Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Building cobaloxime-based metal-organic framework for photocatalytic aerobic oxidation of arylboronic acids to phenols

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1. Materials

Analytical reagents were purchased from Guangdong Guanghua Sci-Tech Co., Ltd. (Shantou, China) and Energy Chemical (Shanghai, China) and used without further purification. The water involved in the experiment is self-made reverse osmosis water in the lab.

2. Instruments and methods

Single crystal X-ray diffraction (SC-XRD) tests were performed on Rigaku XtaLab Pro MM007HF DW X diffractometer at ambient temperature.

Powder X-ray diffraction (PXRD) data were collected on Rigaku MiniFlex600 diffractometer using Cu K_α radiation. Patterns were scanned over 2-30° (2θ) with a scan speed of 10°/min and a step width of 0.02°, respectively (Environment: 25 °C, 50% humidity).

Temperature-dependent powder X-ray diffraction (TD-PXRD) patterns were recorded on Rigaku Ultima IV X-ray diffractometer equipped with graphite-monochromatic Cu Kα radiation (λ = 1.54178 Å) in nitrogen flow at various temperatures.

The morphology of Zr-TCPCo was investigated by using ZEISS Gemini 300 field-emission **scanning electron microscope (SEM)** with an acceleration voltage of 5 kV. EDS mapping analysis was conducted on the same microscope with an voltage of 15 kV.

Infrared spectra (IR) were measured from 400 cm^{-1} to 4000 cm^{-1} by Nicolet AVATAR 360 in transition mode. Samples were diluted in KBr pellets.

Gas adsorption was performed on a ASAP2020 instrument (Micrometrics). Before starting the test, about 120 mg of Zr-TCPCo was degassed at 120 °C for 1 day under dynamic vacuum after 6 days of solvent exchange with DMF and acetone (final mass: 117.2 mg). The surface areas were calculated from the N_2 adsorption isotherms data by applying the linearized BET equation (selective data range: P/P_0 = 0.001~0.05,

with a correlation coefficient of 0.999 and a C value equal to 444.36). Pore size distributions were obtained using NLDFT method.

Diffuse reflection spectra (Solid state UV-Vis spectra) were recorded on PerkinElmer Lambda 950 spectrophotometer using $BaSO_4$ as a reference. Scans were measured from 800 nm to 300 nm with a scan width of 0.5 nm.

X-ray photoelectron spectroscopy (XPS) test was performed on was collected on an Escalab 250XiXPS energy spectrometer using Al Kα radiation. **Thermogravimetric analysis (TGA)** was performed on the TA Instruments Q50 thermogravimetric instrument under N_2 flow (40 $mL \cdot min^{-1}$) and heated from room temperature to 600 °C at a rate of 10 °C min^{-1}.

Electrochemical measurements were recorded on a CHI660E electrochemical workstation (CH Instruments, China). A standard three-electrode system with platinum mesh as the counter electrode, the Ag/AgCl electrode as the reference electrode, and Zr-TCPCo loading on FTO (ink: 5 mg MOF + 0.8 mL EtOH + 0.2 mL Nafion solution, 10 μL on 1×1 cm^2) as the working electrode, respectively. 0.1 M Na_2SO_4 aqueous solution is used as the electrolyte. **Cyclic voltammetry** (CV) measurements were conducted starting from OCP (0.2 V vs Ag/AgCl) and scanning from -1.3 to 1 V vs Ag/AgCl. The scan rate was set at 50 mV/s and the test was conducted for 5 full circles. **AC Impedance measurement** (IMPE) for the Mott-Schottky plot was tested from 0.6 V to -0.6 V vs Ag/AgCl.

Nuclear Magnetic Resonance (NMR) was recorded on the Bruker AscendTM 400 MHz NMR spectrometer with tetramethylsilane (TMS) as an internal standard.

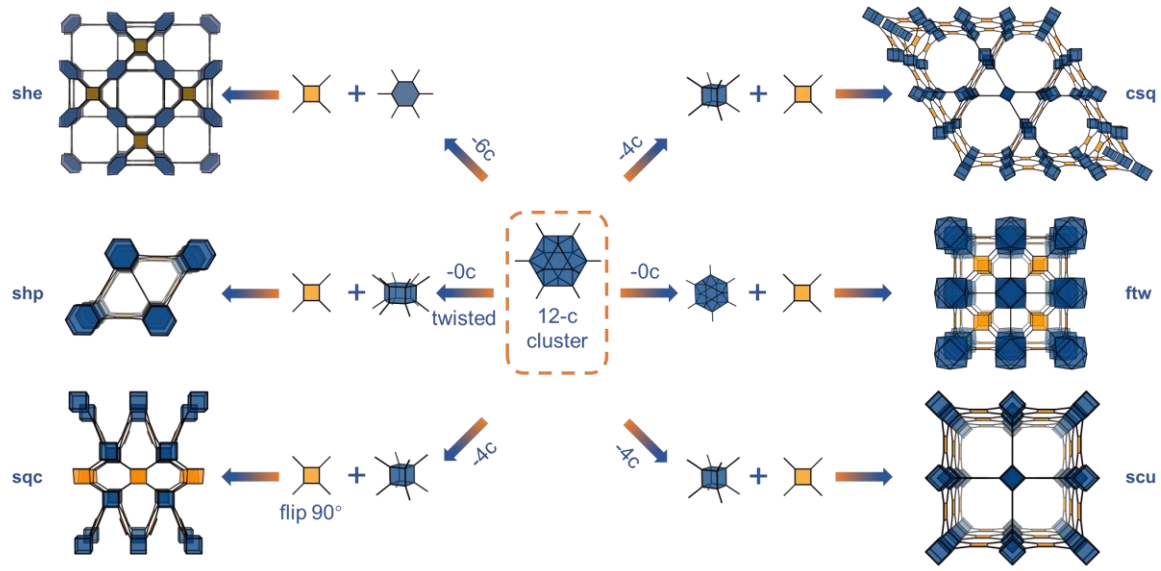
High-Resolution Mass Spectra (HRMS) were recorded using a Q Exactive mass spectrometer (Thermo Fisher Scientific, USA).

Irradiation with visible light was performed using blue LEDs (λ = 450 ± 10 nm) illumination instruments (The instruments were designed by ourselves and the actual output power density of the LEDs at 0.5 cm distance is 33.70 mW/cm^2 detected by CEL-NP2000-10 (Beijing Ceau Light Co. Ltd., China) light power meter). The

material of the reaction vessel is common glass; the distance from the light source is about 0.5 cm.

3. Topology analysis of Zr-based metal-organic frameworks

The topological analysis of Zr-TCPCo was performed by using the computer program Systre[1] and the online database Reticular Chemistry Structure Resource (RCSR).[2]



Scheme S1. Possible networks constructed from planar 4-c ligand and hexanuclear zirconium node with different connectivity. Blue polyhedra and orange squares represent metal clusters and ligands, respectively. -xc (x=0, 4, 6) represents the number of reduced connectivity.

4. Synthesis of Zr-TCPCo

The molecular cobaloxime complex was synthesized based on a previously reported procedure.[3]

26 mg of $ZrCl_4$, 0.5 mL *N*,*N*-dimethylformamide (DMF) and 2 mL of acetic acid (HOAc) were added into a 20 mL vial, which was tightly caped after addition. The glass bottle was heated at 60 °C until all materials were completely dissolved. Next, 30 mg of cobaloxime complex was added to the above-mentioned transparent solution while hot. After ultrasonicating for seconds, a dark green solution formed. The vial was subsequently heated at 120 °C for 24 h to obtain yellow-orange crystals. The crystals were filtered, washed with DMF adequately and preserved in DMF for subsequent characterization.

This procedure can be performed in a ten-time scale by using a 100 mL Duran-Schott vial (See Figure S1).

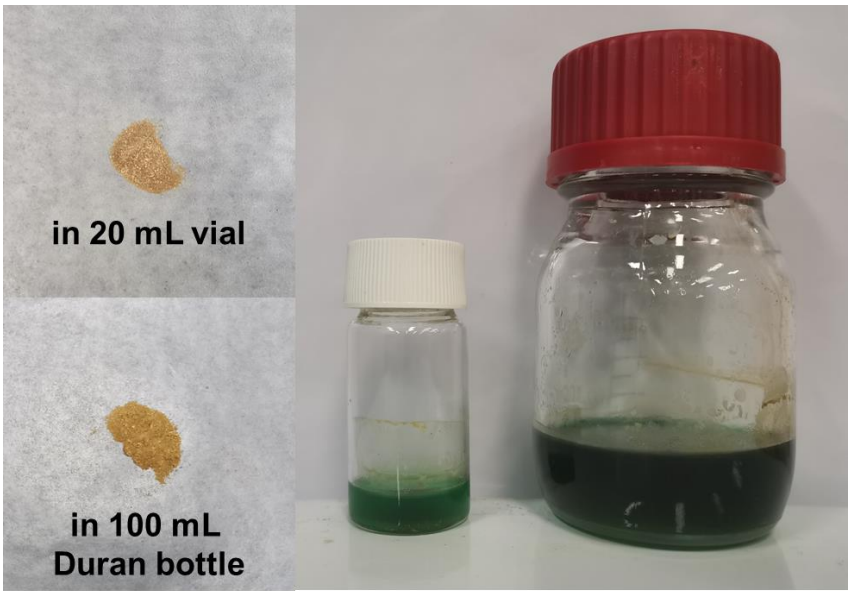


Figure S1. Pictures of small and large scale synthesis of Zr-TCPCo and the final products.

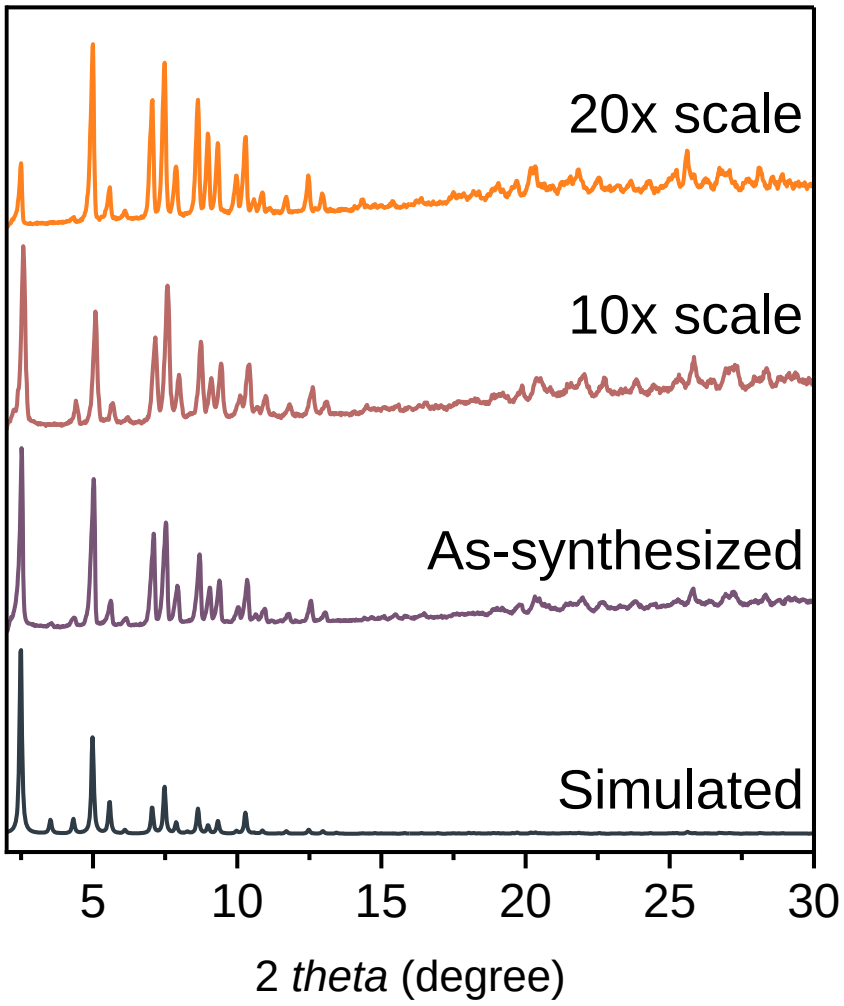


Figure S2. PXRD patterns of Zr-TCPCo synthesized in different scales.

5. Single crystal X-ray crystallography of Zr-TCPCo

Single crystals of Zr-TCPCo were transferred to a microscope slide along with a little mother liquor. A small piece of crystal (about 0.1×0.15×0.2 mm^3) was picked and washed completely in vacuum grease, then mounted using a Dual-Thickness MicroLoop™ (**MiTeGen, Ithaca, New York, USA**).

Data collection was performed on Rigaku Oxford XtaLAB Pro diffractometer equipped with a micro focus sealed X-ray tube (Cu K_α radiation, λ = 1.54178 Å) and PILATUS 200K detector. Data reduction, absorption correction was conducted on CrysAlisPro (Rigaku, V1.171.39.7e, 2015). Absorption correction was based on implanted spherical harmonics in SCALE3 ABSPACK.

The structure was solved by the intrinsic phasing method using *SHELXT*[4] implanted in *Olex2.*[5] Refinement with full matrix least squares techniques on F^2 was performed by using *SHELXL.*[6] Non-hydrogen atoms were refined anisotropically and all hydrogen atoms were generated based on riding mode. Crystallographic data and structure refinement results are given in Table S1. Atomic coordinates and isotropic displacement parameters are shown in Table S2.

Table S1. Crystallographic data of Zr-TCPCo

Complex	Zr-TCPCo
CCDC No.	2222381
Formula	C80 H68 Cl2 Co2 N8 O52.67 Zr8
Formula weight	2902.61
Temperature (K)	200
Crystal system	Cubic
Space group	$Pm\bar{3}m$
a/Å	35.2672(2)
V/Å^3	43864.5(7)
Z	6
D_c /g cm^{-3}	0.659
reflns coll.	50465
unique reflns	8113
R_{int}	0.0358
R_1 [$I > 2\sigma(I)$]	0.0692
wR_2 [$I > 2\sigma(I)$]	0.2155
R_1 (all data)	0.0770
wR_2 (all data)	0.2250
GOF	1.085

Table S2. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for Zr-TCPCo. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr1	3435.2(2)	6564.8(2)	7268.9(2)	56.1(5)
Zr2	2499.6(2)	6795.6(2)	7500.4(2)	62.1(5)
Co1A	0	5000	6875.7(8)	41.4(7)
O3	3317.3(15)	6682.7(15)	6682.7(15)	65(2)
O4	2607.6(14)	7392.4(14)	7392.4(14)	65.2(18)
O6	2253.3(8)	6190.9(9)	6726.9(10)	72.5(9)
O5	2118.3(8)	6326.7(9)	7339.3(10)	76.0(10)
O8A	2868.5(15)	6330(2)	7131.5(15)	46.4(12)
O7A	3090.1(14)	6909.9(14)	7504(2)	44.4(12)
N1A	408.0(16)	5341.6(15)	6861.1(18)	44.0(7)
O2	2987(4)	5989(4)	6563(4)	131(3)
C5	2059.7(11)	6158.8(12)	7025.7(15)	67.0(12)
O9A	350.8(13)	5724.0(13)	7054.2(16)	48.7(9)
O10A	0	5000	7493(3)	50.6(13)
O1	1900(4)	7513(4)	7077(4)	132(2)
C11A	738(2)	5209.0(19)	7032(2)	43.1(8)
C11	1560(4)	5813(4)	6658(5)	75(3)
C10	1234(4)	5593(4)	6642(5)	83(3)
C7	1579(4)	5748(5)	7330(5)	91(5)
C8	1255(4)	5508(5)	7300(6)	101(5)
C4	3292(4)	5863(3)	6782(3)	130(2)
C1	1356(3)	7359(4)	7475(4)	132(2)
C3	3384(4)	5448(3)	6682(5)	131(2)
C2	1785(3)	7283(3)	7369(3)	131(2)
O8B	2837.6(18)	6554(3)	7162.4(18)	63(2)

O7B	3052(2)	6948(2)	7722(3)	72(2)
Cl1A	0	5000	6238(3)	55.2(12)
Co1B	0	5000	7030.6(8)	40.4(7)
N1B	404.6(15)	5349.1(15)	7043.5(18)	43.1(7)
O9B	353.6(13)	5709.7(13)	6835.4(16)	48.7(8)
O10B	0	4865(4)	7623(3)	46.3(12)
C1A	742.1(19)	5202.0(19)	6876(2)	42.6(8)
Cl1B	0	5000	6397(3)	54.7(12)
C8A	1158.8(13)	5652.4(16)	7301.6(13)	93(3)
C7A	1478.4(14)	5882.3(16)	7320.6(12)	91(3)
C6	1727.3(8)	5899.3(10)	7015.5(13)	71.3(11)
C12	1656.6(12)	5686.5(16)	6691.4(12)	85(3)
C10A	1337.0(13)	5456.6(15)	6672.4(13)	92(3)
C9	1088.1(8)	5439.6(9)	6977.5(14)	76.2(12)
O7	3544(3)	5983(2)	7061(3)	95.6(18)
O8	1927(3)	7007(3)	7600(4)	109(2)
Cl2	0	5192.8(14)	6342(3)	102(3)

6. SEM and EDS mapping analysis of Zr-TCPCo

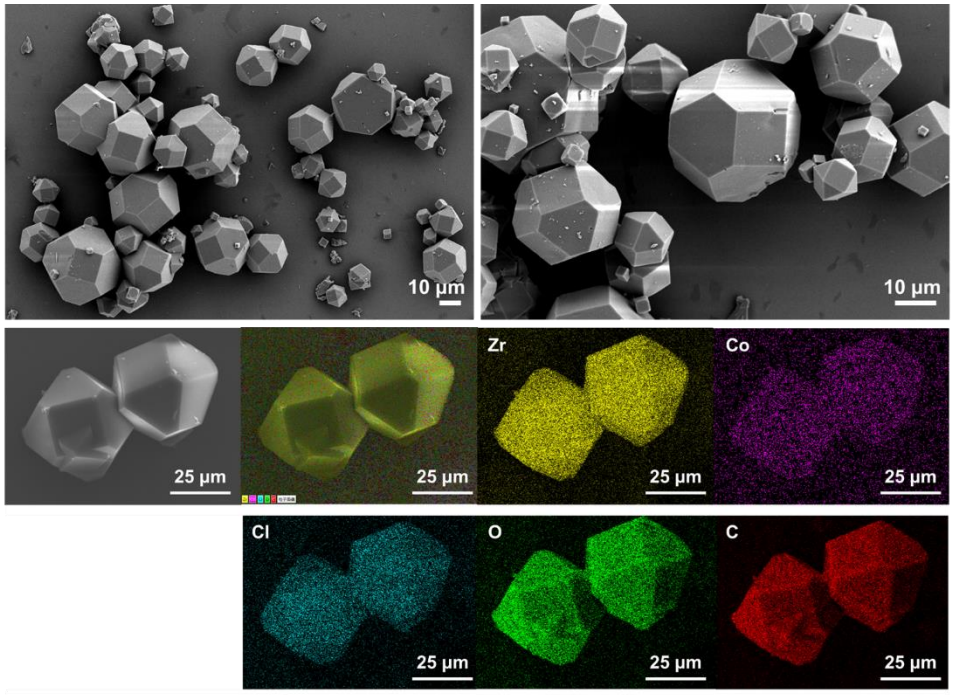


Figure S3. SEM and EDS analysis of Zr-TCPCo before catalysis.

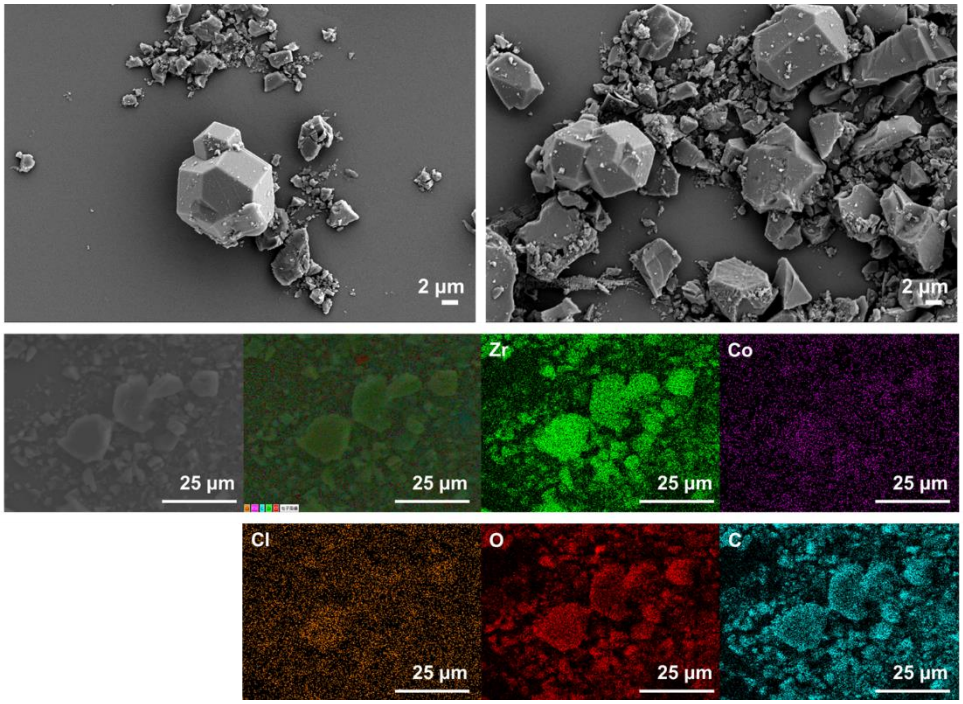


Figure S4. SEM and EDS analysis of Zr-TCPCo after catalysis.

7. XPS test of Zr-TCPCo

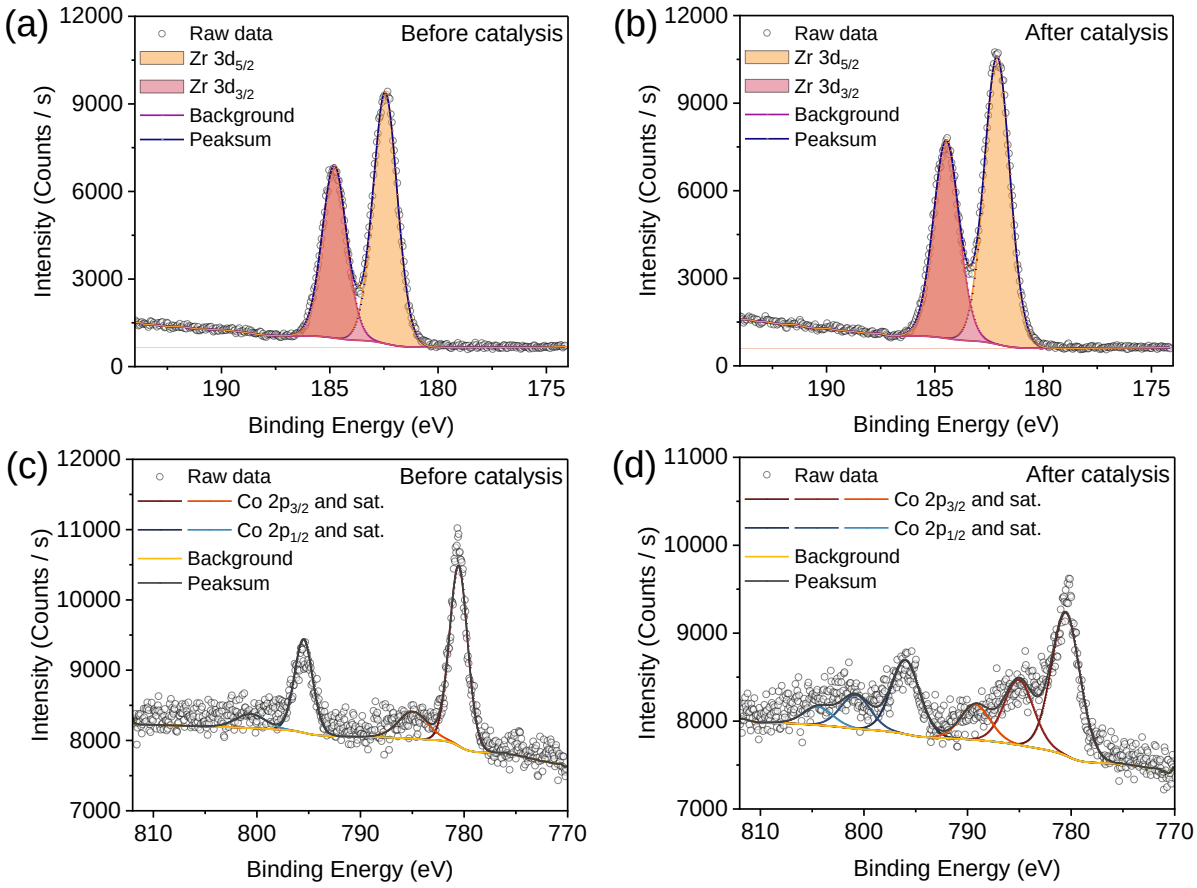


Figure S5. High-resolution XPS spetra of (a-b) Zr 3d and (c-d) Co 2p in Zr-TCPCo before and after catalysis.

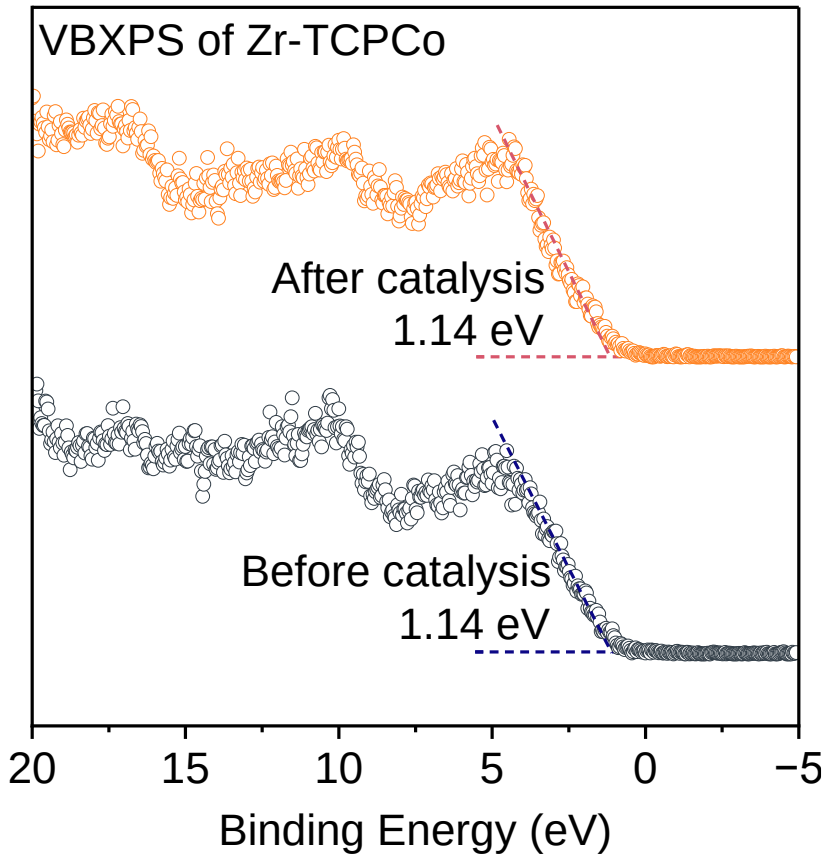


Figure S6. VBXPS spectra of Zr-TCPCo before and after catalysis.

8. Stability test

8.1 Thermostability

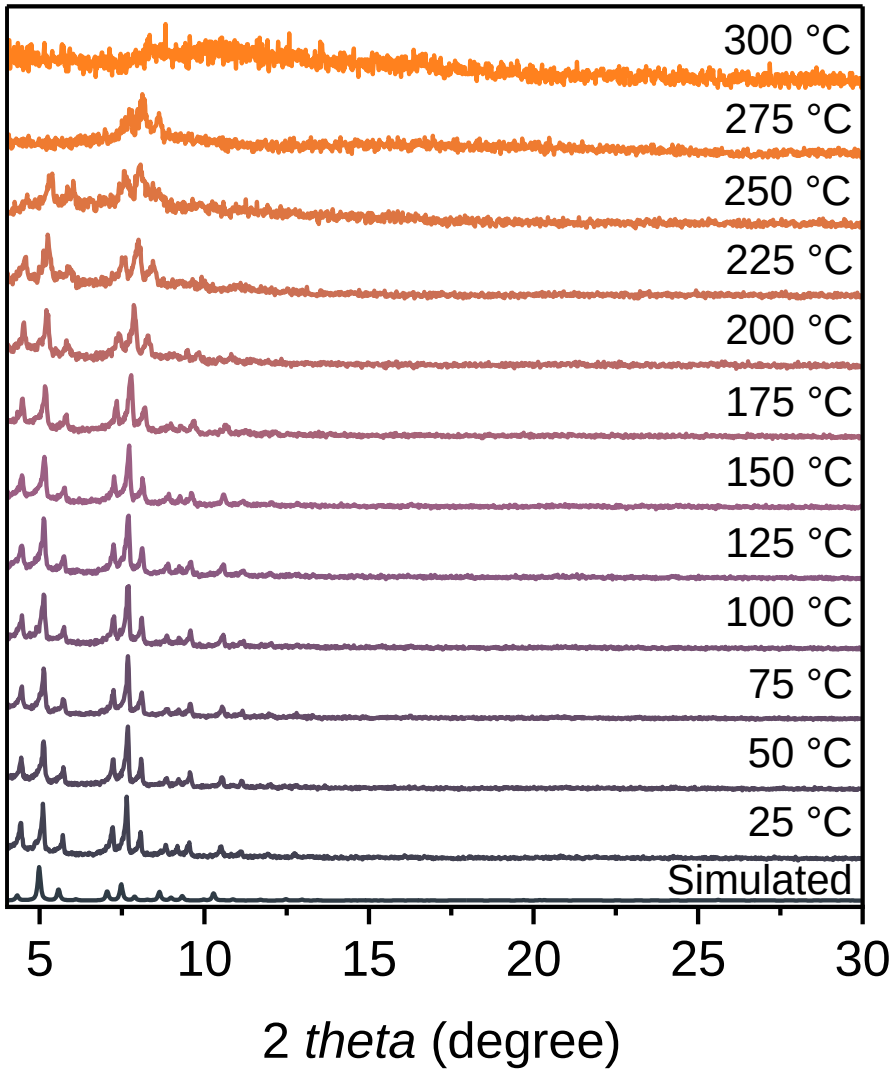


Figure S7. VT-PXRD patterns for Zr-TCPCo.

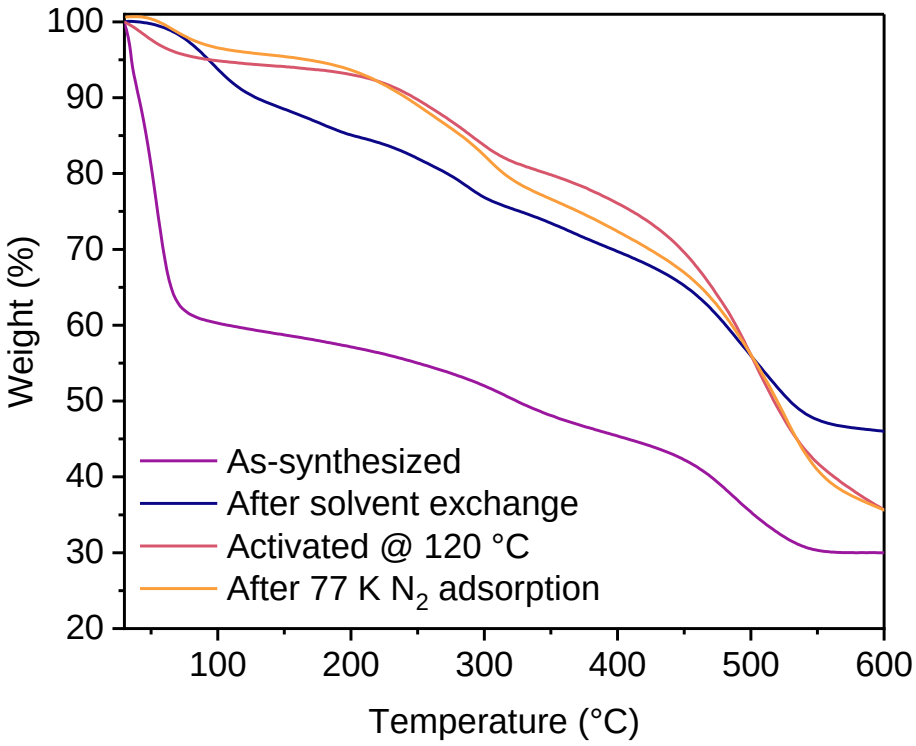


Figure S8. The thermogravimetry curves of Zr-TCPCo.

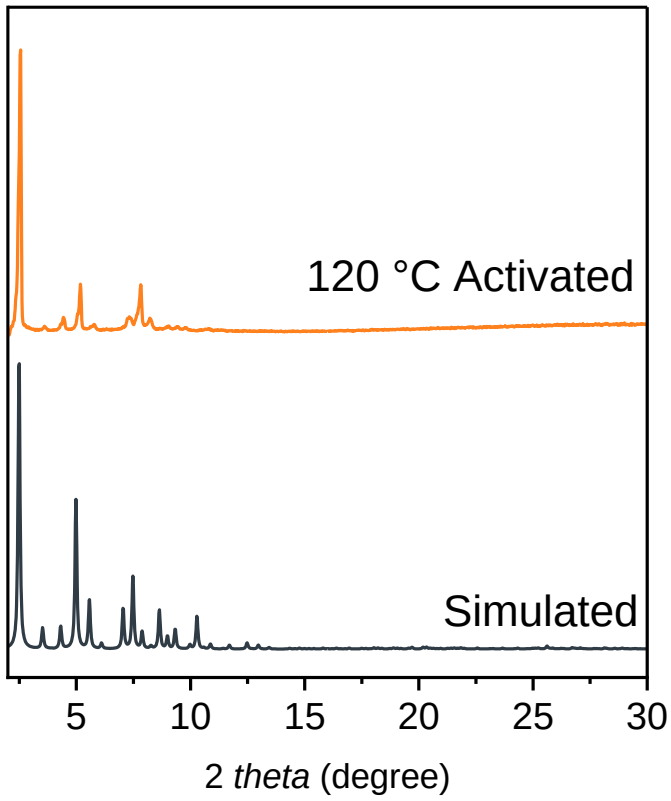


Figure S9. PXRD pattern of activated Zr-TCPCo before gas adsorption test.

8.2 Chemical stability

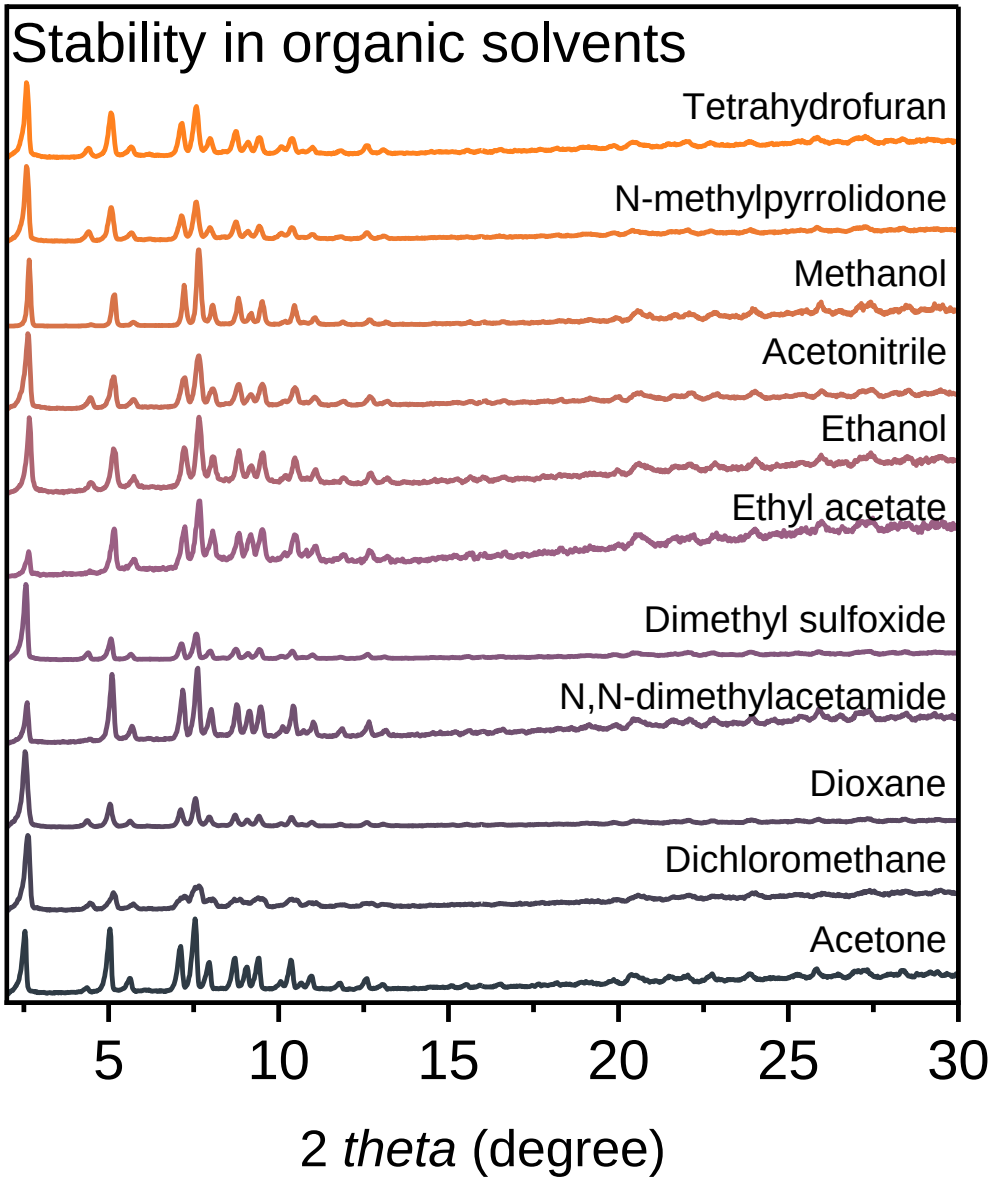


Figure S10. PXRD patterns of Zr-TCPCo after immersing in different organic solvents for 3 days.

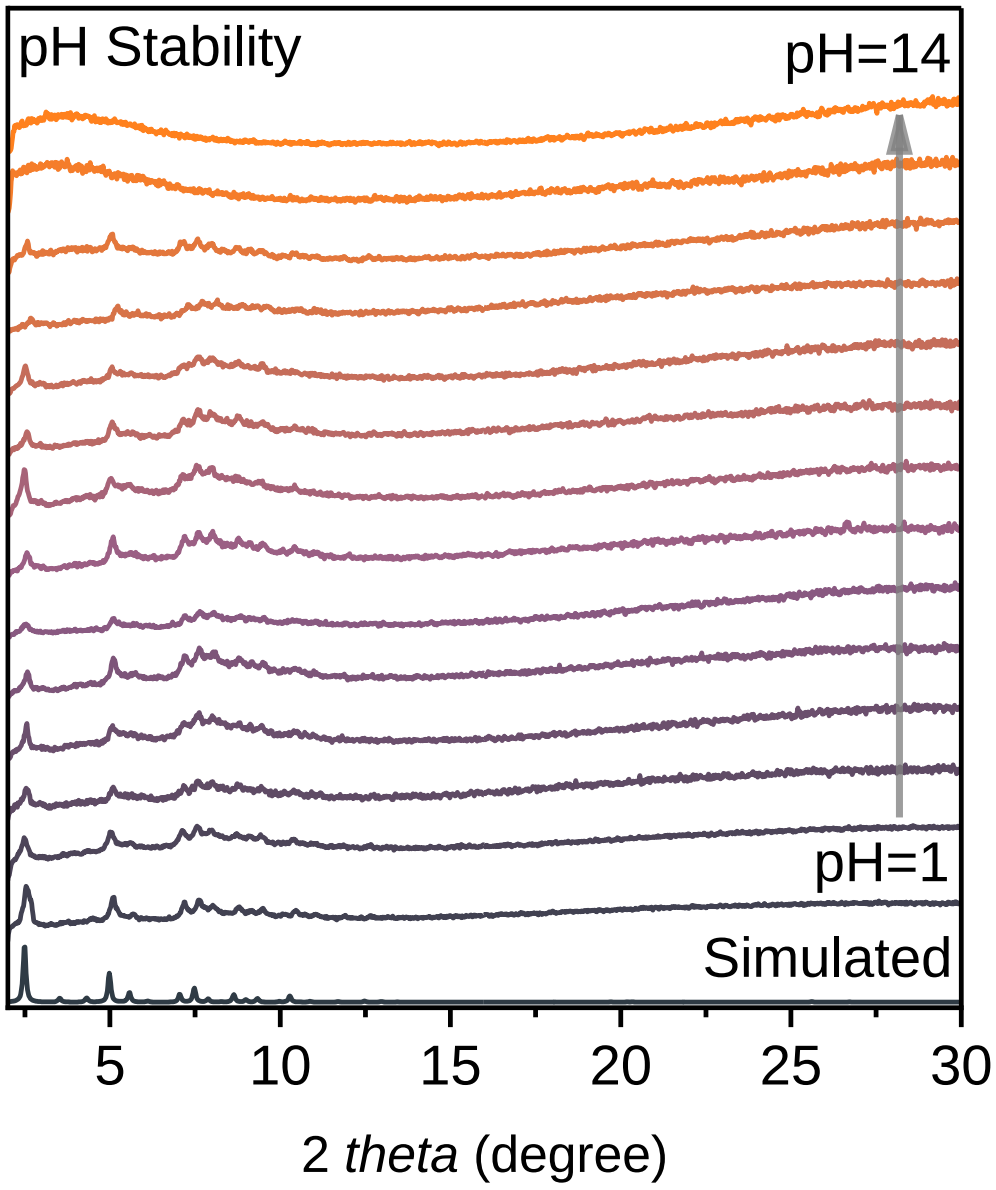


Figure S11. PXRD patterns of Zr-TCPCo after immersing in solutions with different pH values for 1 day.

8.3 Air and water stability

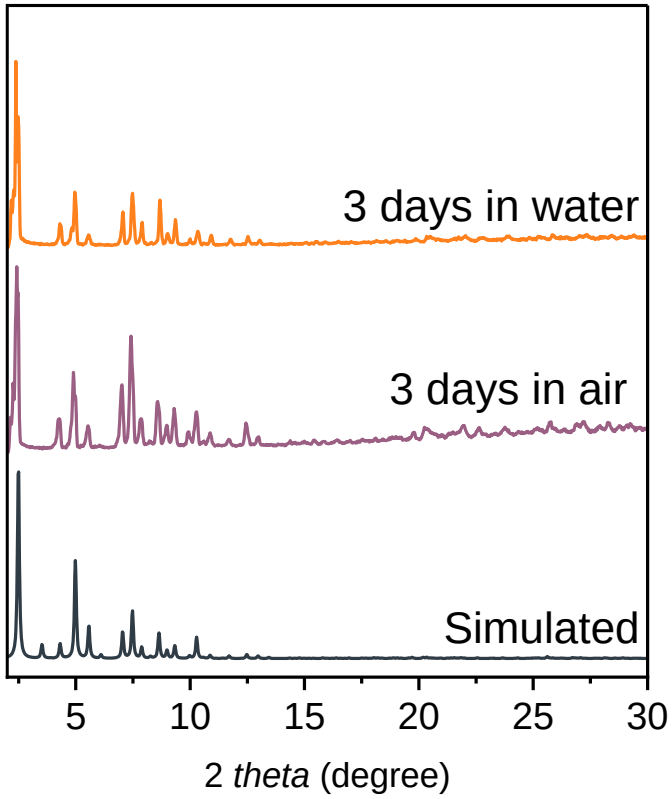


Figure S12. PXRD patterns of Zr-TCPCo after exposure to water and air for 1 day.

9. IR test of Zr-TCPCo

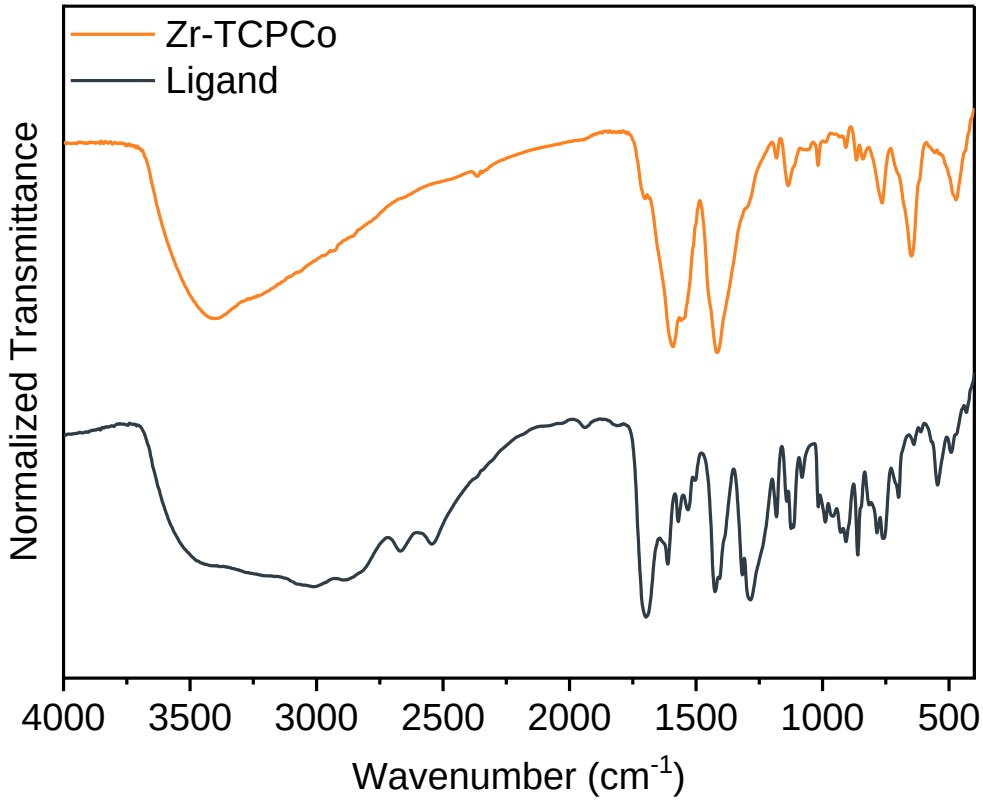


Figure S13. IR spectra of Zr-TCPCo and the cobaloxime ligand.

10. K-M function plot of Zr-TCPCo

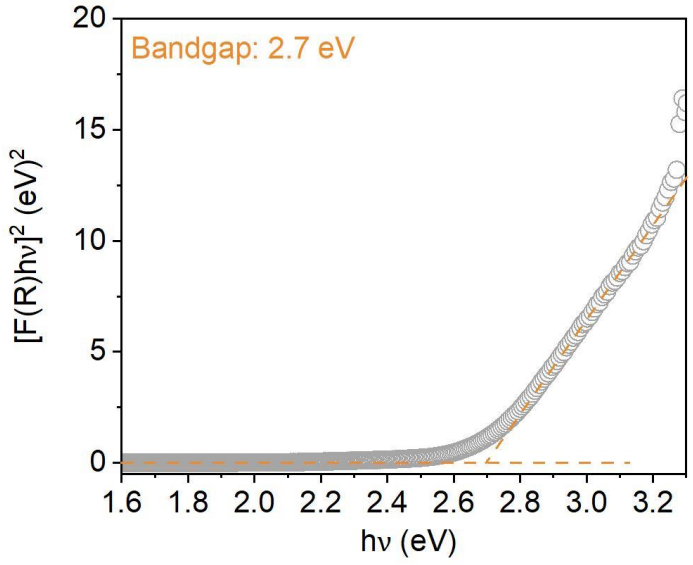


Figure S14. K-M function plot of Zr-TCPCo.

11. Mott-Schottky test

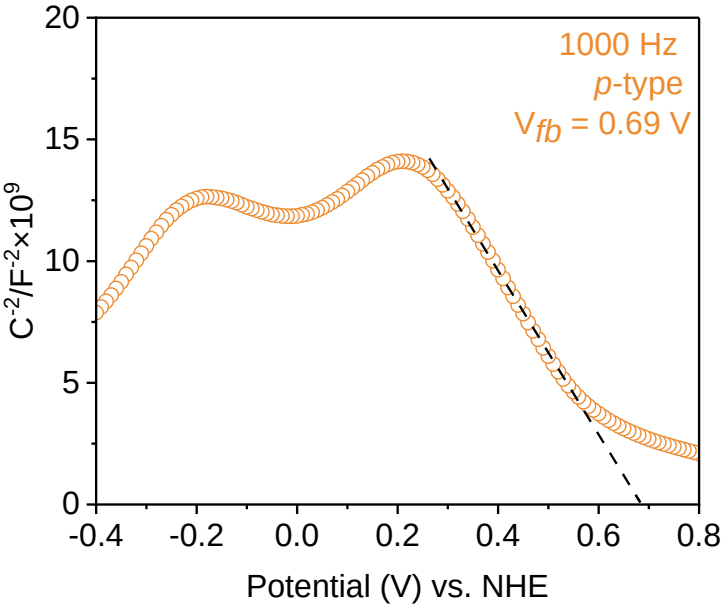


Figure S15. Mott-Schottky plot of Zr-TCPCo.

12. Cyclic voltammetry analysis

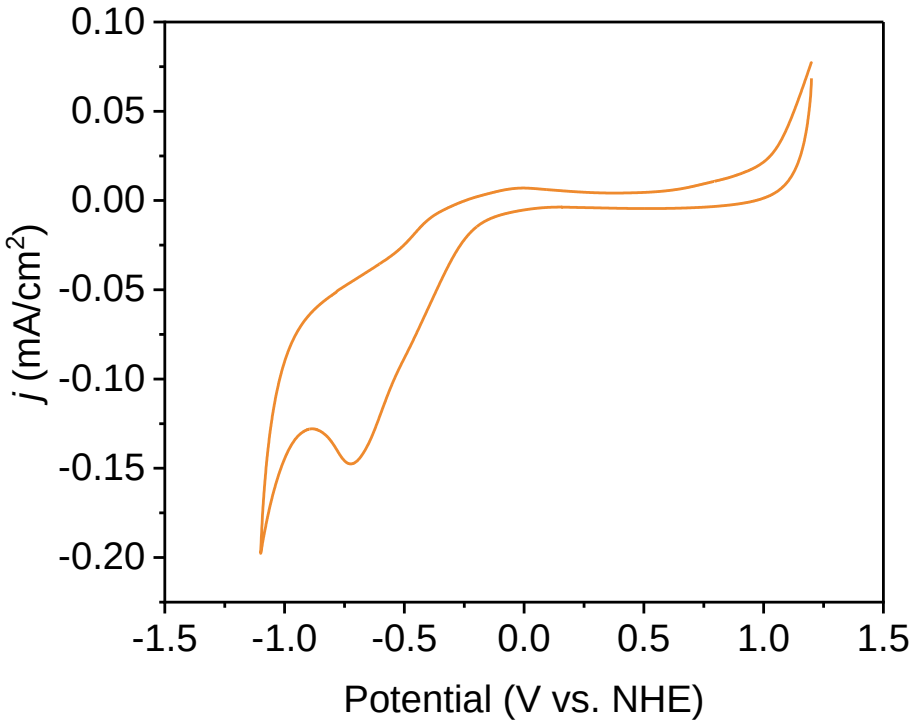
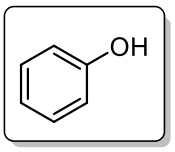


Figure S16. Cyclic voltammetry analysis of Zr-TCPCo.

13. General procedure for the photochemical reactions

a (0.2 mmol), Zr-TCPCo (3.0 mg), Et_3N (55.5 μL, 2.0 equiv.) were dissolved in 2.0 mL DCE in a 10.0 mL flask equipped with a magnetic stirring bar, then degassed with O_2 for 5 min. The reaction tube was irradiated by blue LEDs (λ = 450 ± 10 nm) at room temperature for 12 h. After the reaction, the Zr-TCPCo was separated by centrifugation and washed with a very small amount of DCE, then the solvent was removed by rotary evaporation and purified by column chromatography on silica gel using hexane/ethyl acetate as the eluent to afford the desired product **b**.

14. Characterization data of the products



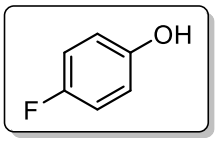
b1

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b1** as off white solid (17.3 mg, 91% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.34 (s, 1H), 7.16 (t, *J* = 7.9 Hz, 2H), 6.80 – 6.72 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 157.8, 129.8, 119.3, 115.7.

HRMS (ESI) calculated for C_6H_7O $[M+H]^+$: 95.0491; Found: 95.0499



b2

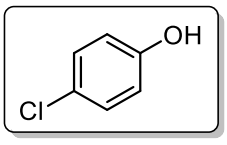
Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b2** as off white solid (13.3 mg, 60% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.36 (s, 1H), 6.97 (t, *J* = 8.9 Hz, 2H), 6.74 (dd, *J* = 9.0, 4.5 Hz, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 156.0 (d, *J* = 233.0 Hz), 154.1 (d, *J* = 1.9 Hz), 116.5 (d, *J* = 8.0 Hz), 116.0 (d, *J* = 22.7 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -128.94 (s, 1F).

HRMS (ESI) calculated for C_6H_6FO $[M+H]^+$: 113.0397; Found: 113.0402



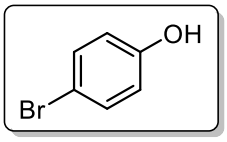
b3

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b3** as pale-yellow solid (19.7 mg, 77% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.67 (s, 1H), 7.19 (d, *J* = 8.8 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 156.8, 129.6, 122.8, 117.4.

HRMS (ESI) calculated for C_6H_6ClO $[M+H]^+$: 129.0102; Found: 129.0099



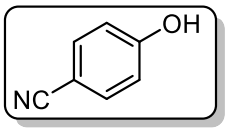
b4

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **O4** as pale-yellow solid (25.5 mg, 74% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.32 (d, J = 8.8 Hz, 2H), 6.74 (d, J = 8.8 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 157.3, 132.5, 118.1, 110.4.

HRMS (ESI) calculated for C_6H_6BrO $[M+H]^+$: 172.9597; Found: 172.9595



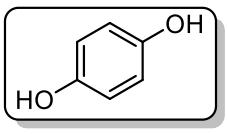
b5

Purification by column chromatography on silica gel (hexane/ethyl acetate = 2/1, v/v) afforded **O5** as pale-yellow solid (12.6 mg, 53% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.33 (s, 1H), 7.81 (d, J = 8.7 Hz, 2H), 6.83 (d, J = 8.6 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 196.5, 162.4, 131.2, 129.1, 115.6.

HRMS (ESI) calculated for C_7H_6NO $[M+H]^+$: 120.0444; Found: 120.0438



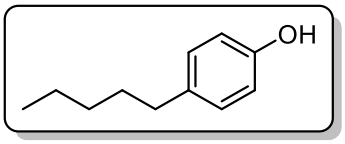
b6

Purification by column chromatography on silica gel (hexane/ethyl acetate = 3/1, v/v) afforded **b6** as off white solid (18.9 mg, 86% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.61 (s, 2H), 6.54 (s, 4H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 150.2, 116.1.

HRMS (ESI) calculated for $C_6H_7O_2$ $[M+H]^+$: 111.0441; Found: 111.0447



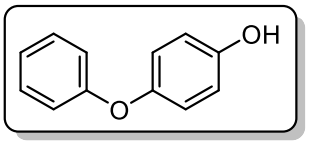
b7

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b7** as off white solid (24.6 mg, 75% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.09 (s, 1H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 2.45 (t, *J* = 7.6 Hz, 2H), 1.52 (p, *J* = 7.4 Hz, 2H), 1.38 – 1.17 (m, 4H), 0.87 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 155.7, 132.8, 129.5, 115.5, 34.8, 31.5, 31.4, 22.5, 14.4.

HRMS (ESI) calculated for $C_{11}H_{17}O$ $[M+H]^+$: 165.1274; Found: 165.1277



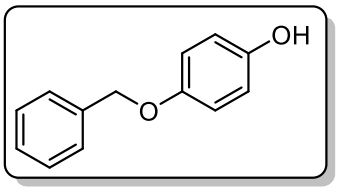
b8

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b8** as white solid (32.9 mg, 88% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.35 (s, 1H), 7.33 (dd, *J* = 8.6, 7.3 Hz, 2H), 7.05 (t, *J* = 7.4 Hz, 1H), 6.90 (d, *J* = 8.9 Hz, 4H), 6.80 (d, *J* = 8.9 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 158.9, 154.4, 148.3, 130.3, 122.7, 121.4, 117.4, 116.8.

HRMS (ESI) calculated for $C_{12}H_{11}O_2$ $[M+H]^+$: 187.0754; Found: 187.0759



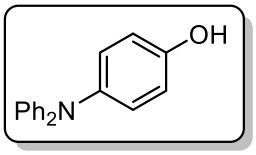
b9

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b9** as white solid (28.0 mg, 70% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.94 (s, 1H), 7.41 (dt, *J* = 14.7, 7.2 Hz, 4H), 7.34 (d, *J* = 7.1 Hz, 1H), 6.84 (d, *J* = 8.9 Hz, 2H), 6.70 (d, *J* = 8.9 Hz, 2H), 5.00 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 151.9, 151.7, 138.1, 128.8, 128.2, 128.1, 116.3, 116.2, 70.2.

HRMS (ESI) calculated for $C_{13}H_{13}O_2$ $[M+H]^+$: 201.0910; Found: 201.0905



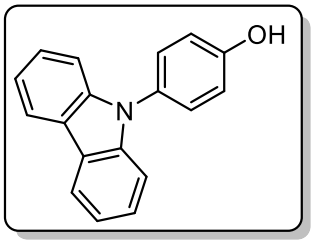
b10

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b10** as pale-green solid (40.2 mg, 77% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.42 (s, 1H), 7.23 (t, *J* = 7.9 Hz, 4H), 6.93 (dd, *J* = 8.7, 6.5 Hz, 8H), 6.78 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 155.1, 148.3, 138.7, 129.7, 128.4, 122.4, 122.0, 116.9.

HRMS (ESI) calculated for $C_{18}H_{16}NO$ $[M+H]^+$: 262.1226; Found: 262.1222



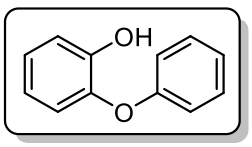
b11

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b11** as off white solid (49.2 mg, 95% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.88 (s, 1H), 8.23 (d, *J* = 7.9 Hz, 2H), 7.46 – 7.33 (m, 4H), 7.28 (dd, *J* = 12.8, 7.7 Hz, 4H), 7.06 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 157.5, 141.3, 128.7, 128.3, 126.6, 122.9, 120.9, 120.1, 117.1, 110.1.

HRMS (ESI) calculated for $C_{18}H_{14}NO$ $[M+H]^+$: 260.1070; Found: 260.1074



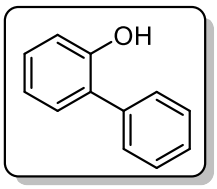
b12

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b12** as white solid (33.3 mg, 74% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.51 (s, 1H), 7.28 (t, *J* = 7.7 Hz, 2H), 6.99 (dq, *J* = 22.3, 7.6, 7.1 Hz, 4H), 6.80 (dd, *J* = 13.5, 7.4 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 158.4, 149.9, 142.9, 130.0, 125.9, 122.4, 122.3, 120.1, 117.8, 116.5.

HRMS (ESI) calculated for $C_{12}H_{11}O_2$ $[M+H]^+$: 187.0754; Found: 187.0760



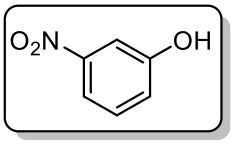
b13

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b13** as white solid (27.5 mg, 81% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.50 (s, 1H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.18 (m, 2H), 7.13 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 154.7, 139.1, 130.8, 129.5, 128.9, 128.3, 128.2, 126.9, 119.9, 116.5.

HRMS (ESI) calculated for $C_{12}H_{11}O$ $[M+H]^+$: 171.0804; Found: 171.0809



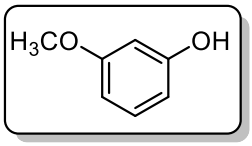
b14

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b14** as light brown solid (13.0 mg, 47% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 7.67 (ddd, *J* = 8.1, 2.2, 0.9 Hz, 1H), 7.57 (t, *J* = 2.3 Hz, 1H), 7.48 (t, *J* = 8.2 Hz, 1H), 7.23 (ddd, *J* = 8.2, 2.4, 0.9 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 158.8, 149.2, 131.1, 122.9, 114.3, 110.1.

HRMS (ESI) calculated for $C_6H_6NO_3$ $[M+H]^+$: 140.0342; Found: 140.0344



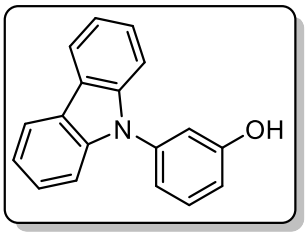
b15

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b15** as off white solid (17.8 mg, 78% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.33 (s, 1H), 7.83 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 166.6, 162.5, 131.9, 120.8, 115.8, 52.1.

HRMS (ESI) calculated for $C_7H_9O_2$ $[M+H]^+$: 125.0597; Found: 125.0562



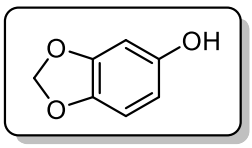
b16

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b16** as off white solid (50.2 mg, 97% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.95 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 8.1 Hz, 1H), 7.47 – 7.42 (m, 4H), 7.29 (ddd, *J* = 8.2, 5.1, 3.3 Hz, 2H), 7.07 – 6.95 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 159.3, 140.6, 138.4, 131.4, 126.7, 123.2, 121.0, 120.5, 117.5, 115.3, 113.8, 110.3.

HRMS (ESI) calculated for $C_{18}H_{14}NO$ $[M+H]^+$: 260.1070; Found: 260.1066



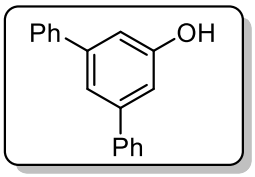
b17

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b17** as colorless oil (17.9 mg, 65% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.10 (s, 1H), 6.70 (d, *J* = 8.3 Hz, 1H), 6.39 (d, *J* = 2.4 Hz, 1H), 6.21 (dd, *J* = 8.3, 2.4 Hz, 1H), 5.90 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 153.0, 148.2, 140.2, 108.7, 106.8, 101.1, 98.4.

HRMS (ESI) calculated for $C_7H_7O_3$ $[M+H]^+$: 139.0390; Found: 139.0398



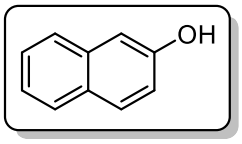
b18

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b18** as white solid (40.8 mg, 83% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.76 (s, 1H), 7.71 (d, *J* = 7.0 Hz, 4H), 7.49 (t, *J* = 7.6 Hz, 4H), 7.38 (dd, *J* = 15.1, 7.8 Hz, 3H), 7.08 (d, *J* = 1.6 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 158.8, 142.8, 140.9, 129.4, 128.1, 127.3, 116.8, 113.3.

HRMS (ESI) calculated for $C_{18}H_{15}O$ $[M+H]^+$: 247.1117; Found: 247.1110



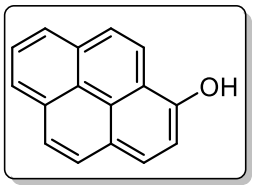
b19

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b19** as white solid (21.8 mg, 75% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.73 (s, 1H), 7.75 (dd, *J* = 8.4, 4.4 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.38 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.25 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.12 (d, *J* = 2.4 Hz, 1H), 7.09 (dd, *J* = 8.7, 2.5 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 155.8, 135.2, 129.8, 128.2, 128.0, 126.6, 126.4, 123.1, 119.1, 109.1.

HRMS (ESI) calculated for $C_{10}H_9O$ $[M+H]^+$: 145.0648; Found: 145.0656



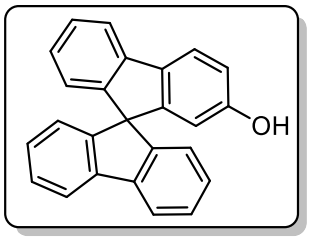
b20

Purification by column chromatography on silica gel (hexane/ethyl acetate = 7/1, v/v) afforded **b20** as white solid (25.8 mg, 59% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.65 (s, 1H), 8.36 (d, *J* = 9.1 Hz, 1H), 8.14 (dd, *J* = 7.7, 5.7 Hz, 3H), 8.07 – 7.97 (m, 3H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 152.7, 131.9, 131.8, 127.9, 126.7, 126.6, 126.00, 125.96, 124.5, 124.4, 124.3, 124.1, 124.1, 121.9, 118.6, 113.8.

HRMS (ESI) calculated for $C_{16}H_{11}O$ $[M+H]^+$: 219.0804; Found: 219.0808



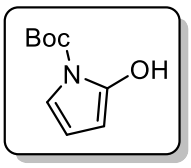
b21

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b21** as off white solid (51.8 mg, 78% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.38 (s, 1H), 8.02 (d, *J* = 7.6 Hz, 2H), 7.84 (dd, *J* = 15.0, 7.9 Hz, 2H), 7.41 (td, *J* = 7.5, 1.1 Hz, 2H), 7.34 (td, *J* = 7.5, 1.1 Hz, 1H), 7.15 (td, *J* = 7.5, 1.1 Hz, 2H), 7.02 (td, *J* = 7.5, 1.1 Hz, 1H), 6.83 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.66 (dd, *J* = 7.6, 0.9 Hz, 2H), 6.57 (d, *J* = 7.5 Hz, 1H), 6.02 (d, *J* = 2.2 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 158.2, 150.6, 149.2, 147.9, 142.3, 141.6, 132.9, 128.5, 128.4, 128.3, 126.8, 124.1, 123.8, 122.0, 121.0, 119.8, 115.7, 110.6, 65.8.

HRMS (ESI) calculated for $C_{25}H_{17}O$ $[M+H]^+$: 333.1274; Found: 333.1271



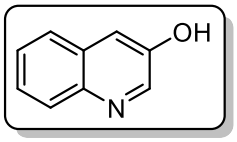
b22

Purification by column chromatography on silica gel (hexane/ethyl acetate = 5/1, v/v) afforded **b22** as colorless oil (32.9 mg, 90% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.02 (s, 1H), 7.29 (dd, *J* = 3.1, 1.5 Hz, 1H), 6.38 (dt, *J* = 3.2, 1.7 Hz, 1H), 6.18 (t, *J* = 3.1 Hz, 1H), 1.50 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ 150.2, 123.3, 120.8, 112.1, 84.4, 27.8.

HRMS (ESI) calculated for $C_9H_{14}NO_3$ $[M+H]^+$: 184.0968; Found: 184.0973



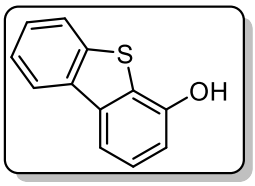
b23

Purification by column chromatography on silica gel (hexane/ethyl acetate = 3/1, v/v) afforded **b23** as off white solid (33.3 mg, 73% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.30 (s, 1H), 8.56 (d, *J* = 2.7 Hz, 1H), 7.88 (d, *J* = 9.1 Hz, 1H), 7.77 (d, *J* = 9.4 Hz, 1H), 7.48 (dd, *J* = 6.5, 3.2 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 151.3, 144.4, 142.9, 129.5, 129.1, 127.2, 127.0, 126.3, 115.7.

HRMS (ESI) calculated for C_9H_8NO $[M+H]^+$: 146.0600; Found: 146.0598



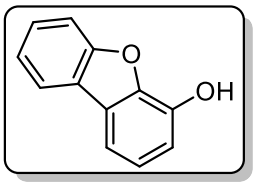
b24

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b24** as off white solid (24.4 mg, 61% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.48 (s, 1H), 8.33 – 8.24 (m, 1H), 8.05 – 7.99 (m, 1H), 7.82 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.56 – 7.43 (m, 2H), 7.36 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.7 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 152.8, 139.2, 137.4, 136.2, 127.4, 126.7, 126.2, 125.1, 125.0, 123.6, 122.7, 113.4, 112.0.

HRMS (ESI) calculated for $C_{12}H_9OS$ $[M+H]^+$: 201.0369; Found: 201.0373



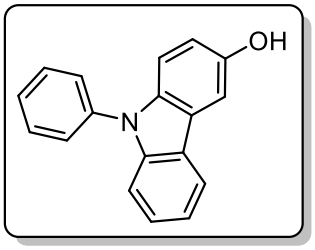
b25

Purification by column chromatography on silica gel (hexane/ethyl acetate = 10/1, v/v) afforded **b25** as off white solid (25.8 mg, 70% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.23 (s, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.47 (m, 2H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.01 (dd, *J* = 7.9, 1.1 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 155.8, 144.6, 143.5, 127.8, 125.7, 124.6, 124.3, 123.4, 121.6, 114.5, 112.2, 111.8.

HRMS (ESI) calculated for $C_{12}H_9O_2$ $[M+H]^+$: 185.0597; Found: 185.0591



b26

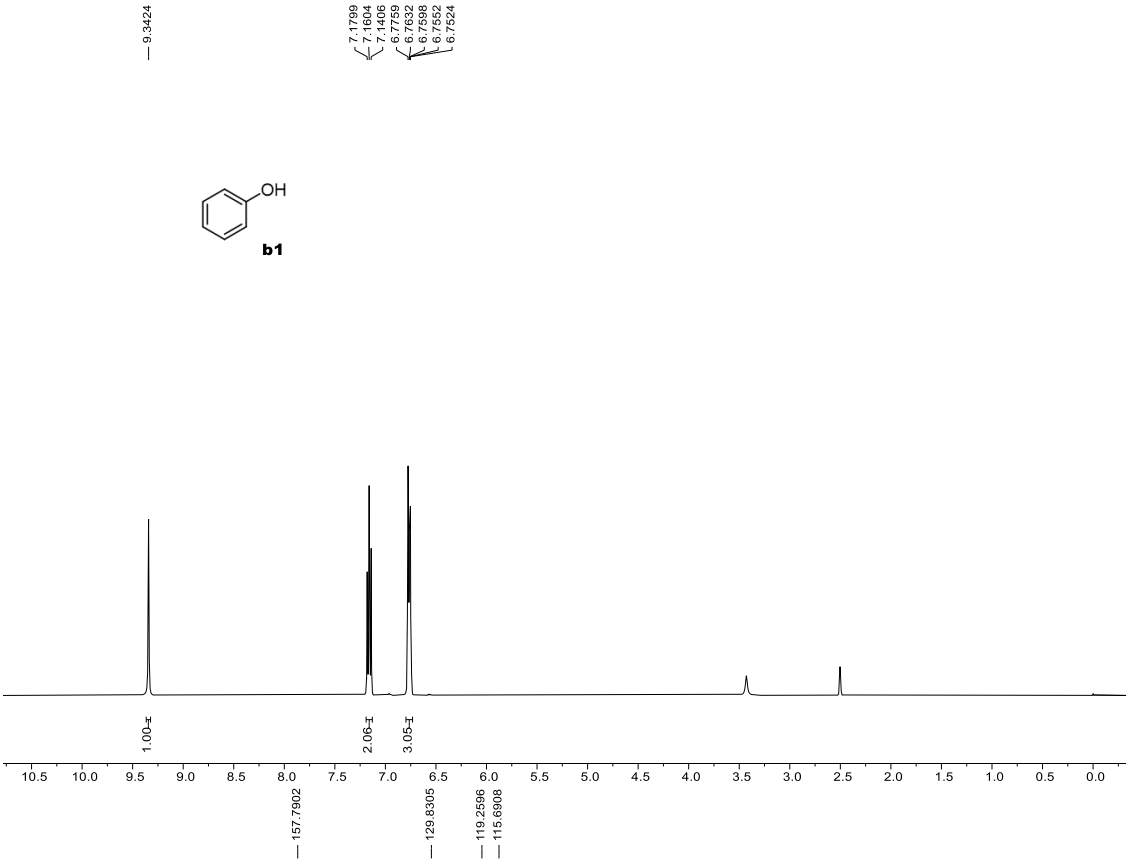
Purification by column chromatography on silica gel (hexane/ethyl acetate = 5/1, v/v) afforded **b26** as light-yellow solid (30.6 mg, 59% yield).

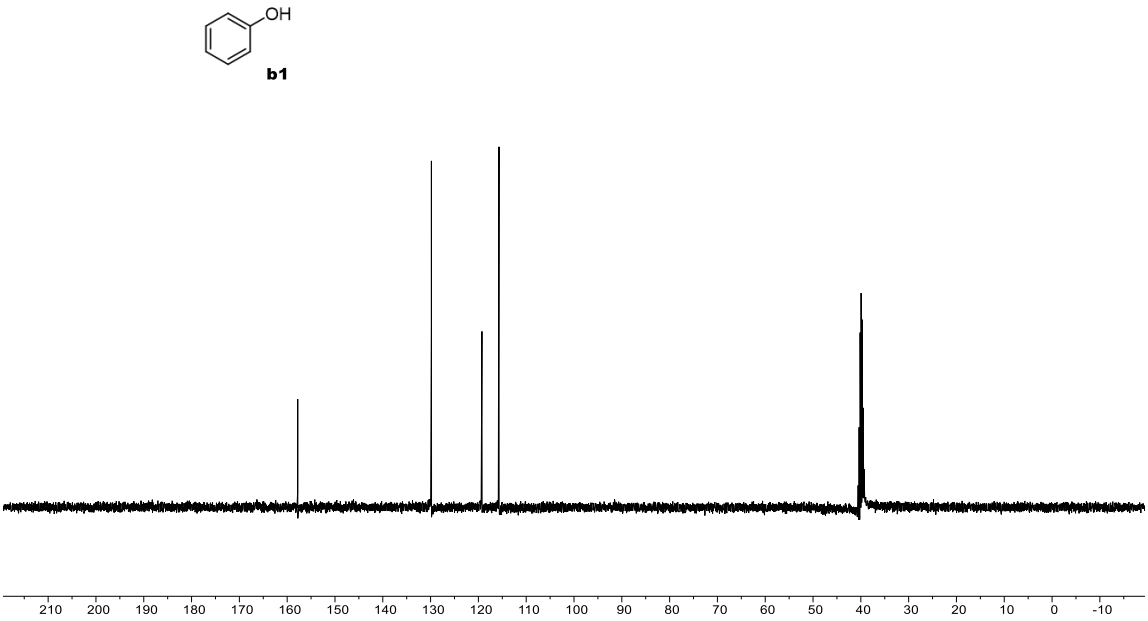
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.20 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 3H), 7.46 (t, *J* = 7.0 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.20 (t, *J* = 7.1 Hz, 2H), 6.93 (d, *J* = 8.8, 1H).

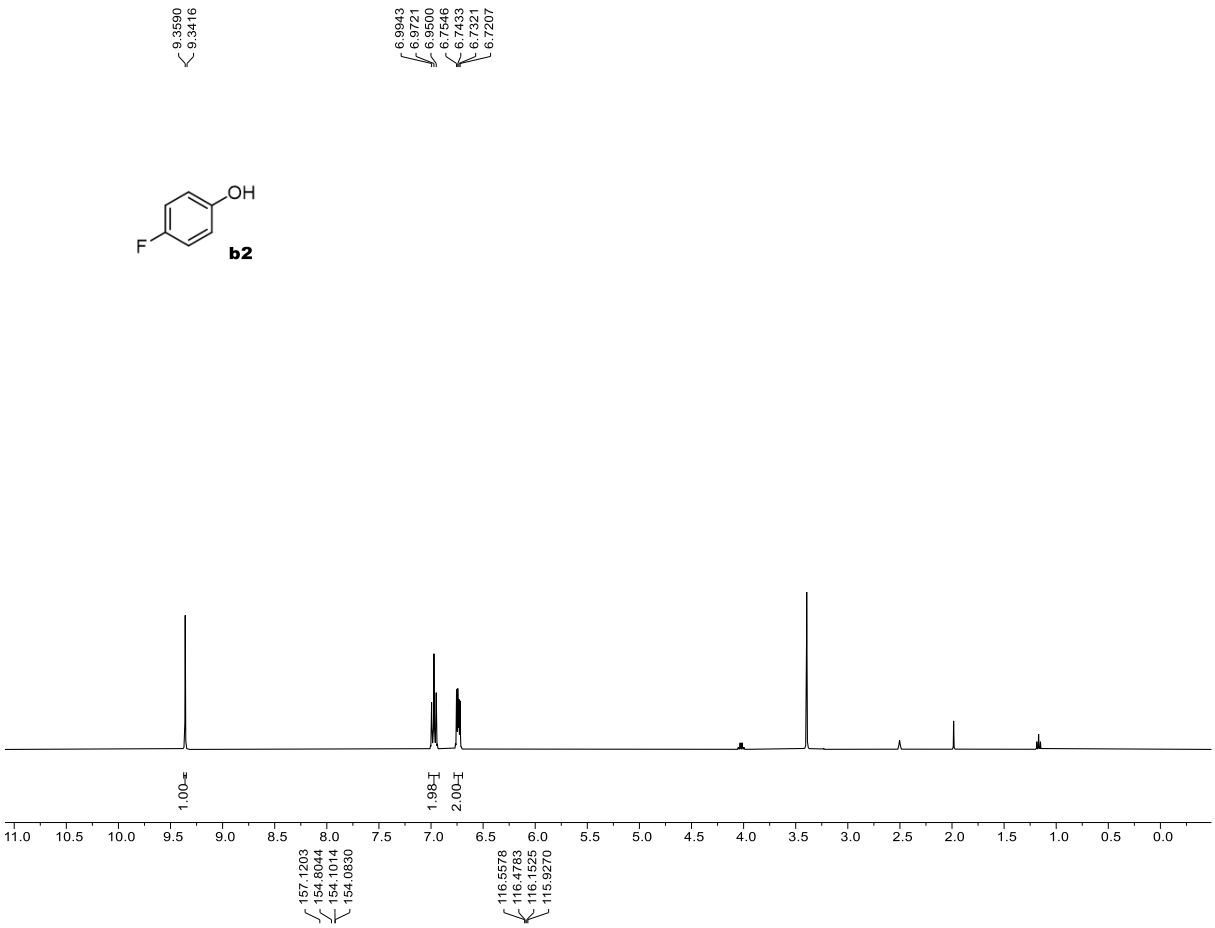
^{13}C NMR (101 MHz, DMSO) δ 152.1, 140.9, 137.8, 134.6, 130.5, 127.6, 126.8, 126.5, 124.0., 123.1, 120.9, 119.8, 115.9, 110.6, 109.9, 105.7.

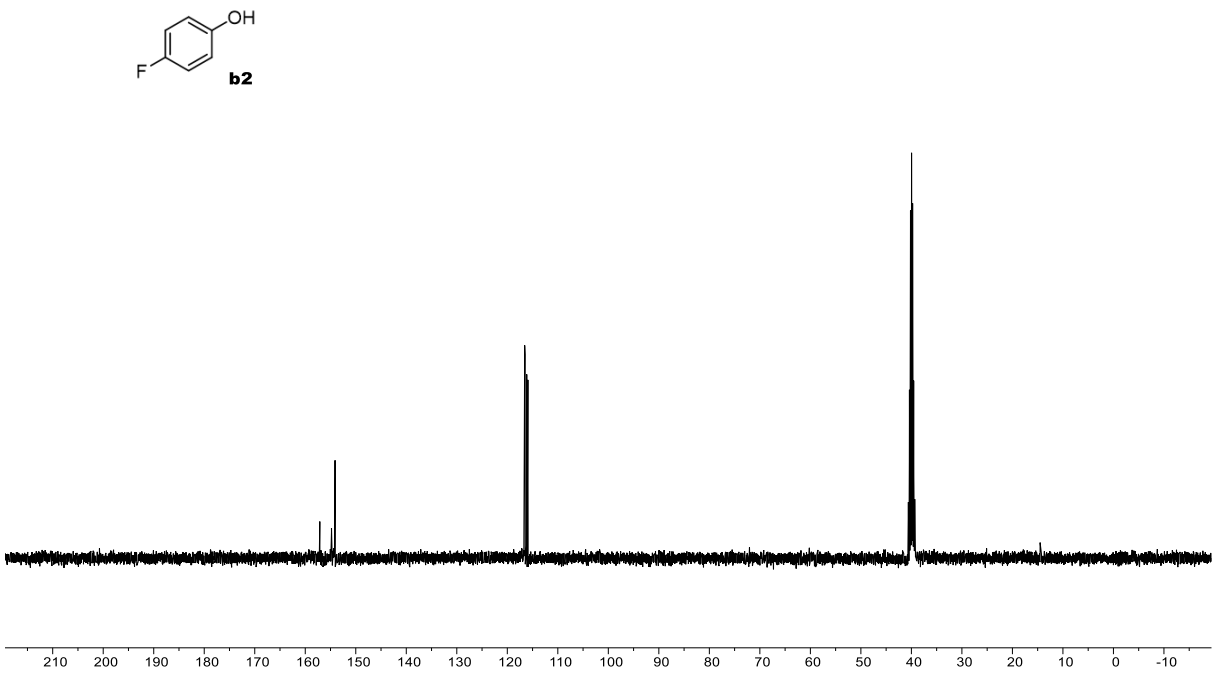
HRMS (ESI) calculated for $C_{18}H_{14}NO$ $[M+H]^+$: 260.1070; Found: 260.1068

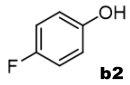
15. NMR spectra for the products






9.3590
9.3416
6.9943
6.9721
6.9500
6.7546
6.7433
6.7321
6.7207
OH
F
b2
1.00
1.98
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
157.1203
154.8044
154.1014
154.0830
116.5578
116.4783
116.1525
115.9270


OH
F
b2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


OH
F

b2

-128.9363
1.00
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
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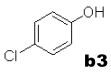
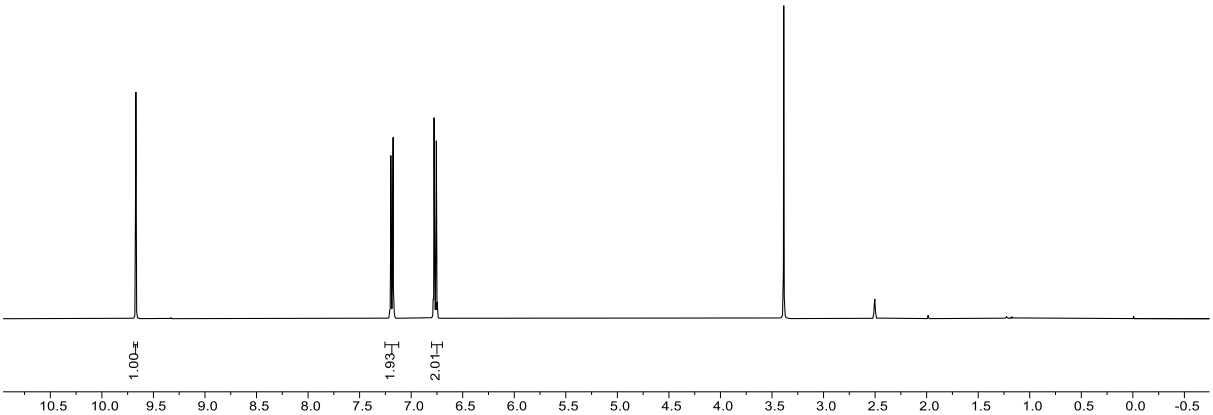
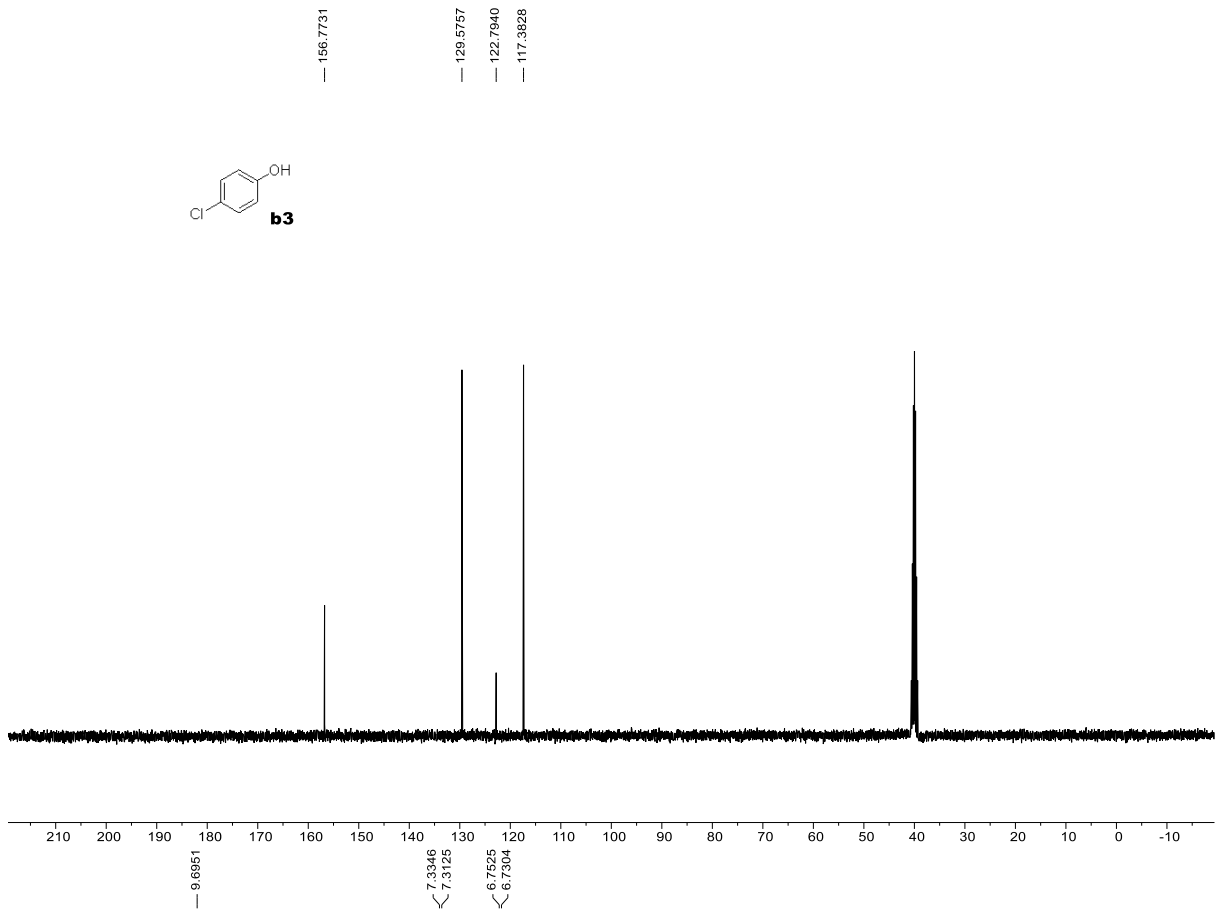
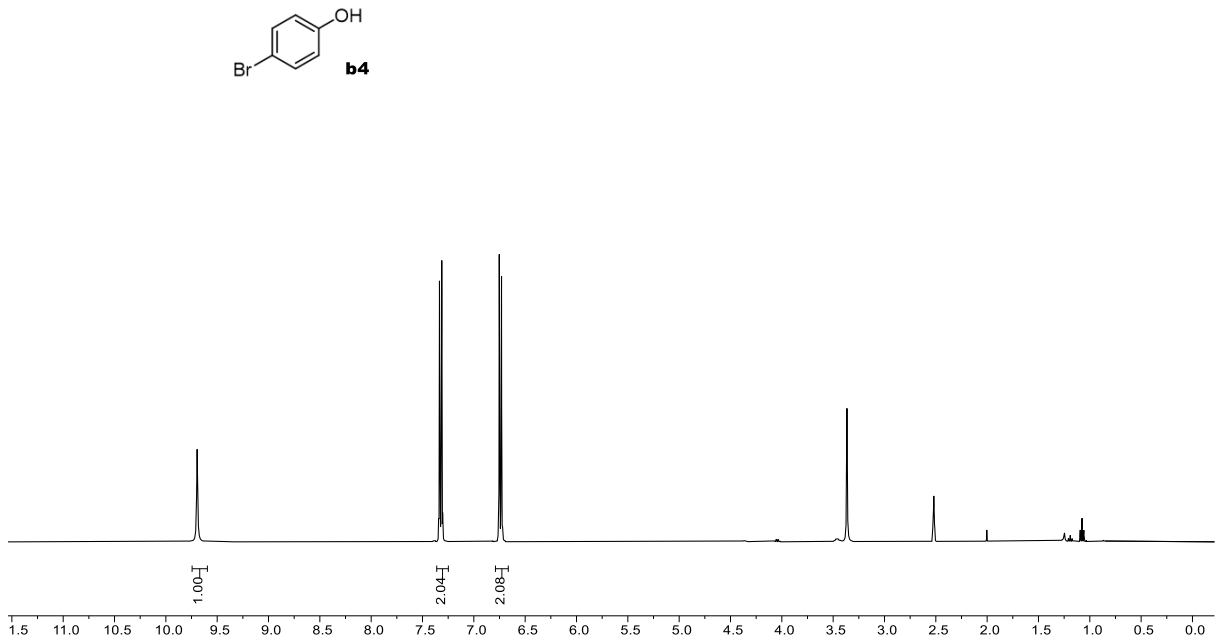
-140
9.6703
7.1972
7.1751
6.7778
6.7558

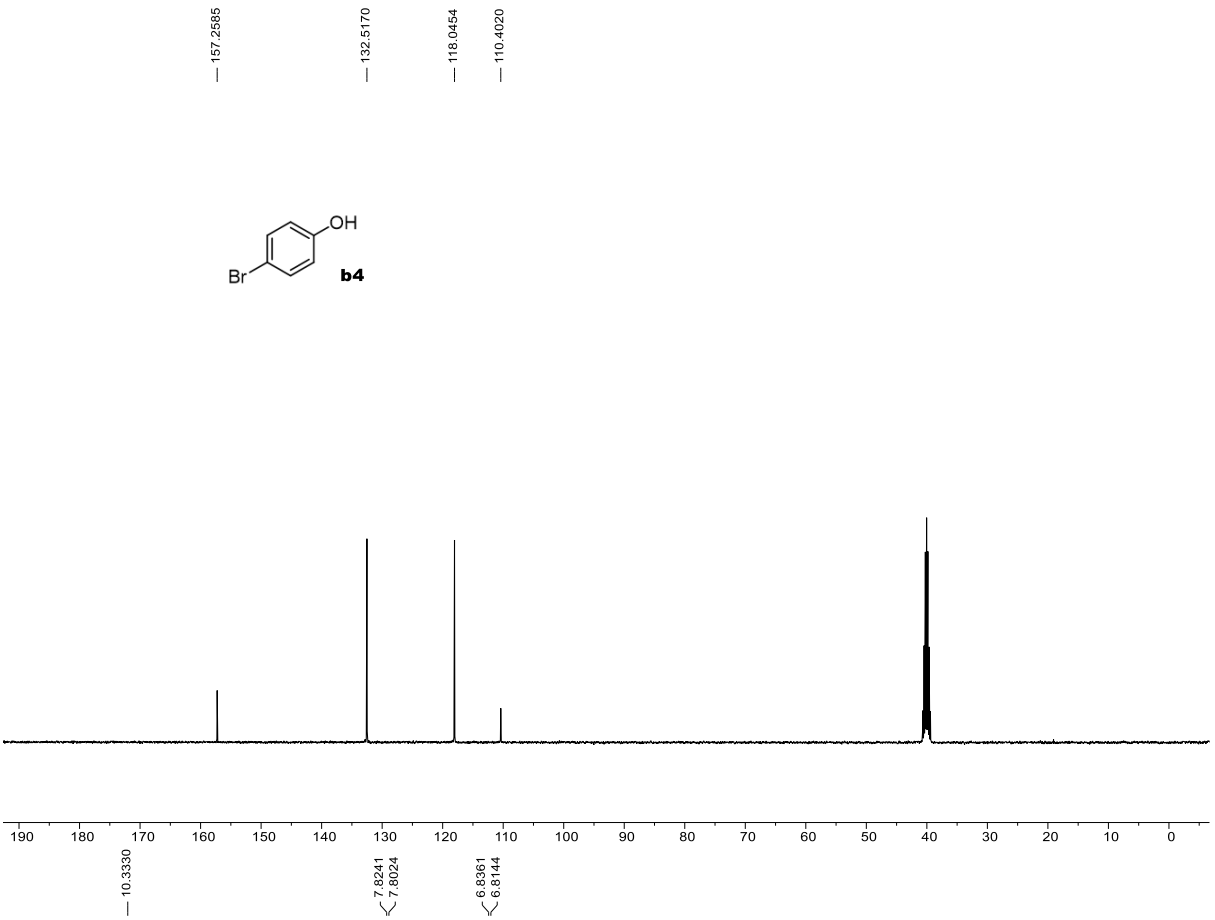

OH
Cl

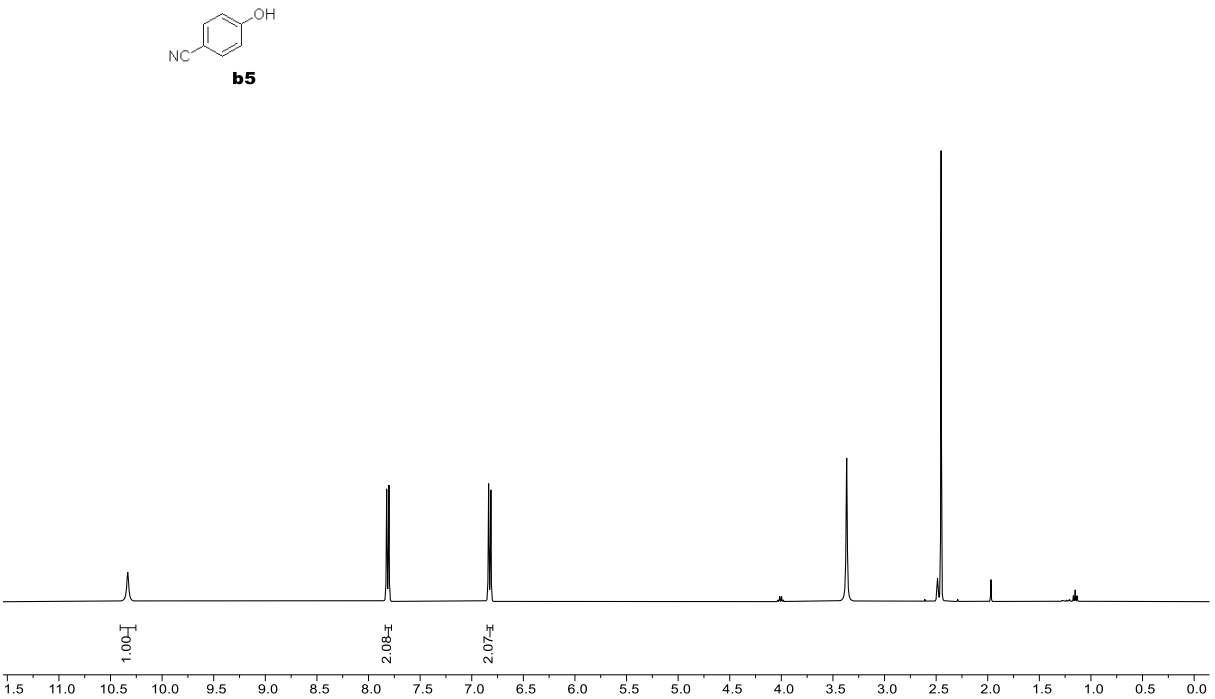
b3

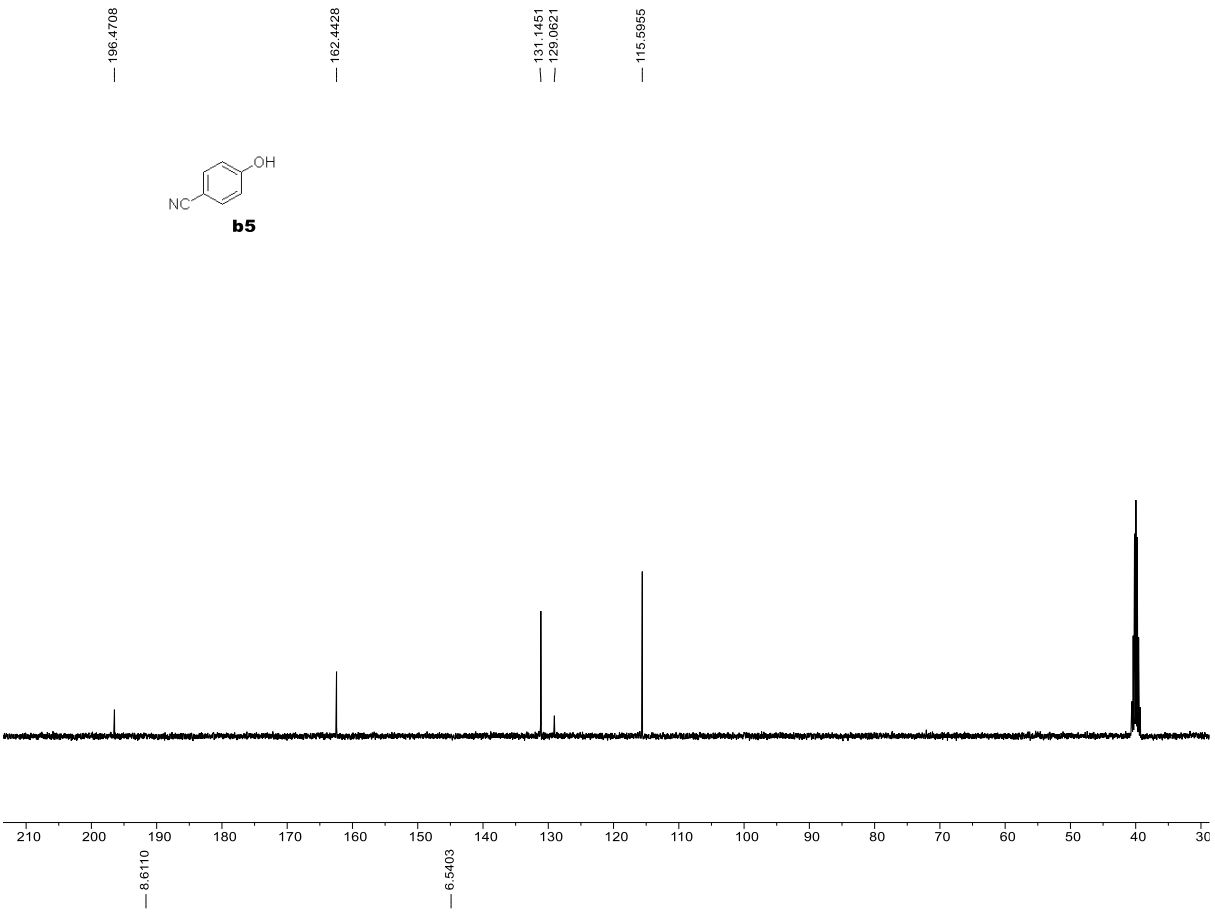

1.00
1.93
2.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


156.7731
129.5757
122.7940
117.3828
OH
Cl
b3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
9.6951
7.3346
7.3125
6.7525
6.7304


OH
Br
b4
1.00
2.04
2.08
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


157.2585
132.5170
118.0454
110.4020
OH
Br
b4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
10.3330
7.8241
7.8024
6.8361
6.8144


OH
NC
b5
1.00
2.08
2.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


196.4708
162.4428
131.1451
129.0621
115.5955
OH
NC
b5
210
200
190
180
170
160
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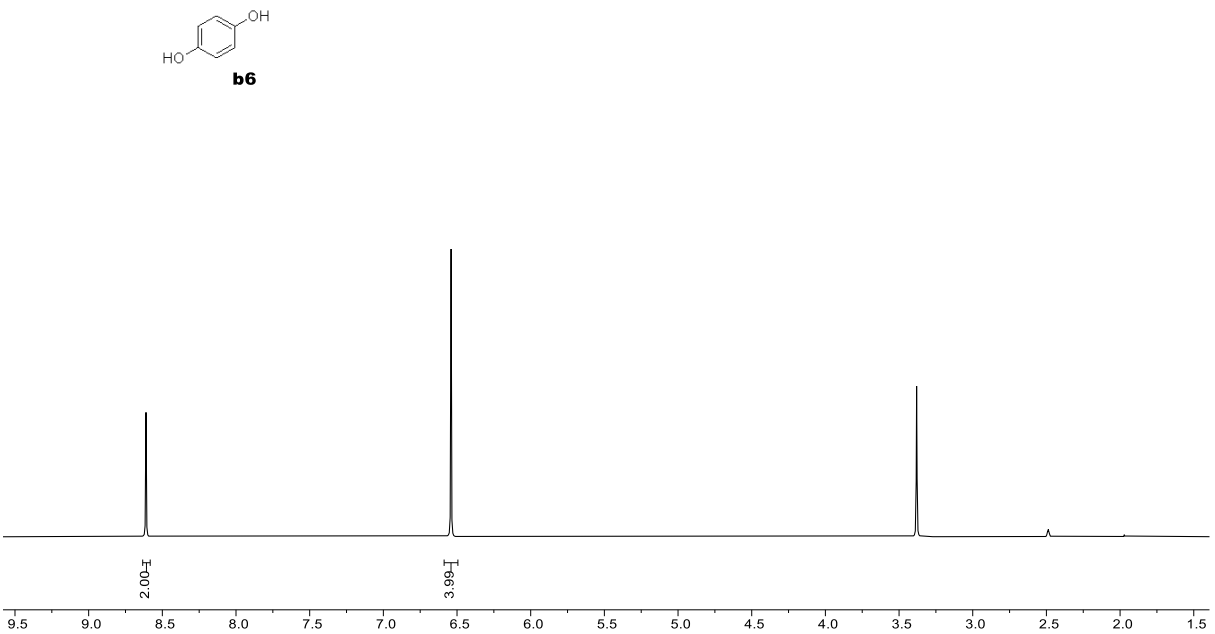
80
70
60
50
40
30
8.6110
6.5403


OH
HO
b6
2.00
3.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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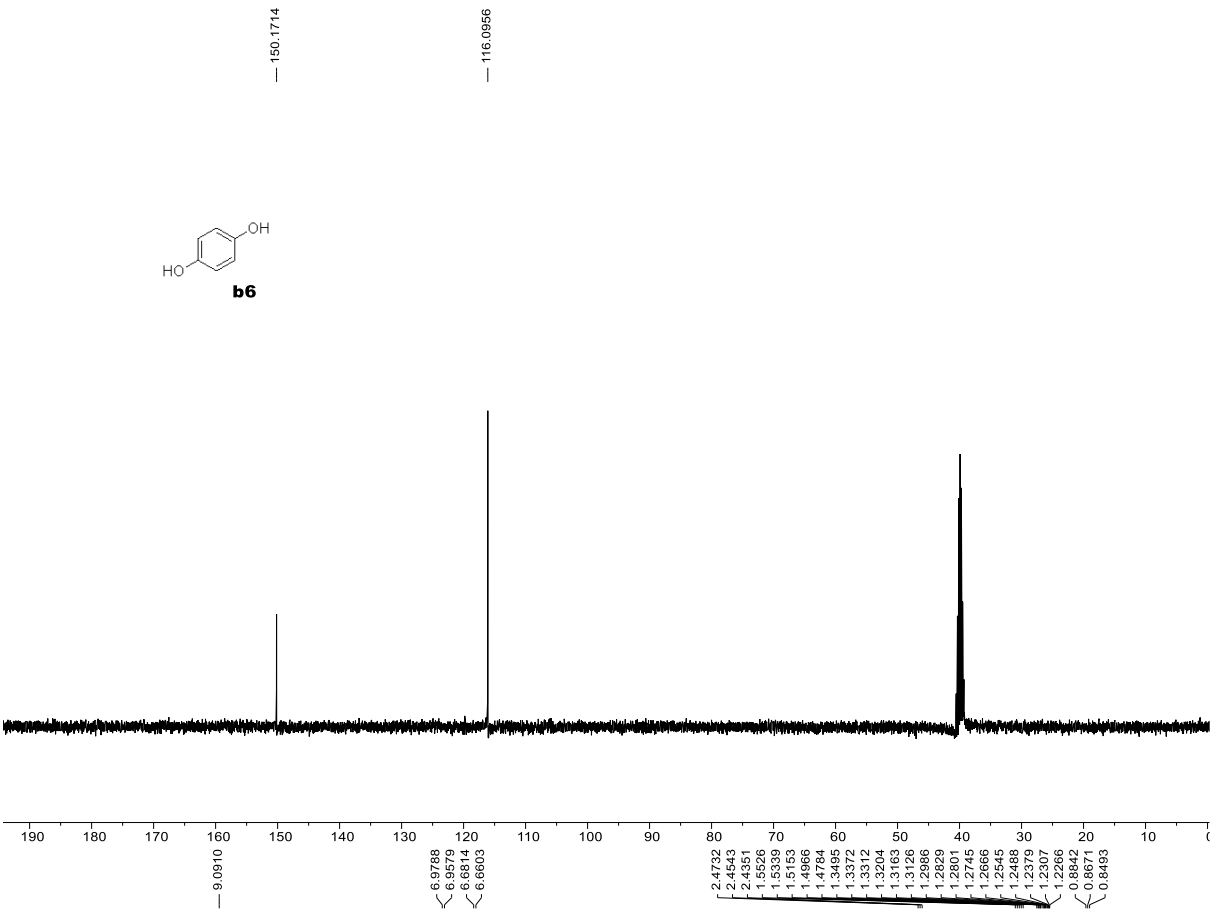
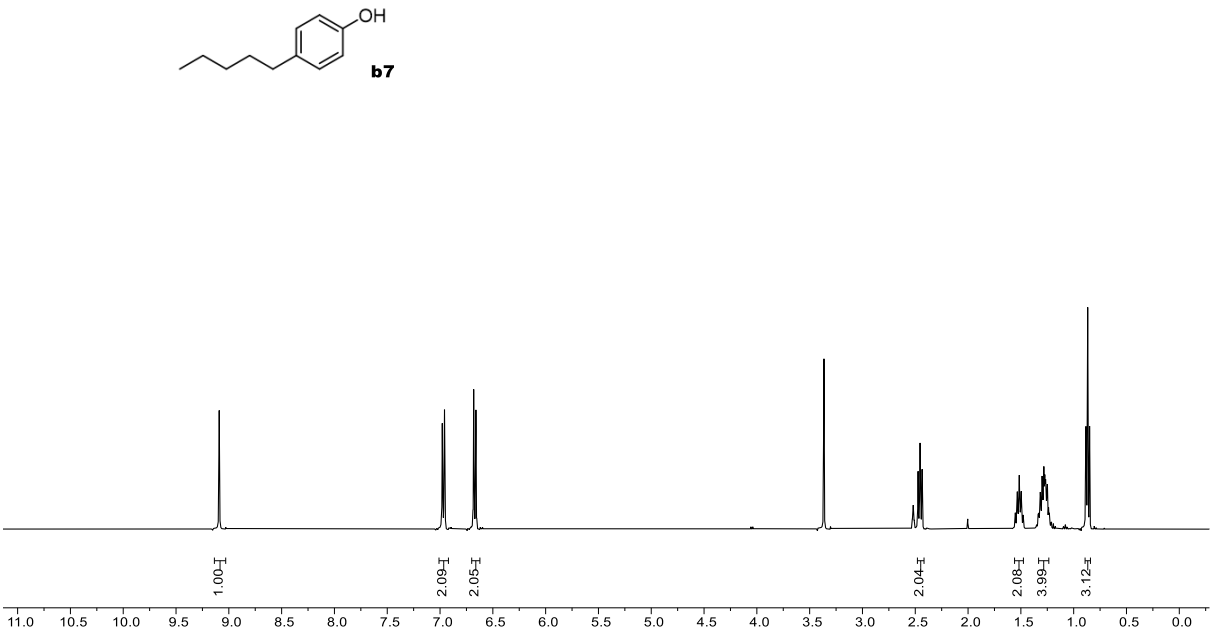
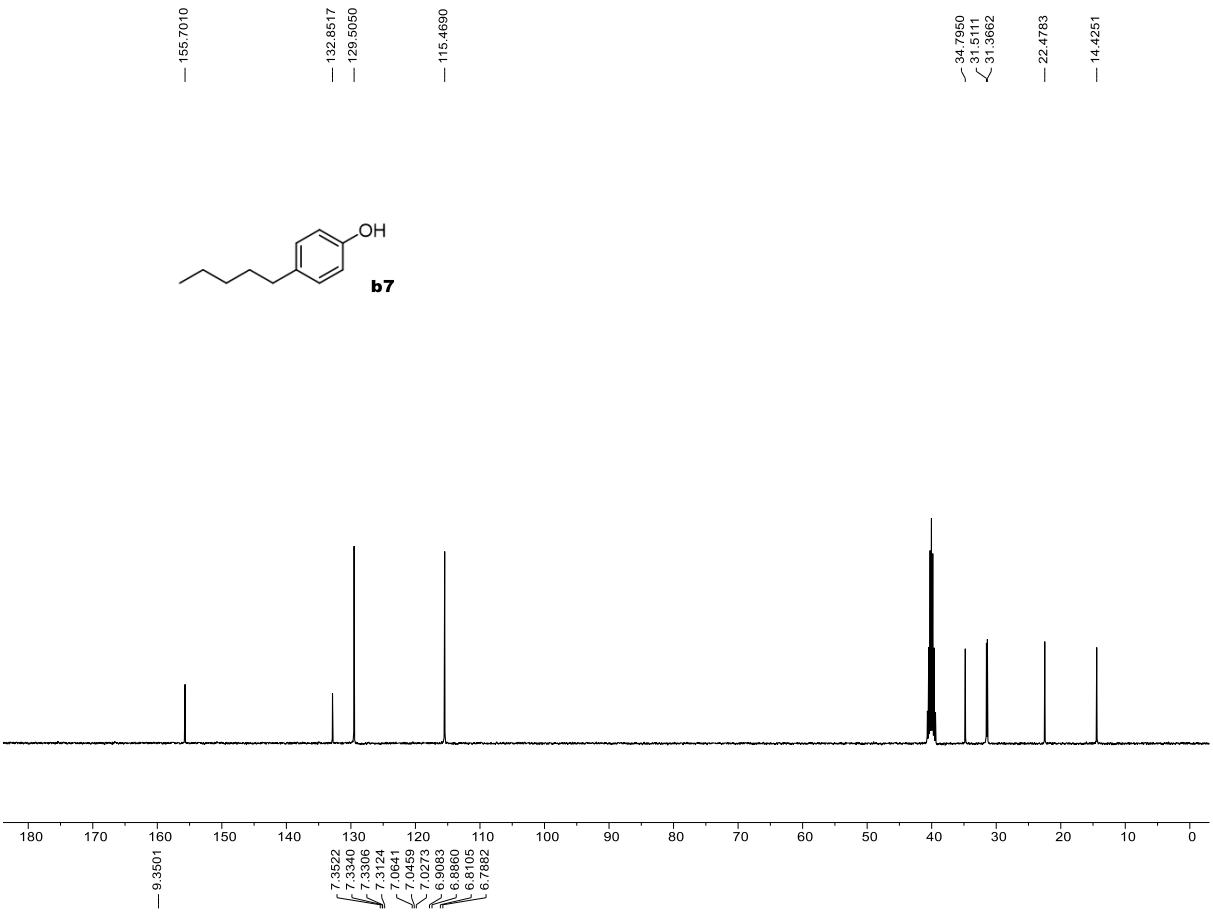
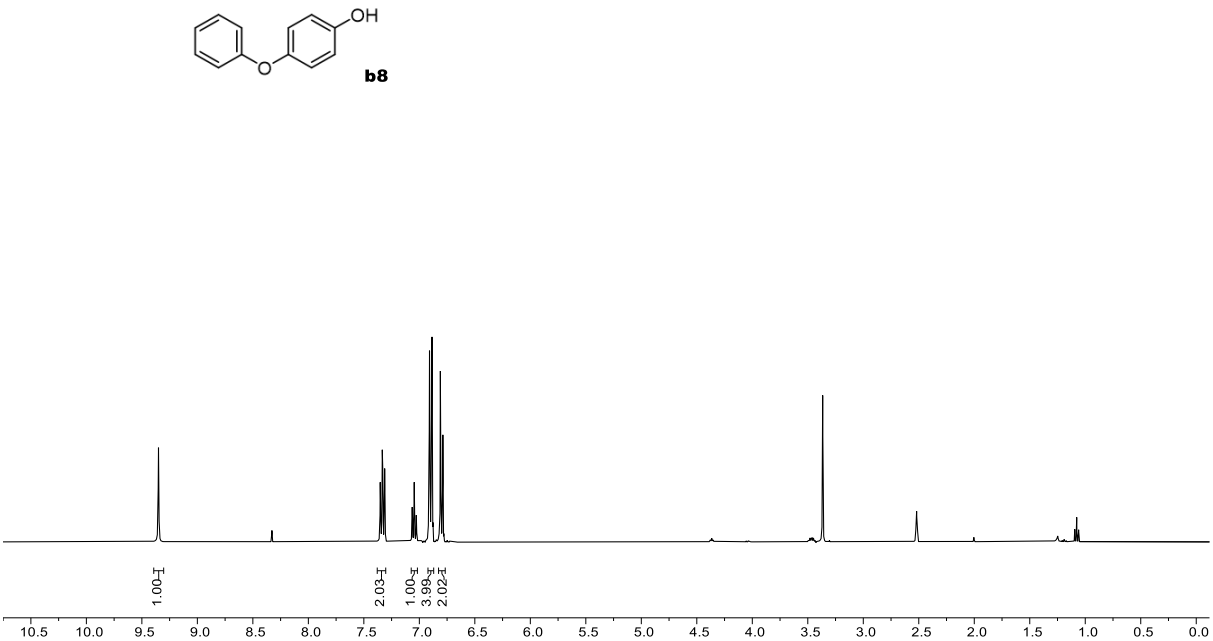
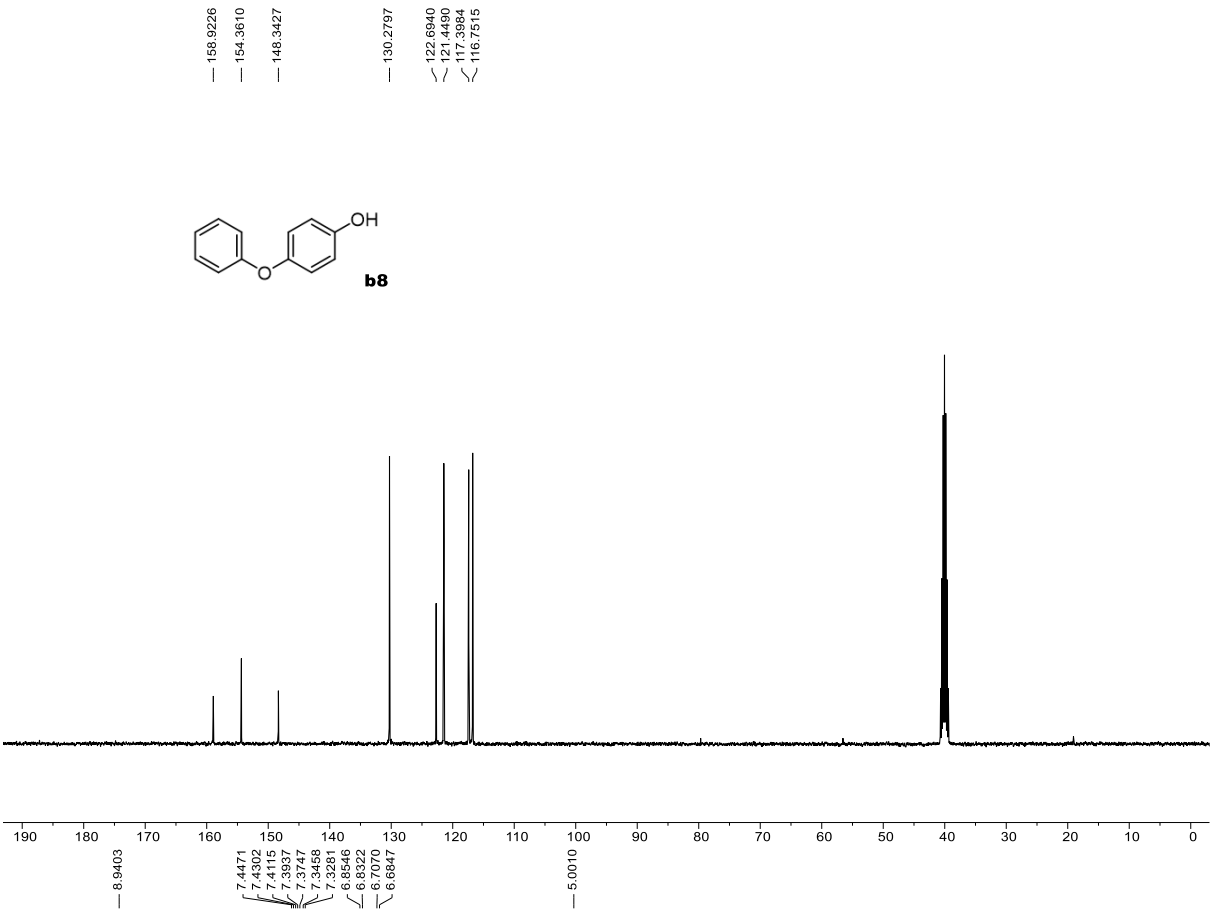
4.0
3.5
3.0
2.5
2.0
1.5

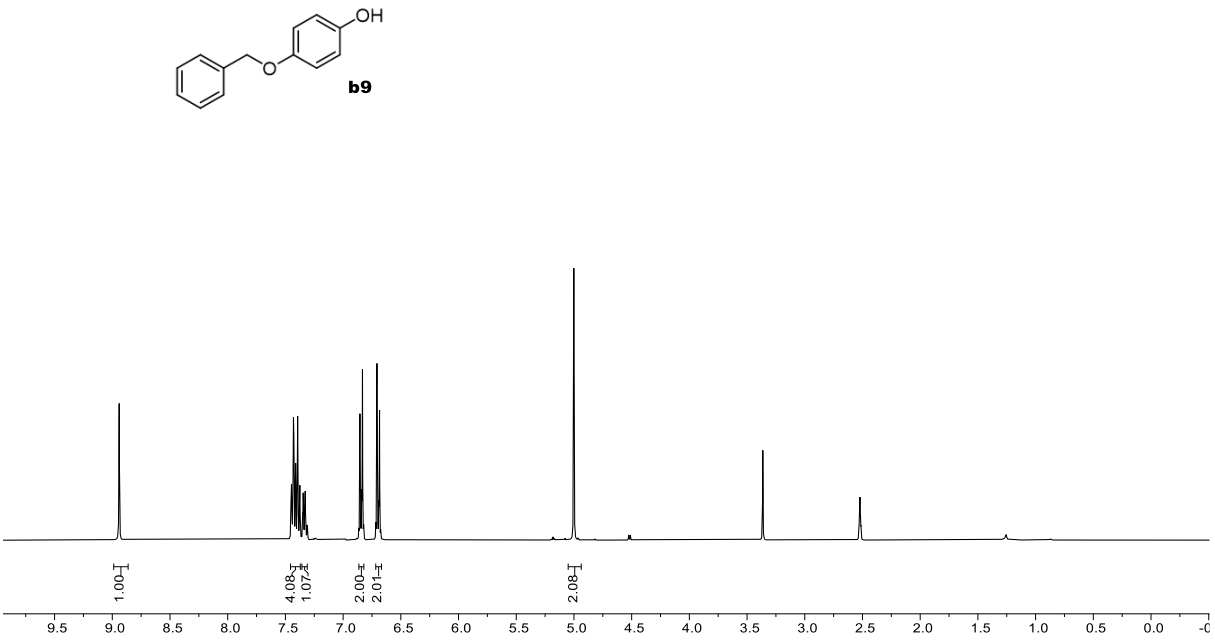

150.1714
116.0956
OH
HO
b6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
9.0910
6.9788
6.9579
6.6814
6.6603
2.4732
2.4543
2.4351
1.5526
1.5339
1.5153
1.4966
1.4784
1.3495
1.3372
1.3312
1.3204
1.3163
1.3126
1.2986
1.2829
1.2801
1.2745
1.2666
1.2545
1.2488
1.2379
1.2307
1.2266
0.8842
0.8671
0.8493

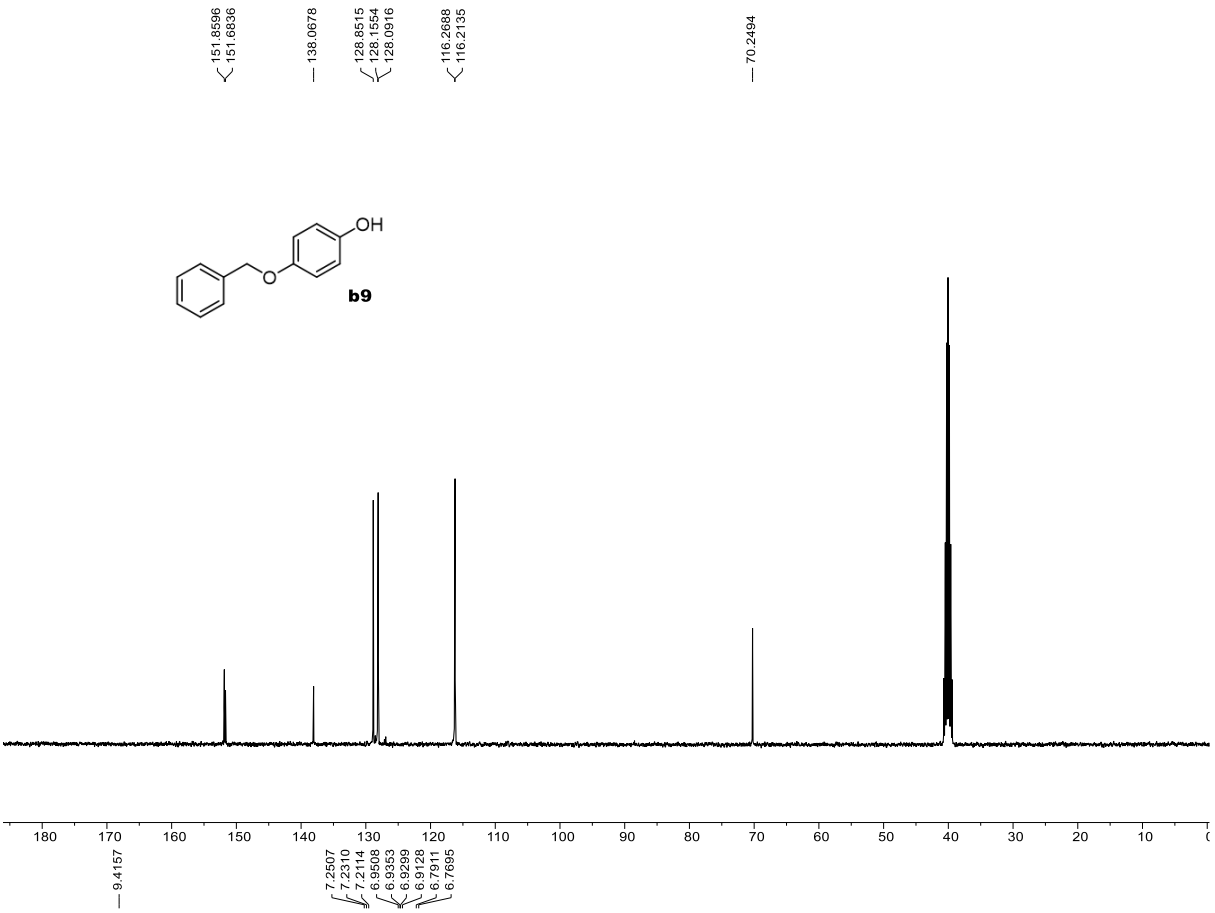

OH
b7
1.00
2.09
2.05
2.04
2.08
3.99
3.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

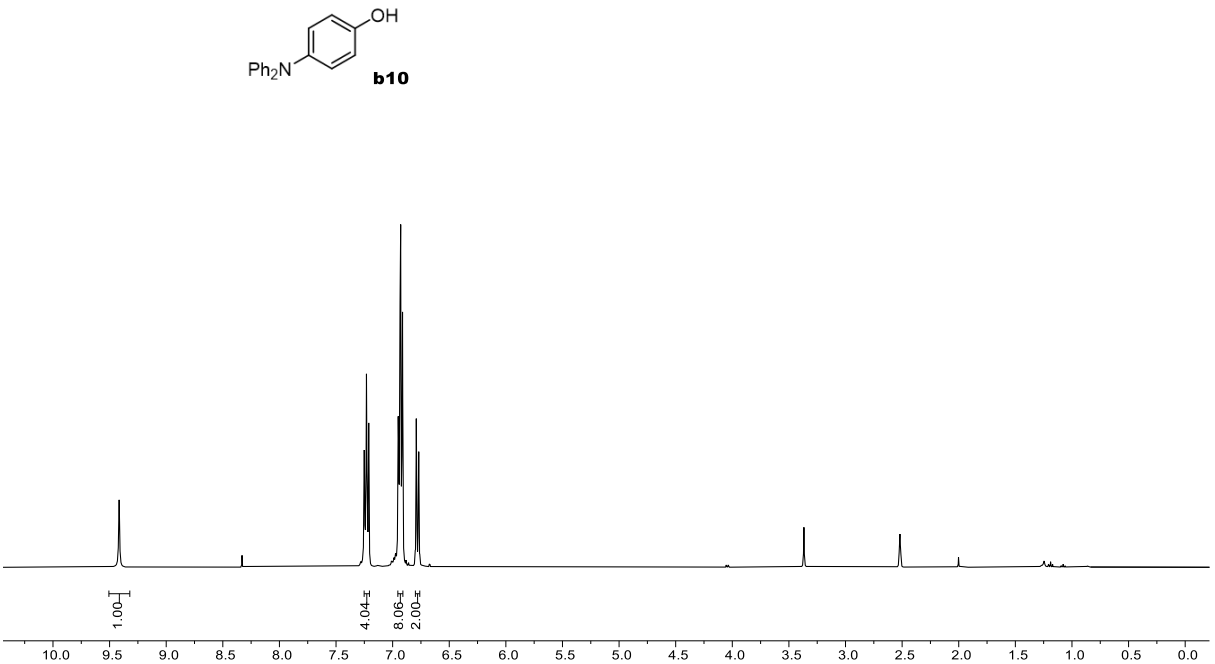

155.7010
132.8517
129.5050
115.4690
34.7950
31.5111
31.3662
22.4783
14.4251
OH
b7
9.3501
7.3522
7.3340
7.3306
7.3124
7.0641
7.0459
7.0273
6.9083
6.8860
6.8105
6.7882

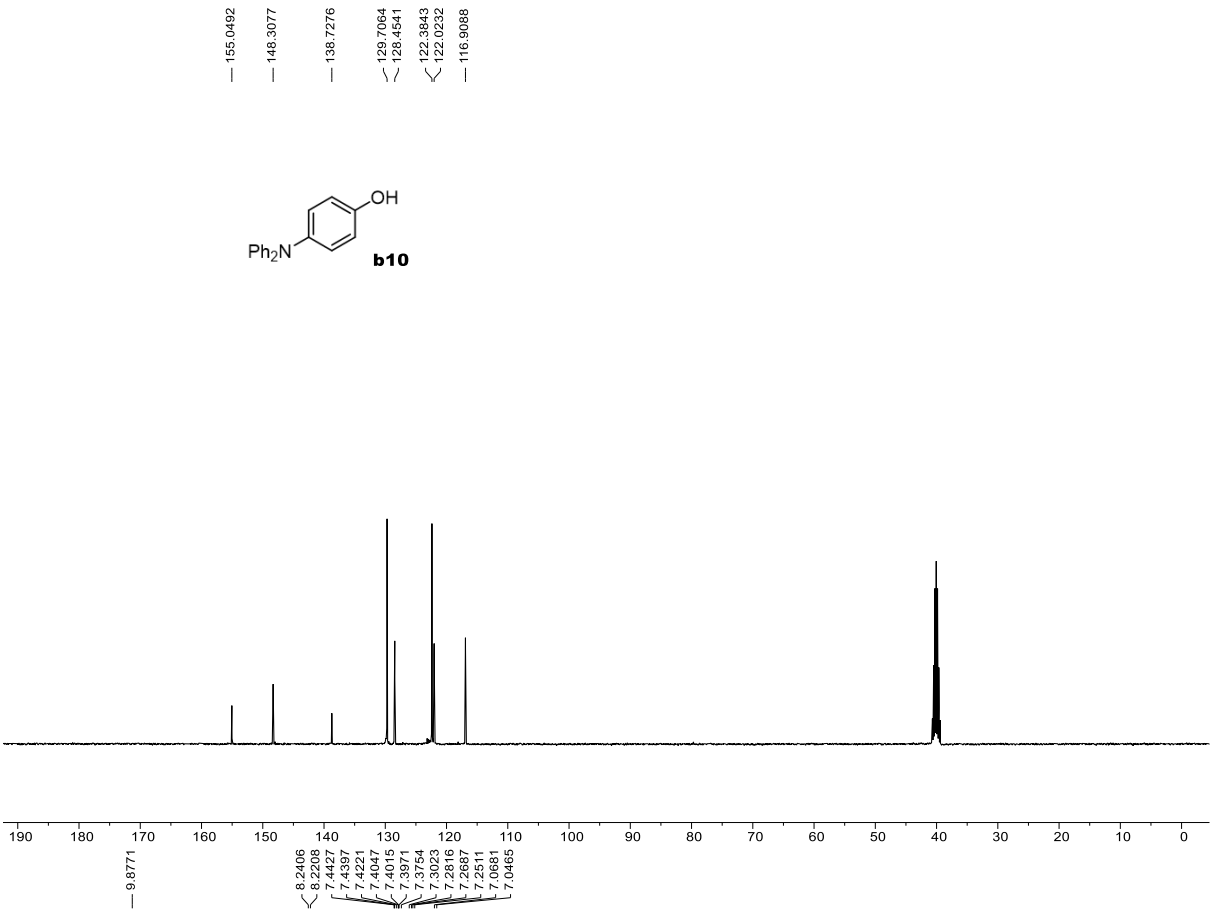

OH
O
b8
1.00
2.03
1.00
3.99
2.02

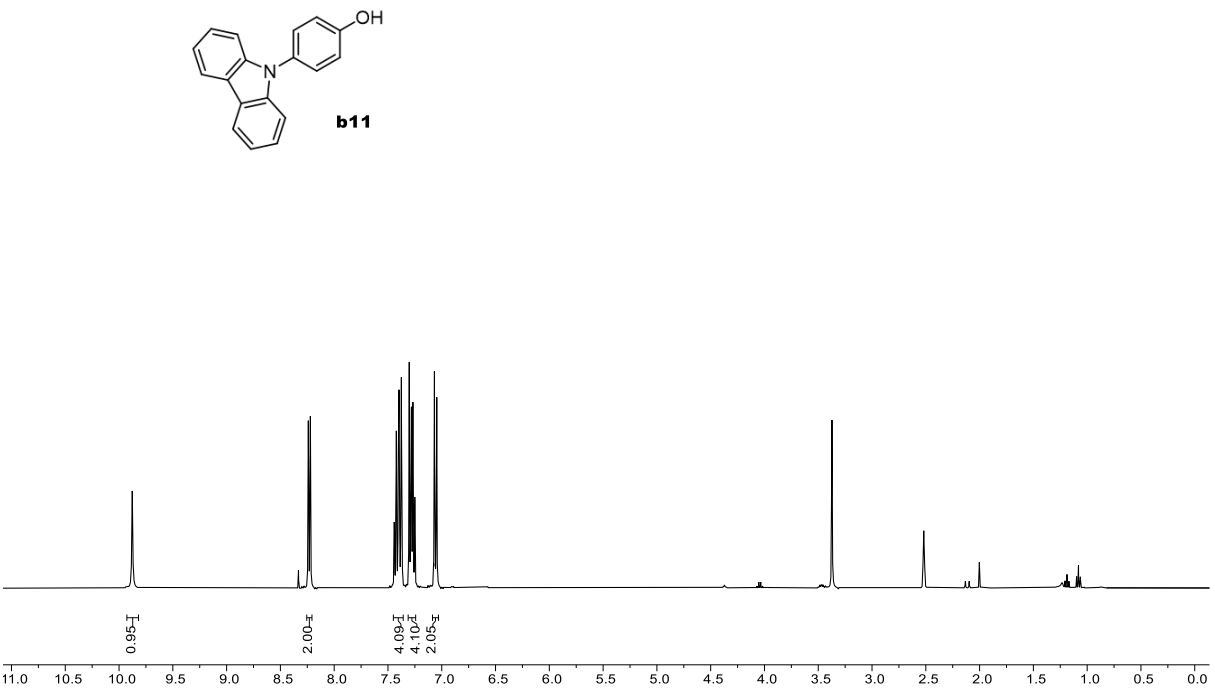

158.9226
154.3610
148.3427
130.2797
122.6940
121.4490
117.3984
116.7515
OH
O
b8
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
8.9403
7.4471
7.4302
7.4115
7.3937
7.3747
7.3458
7.3281
6.8546
6.8322
6.7070
6.6847
5.0010

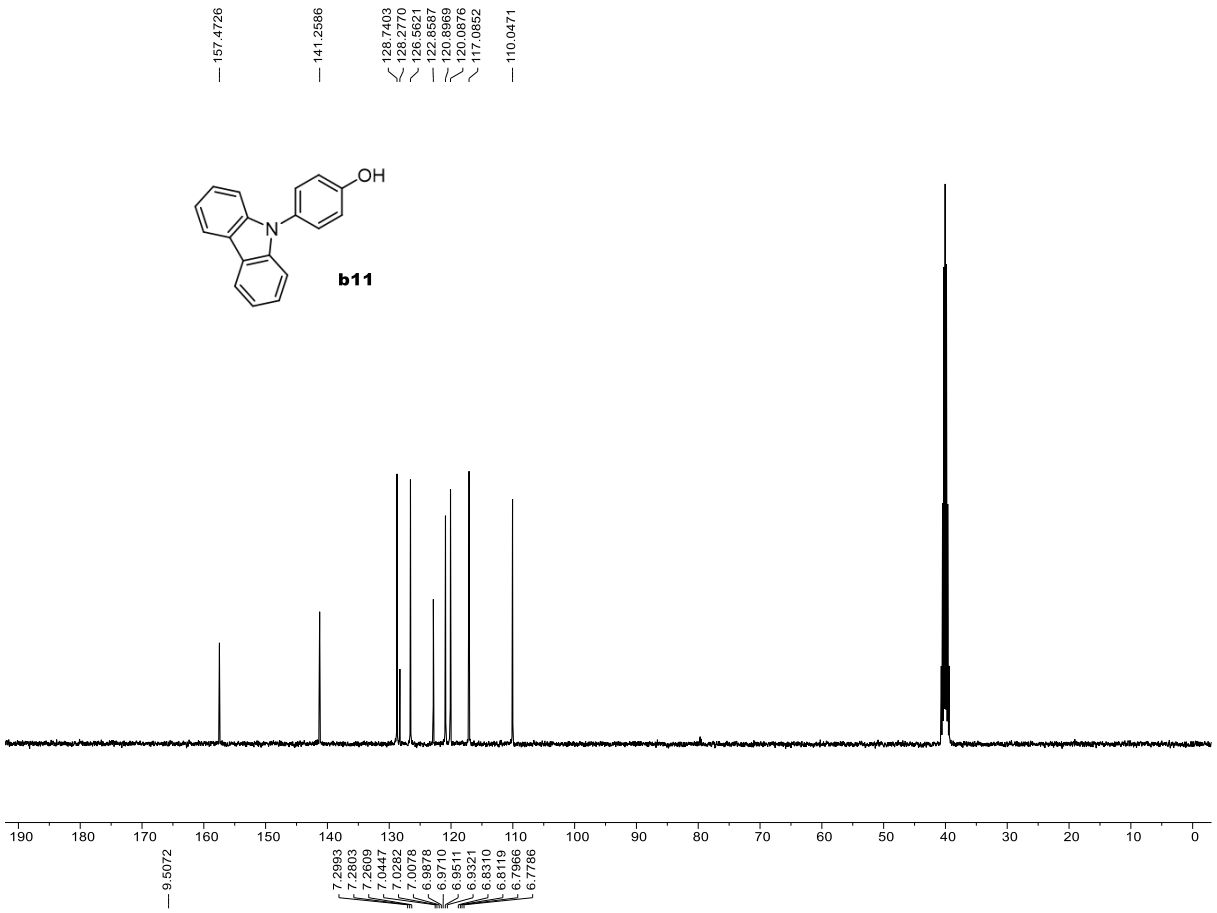

OH
O
b9
1.00
4.08
1.07
2.00
2.01
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


151.8596
151.6836
138.0678
128.8515
128.1554
128.0916
116.2688
116.2135
70.2494
OH
O
b9
9.4157
7.2507
7.2310
7.2114
6.9508
6.9353
6.9299
6.9128
6.7911
6.7695


OH
Ph2N
b10
1.00
4.04
8.06
2.00


155.0492
148.3077
138.7276
129.7064
128.4541
122.3843
122.0232
116.9088
OH
Ph2N
b10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
9.8771
8.2406
8.2208
7.4427
7.4397
7.4221
7.4047
7.4015
7.3971
7.3754
7.3023
7.2816
7.2687
7.2511
7.0681
7.0465


OH
N
b11
0.95
2.00
4.09
4.10
2.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


157.4726
141.2586
128.7403
128.2770
126.5621
122.8587
120.8969
120.0876
117.0852
110.0471
OH
N
b11
9.5072
7.2993
7.2803
7.2609
7.0447
7.0282
7.0078
6.9878
6.9710
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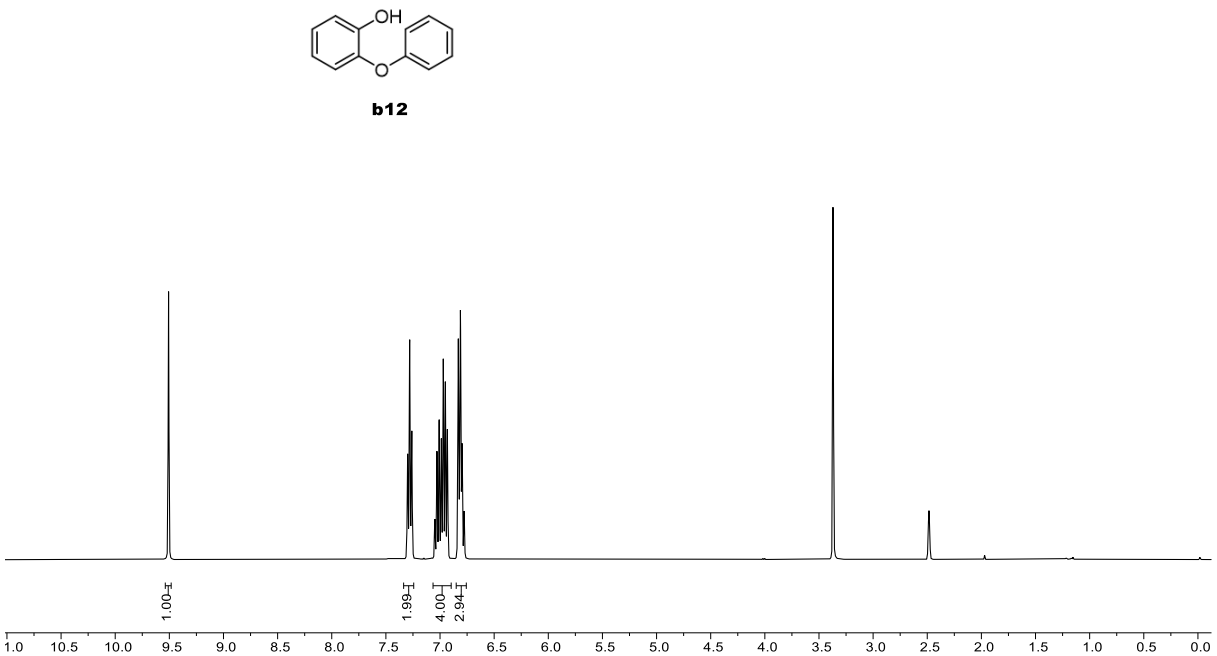
6.9321
6.8310
6.8119
6.7966
6.7786


OH
O
b12
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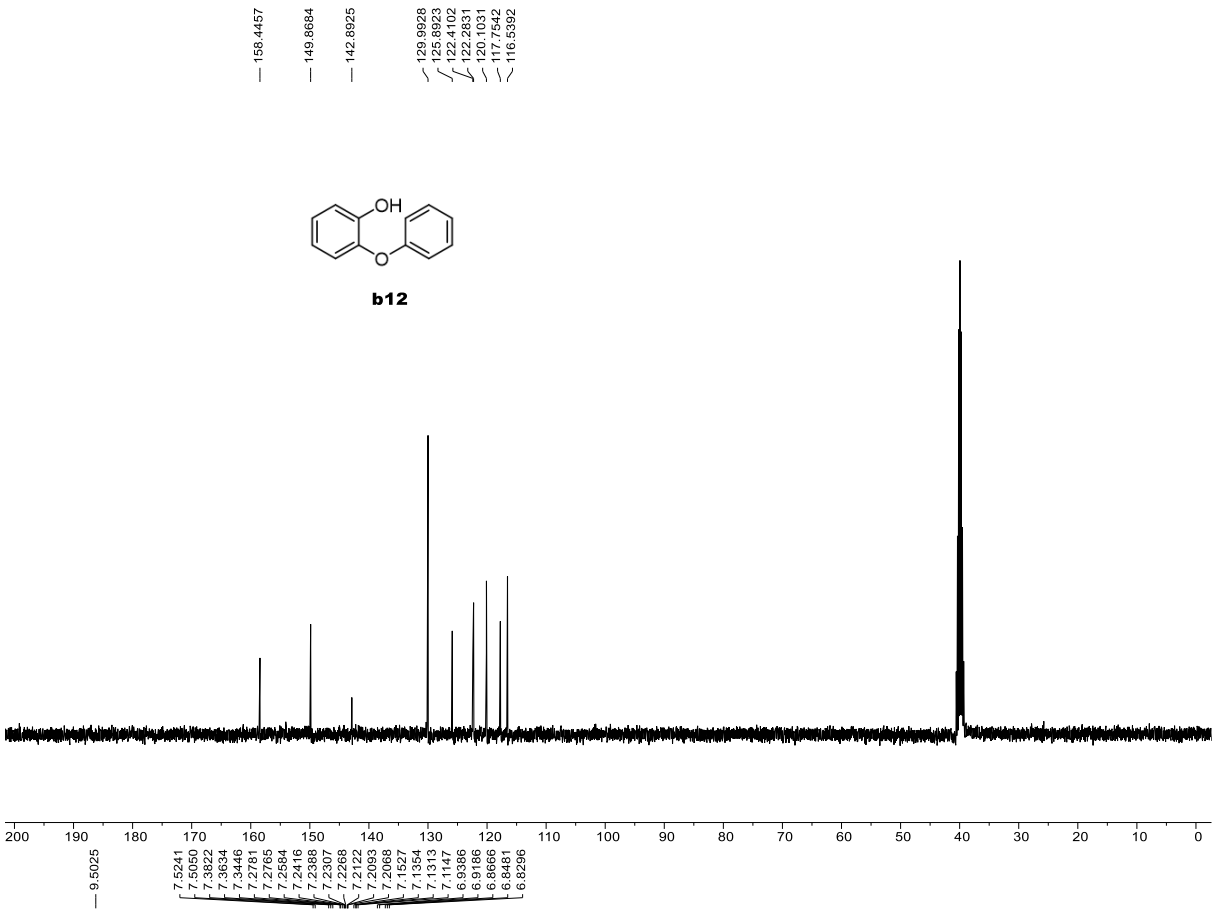
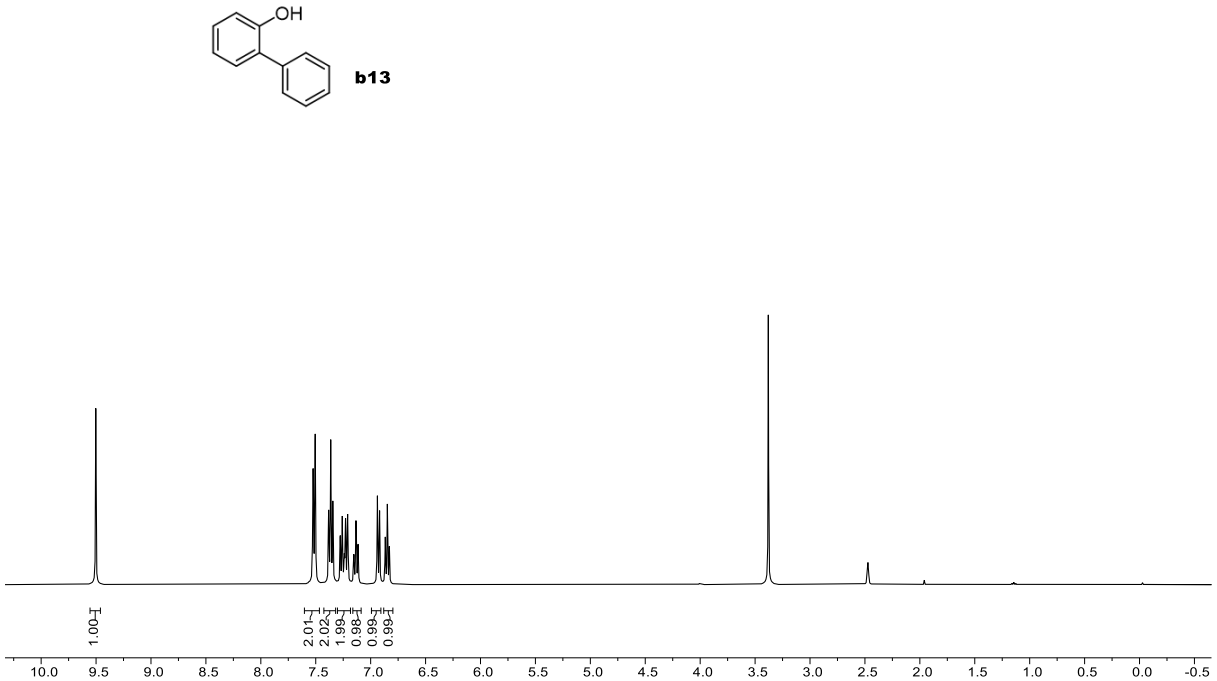
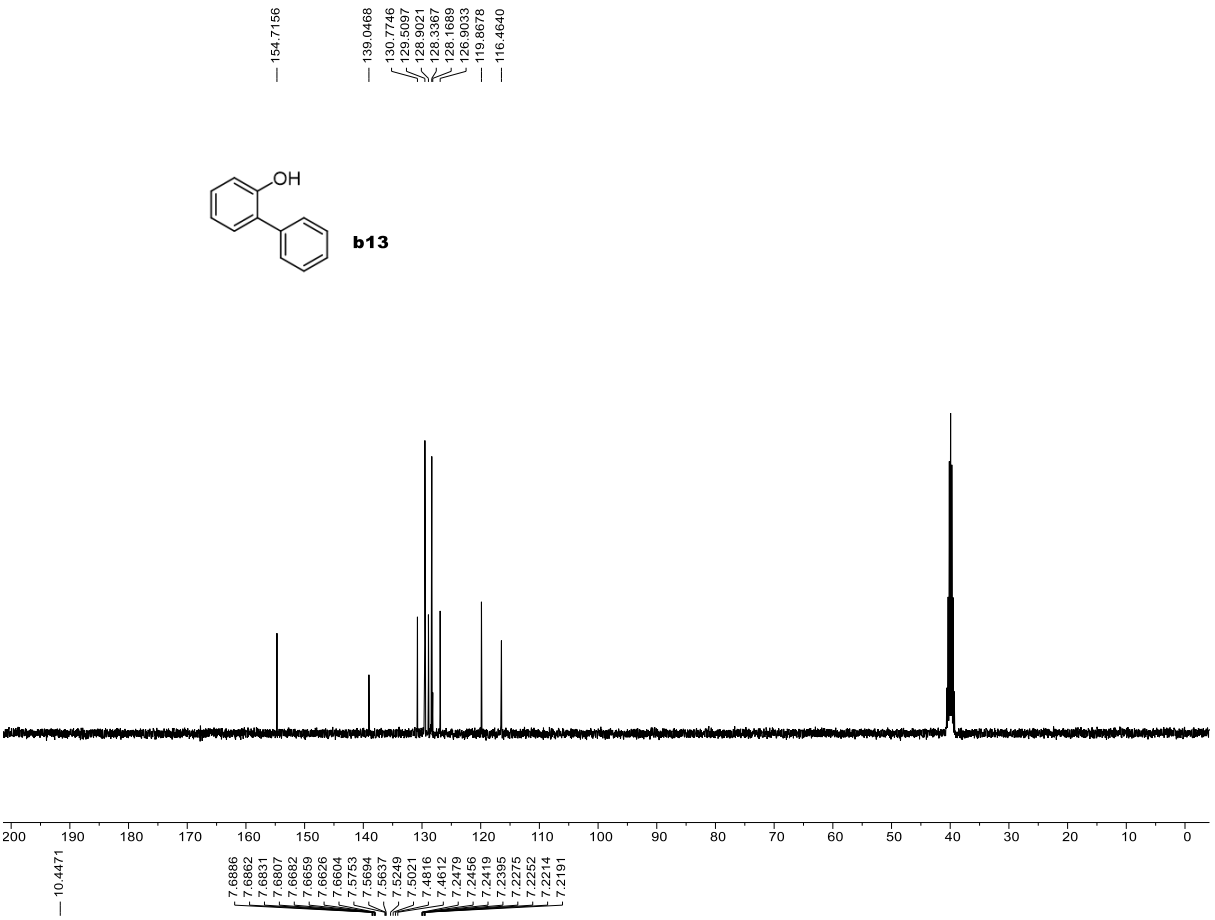
1.99
4.00
2.94


158.4457
149.8684
142.8925
129.9928
125.8923
122.4102
122.2831
120.1031
117.7542
116.5392
OH
O
b12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
9.5025
7.5241
7.5050
7.3822
7.3634
7.3446
7.2781
7.2765
7.2584
7.2416
7.2388
7.2307
7.2268
7.2122
7.2093
7.2068
7.1527
7.1354
7.1313
7.1147
6.9386
6.9186
6.8666
6.8481
6.8296


OH
b13
1.00
2.01
2.02
1.99
0.98
0.99
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


154.7156
139.0468
130.7746
129.5097
128.9021
128.3367
128.1689
126.9033
119.8678
116.4640
OH
b13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
10.4471
7.6886
7.6862
7.6831
7.6807
7.6682
7.6659
7.6626
7.6604
7.5753
7.5694
7.5637
7.5249
7.5021
7.4816
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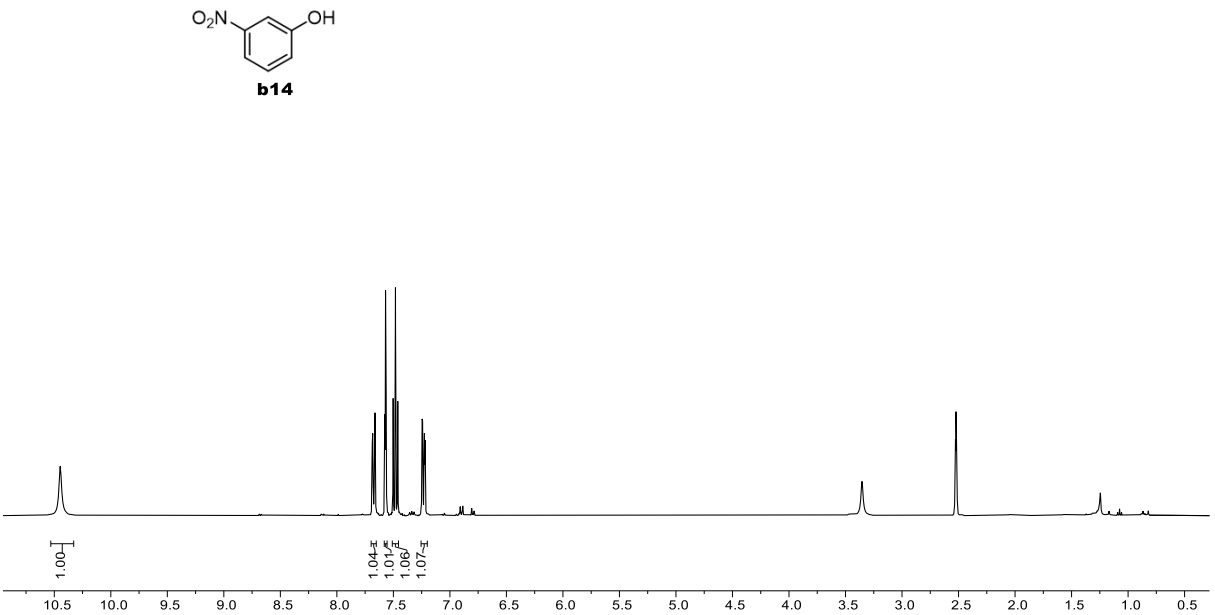
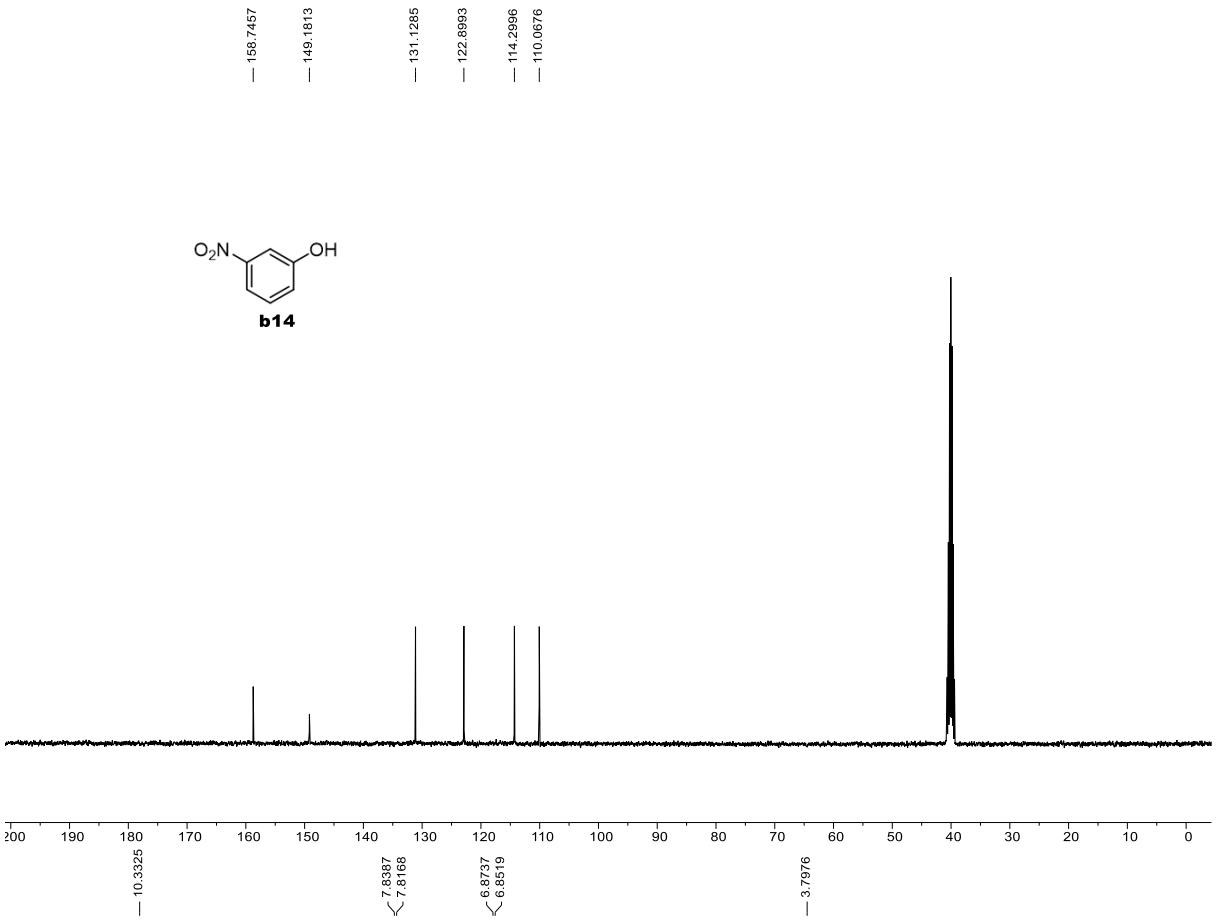
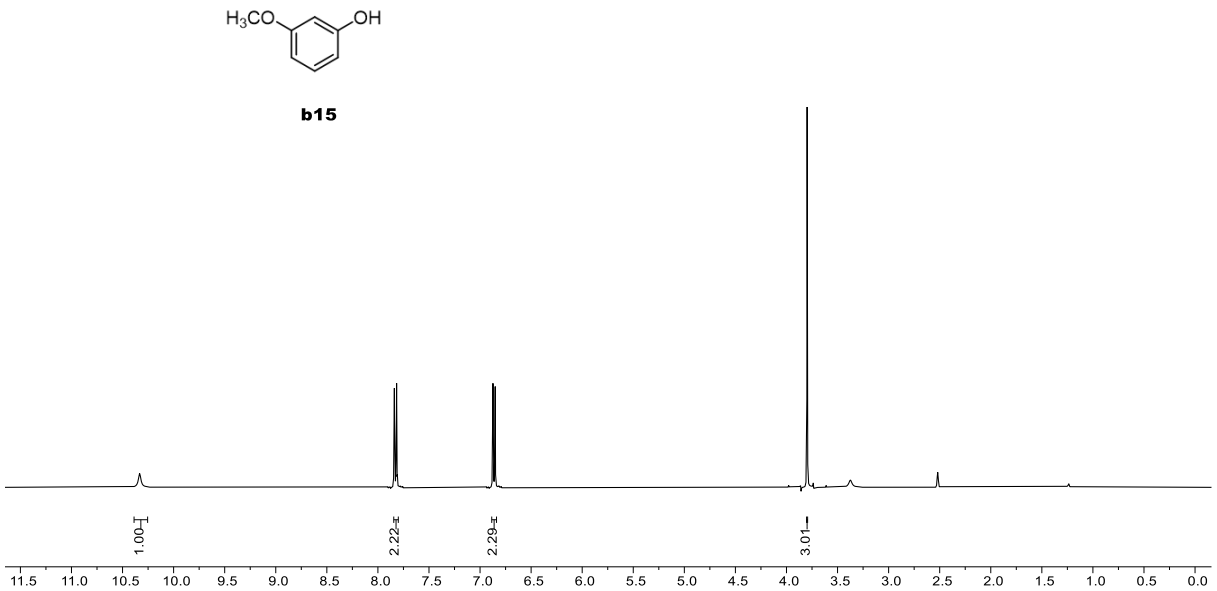
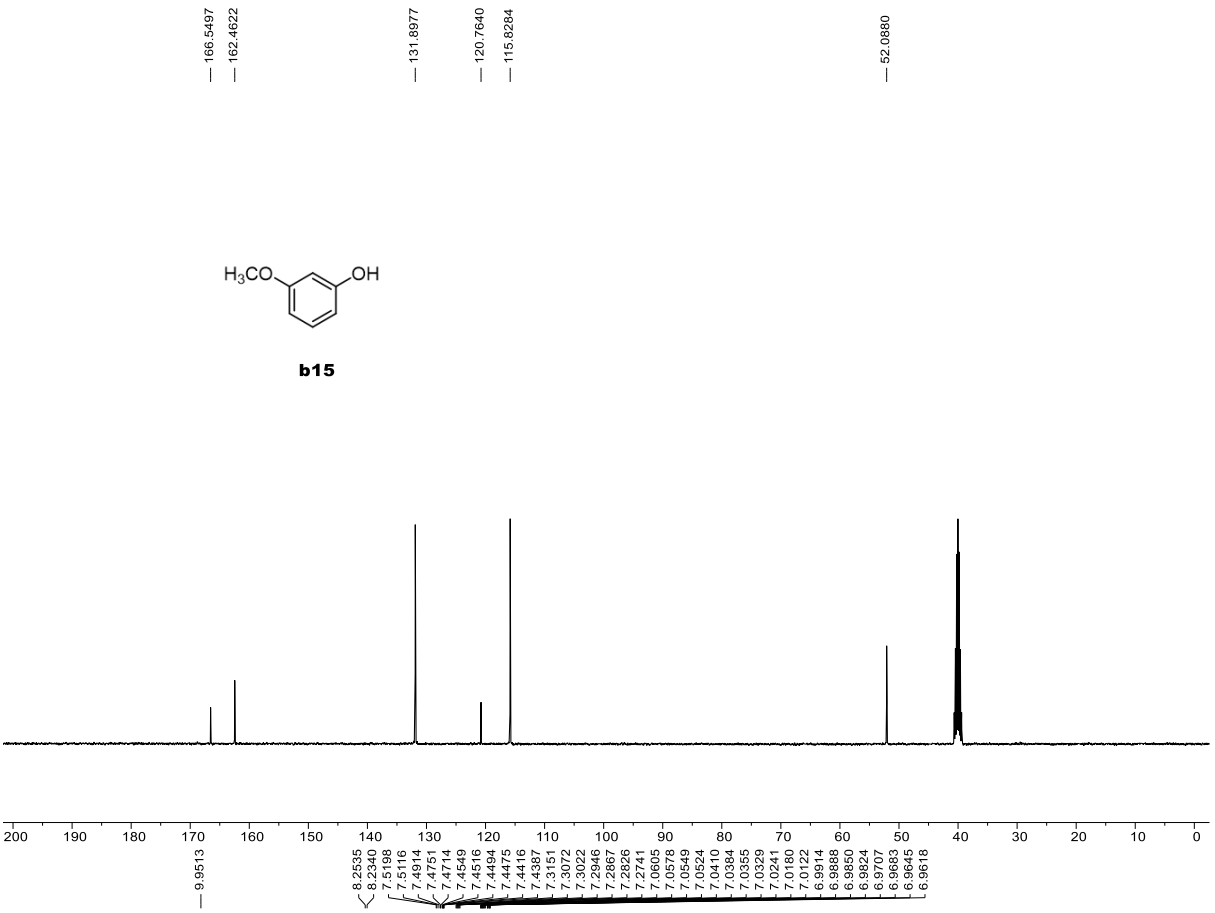
7.2479
7.2456
7.2419
7.2395
7.2275
7.2252
7.2214
7.2191


O2N
OH
b14
1.00
1.04
1.01
1.06
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5


158.7457
149.1813
131.1285
122.8993
114.2996
110.0676
O2N
OH
b14
10.3325
7.8387
7.8168
6.8737
6.8519
3.7976


H3CO
OH
b15
1.00
2.22
2.29
3.01


166.5497
162.4622
131.8977
120.7640
115.8284
52.0880
H3CO
OH
b15
9.9513
8.2535
8.2340
7.5198
7.5116
7.4914
7.4751
7.4714
7.4549
7.4516
7.4494
7.4475
7.4416
7.4387
7.3151
7.3072
7.3022
7.2946
7.2867
7.2826
7.2741
7.0605
7.0578
7.0549
7.0524
7.0410
7.0384
7.0355
7.0329
7.0241
7.0180
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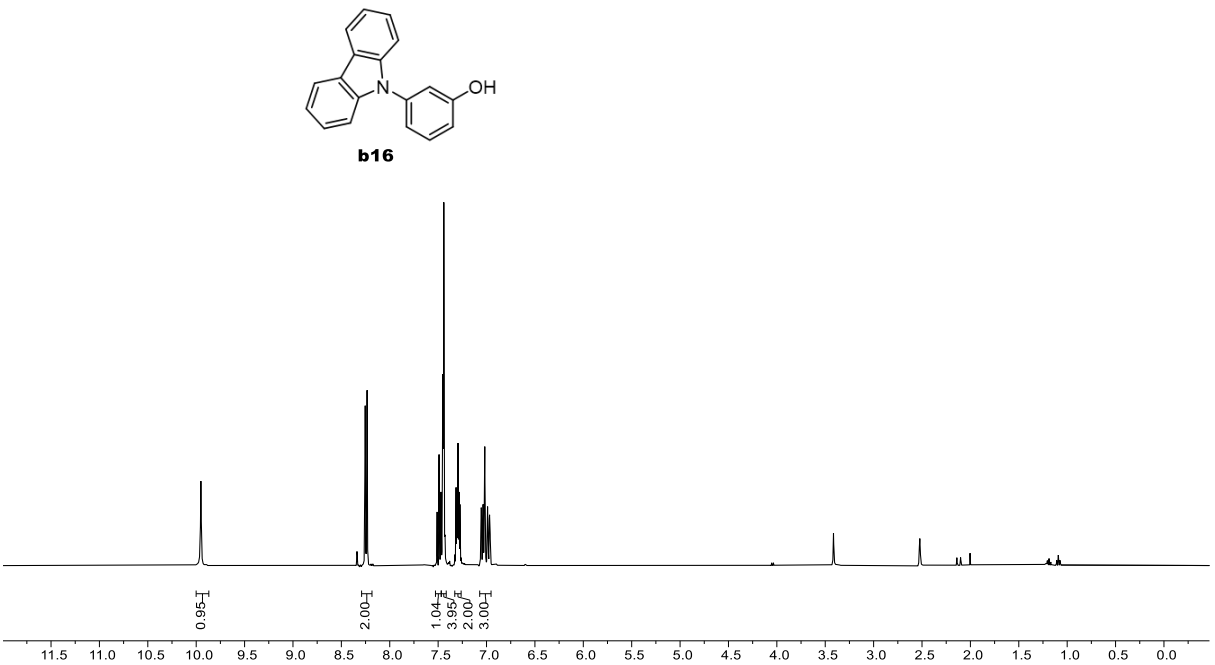
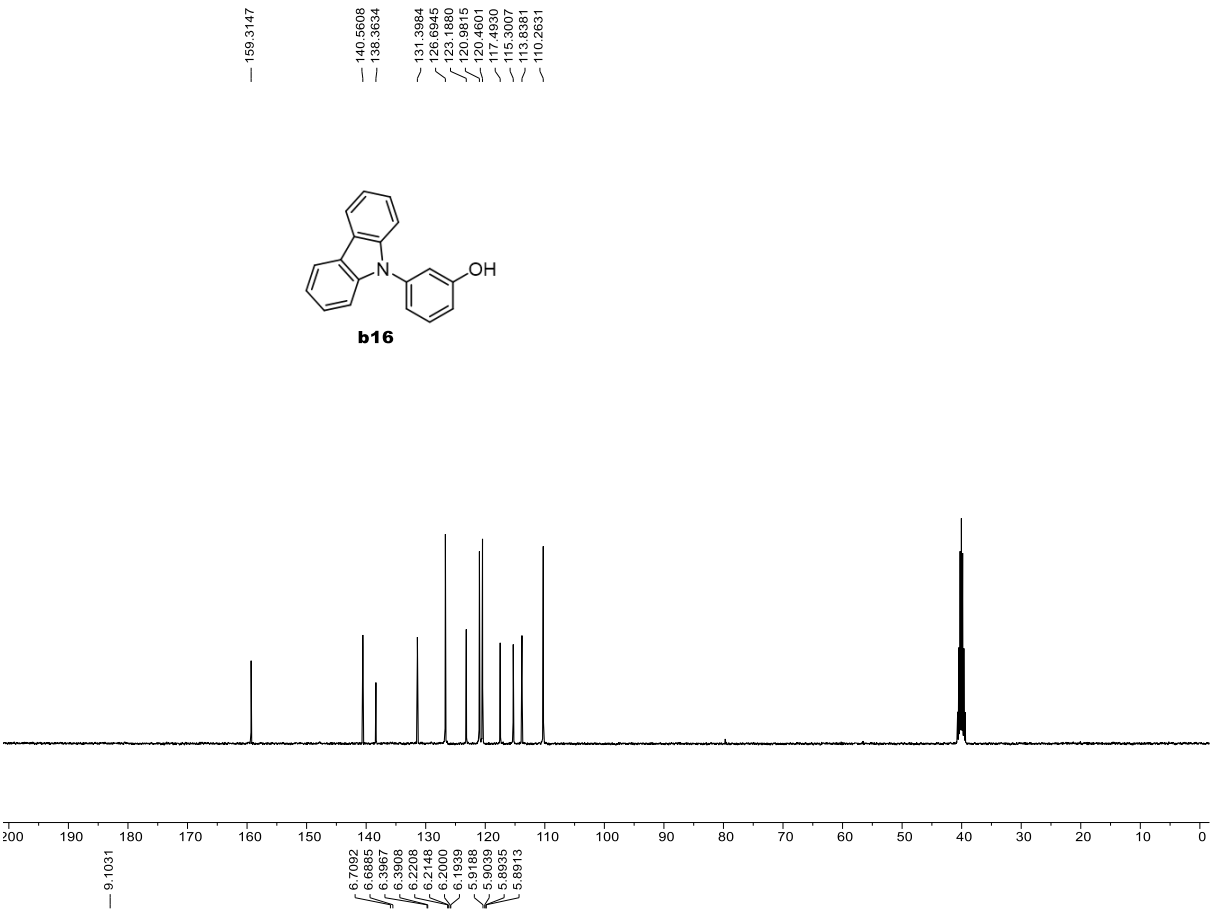
6.9914
6.9888
6.9850
6.9824
6.9707
6.9683
6.9645
6.9618


N
OH
b16
0.95
2.00
1.04
3.95
2.00
3.00


159.3147
140.5608
138.3634
131.3984
126.6945
123.1880
120.9815
120.4601
117.4930
115.3007
113.8381
110.2631
OH
b16
9.1031
6.7092
6.6885
6.3967
6.3908
6.2208
6.2148
6.2000
6.1939
5.9188
5.9039
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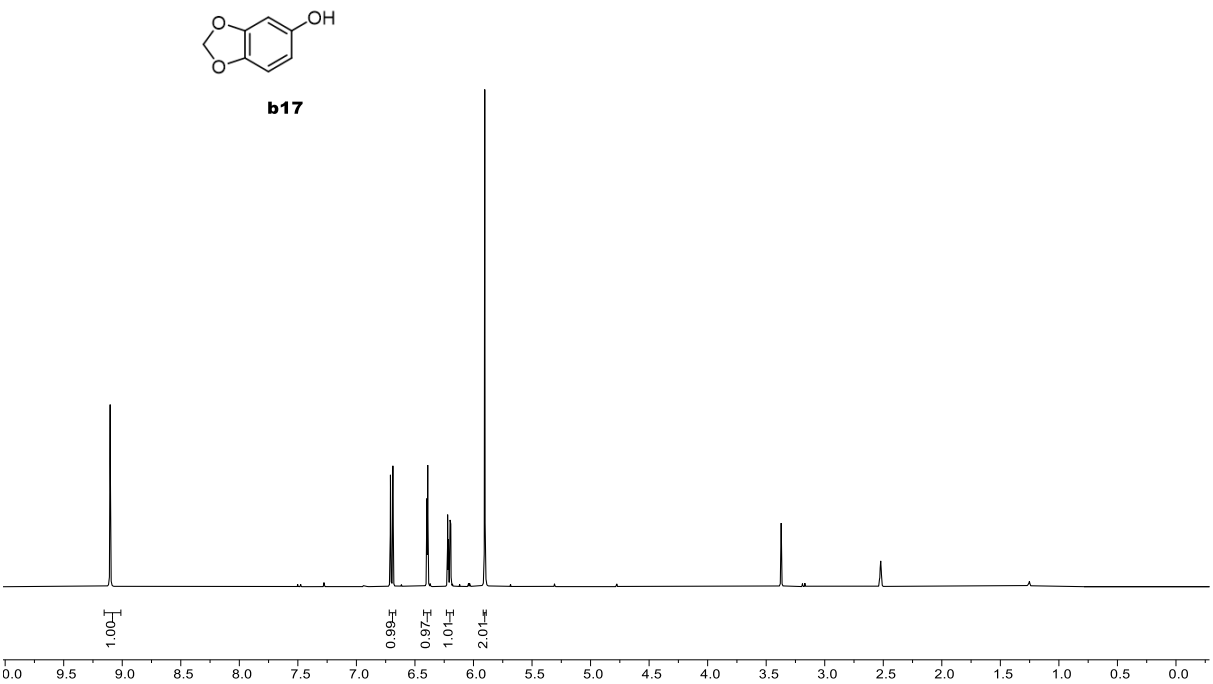
5.8913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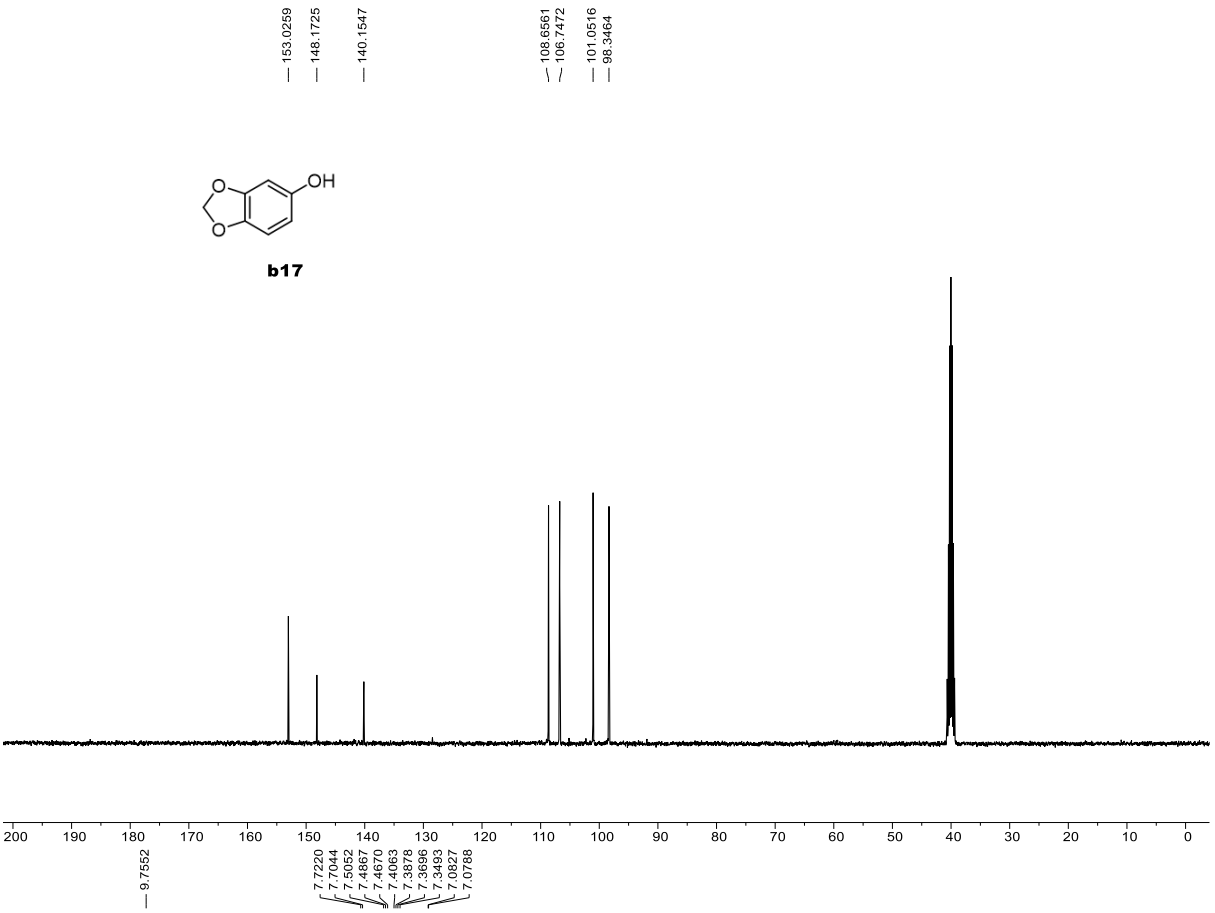
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O
O
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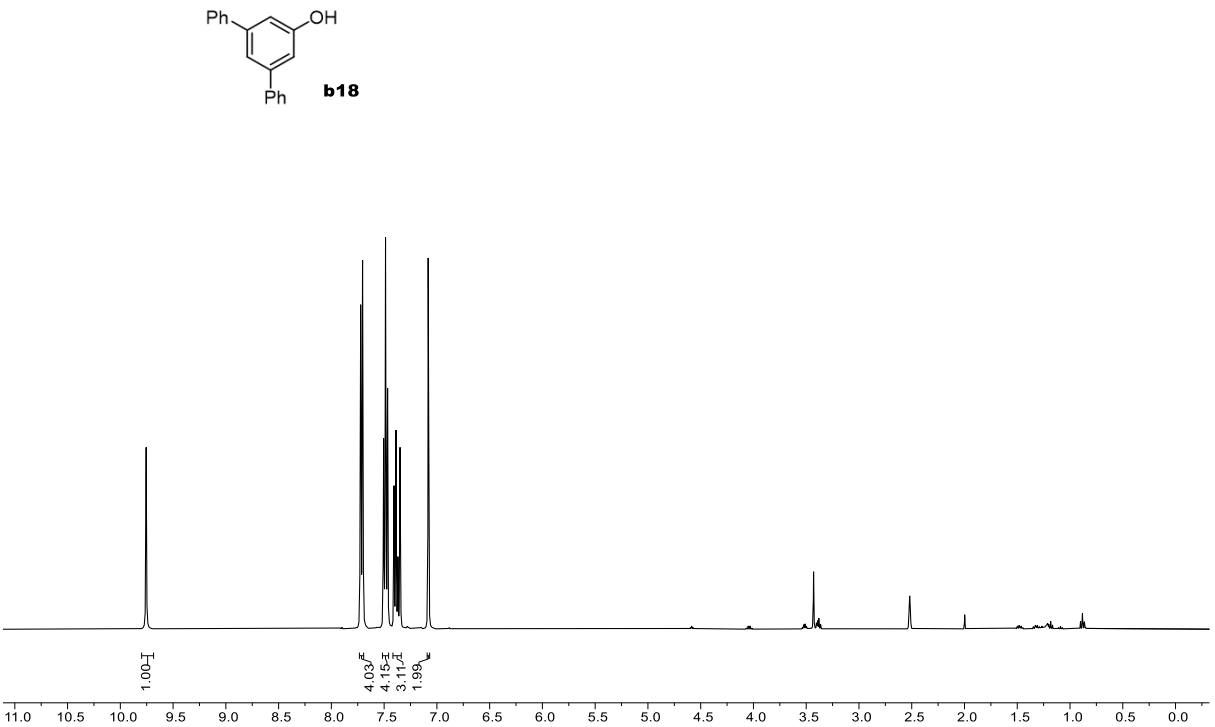
7.3493
7.0827
7.0788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1.99
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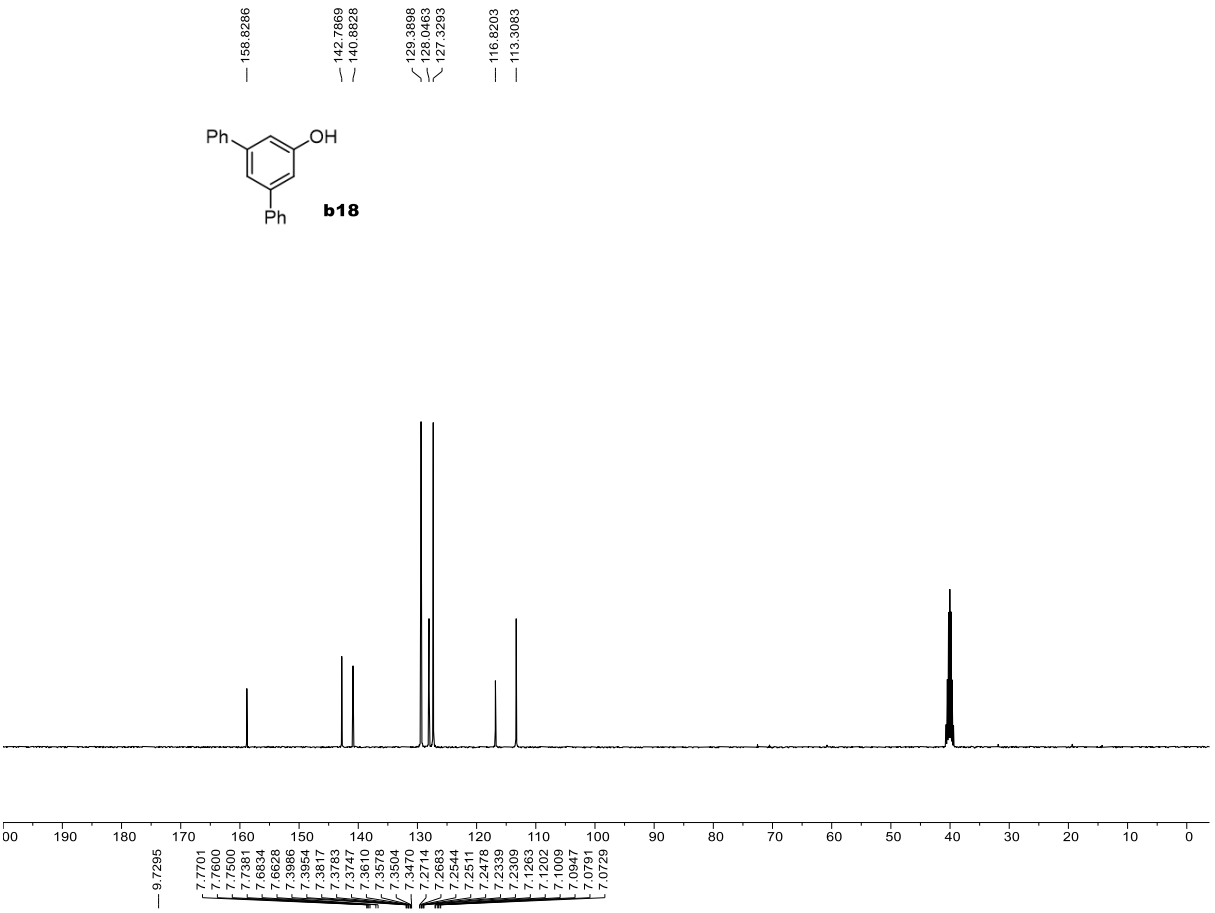
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Ph
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7.7500
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7.3954
7.3817
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7.2683
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1.05
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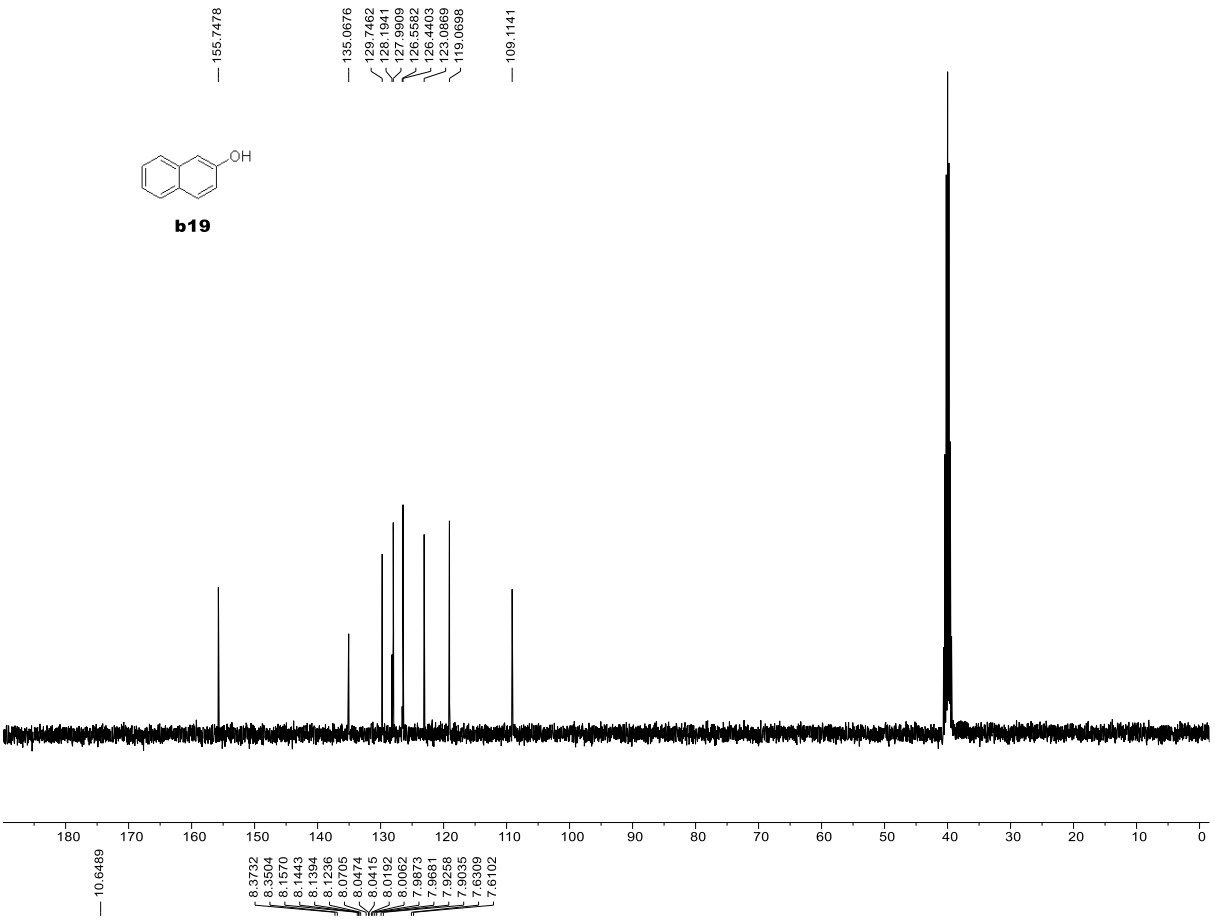
0.99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8.3732
8.3504
8.1570
8.1443
8.1394
8.1236
8.0705
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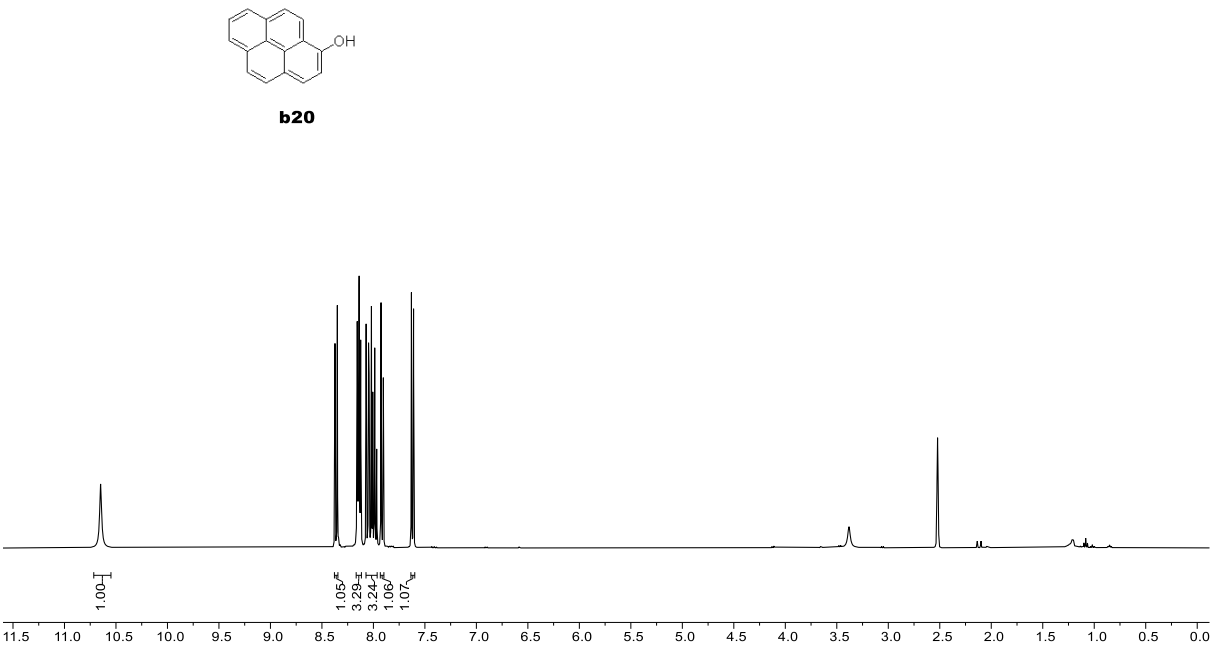
7.9681
7.9258
7.9035
7.6309
7.6102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126.6947
126.6164
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124.4034
124.2971
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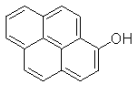
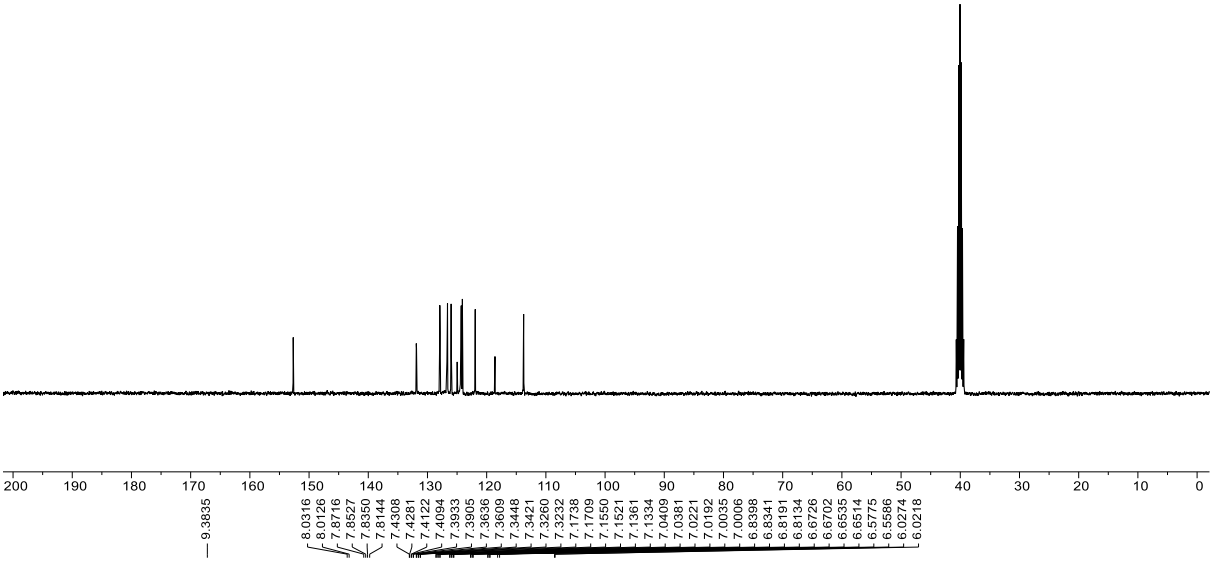
113.7556


OH

b20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7.3933
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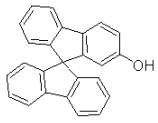
7.3636
7.3609
7.3448
7.3421
7.3260
7.3232
7.1738
7.1709
7.1550
7.1521
7.1361
7.1334
7.0409
7.0381
7.0221
7.0192
7.0035
7.0006
6.8398
6.8341
6.8191
6.8134
6.6726
6.6702
6.6535
6.6514
6.5775
6.5586
6.0274
6.0218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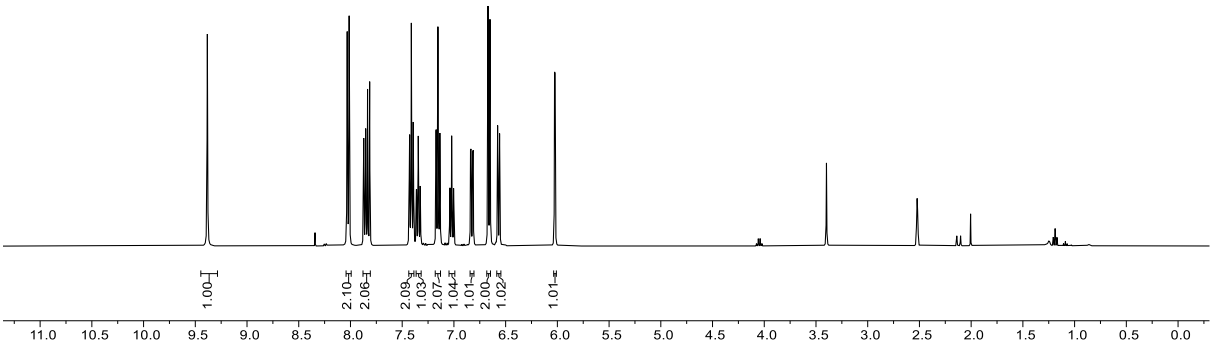
b21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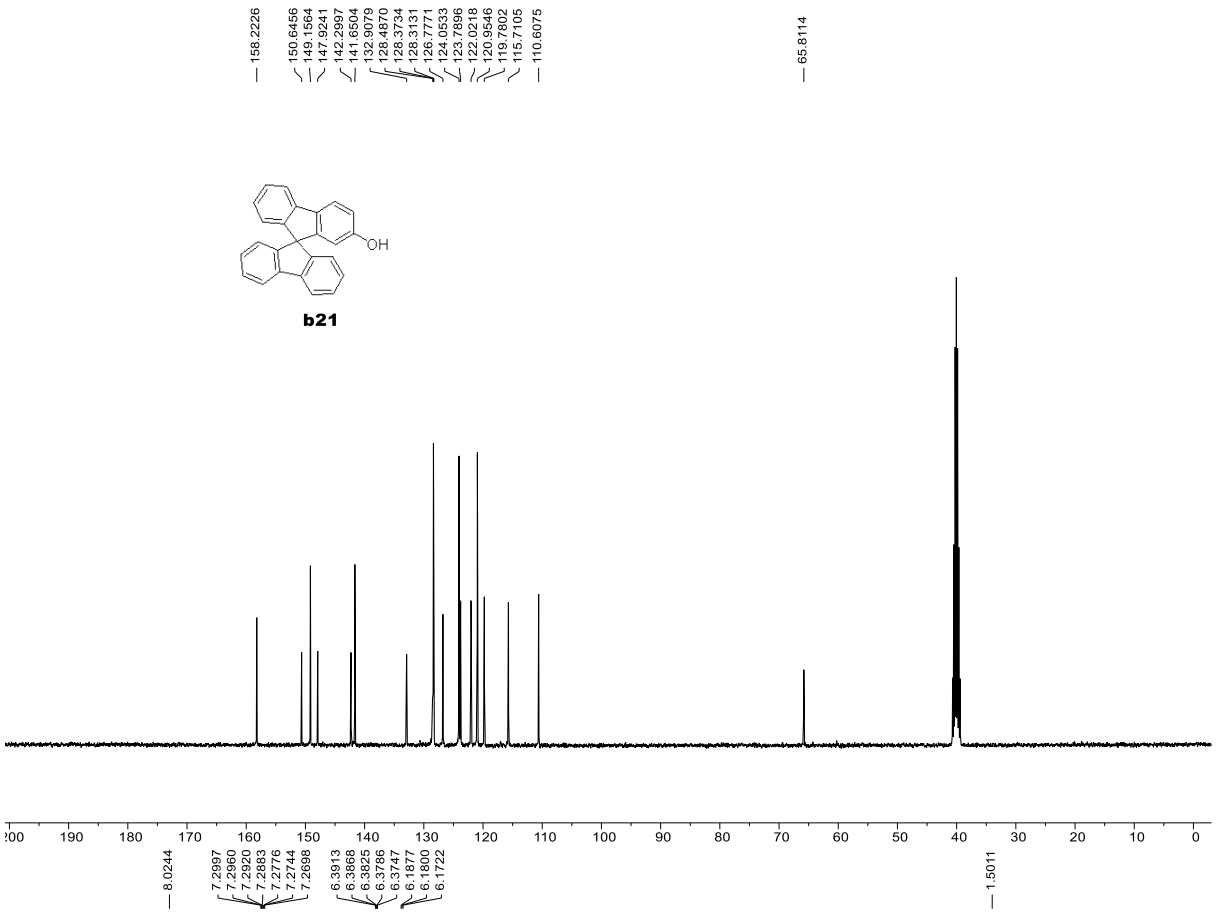
2.07
1.04
1.01
2.00
1.02
1.01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122.0218
120.9546
119.7802
115.7105
110.6075
65.8114
OH
b21
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7.2960
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7.2776
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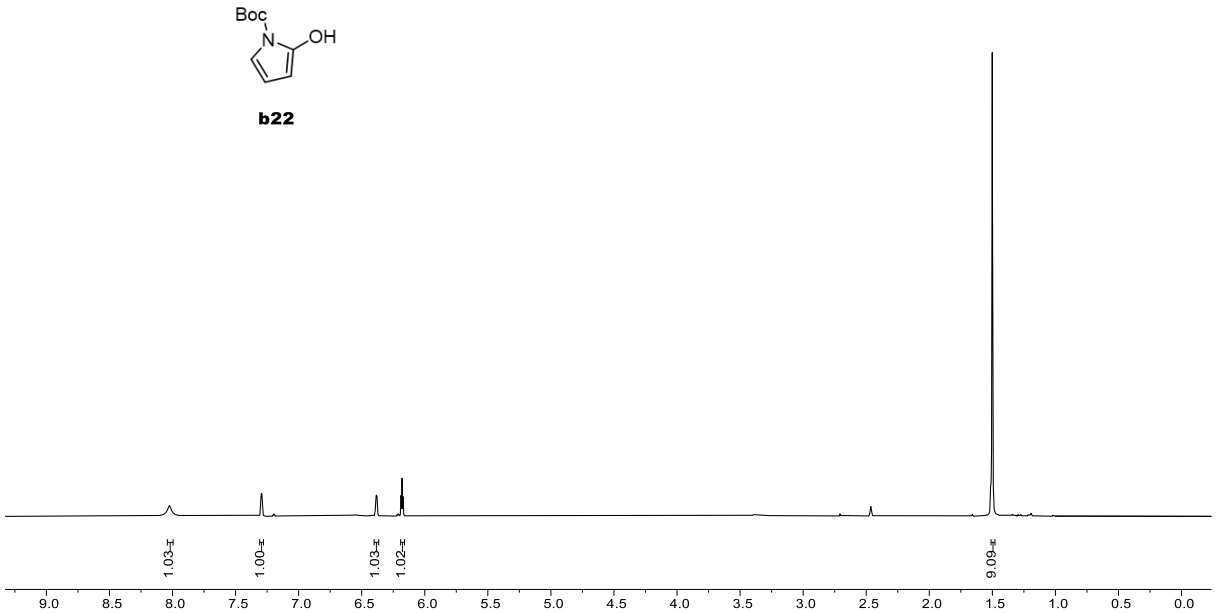
1.5011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b22
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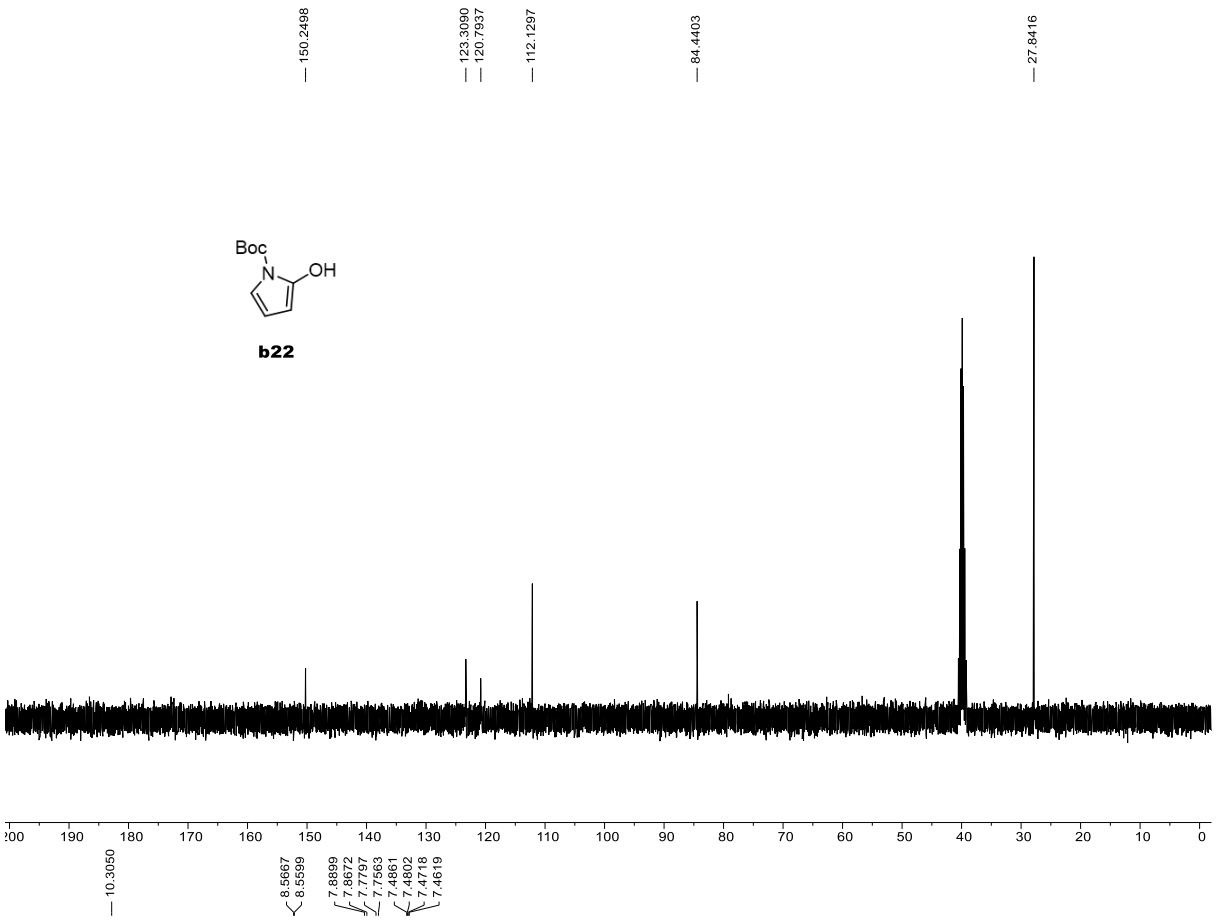
1.03
1.02
9.09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84.4403
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Boc
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OH
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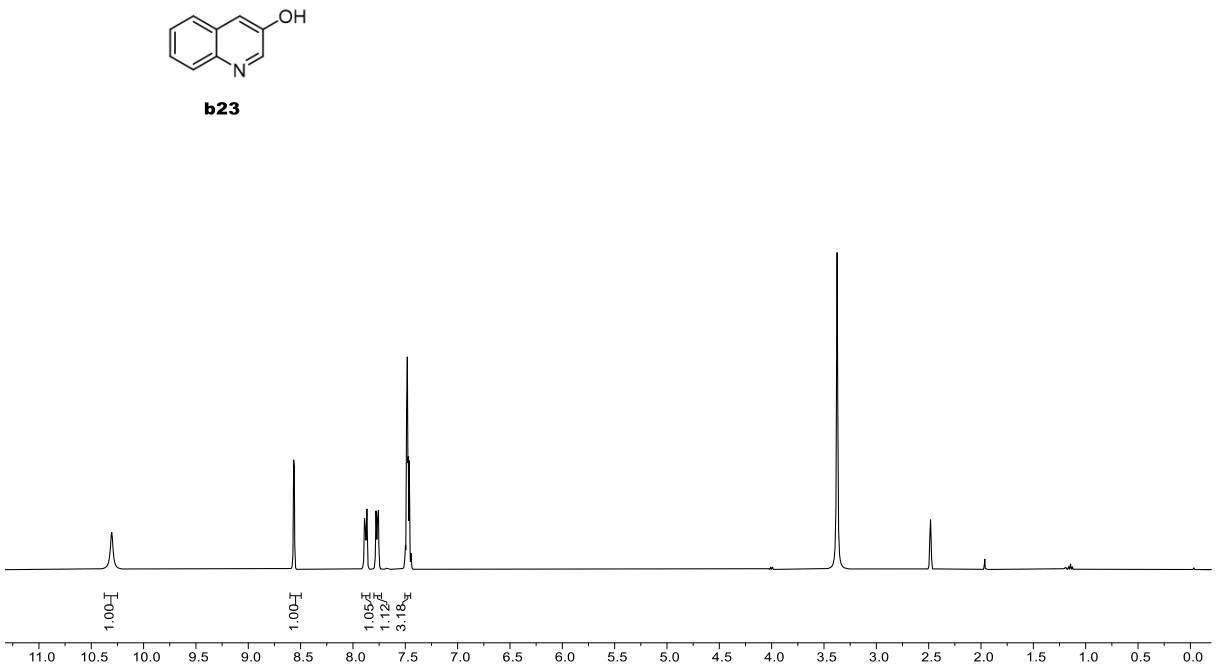
7.8672
7.7797
7.7563
7.4861
7.4802
7.4718
7.4619

b22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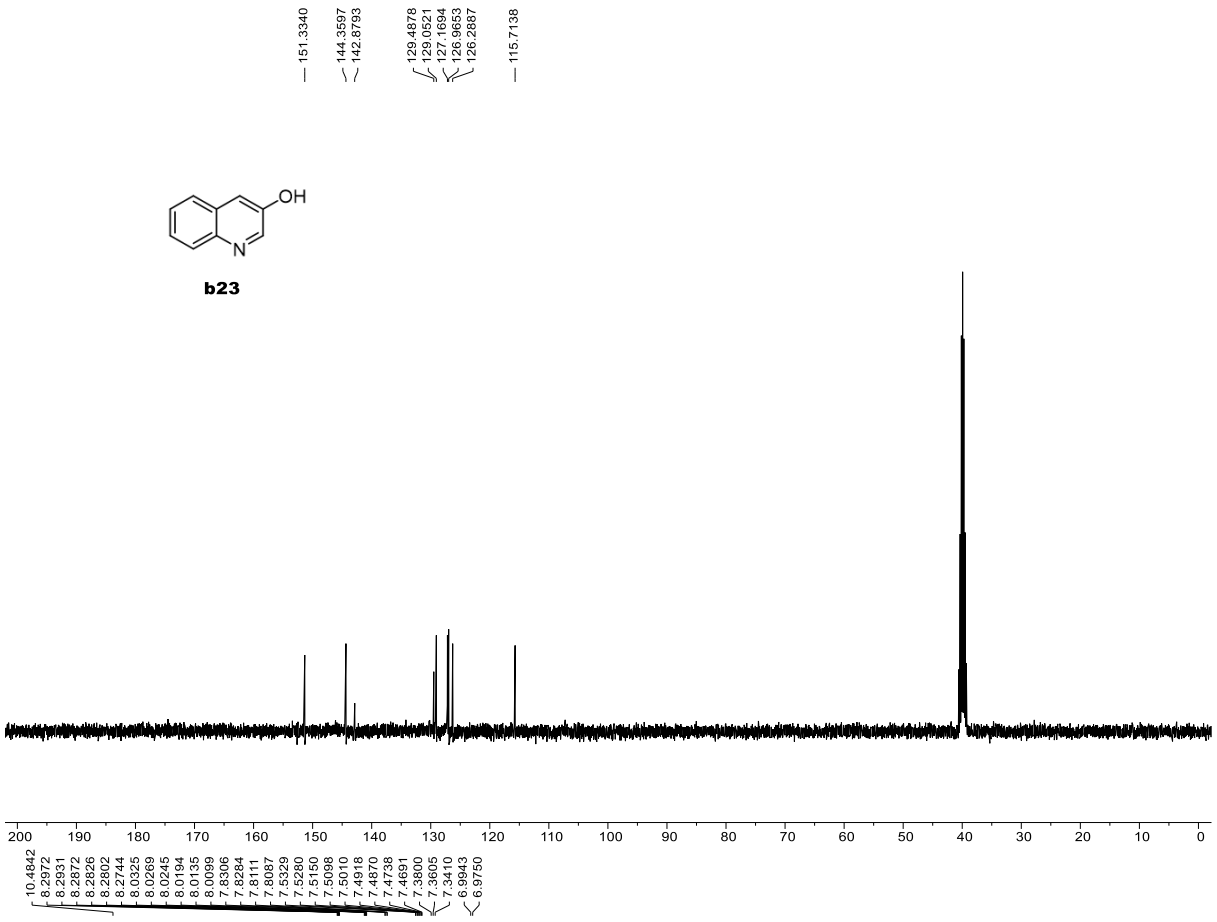
3.18

b23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126.9653
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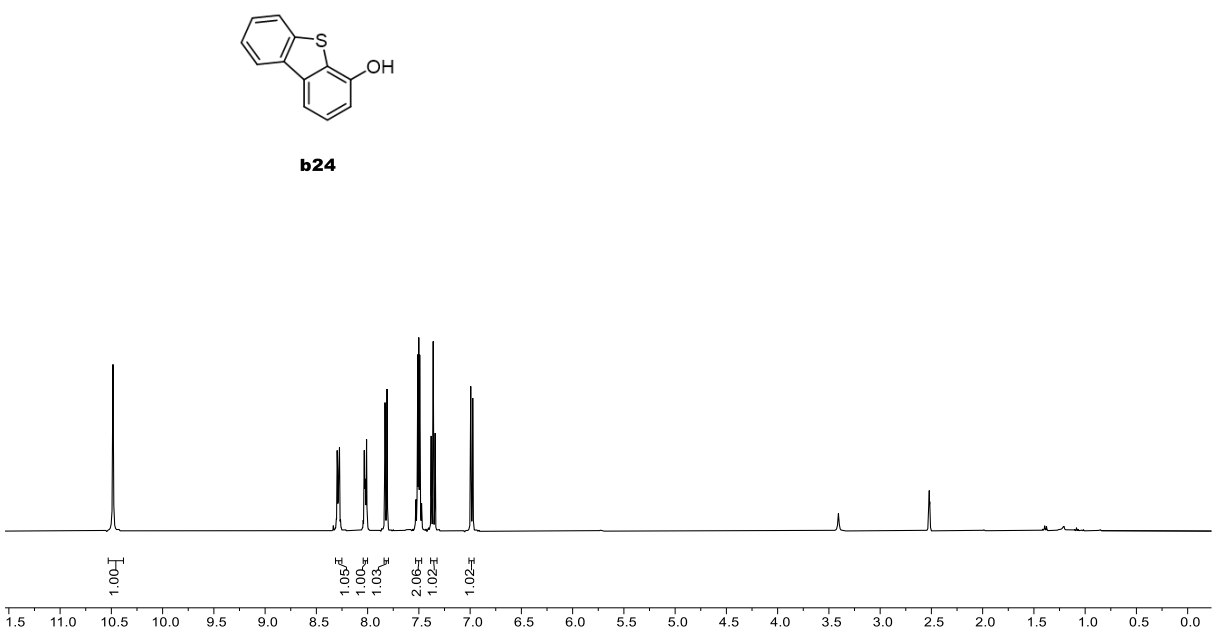
b23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8.0245
8.0194
8.0135
8.0099
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7.8284
7.8111
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7.5098
7.5010
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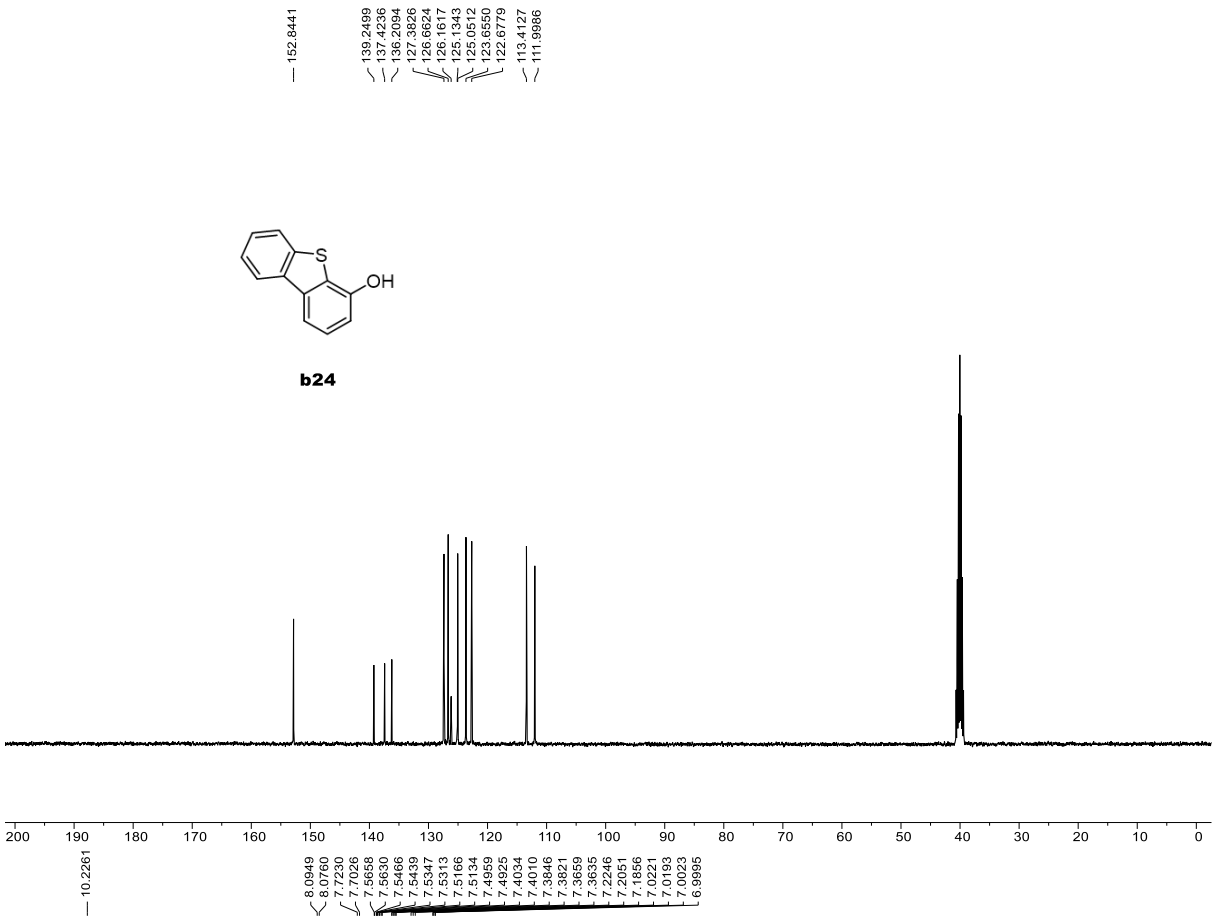
7.4870
7.4738
7.4691
7.3800
7.3605
7.3410
6.9943
6.9750
S
OH
1.00
1.05
1.00
1.03
2.06
1.02
1.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

b24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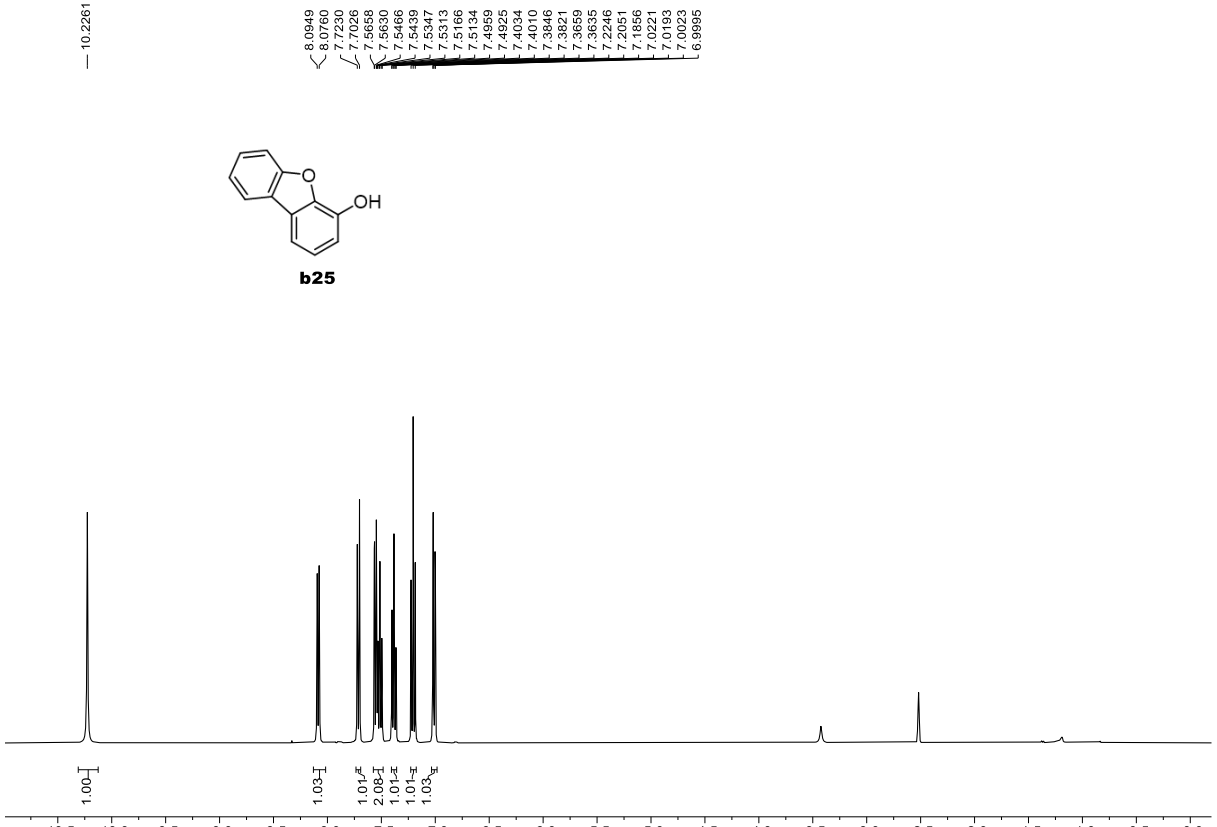
126.1617
125.1343
125.0512
123.6550
122.6779
113.4127
111.9986
S
OH
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

b24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7.5630
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7.5313
7.5166
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7.4010
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7.3659
7.3635
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7.2051
7.1856
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7.0023
6.9995
O
OH
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1.01
2.08
1.01
1.01
1.03
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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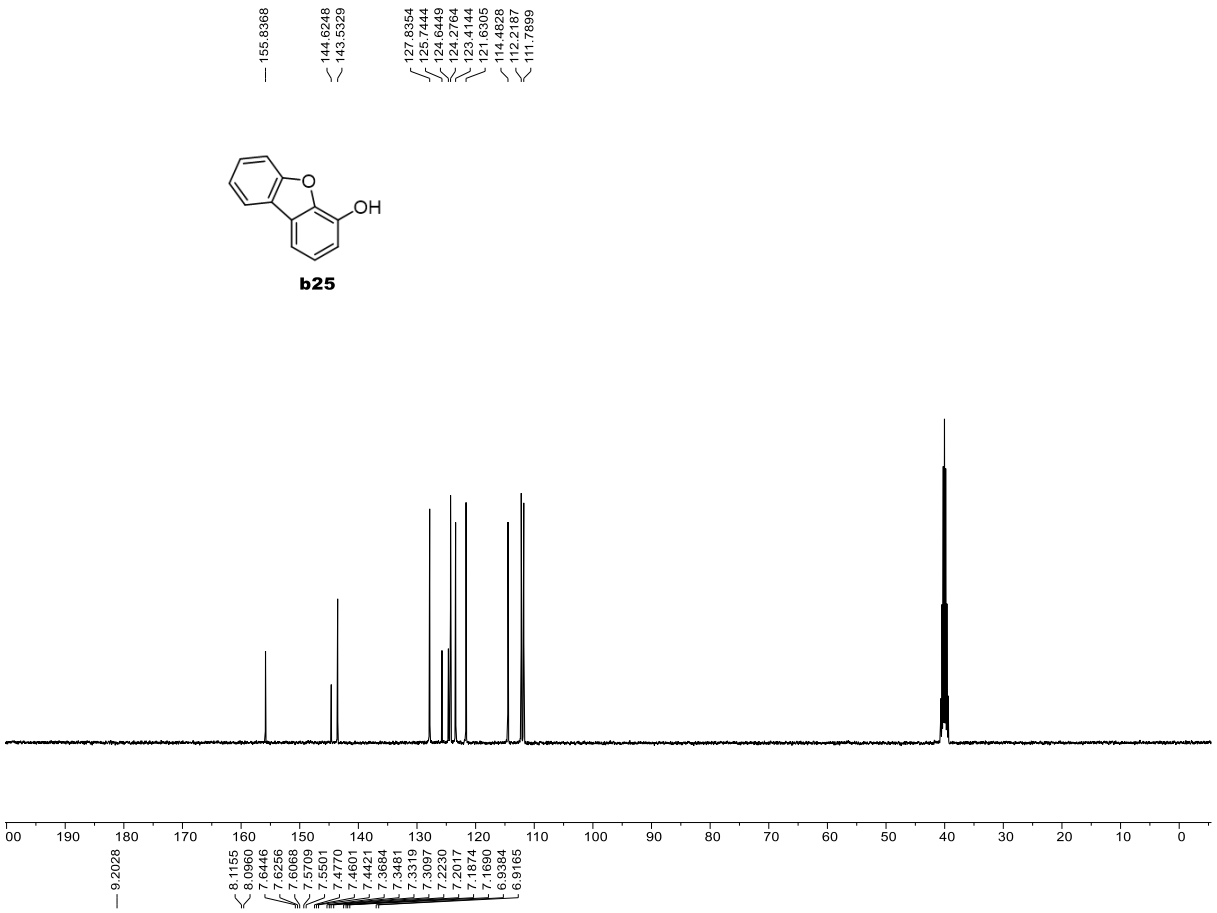
b25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111.7899
O
OH
b25
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8.0960
7.6446
7.6256
7.6068
7.5709
7.5501
7.4770
7.4601
7.4421
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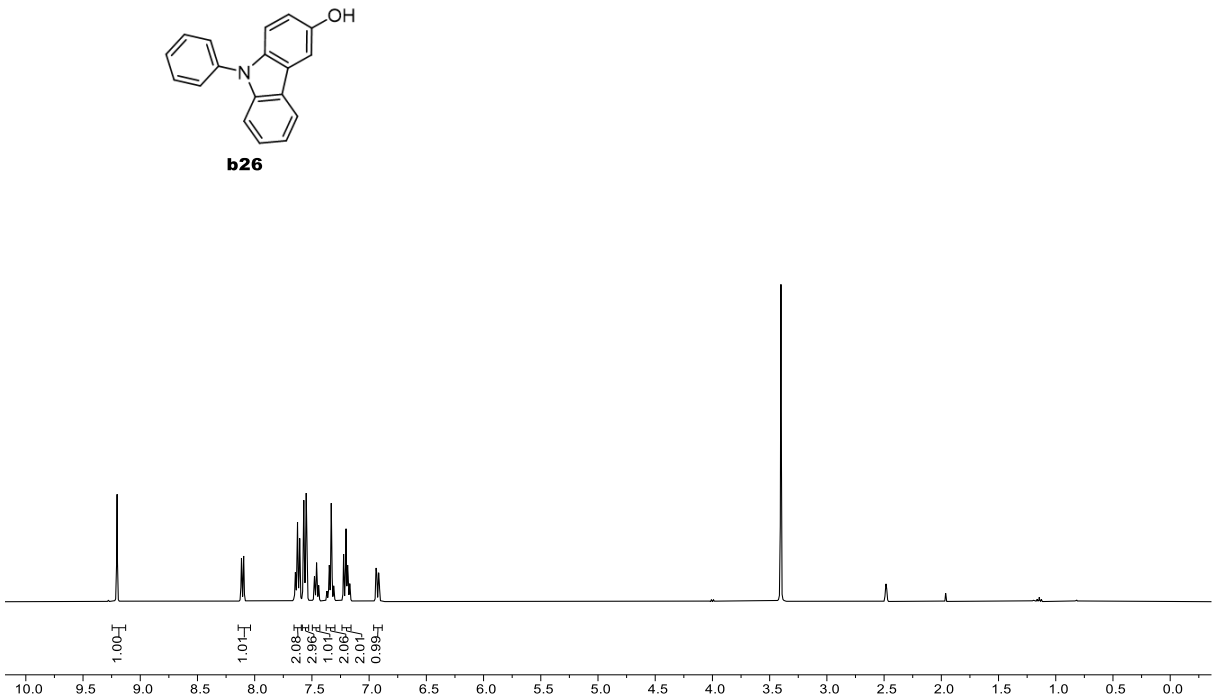
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1.01
2.06
2.01
0.99
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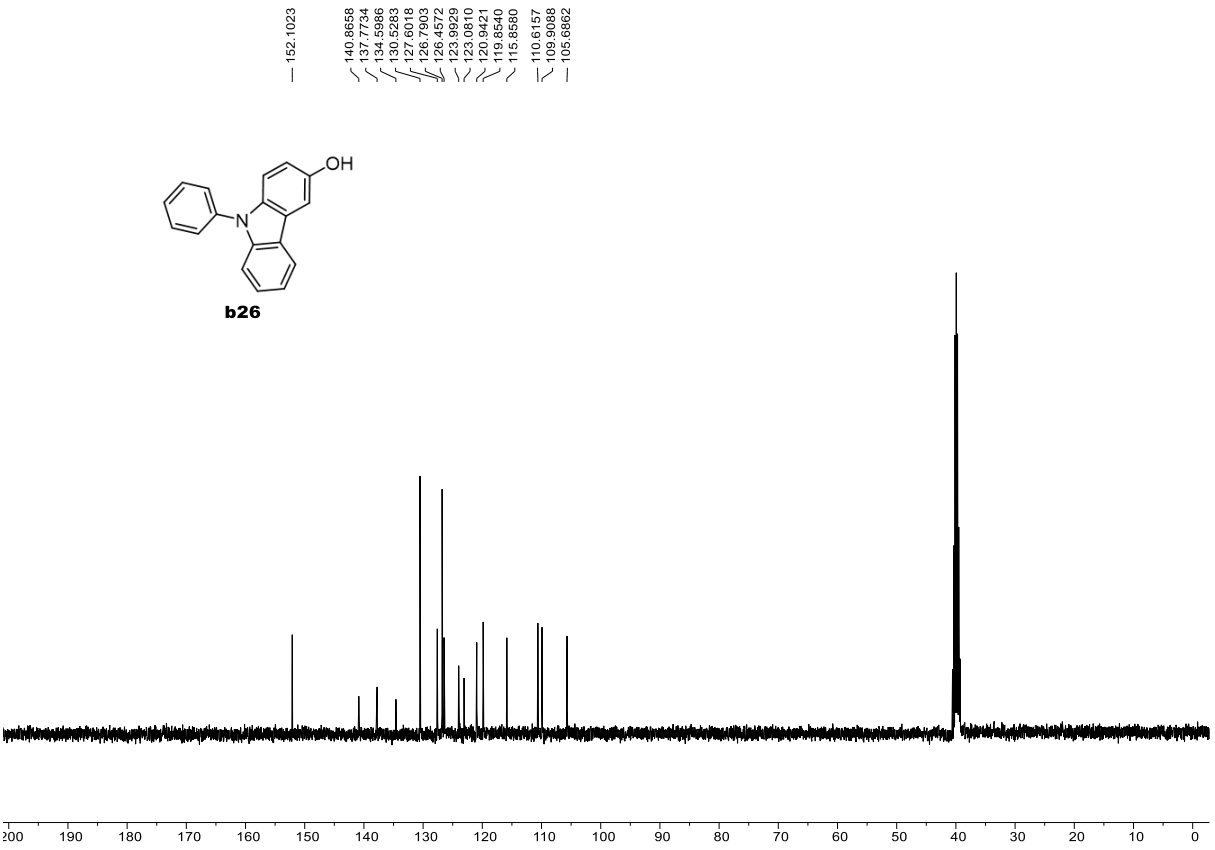
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120.9421
119.8540
115.8580
110.6157
109.9088
105.6862
OH
N
b26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

16. Single crystal X-ray crystallography of product b21

A single crystal of **b21** was mounted and tested as Zr-TCPCo. Data collection, data reduction, structure solution, and refinement method were all following the same procedure as Zr-TCPCo. Crystallographic data and structure refinement results are given in Table S3.

Table S3. Crystallographic data of b21

Compound	**b21**
CCDC No.	2222429
Formula	C25 H16 O
Formula weight	332.38
Temperature (K)	298
Crystal system	Trigonal
Space group	$P3_2$
a/Å	10.8049(2)
c/Å	12.9961(2)
V/Å^3	1313.97(5)
Z	3
D_c /g cm^{-3}	1.260
reflns coll.	8564
unique reflns	3271
R_{int}	0.0265
R_1 [$I > 2\sigma(I)$]	0.0601
wR_2 [$I > 2\sigma(I)$]	0.1701
R_1 (all data)	0.0610
wR_2 (all data)	0.1717
GOF	1.078

17. UV-Vis spectrum of the recycled Zr-TCPCo

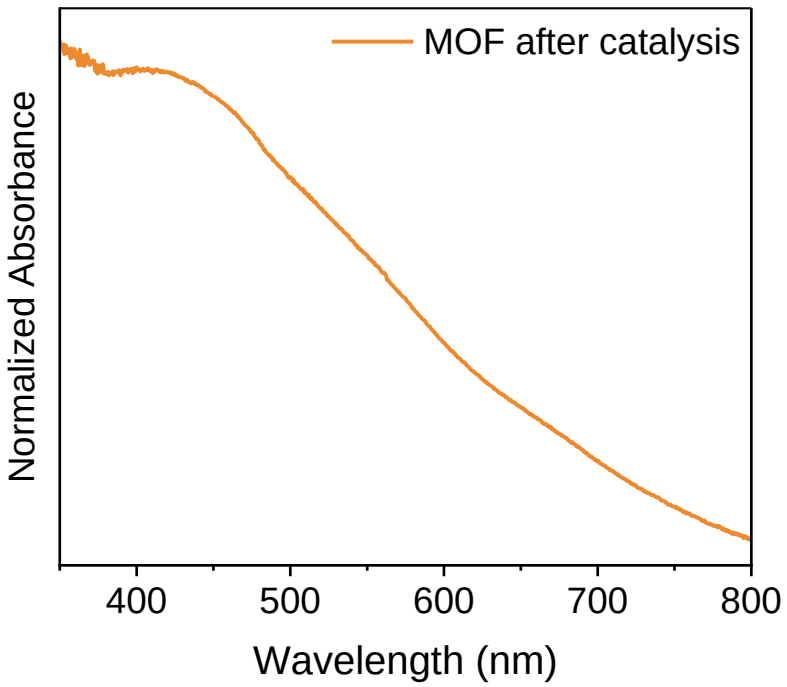

Figure S17. UV-Vis spectrum of Zr-TCPCo after catalysis.

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[2] M. O'Keeffe, M. A. Peskov, S. J. Ramsden and O. M. Yaghi, *Acc. Chem. Res.*, 2008, **41**, 1782–1789.

[3] S. Roy, Z. Huang, A. Bhunia, A. Castner, A. K. Gupta, X. Zou and S. Ott, *J. Am. Chem. Soc.*, 2019, **141**, 15942–15950.

[4] G. Sheldrick, *Acta Crystallogr. Sect., A* 2015, **71**, 3–8.

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[6] G. Sheldrick, *Acta Crystallogr. Sect., A* 2008, **64**, 112–122.