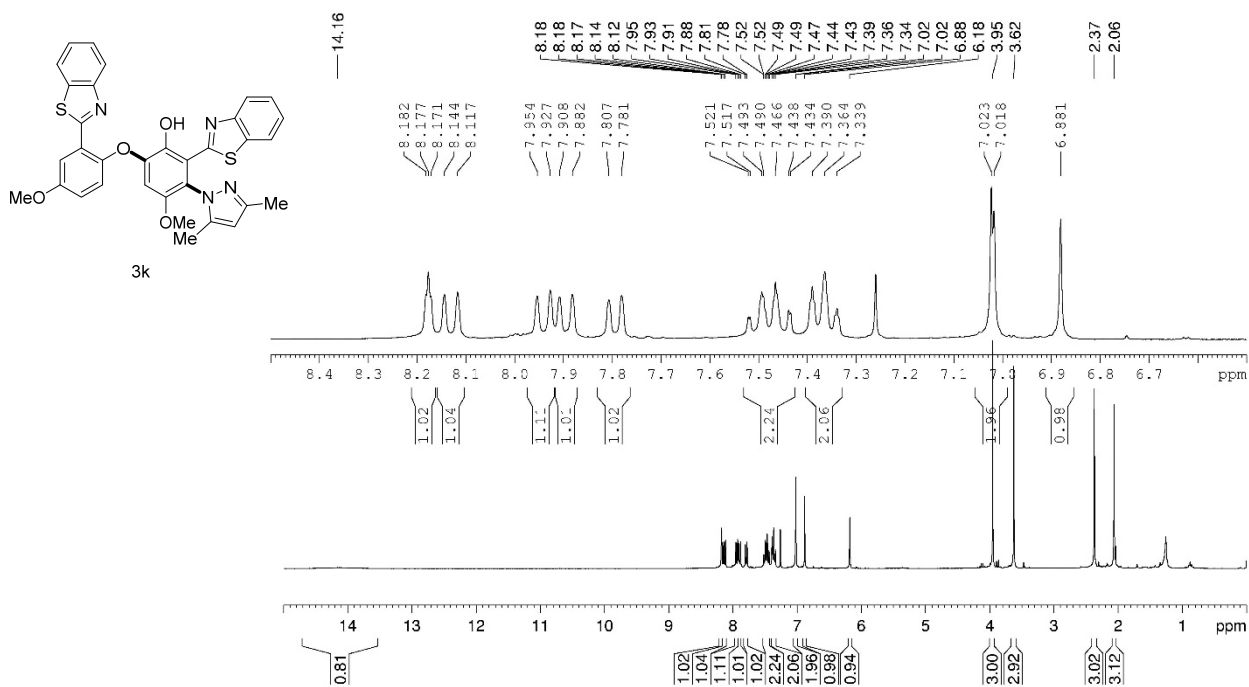


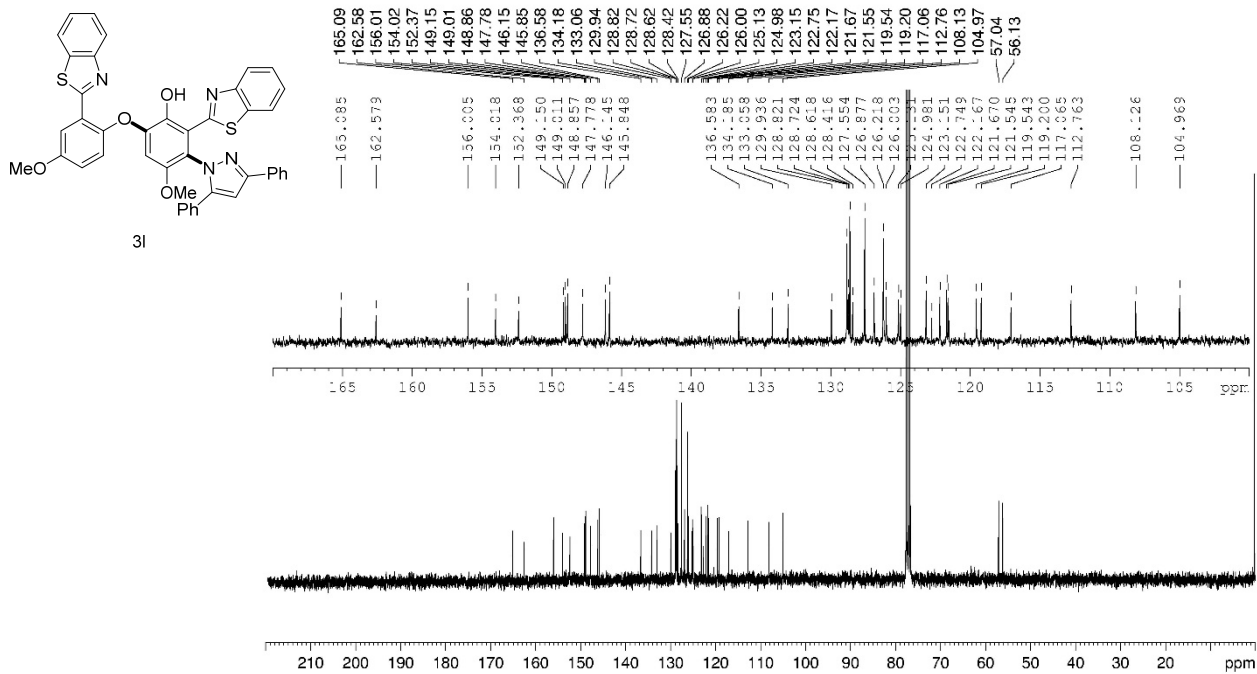
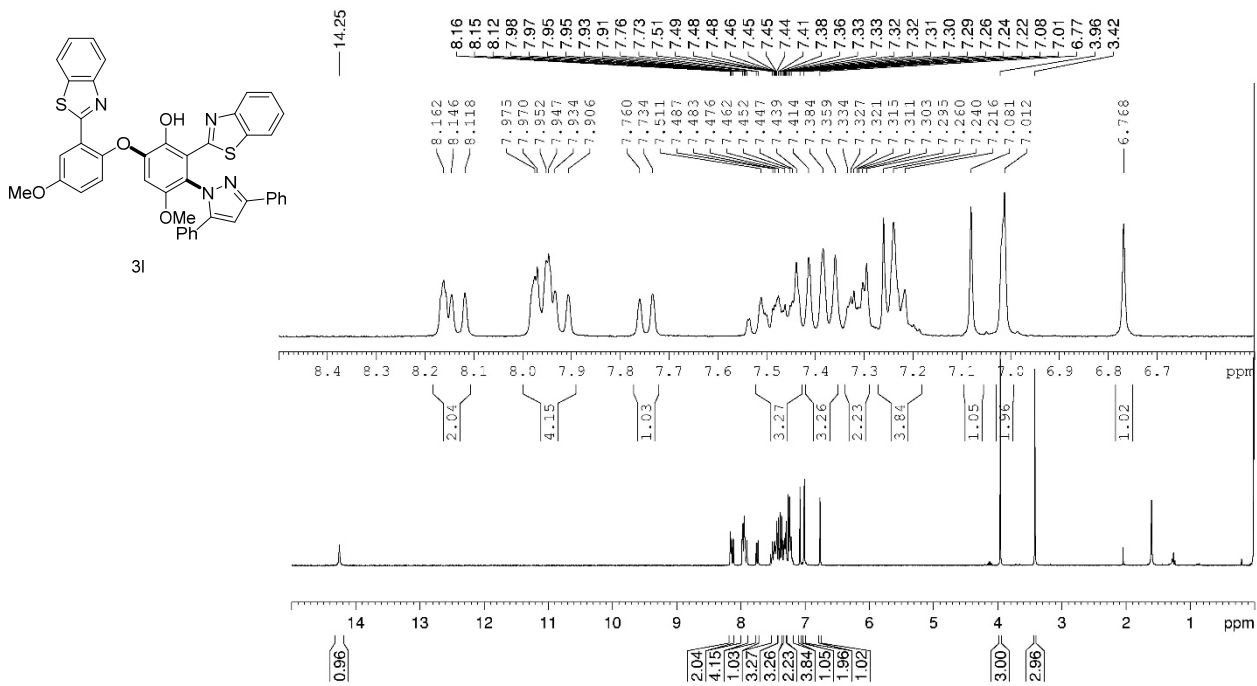


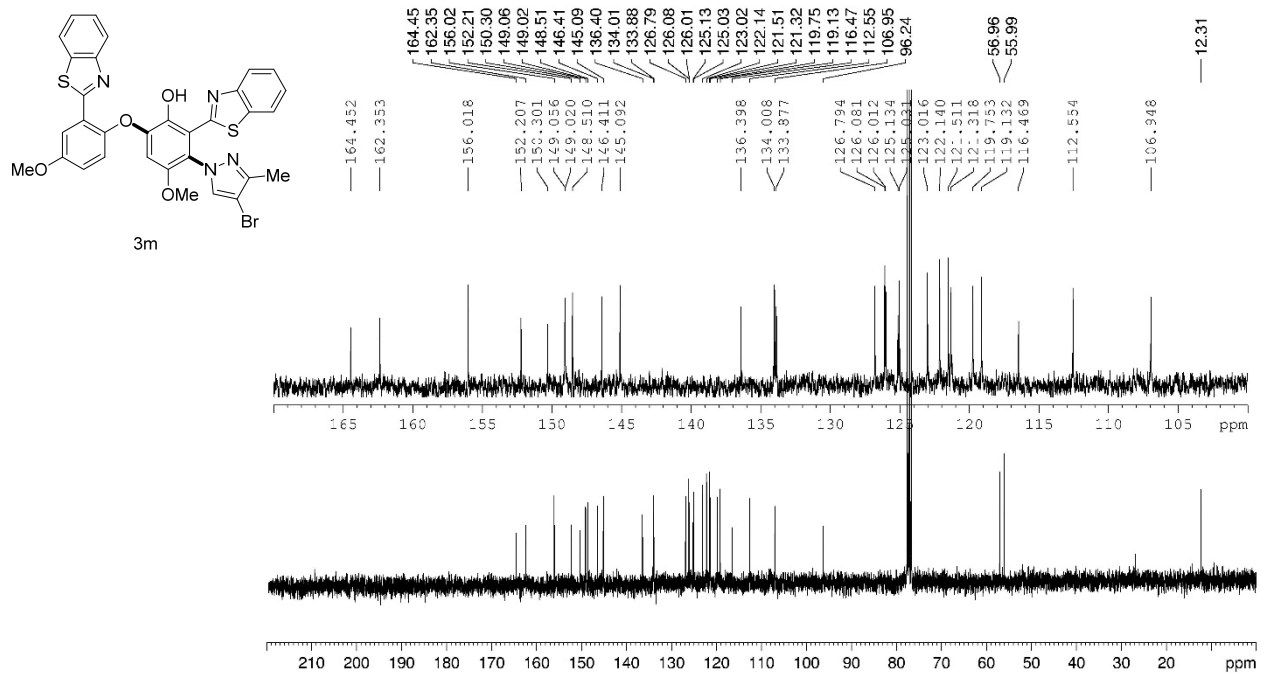
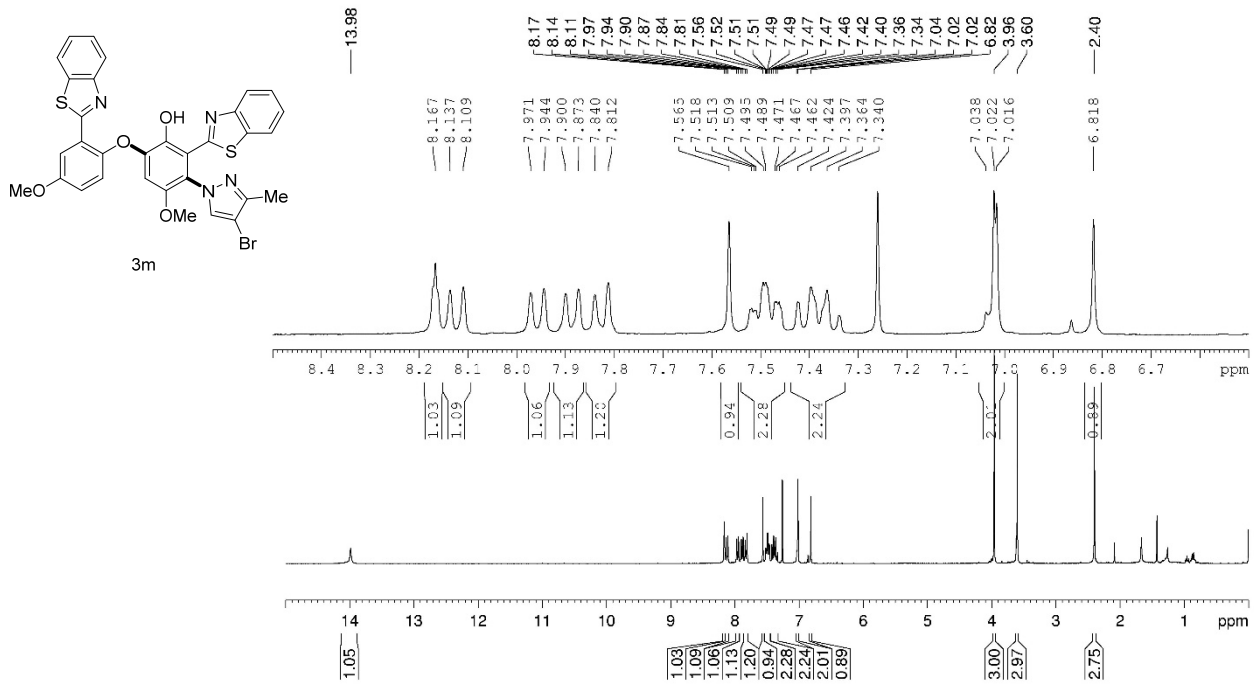


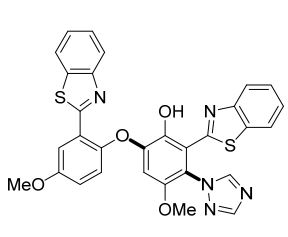




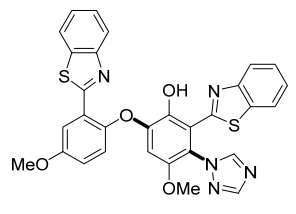
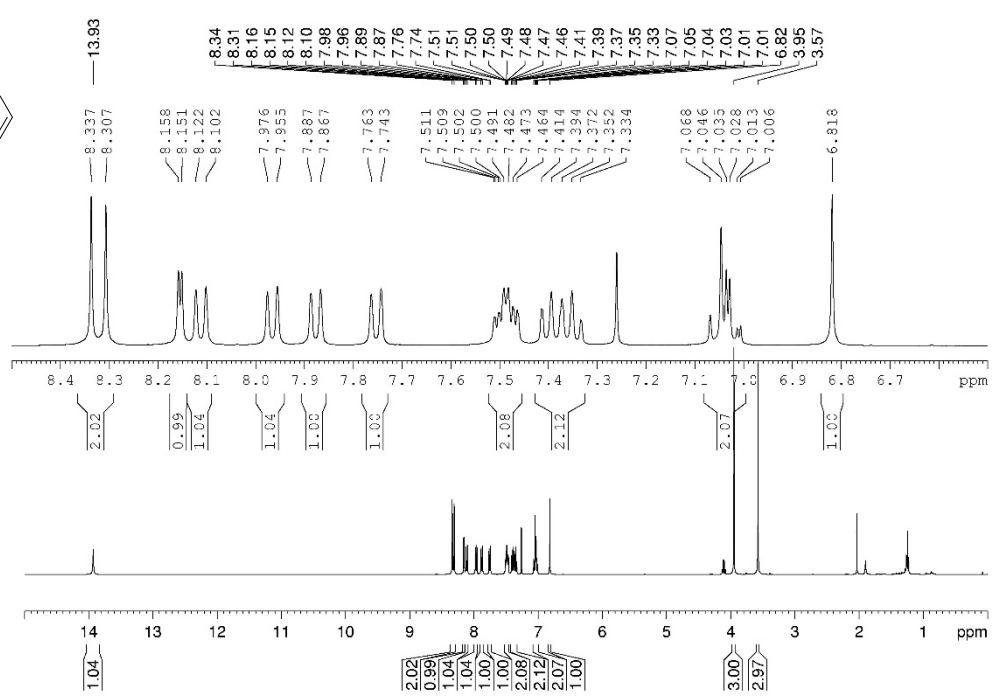




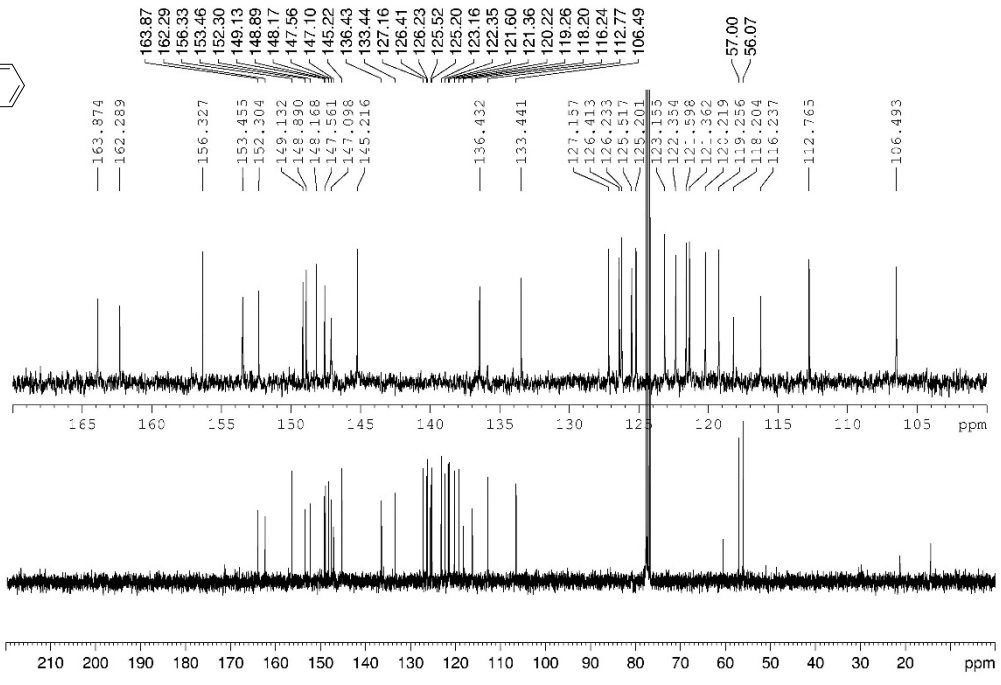


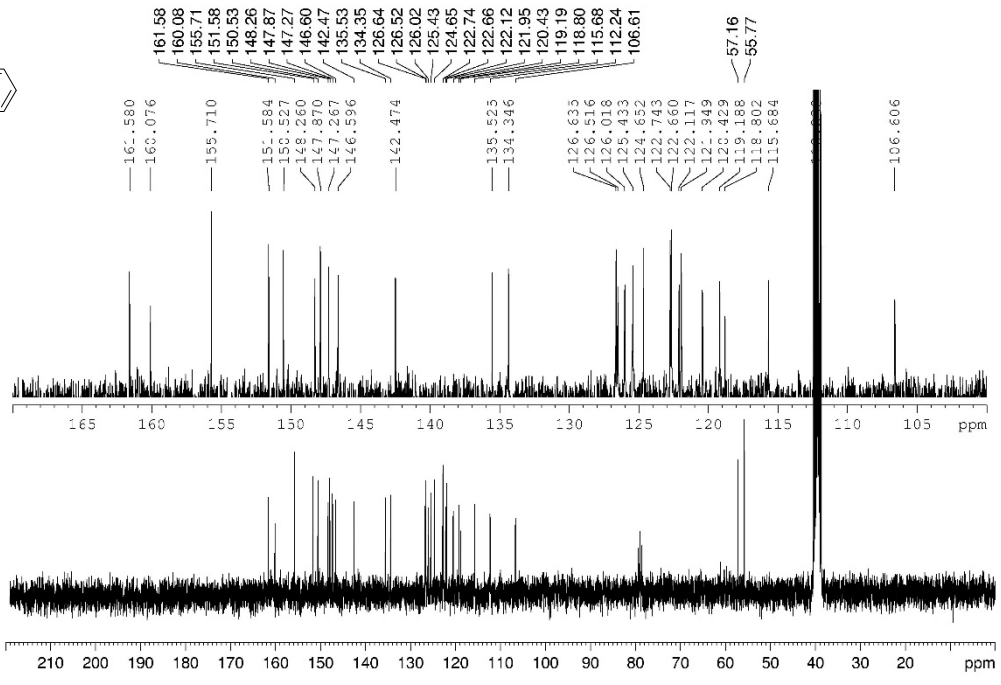
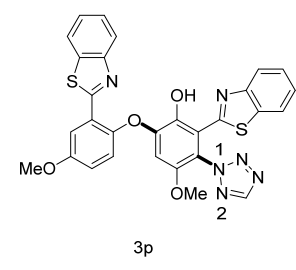
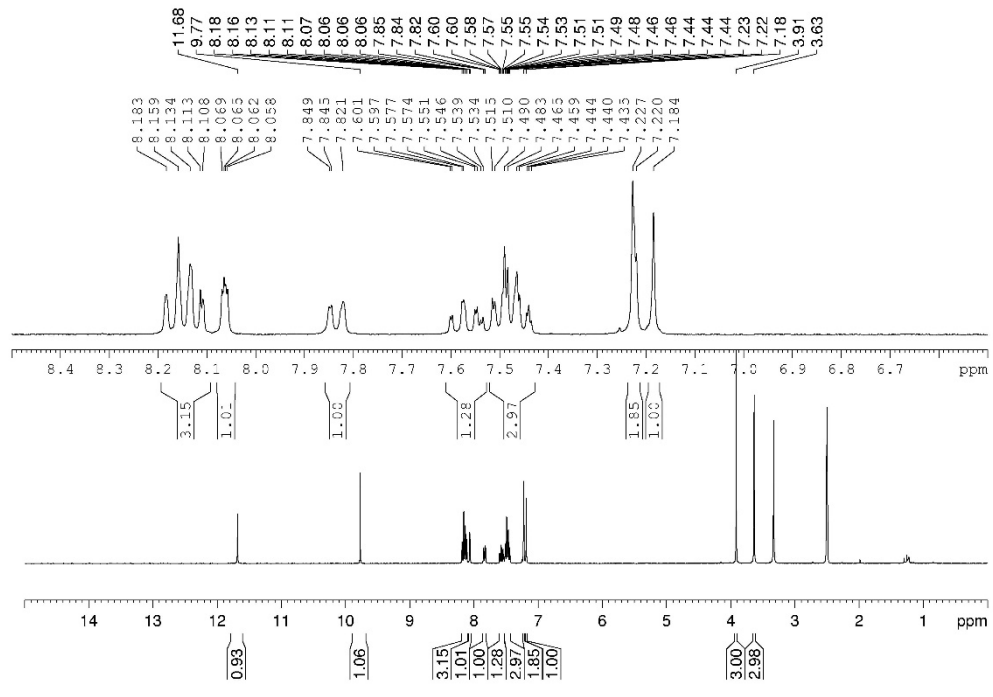
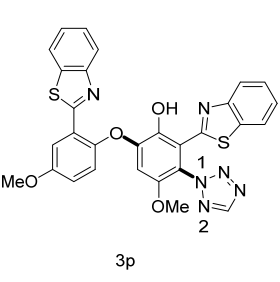


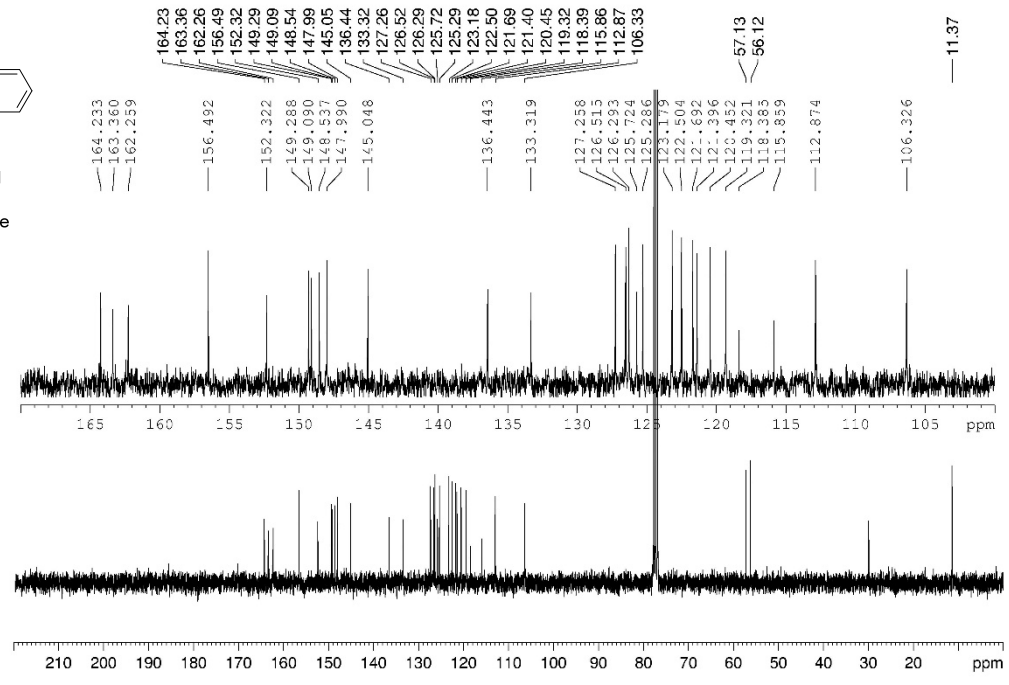
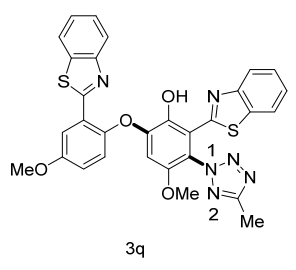
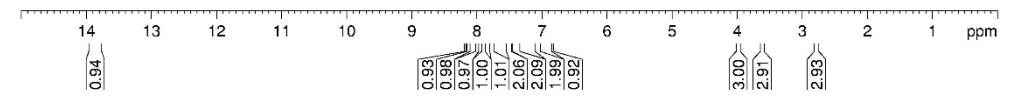
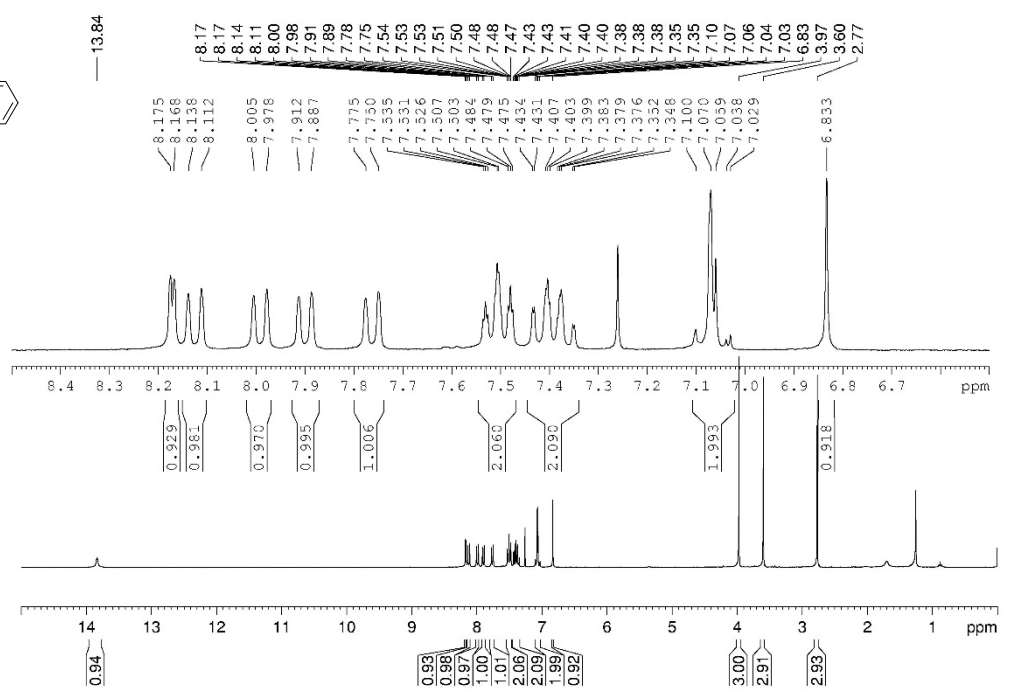
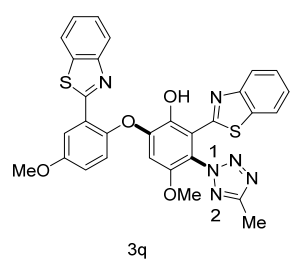
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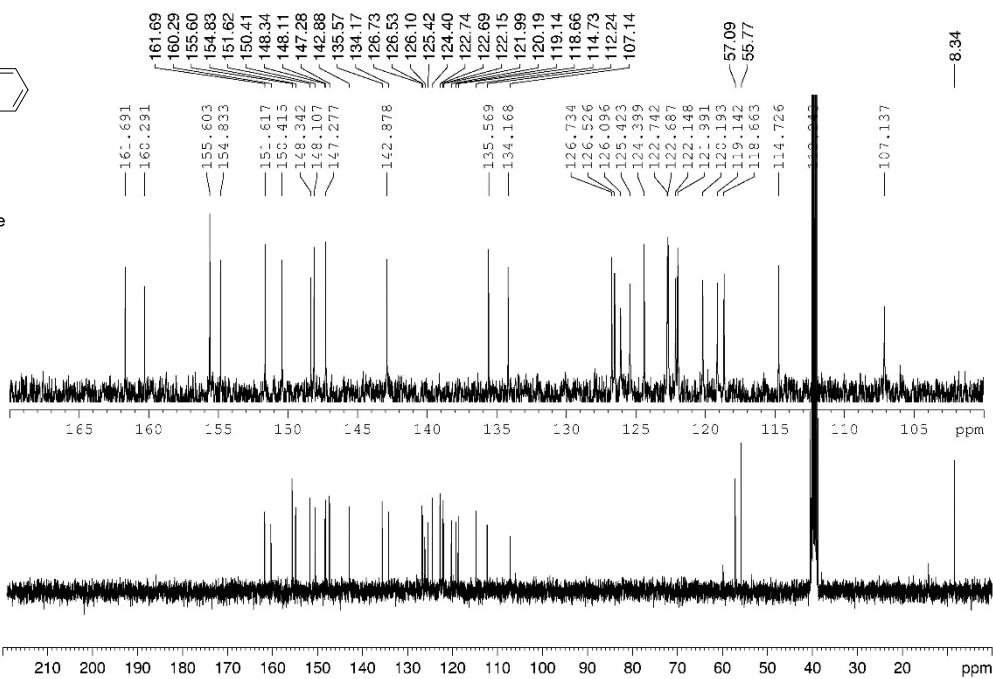
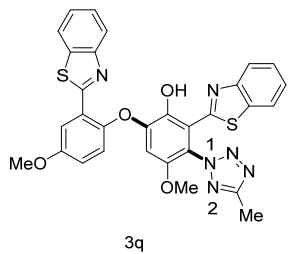
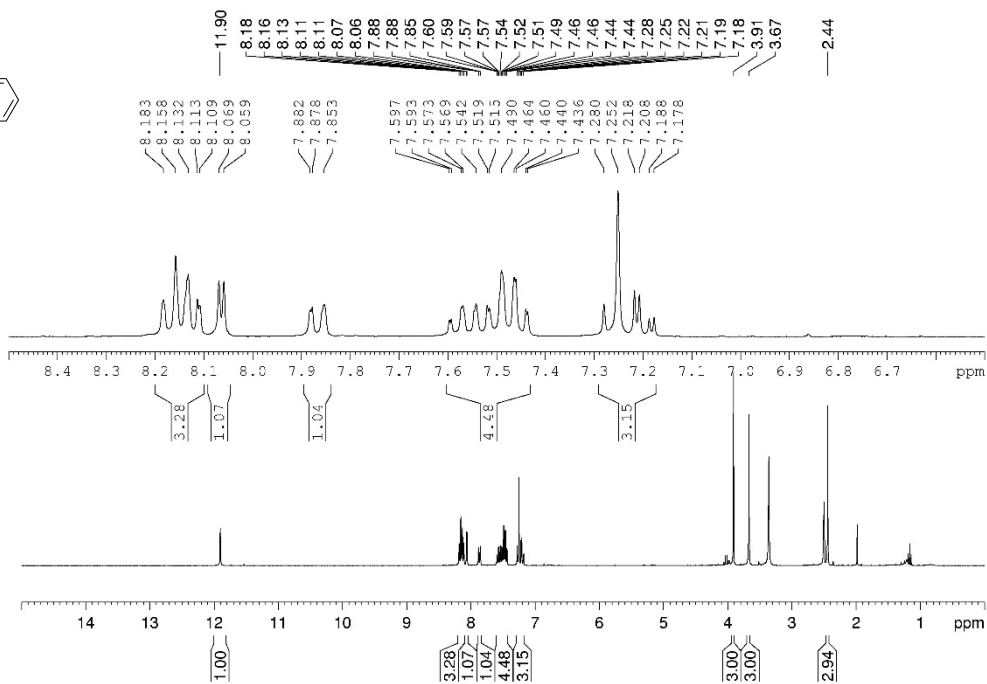
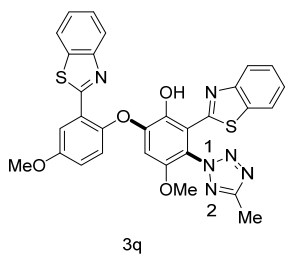


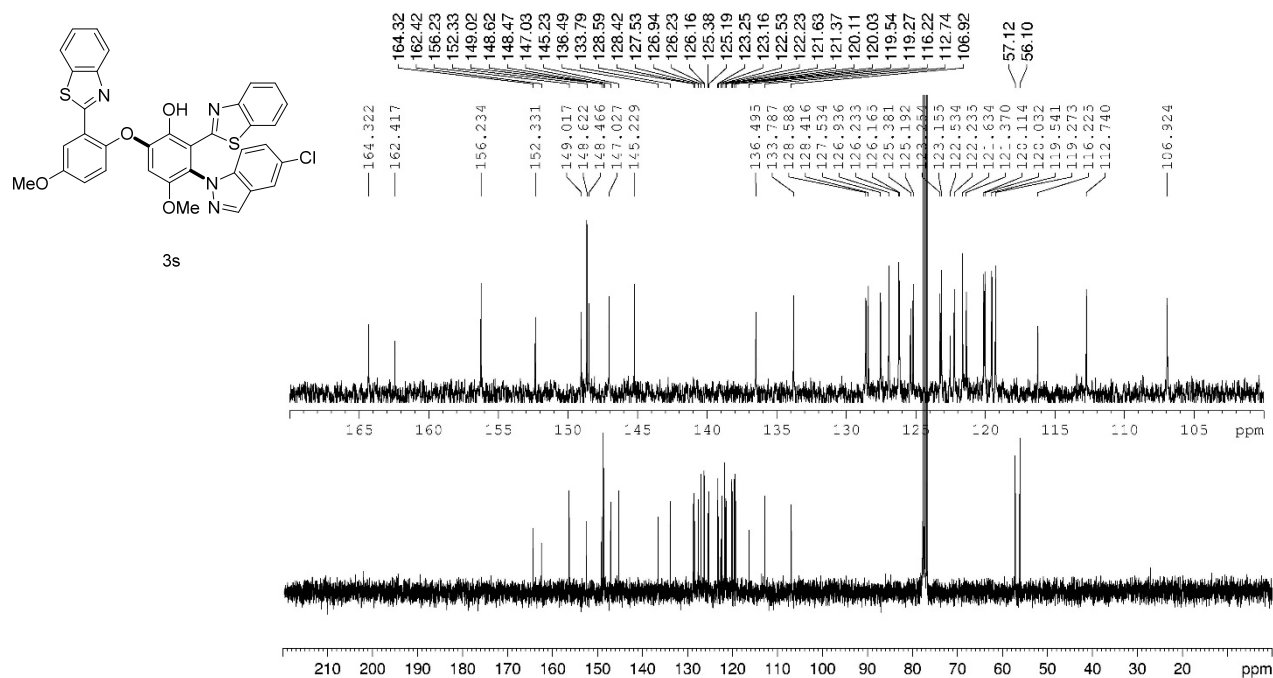
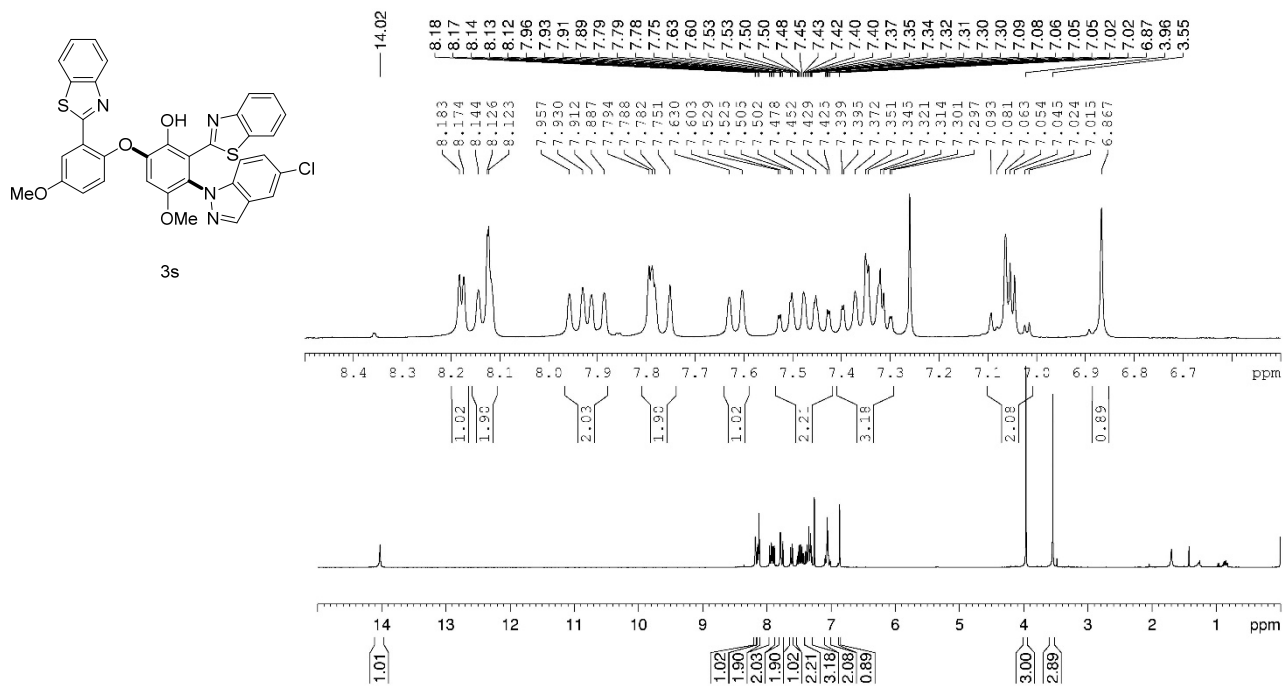
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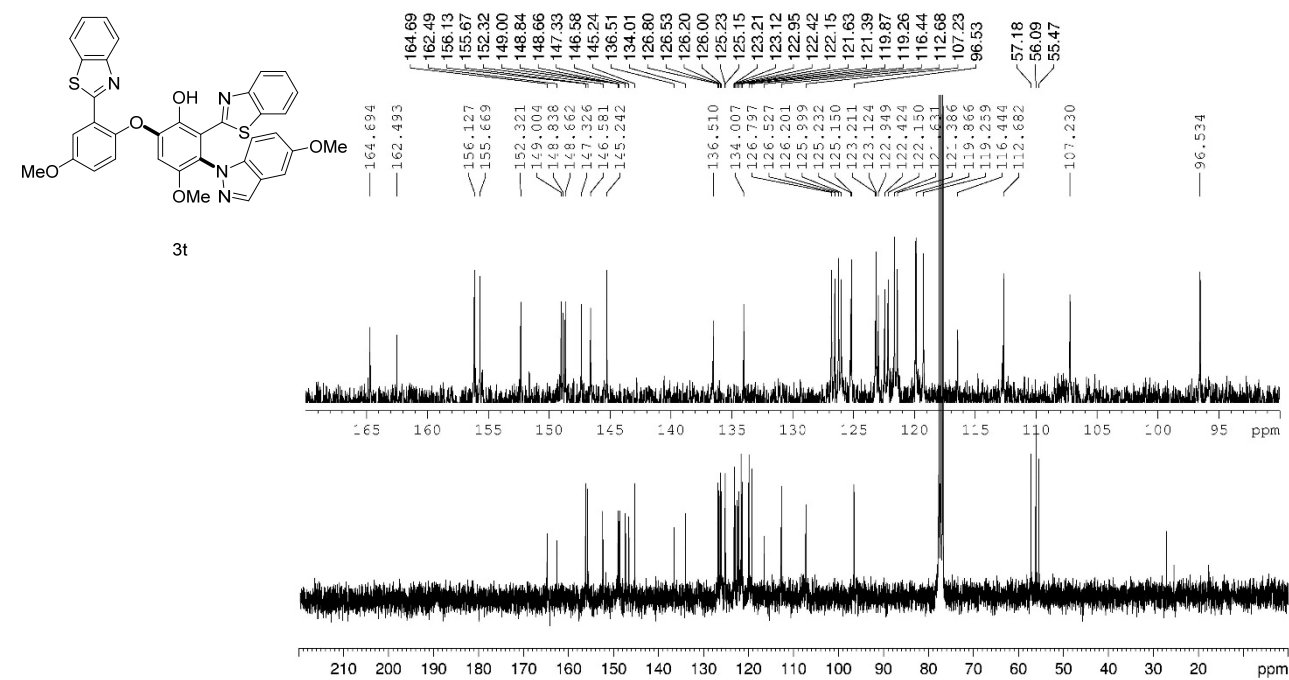
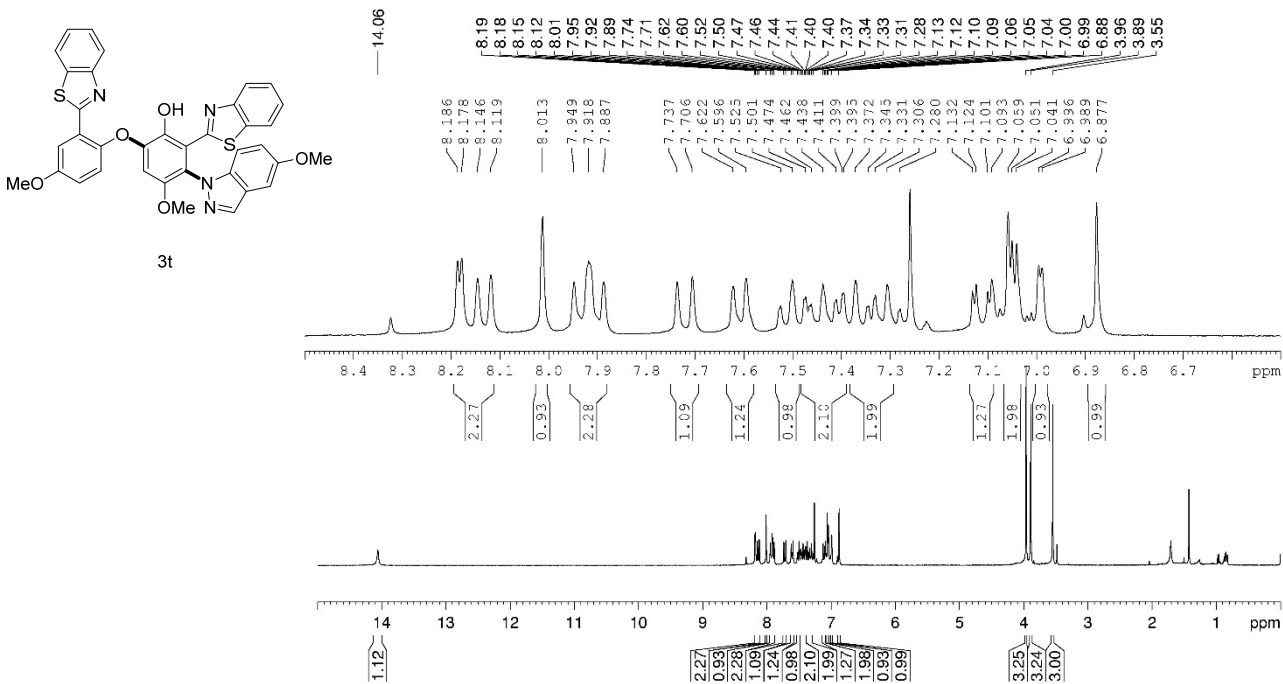


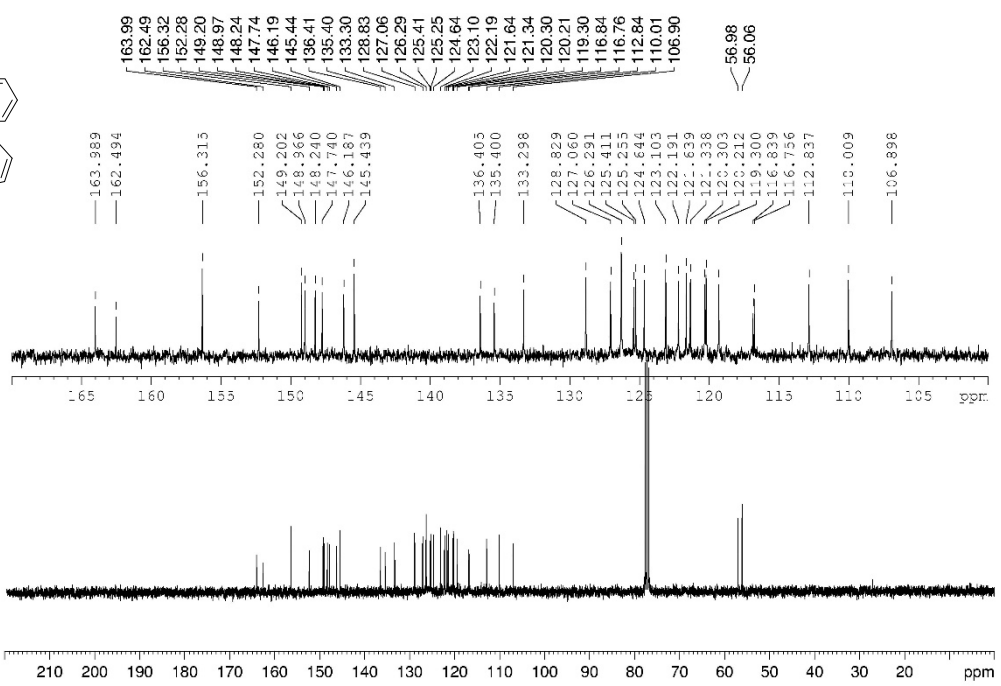
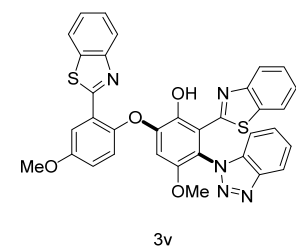
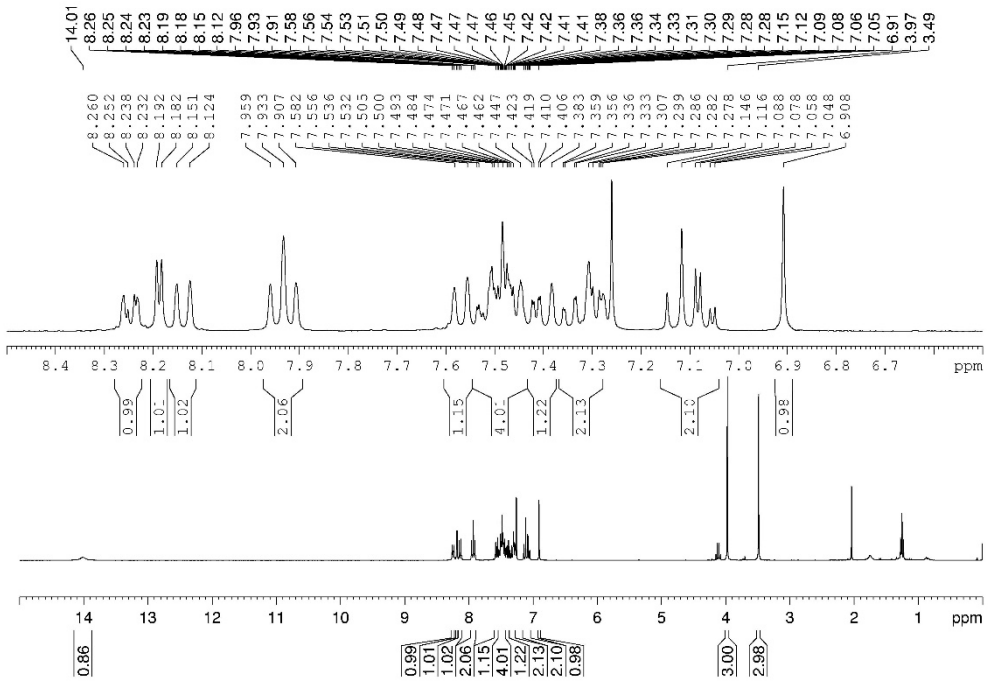
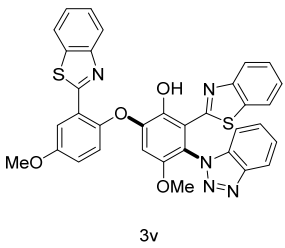


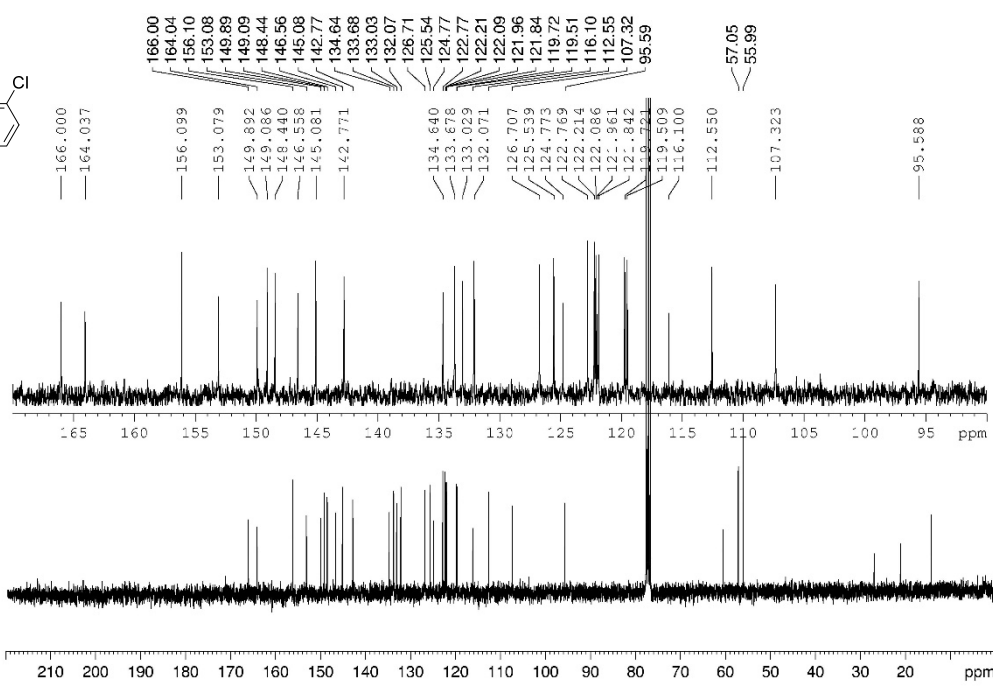
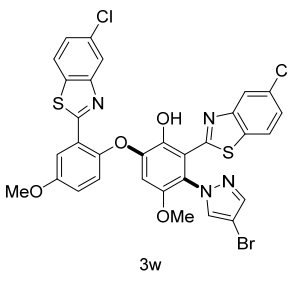
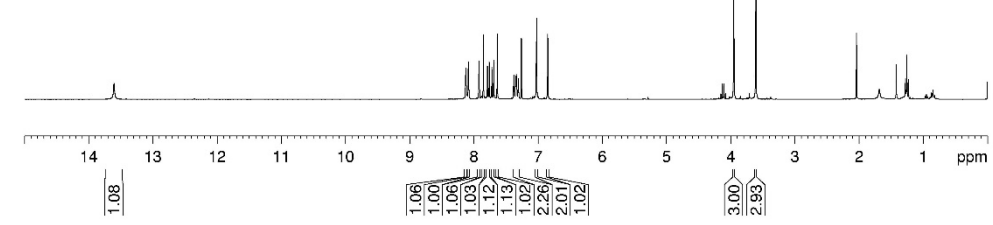
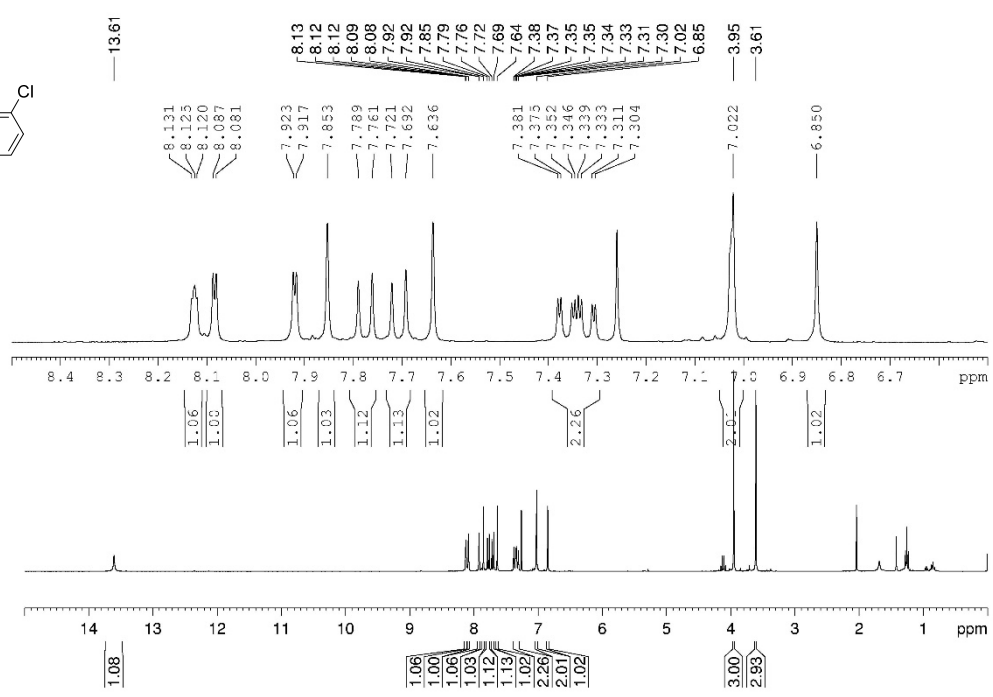
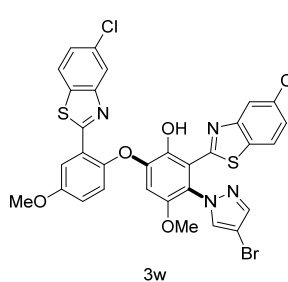


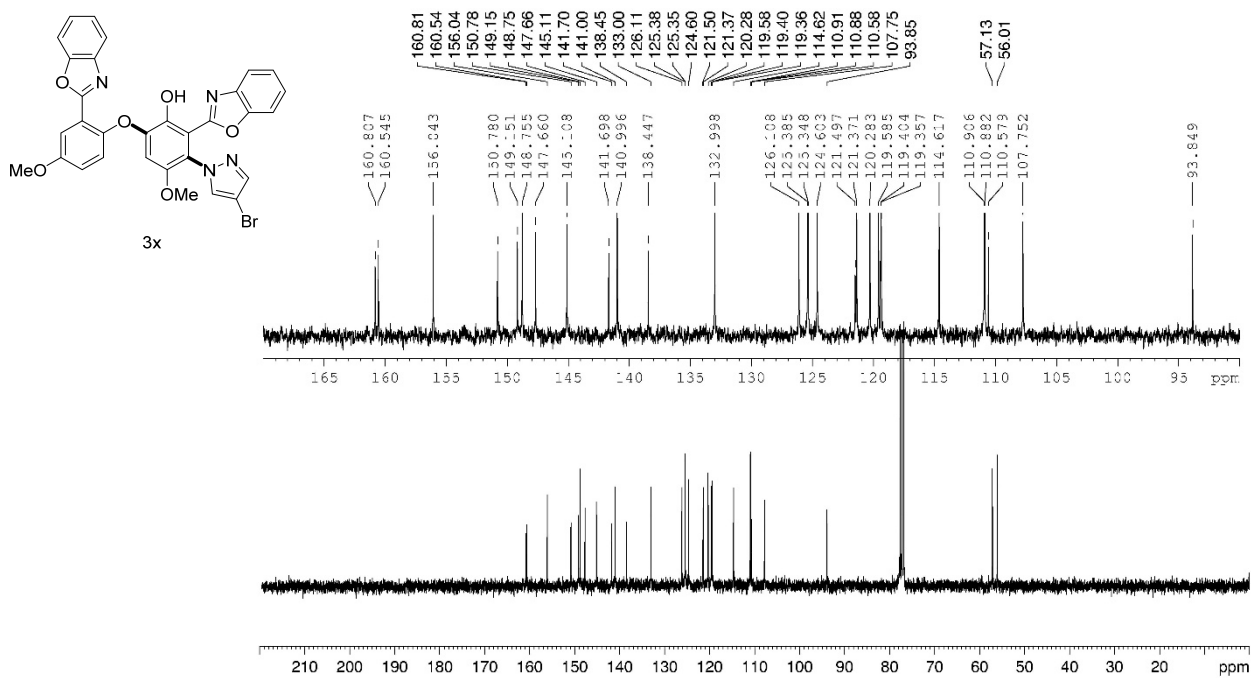
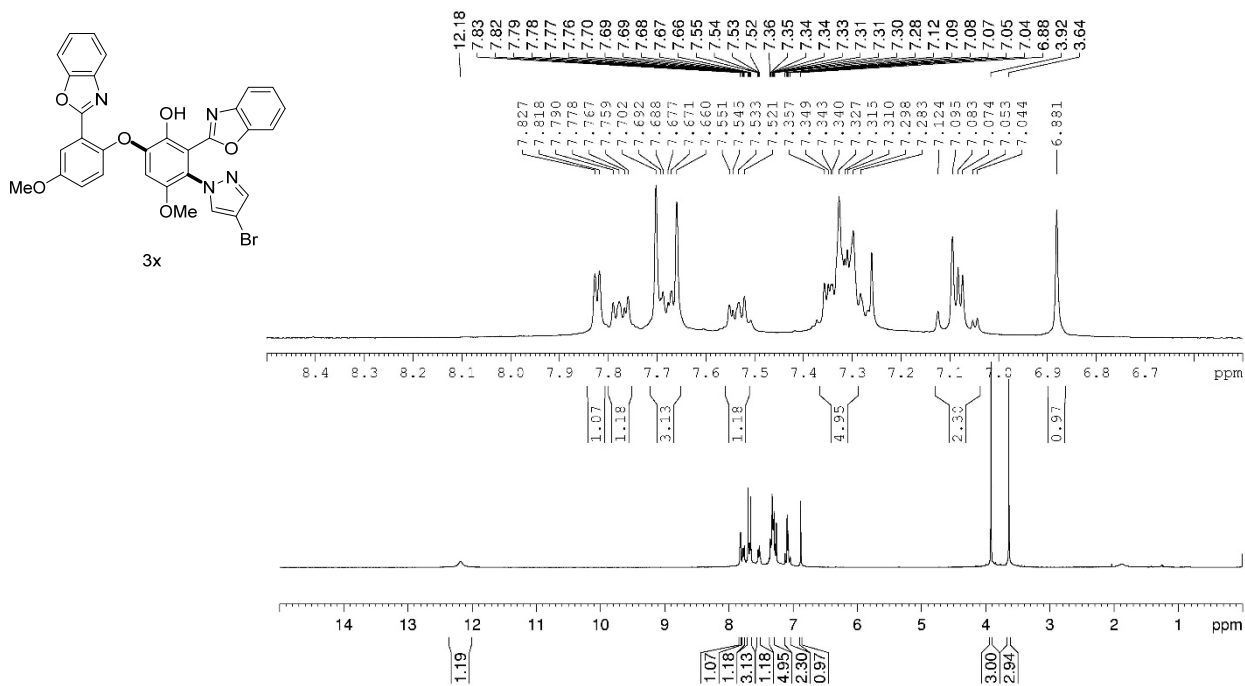


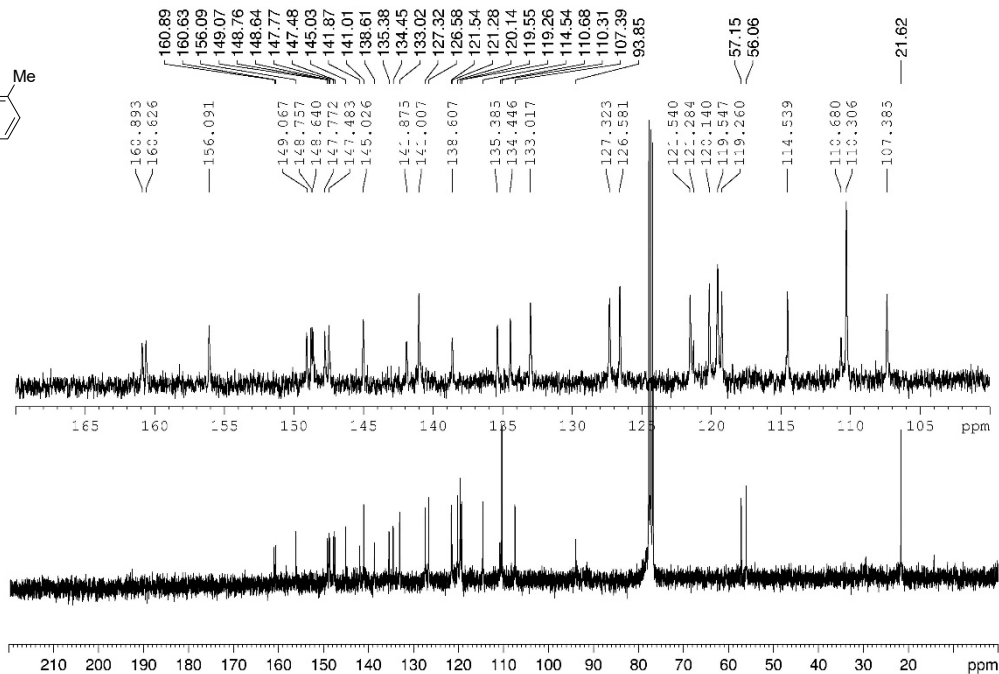
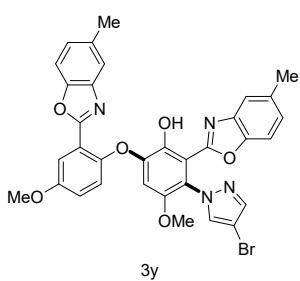
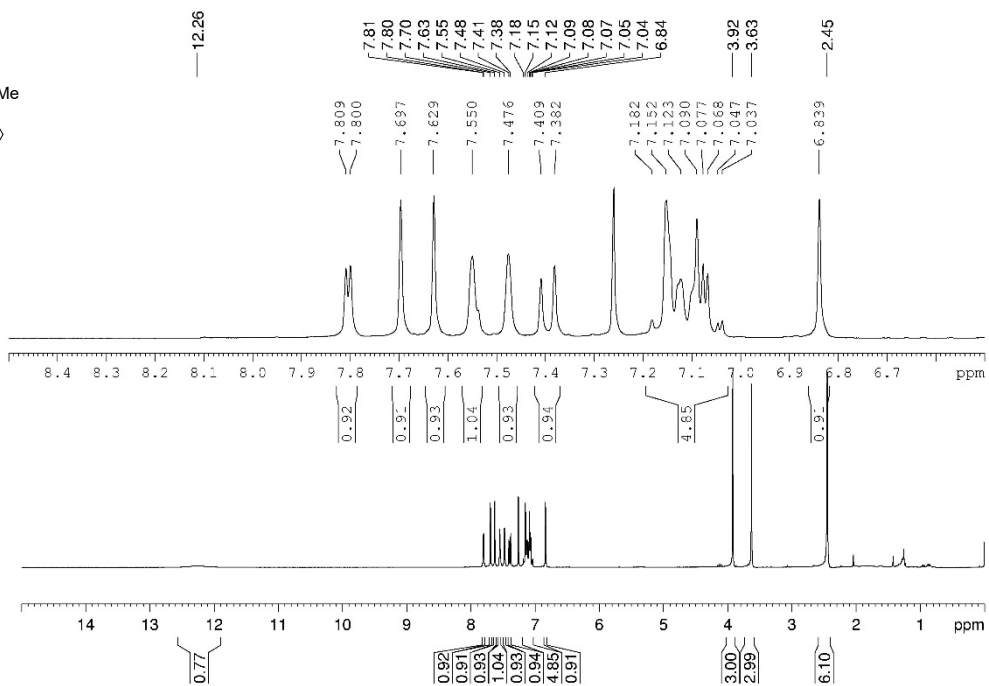
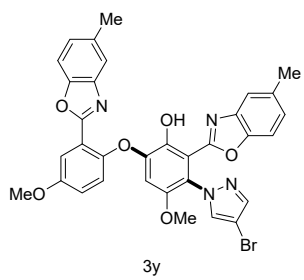


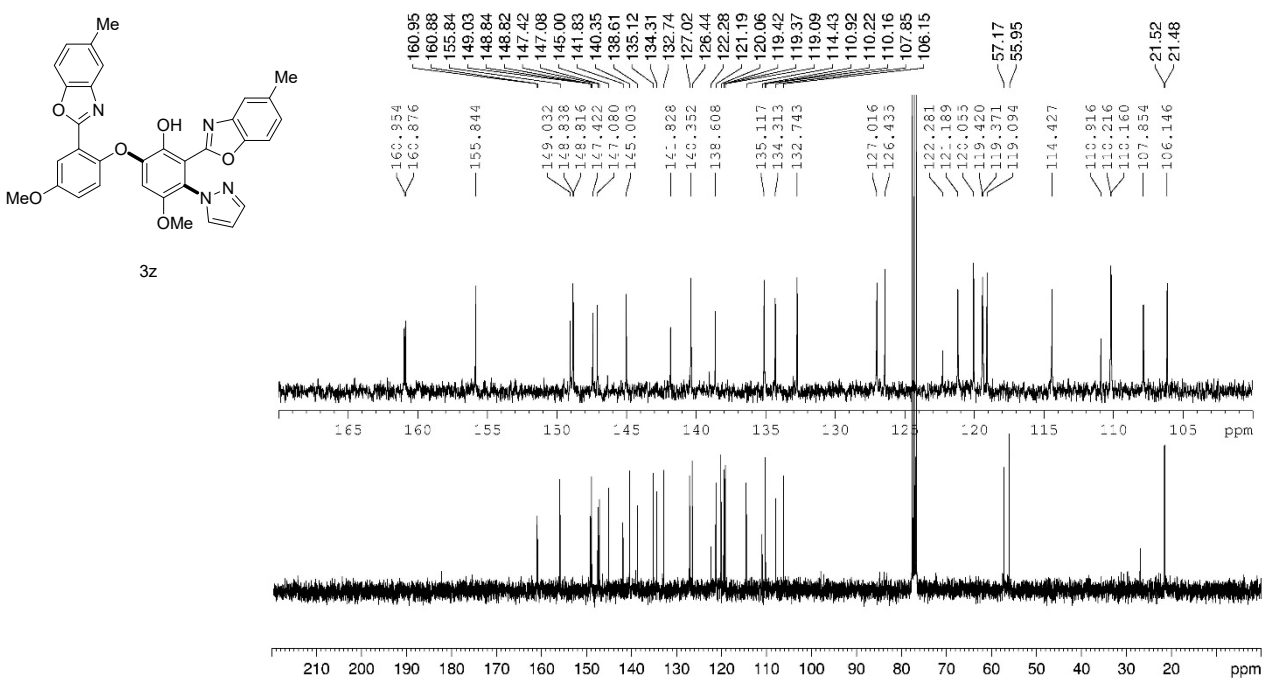
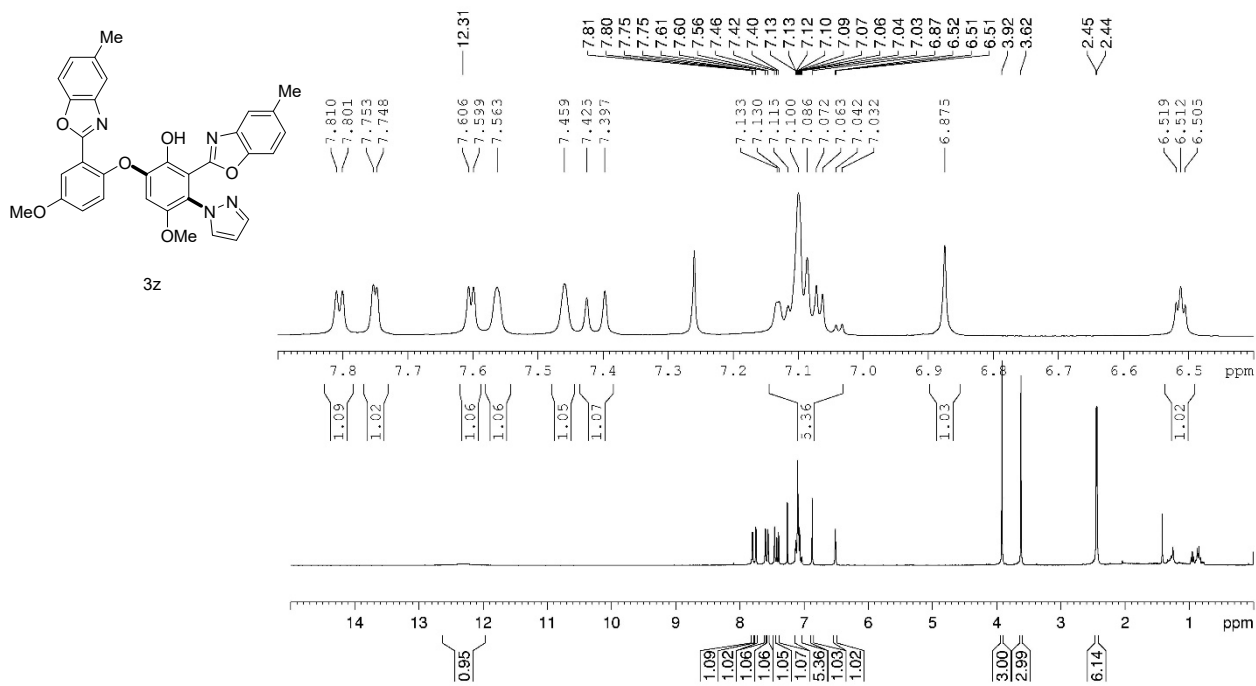


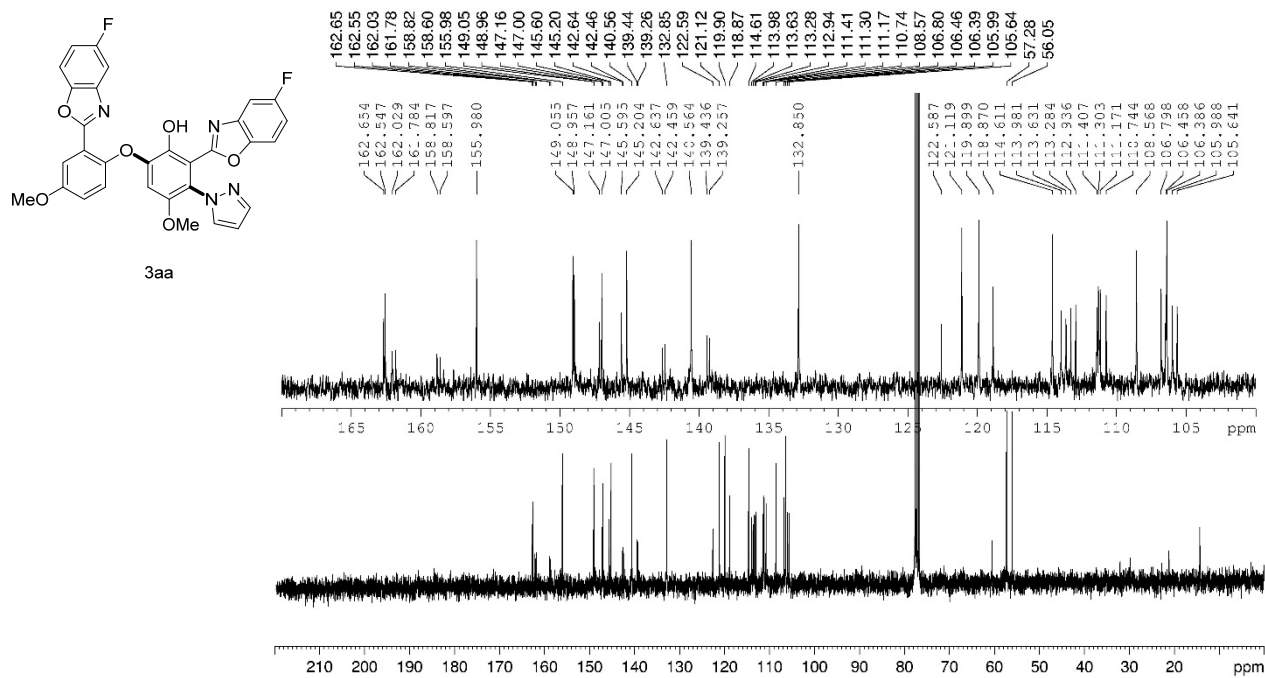
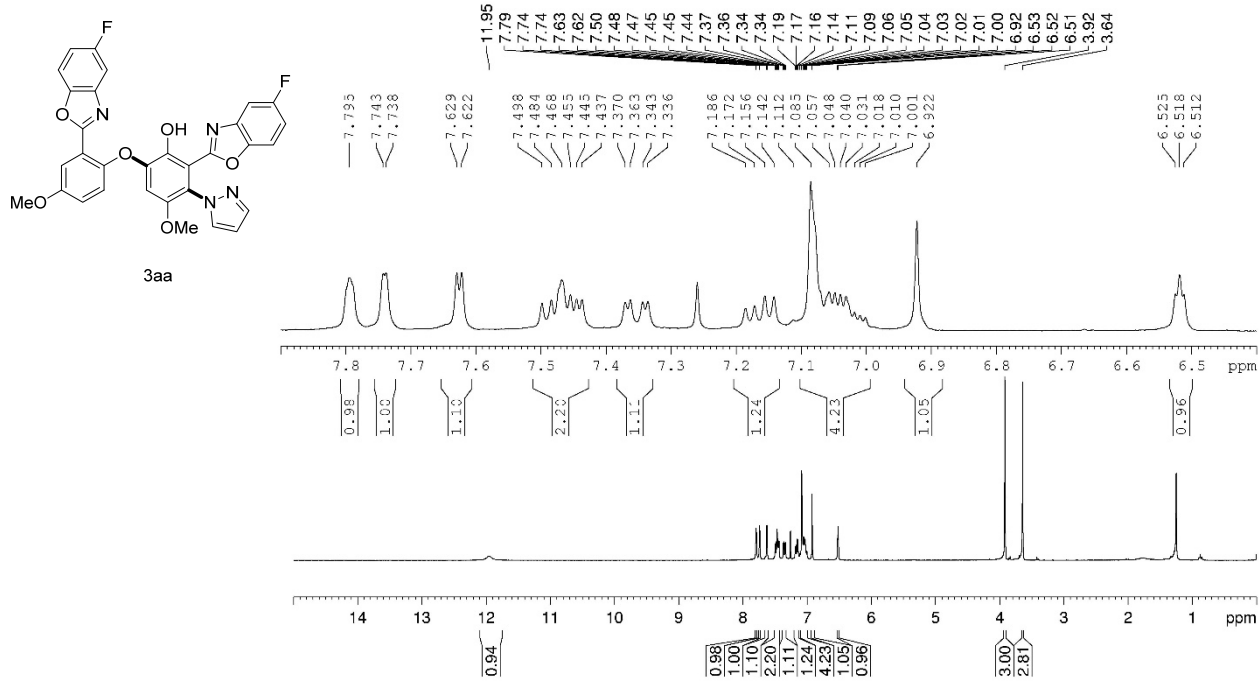


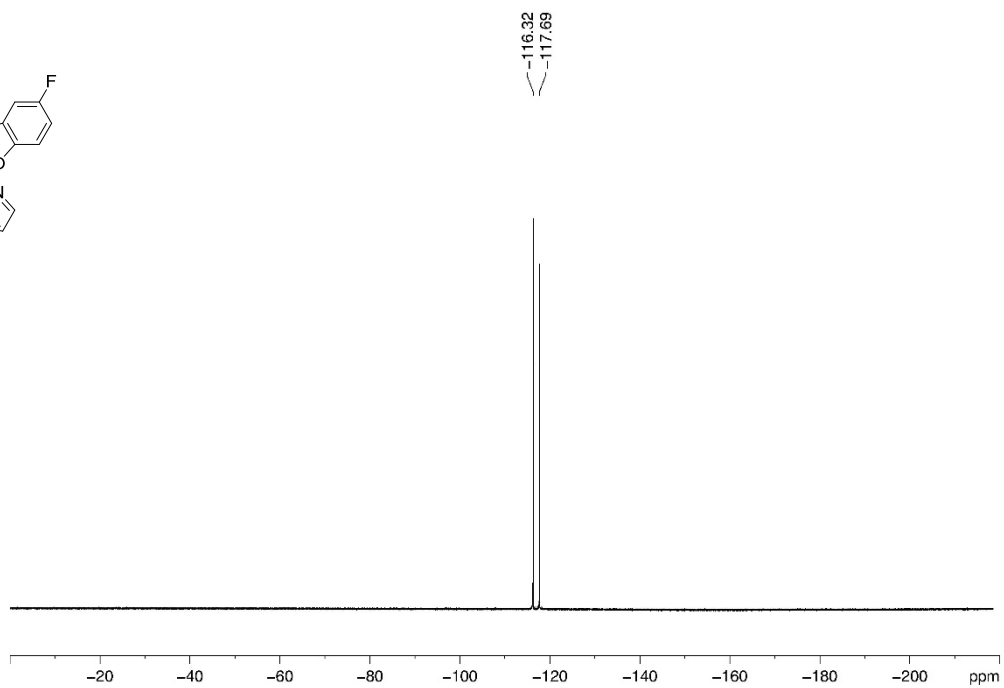
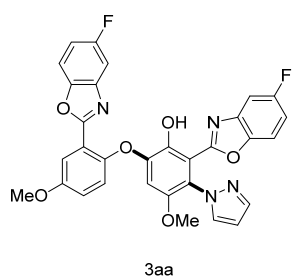


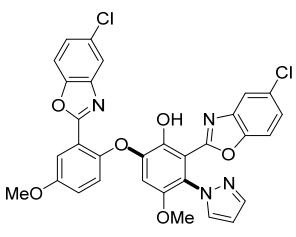




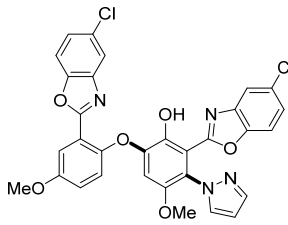
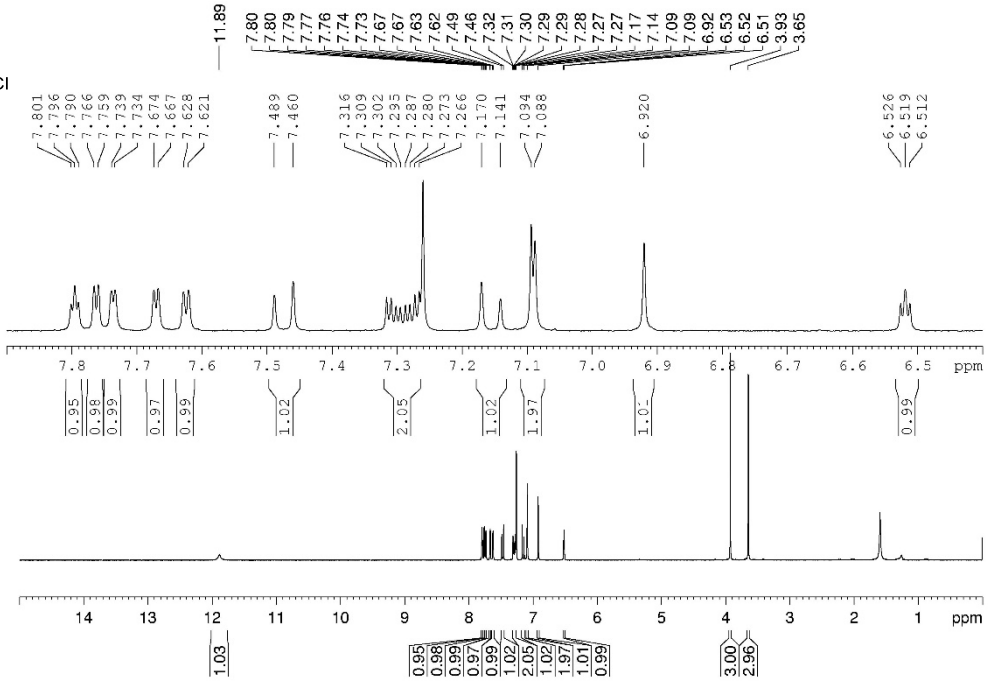








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