

Supporting Information

Ru-nanos at zeolite-Y for *ortho*-benzylation of phenols and activation of H₂O₂ for selective synthesis of BINOLs

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Reagents, Chemicals and Solvents

Catalyst support (like- zeolites, alumina, silica) used here to prepare the materials were obtained from Sigma-Aldrich. Various salts (e.g. ruthenium chloride, $\text{RuCl}_3 \cdot x\text{H}_2\text{O}$ anhydrous basis) were purchased from Sigma-Aldrich. Stated all the organic reactions were performed in various oven or flame-dried glassware with magnetic stirring bar using optimized reaction conditions under nitrogen or argon atmosphere. The organic substrates used here i.e. phenol derivatives, naphthols derivatives and various aromatic alcohols were procured from Sigma-Aldrich, ThermoFisher Scientific (Alfa Aesar). Various organic solvents and reagents were used here dried and HPLC grade procured from E-Merck and stored over molecular sieves (whether applicable) under dry atmosphere. Dried and clean measuring apparatus, needle and syringes were used whenever required to transfer solvents and reagents.

Physical Measurements

After synthesizing the materials and overnight vacuum dried the physical measurements were done by several analytical approaches. The powder X-ray diffraction (PXRD) of all materials were performed in a Philips PANalytical Empyrean instrument, enabling low-angle measurement from $0-70^\circ$ with a minimum step size (2θ) of 0.0001, and BRUKER AXS, GERMANY and Rigaku Corporation, Japan, Model: D8 FOCUS and MINIFIEX instrument in the 2θ value range of $5-80^\circ$. Determination of crystal structure powder samples were carried out by XRD COMMANDER 2, DIFFAC.EVA and Rigaku software. The Fourier transform infrared (FTIR) analyses of solid sample and liquid sample were investigated through PerkinElmer Spectrum Version 10.4.3 instrument. The NH_3 -Temperature-programmed desorption (NH_3 -TPD) and H_2 -Temperature-programmed reduction (H_2 -TPR) analysis was executed in ChemBET Pulsar TPR/TPD (automated chemisorption analyzer) from Quantachrome Instruments. The NH_3 -TPD study was performed by taking 0.050 g of the synthesized materials placed in a U-shaped quartz tube, heated with the $80-800^\circ\text{C}$ with rate of $10^\circ\text{C}/\text{min}$. The SU8200 Cold FE-SEM (Hitachi High-Technologies) instrument was used for record Field emission scanning electron microscopy (FESEM) of the synthesized materials with acceleration voltage: $0.1 \sim 30\text{kV}$ ($0.01\text{kV}/\text{step}$), resolution: $0.8\text{nm}/15\text{kV}$, $1.1\text{nm}/1\text{kV}$, magnification: LM $20 \sim 2,000\text{X}$, HM $100 \sim 800,000\text{X}$ and electrical image shift: $\pm 12\mu\text{m}$ ($\text{WD}=8\text{mm}$). The transmission electron microscopy (TEM), STEM imaging (HAADF), energy dispersive X-ray (EDX) were recorded on a model: JEM-2100F, JEOL, instrument with Lattice resolution: 0.102, with a 200 kV accelerating voltage and having HAADF-STEM resolution: 0.096 nm. The HR-TEM (TEM, STEM-HAADF, EDX) of the samples (*viz* Ru-NaY-1, Ru-NaY-2 and Ru-NaY-3) were carried out taking $0.1 \text{ mg}/1000 \mu\text{L}$ (samples/ethanol solution) in a bath sonication for 45. Then samples/ethanol solution was taken in TEM grid, Lacey carbon film 300 mesh, Nickel and evaporated at 40°C for 30 min. After that the imaging technique was done taking various image resolution. The EDX analysis of optimal Ru-content in different concentration of $\text{RuCl}_3 \cdot x\text{H}_2\text{O}$ (0.001M, 0.005, 0.02M and 0.05M) in Ru-NaY-1 material was done in Material Science and Technology Division (CSIR-North East Institute of Science & Technology, Jorhat, India) using Oxford XMax 20 detector. Shimadzu, UV-2550 spectrophotometer was used for UV-Visible

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study of reactions. Inductively Coupled Plasma Optical Emission Spectrophotometer (ICP-OES) analysis was performed in PERKIN ELMER, USA, Model: AVIO 220 MAX. Syngistic software was used. Bruker Multi-mode V (Model) instrument with Contact, Tapping, and ScanAsyst imaging modes were used for Atomic force microscopy (AFM) analysis of the materials. The instrument having resolution of < 5 nm and measuring up to $120 \mu\text{m} \times 120 \mu\text{m}$ areas with vertical range of nearly $5 \mu\text{m}$, maximum sample size: $1 \text{ cm} \times 1 \text{ cm}$. The AFM analyses of samples were prepared by sonication followed by drop casting method. For sample preparation 0.1 g of sample or zeolite-Y was mixed with 1 mL of ethanol solution, and then the mixture was sonicated for 100 min . After forming fine slurry, the suspension was drop casted on mica disc (12 nm) and then evaporated at $60 \text{ }^\circ\text{C}$ for 30 min . After that the dried samples were ready for AFM analysis. The synthesized and oven-dried samples (finely ground) were dusted on a graphite sheet (double side stick) and mounted over the sample holder, before being transferred to an analysis chamber. The sample was degassed overnight in a vacuum oven before recording the X-ray photoelectron spectroscopy (XPS) The XPS analysis was performed with KRATOS (ESCA AXIS 165) spectrometer using $\text{Mg K}\alpha$ (1253.6 eV) radiation as a source. The binding energy values were corrected with reference to $\text{C } 1\text{s}$ peak at 284.8 eV . The electrochemical measurements of all the materials were executed in CH Instruments, model: CHI-600E potentiostat meter. Glassy Carbon Electrode (GCE) and also platinum (Pt) electrode were used as working electrode in electrochemical cell for cyclic voltammetry analysis. The Ag/AgCl and Pt wire were used as reference electrode and as a counter electrode respectively. Thermo Gravimetric Analysis (TGA) of all the materials were carried out on Mettler Toledo simultaneous TG thermo analyzer. The analyzer was equipped with a platinum (Pt) crucible, 13% thermocouples of Pt/Pt-Rh with flow rate of $20 \text{ mL}/\text{min}$ of controlling gas (air). Thin-layer chromatography (TLC) technique was executed to monitor the progress of the reaction by taking TLC Silica gel 60 F₂₅₄ aluminum pre-coated plates (layer thickness $\sim 0.25 \text{ mm}$) from Merck. The TLC plates (chromatograms) were visualized under UV light at 254 nm (short range) using Relitech UV chamber with using suitable TLC stains (e.g. iodine chamber). GC analysis was performed for the calculation of % conversion of phenol and 2-naphthol for benzylation and oxidative coupling reaction respectively. GC-MS Aglient 7980 series with HP-5 column and flame ionization detector was used for the analysis. The results are predicted in mol % using the following formula: % conversion reactant = $[\text{moles of reactant} \times 100/\text{Initial moles of reactant}]$. After successful separation of the product the following equation is used for calculation of the % isolated product yield as: % yield = $[\text{mole of isolated product}/\text{mole of limiting reactant}] \times 100$. After purification of the product, NMR spectra were recorded on 400, 500 and 600 MHz spectrometers (for ^1H NMR spectra) and 101, 126 and 151 MHz (for ^{13}C NMR spectra). The ^1H and ^{13}C NMR analyses were done by DRX-400 Varian, Bruker AVANCE III HD 600 MHz, 500 MHz and 400 MHz spectrometers. In NMR analysis, various chemical shifts (δ -value) are described in unit of ppm from tetramethylsilane (TMS) as the internal standard (for CDCl_3 solvent: $\delta 7.26$ for ^1H NMR and CDCl_3 : $\delta 77.16$ for ^{13}C NMR analysis). The spin-spin coupling constants (J) were in hertz (Hz) unit, and other data were represented as follows: s (singlet), d

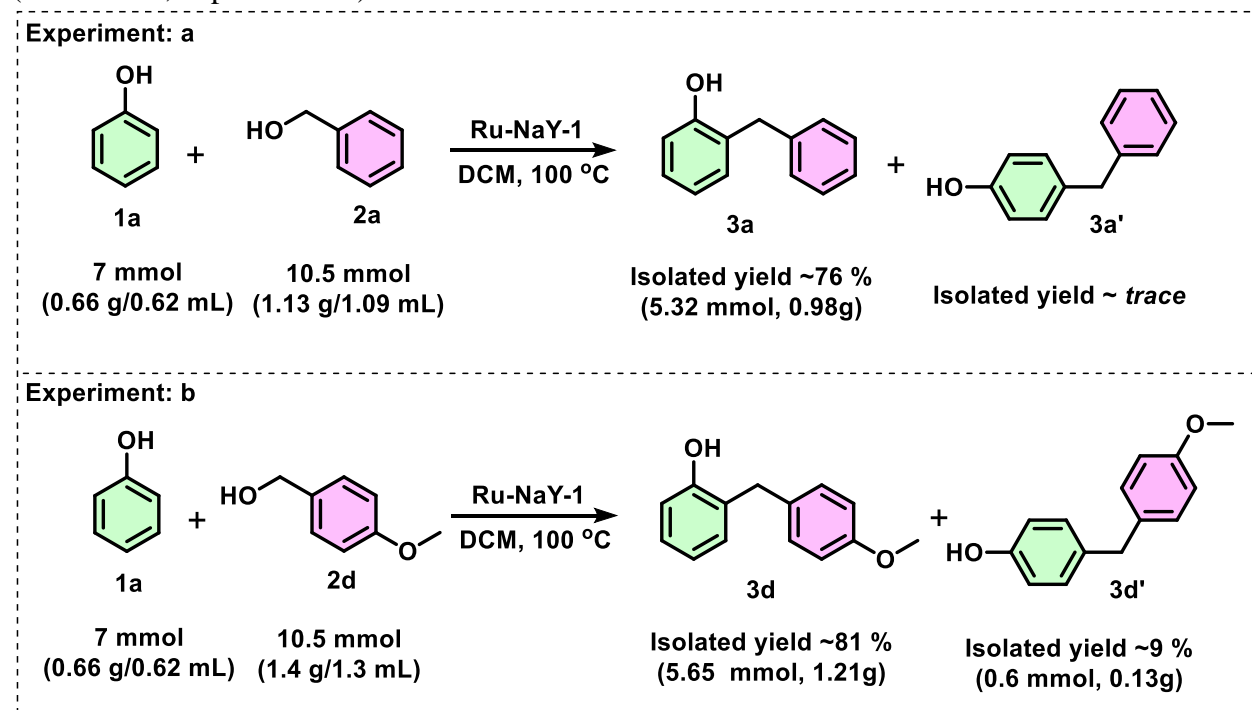
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(doublet), dd (doublet of doublet), ddd (doublet of doublet of doublet) t (triplet), m (multiplet) q (quartet). The ^1H NMR data were reported as follow: chemical shift (δ) (multiplicity, coupling constant, integration i.e., number of protons). The mass of the organic molecules was determined by Low-resolution mass spectra (LRMS) for all the compounds. Mass spectra (MS) of the samples were recorded in Thermo Scientific Q-Exactive, Accela 1250 pump. Perkin Elmer 2400 (series II) CHN analyzer was used for elemental analysis (wt% C, H) in the synthesized compounds (taking acetanilide as internal organic analytical standard: C= 71.09%, H= 6.7%1, N=10.36%, PerkinElmer). LRMS were recorded on an Agilent InfinityLab LC/MSD 6125SQ LCMS system using 1260 Quat Pump. Bruker SMART Apex II CCD diffractometer using Mo $\text{K}\alpha$ ($\lambda = 0.71073 \text{ \AA}$) radiation was used for X-ray diffraction study and data collection.¹ Bruker SMART software was used to collect the X-ray diffraction data of all crystals and also utilized for indexing and determination of the unit cell parameters of the crystals. SHELXTL software was used for solving the cell structures by direct method after refined by full-matrix least squares against F2 of all results. All H-atoms in isotropic approximation, against F2 of all reflections along with all other the non-H-atoms were refined by full-matrix least squares in anisotropic.

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General procedure for synthesis of gram scale substrate study for benzylation of phenol with aromatic alcohol

In scale-up reaction of phenol and BA, in a 50 mL RB with phenol, 1a (7 mmol, 0.66g, 1 equiv.) and benzyl alcohol 2a (10.5 mmol, 1.13g, 1.5 equiv.) with ~ 200 mg Ru-NaY-1 in 7 mL of DCE were refluxed at 100 °C for 6 h. After completion, the *ortho*-substituted product 3a was obtained as the major product (~76 %) while the *para*-substituted adduct, 3a' was detected as trace amount and was not isolated (Scheme S1, experiment: a). Another gram-scale study was performed by taking 1a (7 mmol, 0.66g, 1 equiv.) and 4-methoxy benzyl alcohol, 2d (10.5 mmol, 1.4g, 1.5 equiv.) under same condition. The products 3d (5.65 mmol, 1.21 g, isolated yield: 81%) along with *para*-substituted product was also obtained as 3d', white solid, yield ~ 9% (0.6 mmol) (Scheme S1, experiment: b).



Scheme S1. Gram-scale reaction of (a) phenol and benzyl alcohol, (b) phenol and 4-methoxybenzyl alcohol.

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Table S1. ICP-OES (EDX-elemental analysis) data for the synthesized materials. The values are given in weight%. The values in the parenthesis are from EDX elemental analysis.

Materials	Elements (wt%)				Metal loading ^a (mmol g ⁻¹ of support)
	Si	Al	O	Ru	
Ru-NaY-1	- (29.61)	- (5.40)	- (41.56)	3.60 (23.53)	0.35 -
Ru-NaY-2	- (30.71)	- (3.28)	- (43.56)	3.45 (22.45)	0.34 -
Ru-NaY-3	- (30.54)	- (11.28)	- (37.41)	3.41 (20.76)	0.33 -

$${}^a \text{Metal loading} = \frac{\text{Observed metal \%} \times 10}{\text{Atomic weight of metal}} \text{ (in mmol g}^{-1}\text{)}^2$$

Table S2. Detected amount of Ru-content in Ru-NaY-1 materials at different concentration of RuCl₃.xH₂O (0.001M, 0.005M, 0.01M, 0.02M and 0.05M) from ICP-OES analysis (in wt%).

Entry	Conc. of RuCl ₃ (in M)	Ru-loading (wt%)
1	0.001	0.39
2	0.005	1.87
3	0.01	3.60
4	0.02	5.32
5	0.05	7.14

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X-ray Crystallographic analysis: All the crystallographic information of crystals is given in the crystallographic table, **Table S3** which contains the crystal parameters and the refinement factor. The structure of **5e** was drawn at MERCURY software.³ The CIF files of compound **5e** having the whole information of the studied structure was deposited with CCDC, deposition number **2295241** which are easily accessible upon request from the Director, CCDC, 12 Union Road, Cambridge CB21EZ, UK (Fax: +44-1223-336033; email:deposit@ccdc.cam.ac.uk) or from the following website: www.ccdc.cam.ac.uk/data_request/cif.

Table S3. Crystallographic data and refinement parameters for the compound **5e**

Compound name	Compound 5e <i>(Dimethyl 2,2'-dihydroxy-[1,1'-binaphthalene]-6,6'-dicarboxylate</i>
chemical formula	C ₂₄ H ₁₈ O ₆
CCDC deposition number	2295241
formula mass	402.38
crystal system	monoclinic
space group	I2/c
a/Å, b/Å, c/Å	13.71(3), 8.846(19), 16.24(3)
α/°, β/°, γ/°	90.00, 93.51(18), 90.00
V/Å ³	1966(7)
Density (g cm ⁻³)	1.360
T/K	296(2)
Z	4
radiation type	Mo Kα
absorption coefficient, μ/mm ⁻¹	0.098
Total no. of reflections measured	2385
Reflections, I > 2σ(I)	612
Complete to 2θ (%)	99.1
Ranges (h, k, l)	-17 ≤ h ≤ 18

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	$-11 \leq k \leq 11$ $-21 \leq l \leq 21$
Data/ Restraints/Parameters	2385/0/137
R indices [$I > 2\sigma(I)$]	0.0953
R indices (all data)	0.3392
wR2 (all data)	0.1902
Goodness of fit	1.063

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Table S4. Comparison study for (a) for benzylation of phenol with PBA and (b) oxidative C-C coupling of 2-naphthol using H₂O₂ with previous reports.

(a) Comparative study for benzylation of phenol with PBA						
Entry	Catalyst	Conditions	Product (specific to this scheme)	Yield of 3a (%)	Selectivity	Ref.
1	[(C ₆ H ₆)(PCy ₃)(CO)RuH] ⁺ BF ₄ ⁻	100 °C, Toluene, C ₅ H ₈ , 6-12 h	1 (22 overall, both 1° and 2° alcohol)	92	3a	4
2	Zr-Modified Superacid:U DCaT-5	140 °C, 1 h	15 (both 1° and 2° alcohol)	65	3a + 3a'	5
3	HCl	180 °C, 0.05 M HCl, 16 h	11 (both 1° and 2° alcohols)	78	3a + 3a'	6
4	Bi(OTf) ₃	-, MeNO ₂ , 2 h	2 (22 overall, both 1° and 2°)	66	3a + 3a' + 3a''	7
5	ZrO ₂ /SBA-15	90 °C, 12-Tungstophosphoric acid, Silica; 3 h	1	77	3a + 3a'+ ethers	8
6	<i>Ru-NaY-1</i>	<i>100 °C, DCE, 6 h</i>	<i>15</i>	<i>82</i>	<i>3a + trace 3a'</i>	<i>This work</i>
(b) Comparative study for oxidative C-C coupling of 2-naphthol using H ₂ O ₂						
Entry	Catalyst	Conditions	No. Product	Yield of 5a (%)	Ref.	
1	Au/SrTiO ₃	rt, dark	1	-	9	
2	Benzothioephene S-oxide	DCM/TFA, TFAA, ligand 0°C to rt, >2 h	27	84	10	
3	Pd-Au-Y	Toluene, 60 °C, 4h	1	58	11	
4	AuVOx-MWCNT	Toluene, 60 min, MW-450	1	78	12	
5	<i>Ru-NaY-1</i>	<i>Toluene, rt, 15 min</i>	<i>8</i>	<i>91</i>	<i>This study</i>	

This comparative study is only based on reactions which utilized H₂O₂ as oxidant.

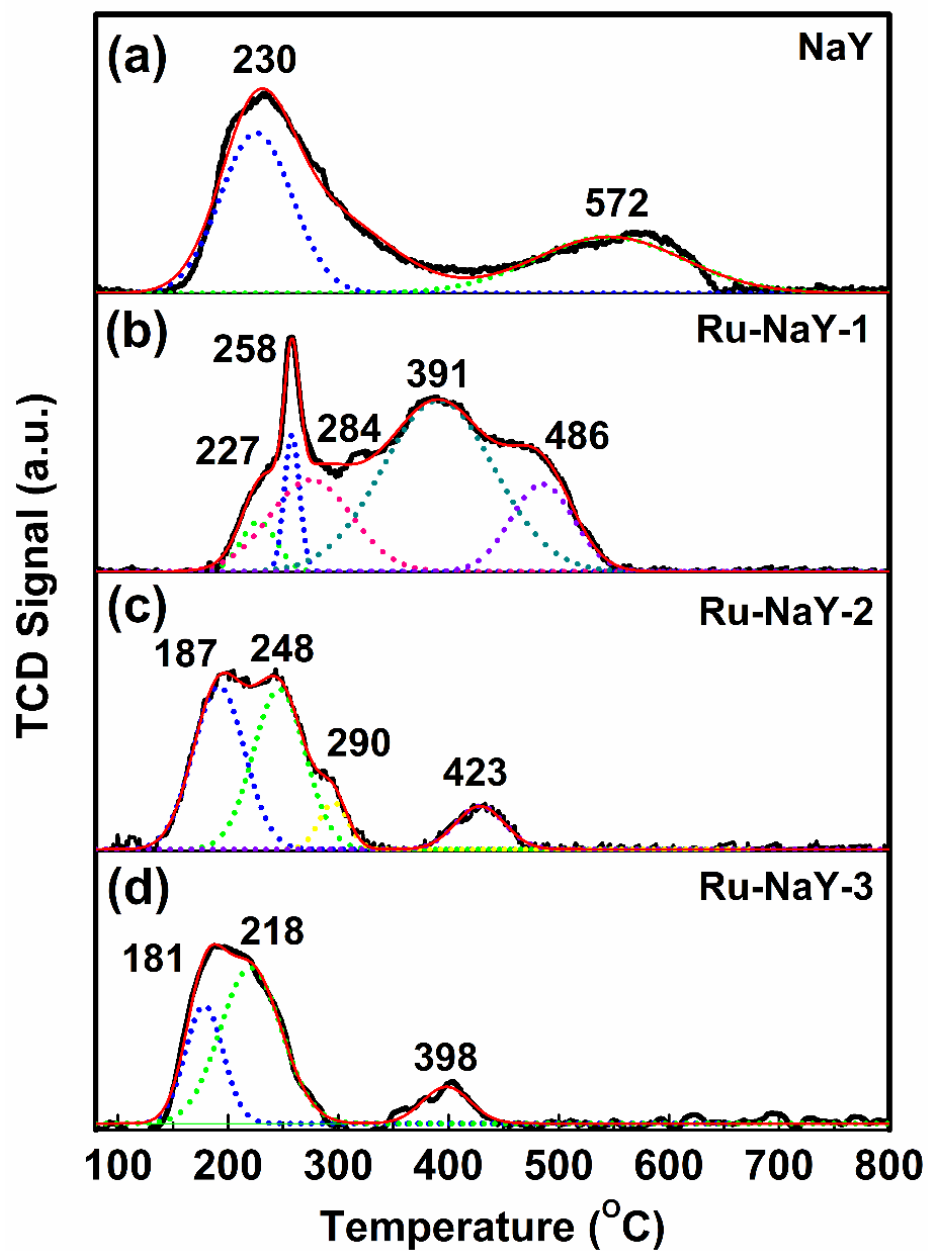
NH₃-Temperature Programmed Desorption (NH₃-TPD) plots of synthesized materials

Fig. S1 NH₃-Temperature Programmed Desorption (NH₃-TPD) plots for (a) neat zeolite-NaY, (b) Ru-NaY-1, (c) Ru-NaY-2 and (d) Ru-NaY-3.

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Characterization of the synthesized materials HADDF-STEM image and EDX mapping and elemental analysis Ru-NaY-2

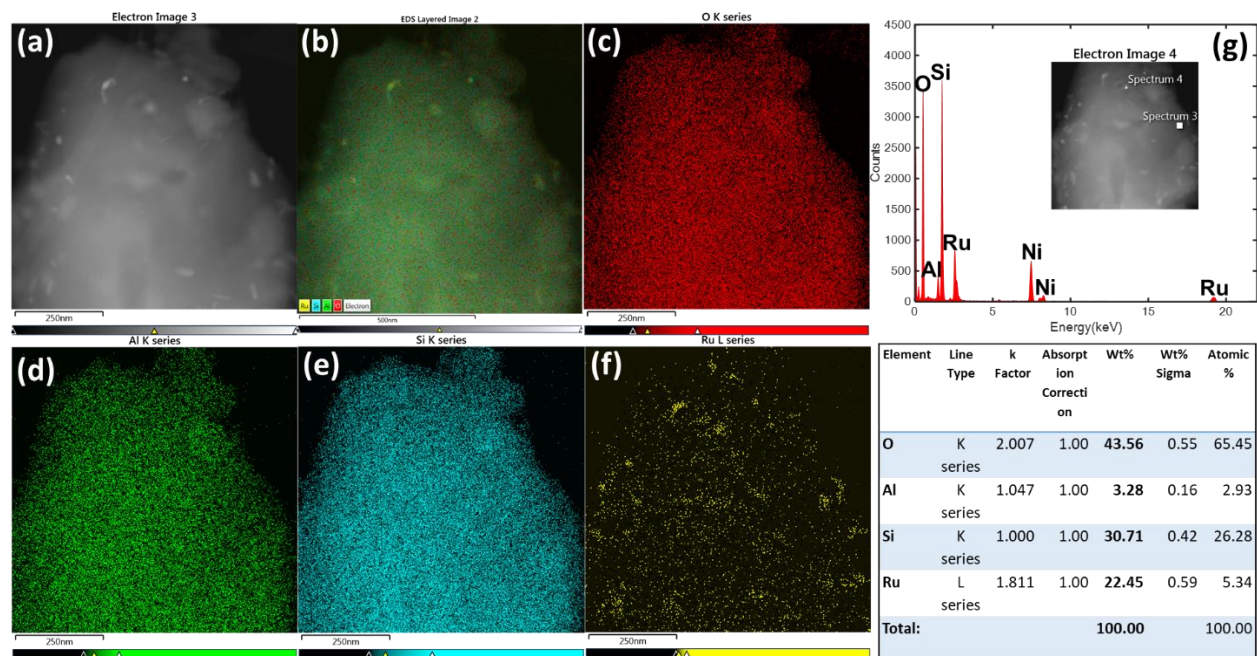


Fig. S2 (a-b) HADDF-STEM images showing the Ru-NPs located on Ru-NaY-2, (c-f) EDX mapping showing the presence of all the elements in Ru-NaY-2 (g) EDX spectra and details of all elements.

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HADDF-STEM image and EDX mapping and elemental analysis of Ru-NaY-3

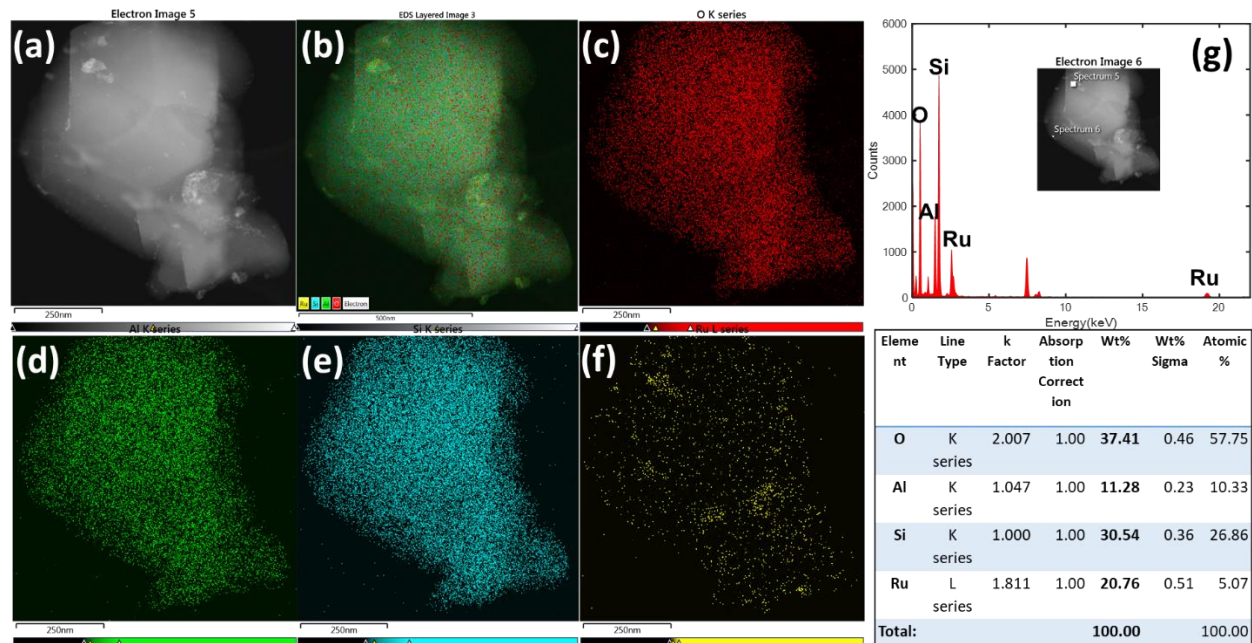


Fig. S3 (a-b) HADDF-STEM images showing the Ru-NPs located on Ru-NaY-3, (c-f) EDX mapping showing the presence of all the elements in Ru-NaY-3 (g) EDX spectra and details of all elements.

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XPS analysis

XP spectrum of Al 2p, Si 2p and O 1s of Ru-NaY-1, Ru-NaY-2 and Ru-NaY-3 catalyst

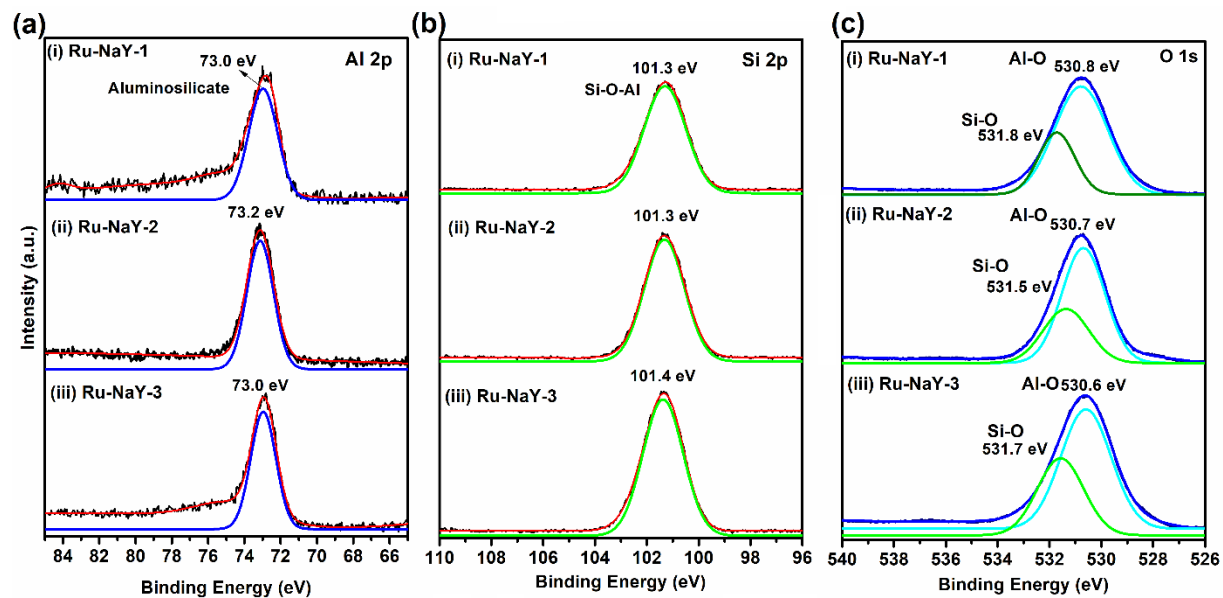


Fig. S4 The XP spectra of (a) Al 2p, (b) Si 2p and (c) O 1s in of Ru-NaY-1, Ru-NaY-2 and Ru-NaY-3 catalyst.

XPS Survey scan of Ru-NaY-1, Ru-NaY-2 and Ru-NaY-3 materials

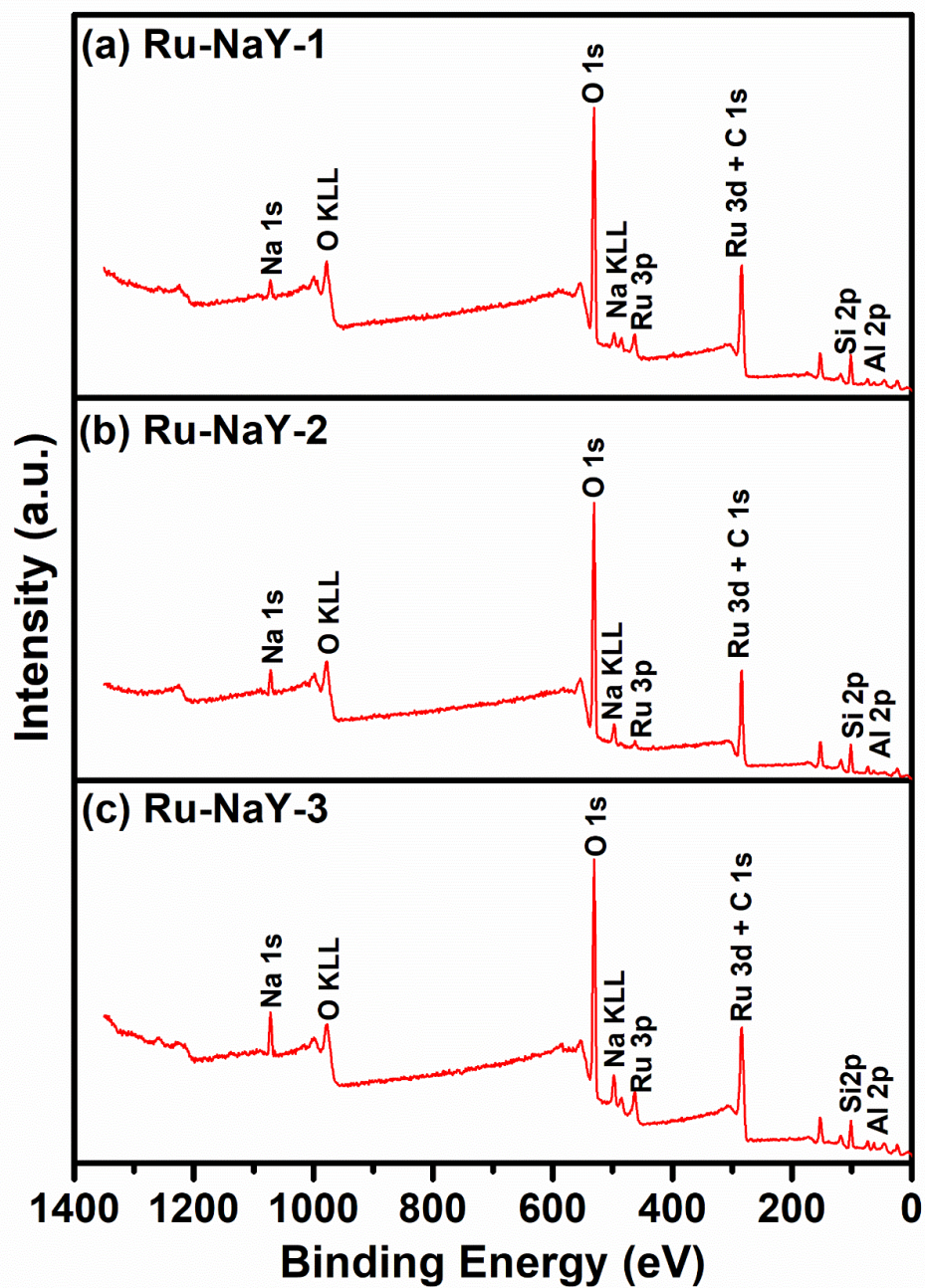


Fig. S5 Full XPS survey scan of (a) Ru-NaY-1, (b) Ru-NaY-2 and (c) Ru-NaY-3 materials.

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EDX analysis of synthesized materials

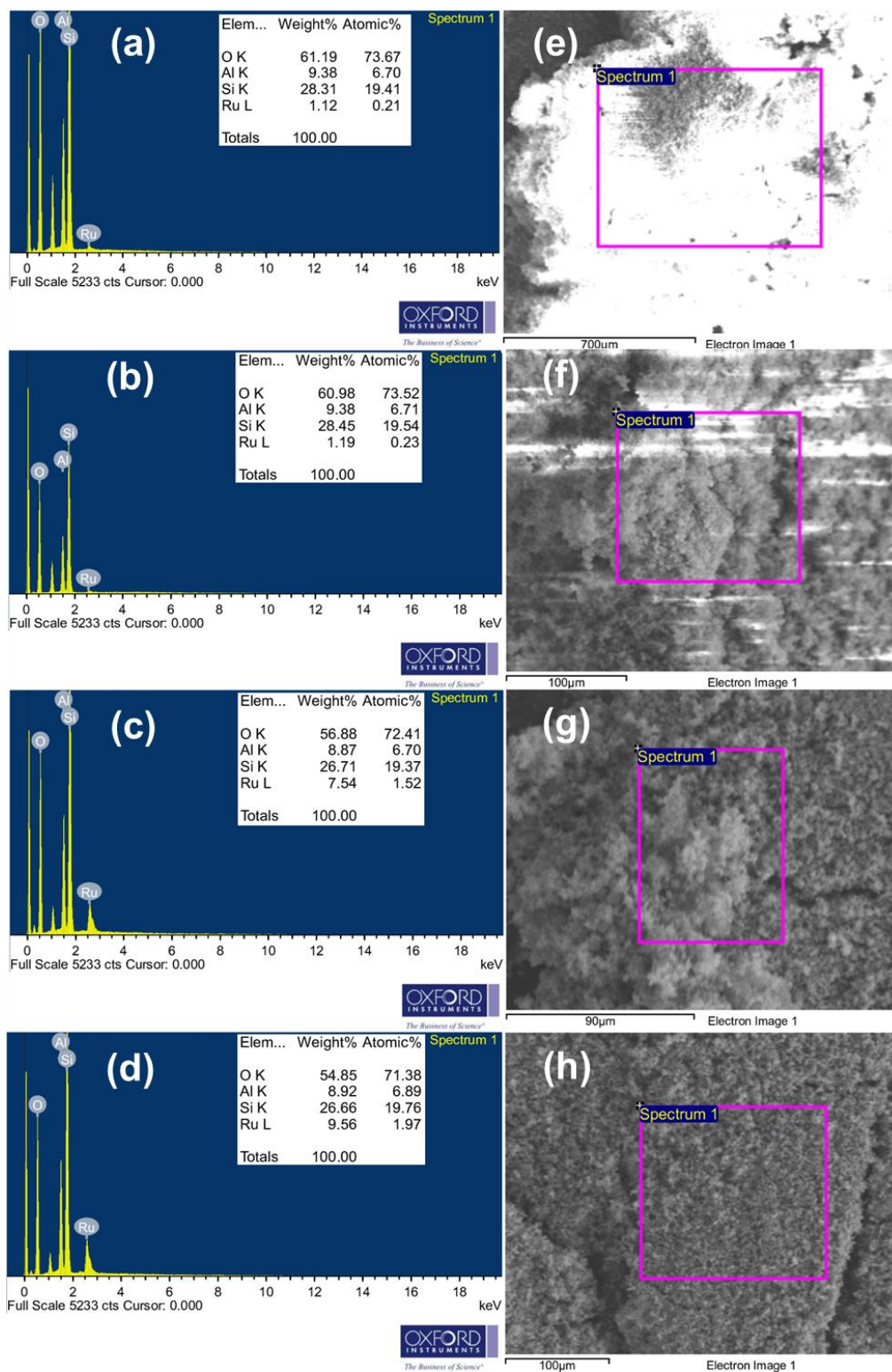


Fig. S6 (a-d) EDX spectra of Ru-NaY-1 catalyst prepared with different of $\text{RuCl}_3 \cdot x\text{H}_2\text{O}$ 0.001M, 0.005M, 0.02M and 0.05 M, respectively, (e-f) particular region chosen for EDX analysis for respective catalysts.

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Optimization of Ru content in Ru-NaY-1 catalyst for optimum catalytic performance for benzylation reaction

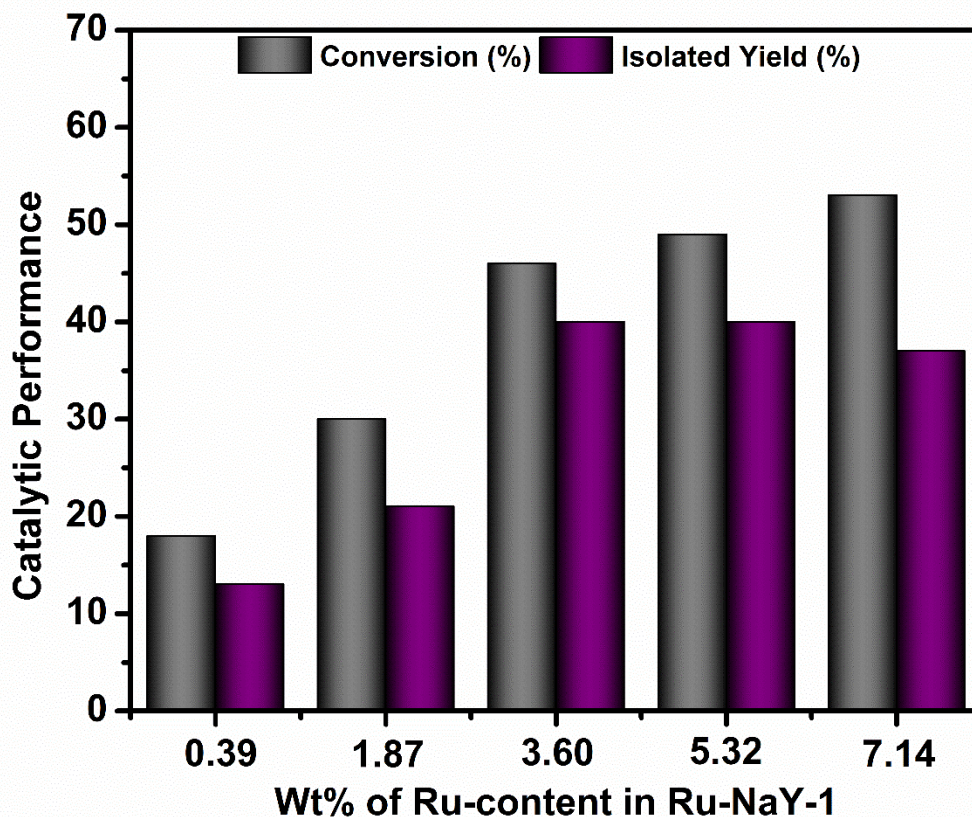


Fig. S7 Graphical representation of optimized wt % Ru content in Ru-NaY-1 catalyst for optimum catalytic activity. % conversions obtained from GC analysis. % yields calculated after separating through column chromatography.

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UV-visible spectra

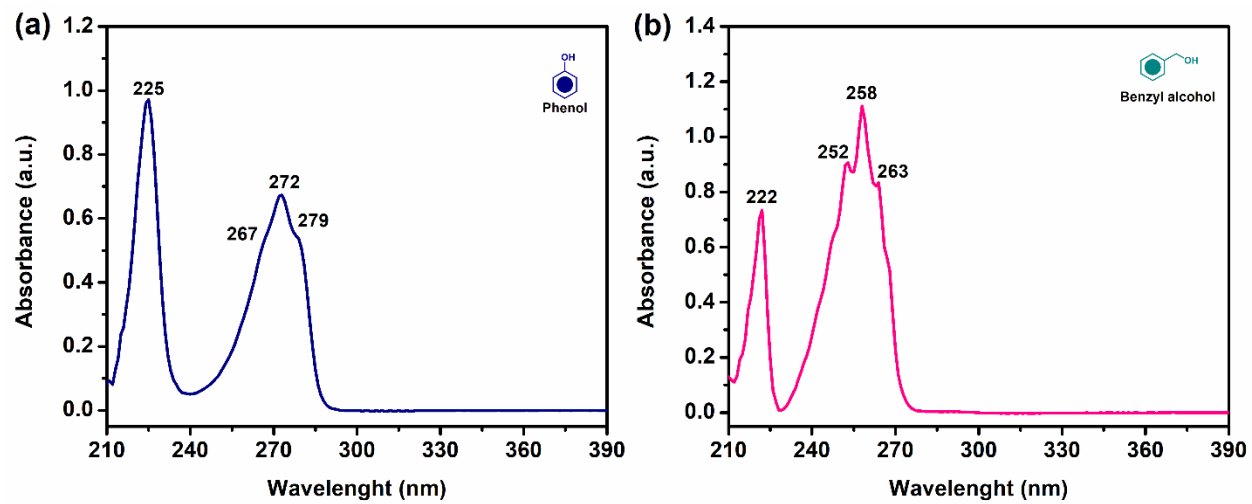


Fig. S8 UV-visible spectra of the (a) phenol and (b) BA

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Optimized structures for the benzylation of phenol with benzyl alcohol

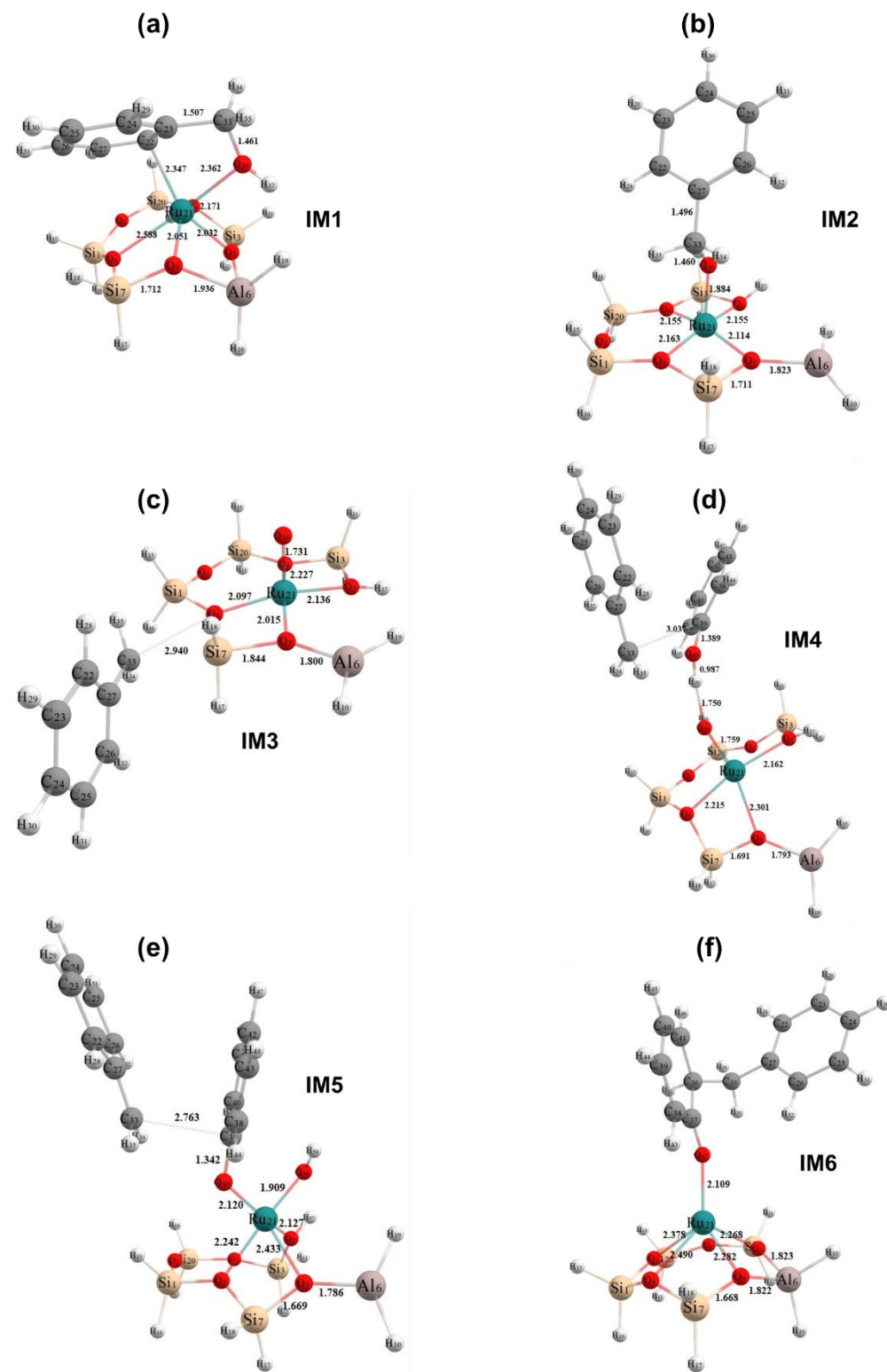


Fig. S9 Optimized structures for the benzylation of phenol with benzyl alcohol at B3LYP/6-311+G(d,p)/SDD level of theory.

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Optimization of Ru content in Ru-NaY-1 catalyst for optimum catalytic performance for 2-naphthol oxidation reaction

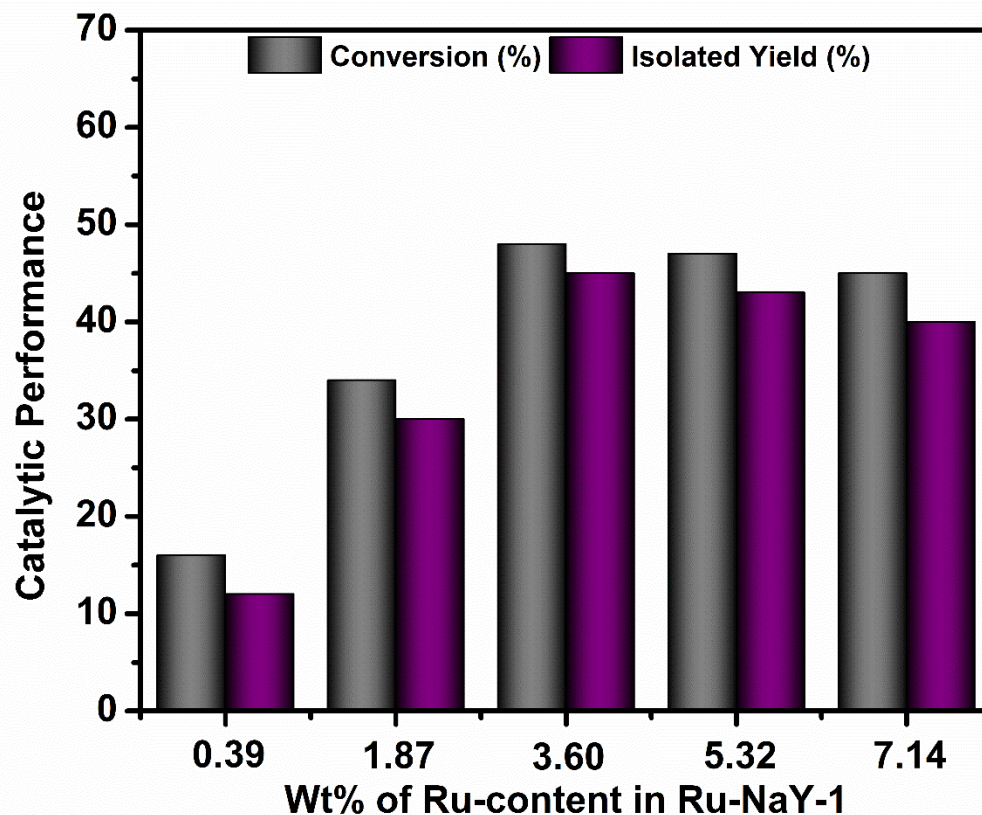


Fig. S10 Graphical representation of optimized wt % Ru content in Ru-NaY-1 catalyst for optimum catalytic activity. % conversions obtained from GC analysis. % yields calculated after separating through column chromatography.

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NMR spectra of solvent after reaction

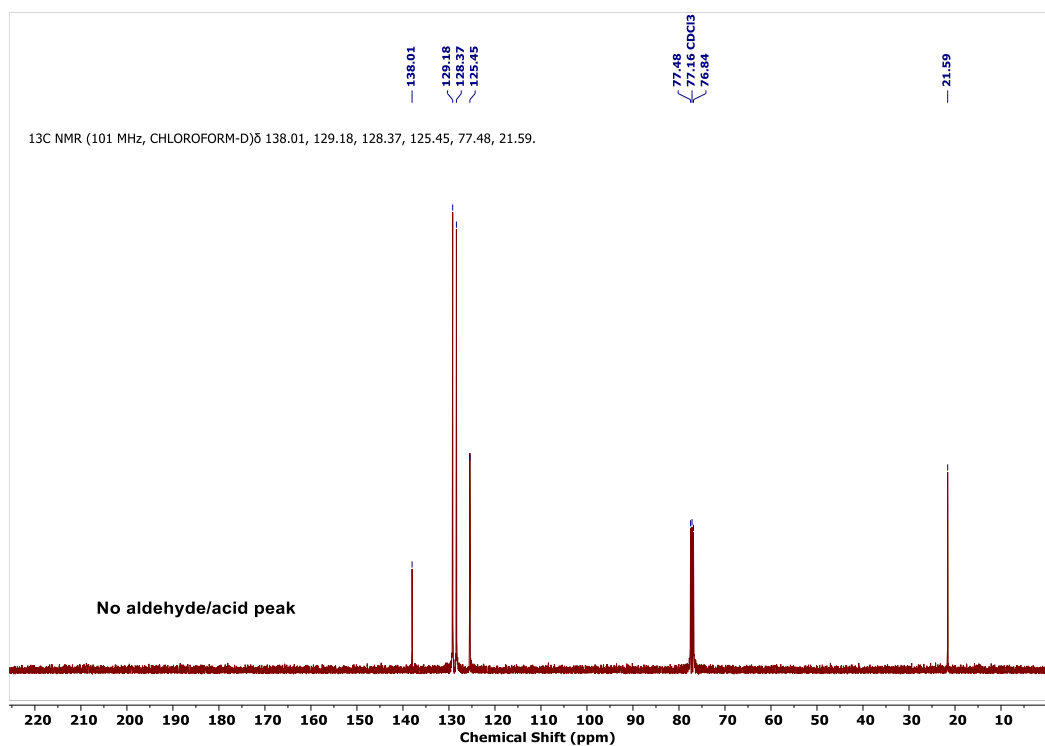
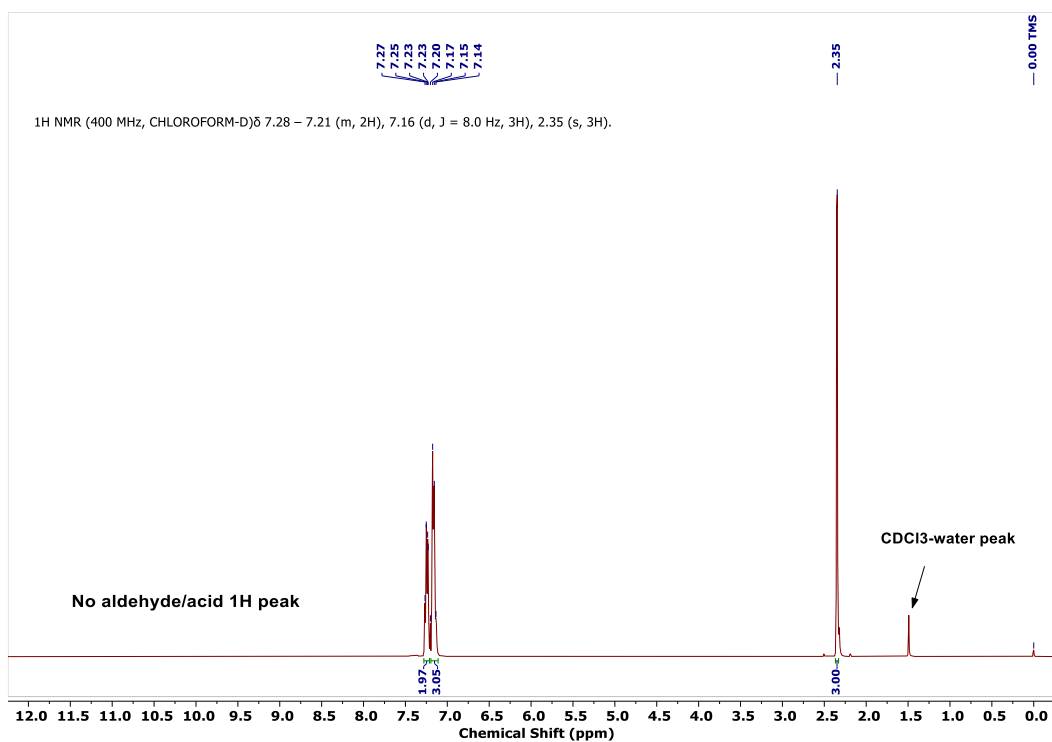


Fig. S11 ¹H and ¹³C NMR spectra for reaction solvent recorded after separating the catalyst (Ru-NaY-1) from solvent (toluene).

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X-ray structure of 5e

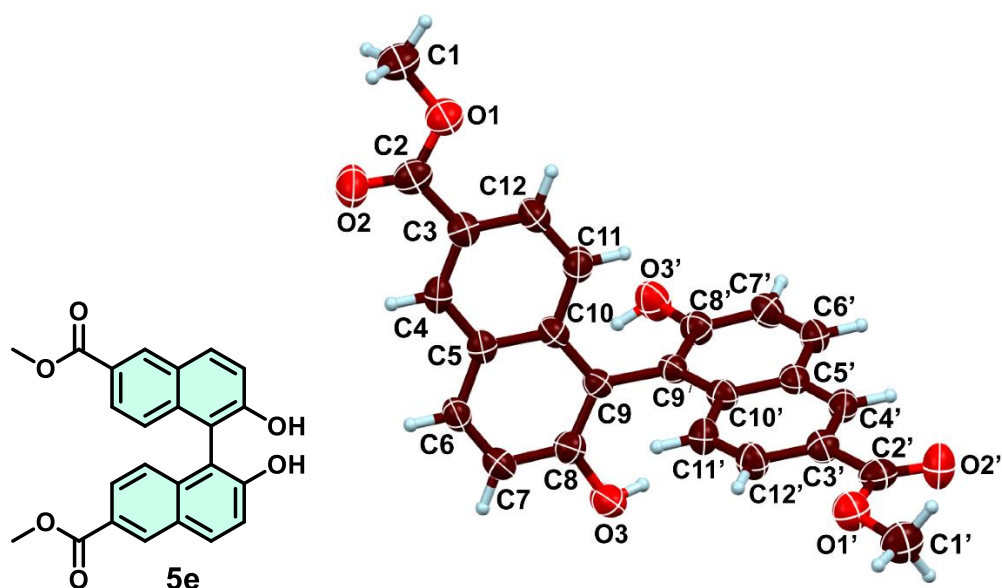


Fig. S12 ORTEP view (40% thermal ellipsoid probability) of **5e** (CCDC 2295241).

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Raman study

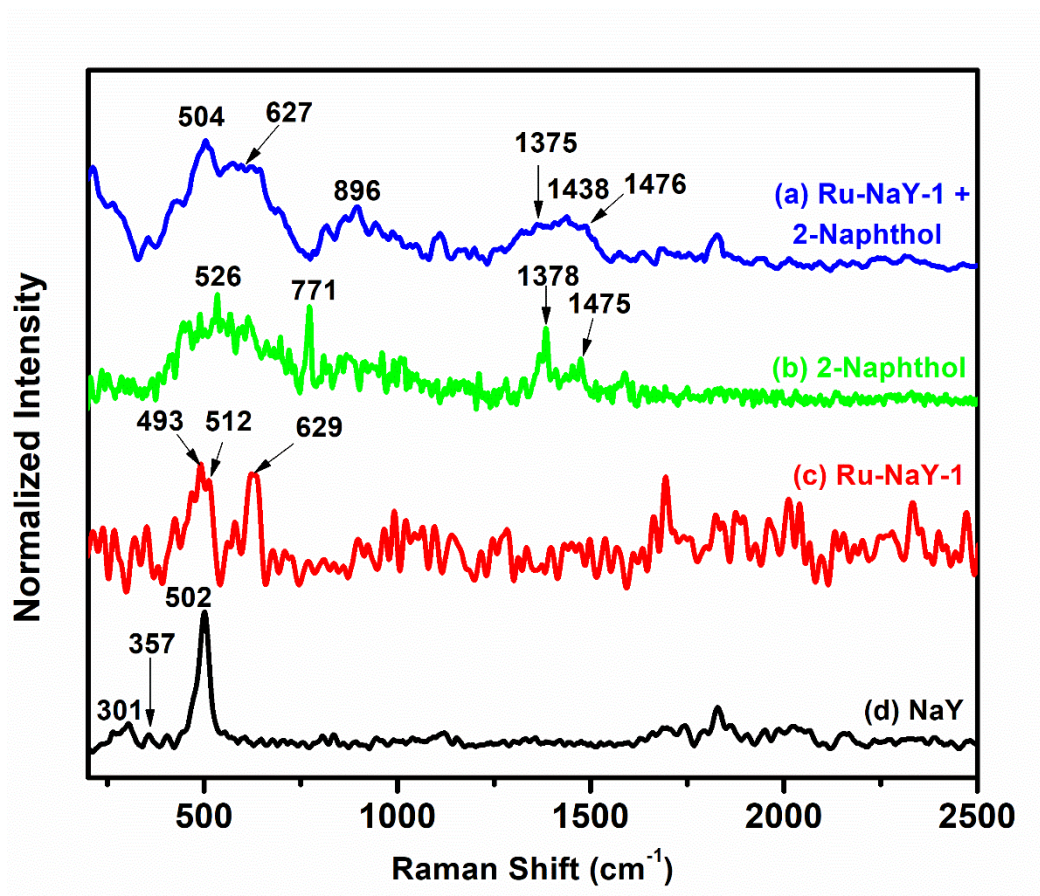


Fig. S13 Raman spectra of (a) Ru-NaY-1 + 2-naphthol, (b) 2-naphthol, (c) Ru-NaY-1 and (d) neat zeolite-NaY.

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Mass spectra of radical trapping experiment

Print of window 80: MS Spectrum

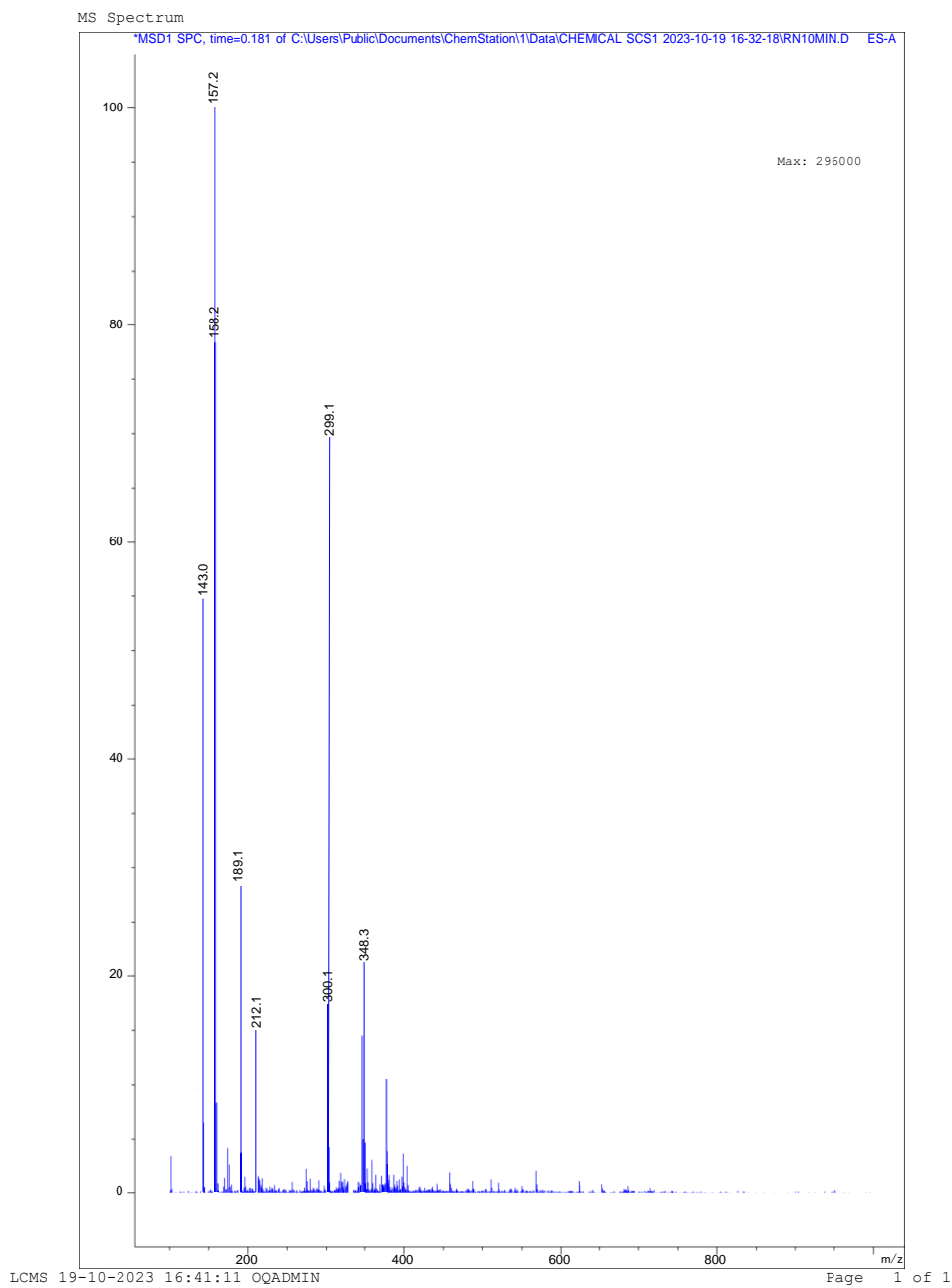


Fig. S14 LCMS spectra of reaction mixture after 10 min.

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Catalytic recyclability study

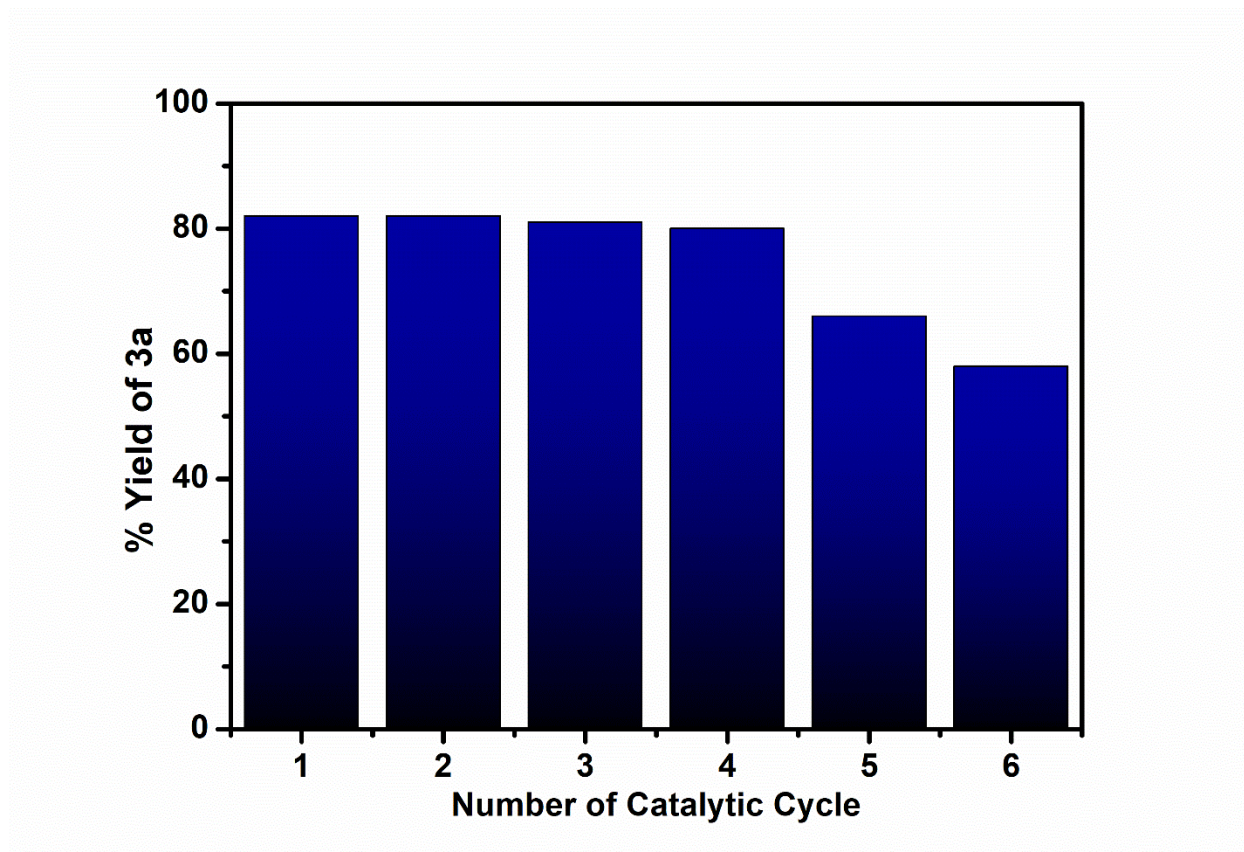


Fig. S15 Graphical representation of each consecutive run (catalytic cycle 1-6) showing % yield of 3a using Ru-NaY-1 catalyst.

Supporting Information

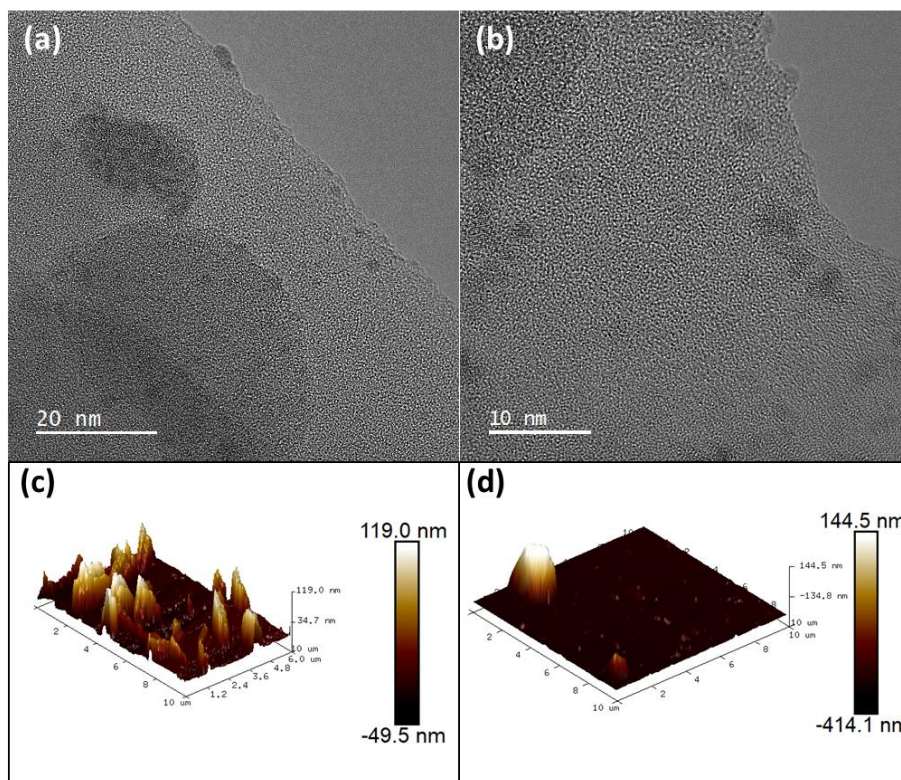


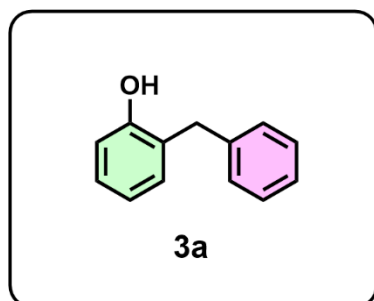
Fig. S16 (a) TEM images of reused catalyst after 6th cycle; (b) AFM images of reused catalyst after 6th cycle.

Characterization of the compound

Spectral data of synthesized compounds (3a-3o)

After the monitoring the reaction at optimized conditions the different isolated benzylated products are characterized by ¹H, ¹³C NMR, FTIR, mass and elemental analysis.

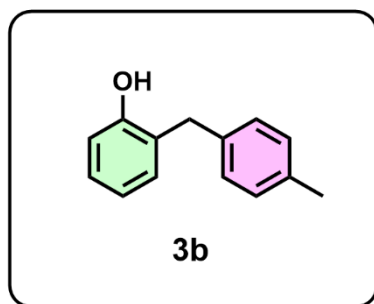
Compound 3a: 2-benzylphenol ⁴



The titled compound (Compound 3a) was synthesized by using GP-A using phenol (1 mmol) and benzyl alcohol (1.5 mmol). After completion, the product was separated and purified by column chromatography on 100-200 mesh silica gel (gradient from 0-5% ethyl acetate/n-hexanes solvent system) to afford 3a as a light brown semi-solid (82% yield). **NMR Analysis:** ¹H NMR (400 MHz, CDCl₃): δ 8.04 (d, *J* = 8.6 Hz NMR Analysis: ¹H NMR (400 MHz, CDCl₃): δ 7.32 – 7.26 (m, 2H), 7.24 – 7.18 (m, 3H), 7.13 (dd, *J* = 11.9, 4.4 Hz, 2H), 6.89 (t, *J* = 7.8 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 4.64 (s, 1H), 4.00 (s, 2H). ¹³C NMR (126 MHz, CDCl₃): δ 153.8, 140.0, 131.1, 128.8, 128.0, 127.1, 126.5, 121.1, 115.8, 36.5. **FTIR (KBr):** 3293, 3063, 3026, 2920, 2842, 1602, 1589, 1494, 1350, 1273, 1210, 1205, 1088, 850, 766, 698 cm⁻¹. **LRMS (ESI):** *m/z* calculated for C₁₃H₁₁O [M-H]⁺: 183.1, found 183.1 (100%). **Elemental Analysis:** Anal. calcd for C₁₃H₁₂O: C, 84.75; H, 6.57; found: C, 85.01.58, H, 6.51. The characterization data of synthesized compound are in accordance with the reported one.

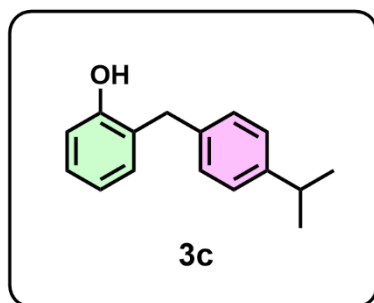
Supporting Information

Compound 3b: 2-(4-methylbenzyl)phenol ¹³



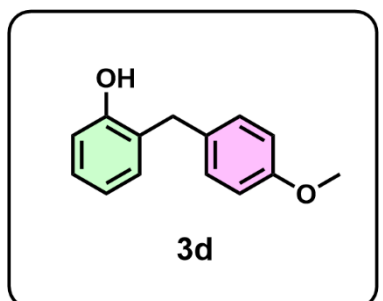
The titled compound (3b) was synthesized by using GP-A using phenol (1.0 mmol) and 4-methylbenzyl alcohol (1.5 mmol). The final crude was purified by column chromatography on 100-200 mesh silica gel (gradient from 0-5% ethyl acetate/n-hexanes solvent system) to afford 3b as a yellow liquid (85% yield). **NMR Analysis:** ¹H NMR (400 MHz, CDCl₃): δ 7.17 – 7.06 (m, 6H), 6.88 (t, *J* = 7.8 Hz, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 4.63 (s, 1H), 3.95 (s, 2H), 2.31 (s, 3H). ¹³C NMR (126 MHz, CDCl₃): δ 153.9, 136.7, 136.1, 131.1, 129.5, 128.7, 127.9, 127.3, 121.1, 115.9, 36.2, 21.2. **FTIR (KBr):** 3291, 3044, 3019, 2920, 2857, 1610, 1590, 1513, 1504, 1357, 1232, 1169, 1096, 911, 815, 760, 709 cm⁻¹. **LRMS (ESI):** m/z calculated for C₁₄H₁₃O [M-H]⁺: 197.1, found 197.1 (100%). **Elemental Analysis:** Anal. calcd for C₁₄H₁₄O: C, 84.81; H, 7.12; found: C, 84.98, H, 7.36. The reported data of synthesized compound are in accordance with the literature one.

Compound 3c: 2-(4-isopropylbenzyl)phenol ¹⁴



The titled compound (3c) was synthesized by using GP-A using phenol (1.0 mmol) and 4-isopropylbenzyl alcohol (1.5 mmol). Crude was separated and purified by chromatographic method on 100-200 mesh silica gel (gradient from 0.5-2% ethyl acetate/n-hexanes solvent system) to afford 3c as a brown-yellow liquid (86% yield). **NMR Analysis:** ¹H NMR (400 MHz, CDCl₃): δ 7.16 – 7.09 (m, 6H), 6.88 (t, *J* = 7.4 Hz, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 4.75 (s, 1H), 3.96 (s, 2H), 2.92 – 2.81 (m, 1H), 1.22 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃): δ 153.9, 147.1, 137.1, 131.1, 128.7, 127.9, 127.2, 126.9, 121.0, 115.9, 36.2, 33.8, 24.2. **FTIR (KBr):** 3531, 3021, 2960, 2926, 2870, 1607, 1592, 1511, 1489, 1455, 1328, 1257, 1212, 1090, 814, 752 cm⁻¹. **LRMS (ESI):** m/z calculated for C₁₆H₁₇O [M-H]⁺: 225.1, found 225.1 (100%). **Elemental Analysis:** Anal. calcd for C₁₆H₁₈O: C, 84.91; H, 8.02; found: C, 85.13, H, 8.16. The reported data of synthesized compound 3c are in accordance with the literature report.

Compound 3d: 2-(4-methoxybenzyl)phenol ¹⁵

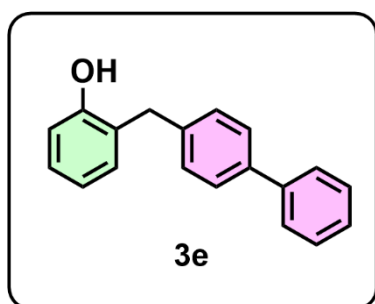


The compound 3d was synthesized by using GP-A using phenol (1.0 mmol) and 4-methoxybenzyl alcohol (1.5 mmol). After completion of the reaction under standard optimized parameters, the final product was collected after column chromatography on 100-200 mesh silica gel (gradient from 0-5% ethyl acetate/n-hexanes solvent system). Isolated pure product appeared as a brown-white solid (89% yield). **NMR Analysis:** ¹H NMR (400 MHz, CDCl₃): δ 7.13 (dd, *J* = 11.8, 8.9 Hz, 4H), 6.89 (t, *J* = 7.0 Hz, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.0 Hz, 1H), 4.66 (s, 1H), 3.94 (s, 2H), 3.78 (s, 3H). ¹³C NMR (126 MHz, CDCl₃): δ 158.3, 153.9, 131.8, 131.0, 129.8, 127.9, 127.4, 121.0,

Supporting Information

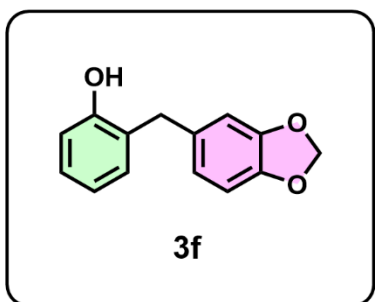
115.9, 114.2, 55.4, 35.7. **FTIR (KBr):** 3354, 3033, 2991, 2919, 2841, 1607, 1593, 1508, 1454, 1357, 1238, 1179, 1027, 912, 812, 759, 675 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{14}\text{H}_{13}\text{O}_2$ $[\text{M}-\text{H}]^+$: 213.1, found 213.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{14}\text{H}_{14}\text{O}_2$: C, 78.48; H, 6.59; found: C, 78.72, H, 6.62. The reported characterization data of compound 3d are in matched with the literature.

Compound 3e: 2-([1,1'-biphenyl]-4-ylmethyl)phenol ¹⁶



The compound 3e was synthesized by using GP-A using phenol (1.0 mmol) and biphenyl-4-methanol (1.5 mmol). The crude was separated after completion of the reaction under optimized conditions and purified by silica gel column chromatographic method (gradient from 100% n-hexanes to 1.5% ethyl acetate/n-hexanes solvent system) to give 3e as a white solid (72% isolated yield). **NMR Analysis:** ^1H NMR (400 MHz, CDCl_3): δ 7.59 – 7.49 (m, 4H), 7.42 (t, $J = 7.6$ Hz, 2H), 7.31 (dd, $J = 12.6, 7.7$ Hz, 3H), 7.15 (dd, $J = 9.8, 7.6$ Hz, 2H), 6.91 (t, $J = 7.4$ Hz, 1H), 6.80 (d, $J = 7.9$ Hz, 1H), 4.69 (s, 1H), 4.04 (s, 2H). ^{13}C NMR (126 MHz, CDCl_3): δ 153.9, 141.1, 139.5, 139.2, 131.2, 129.2, 128.9, 128.0, 127.5, 127.2, 121.2, 115.9, 36.1. **FTIR (KBr):** 3366, 3055, 3030, 2925, 2852, 1588, 1499, 1486, 1454, 1232, 1111, 1040, 861, 752, 696 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{19}\text{H}_{15}\text{O}$ $[\text{M}-\text{H}]^+$: 259.1, found 259.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{19}\text{H}_{16}\text{O}$: C, 87.66; H, 6.20; found: C, 87.90, H, 6.53. All the characterization data are in good matched with the previous report.

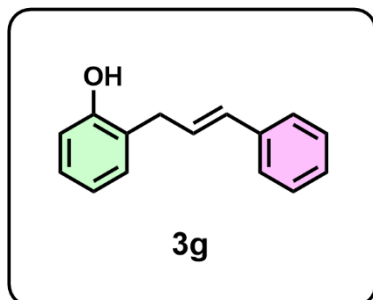
Compound 3f: 2-(benzo[d][1,3]dioxol-5-ylmethyl)phenol



Compound 3f was prepared by using the GP-A taking phenol (1.0 mmol) along with benzo[d][1,3]dioxol-5-ylmethanol (1.5 mmol) under optimized condition. The organic product was isolated and separated by column chromatographic technique using 100-200 mesh silica gel (gradient from 0-5% ethyl acetate/n-hexanes solvent system), afforded to 3f as brown semi-solid (65% yield) **NMR Analysis:** ^1H NMR (400 MHz, CDCl_3): δ 7.14 – 7.08 (m, 2H), 6.89 (t, $J = 7.4$ Hz, 1H), 6.73 (ddd, $J = 13.5, 12.1, 6.2$ Hz, 4H), 5.91 (s, 2H), 4.74 (s, 1H), 3.91 (s, 2H). ^{13}C NMR (126 MHz, CDCl_3): δ 154.0, 148.1, 146.3, 133.8, 131.0, 128.0, 127.2, 121.5, 121.1, 115.9, 109.3, 108.4, 101.0, 36.3. **FTIR (KBr):** 3460, 3067, 2920, 1607, 1501, 1488, 1455, 1443, 1243, 1186, 1039, 927, 846, 810, 754 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{14}\text{H}_{11}\text{O}_3$ $[\text{M}-\text{H}]^+$: 227.1, found 227.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{14}\text{H}_{12}\text{O}_3$: C, 73.67; H, 5.30; found: C, 73.85, H, 5.39.

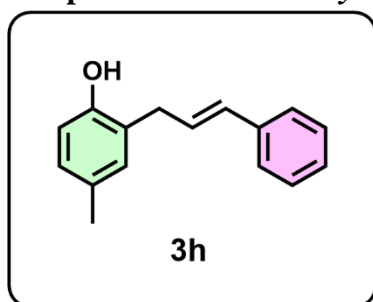
Compound 3g: 2-cinnamylphenol ¹⁷

Supporting Information



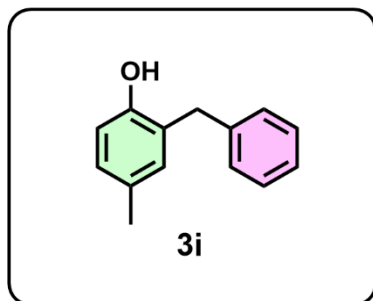
Prepared the compound (3g) using GP-A taking phenol (1.0 mmol), and cinnamyl alcohol (1.5 mmol) in 1 mL DCE at 80 °C for 6 h. The final organic product was purified by silica gel column chromatographic method (30 cm long column pack) 100-200 mesh silica gel (n-hexanes/EtOAc 100:0 to 99:1 v/v). The obtained product 3g was collected as a yellow liquid (88% yield). **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.37 – 7.26 (m, 4H), 7.24 – 7.10 (m, 3H), 6.90 (t, $J = 7.4$ Hz, 1H), 6.81 (d, $J = 8.0$ Hz, 1H), 6.51 (d, $J = 15.9$ Hz, 1H), 6.38 (dt, $J = 15.9, 6.4$ Hz, 1H), 4.92 (s, 1H), 3.57 (d, $J = 6.3$ Hz, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 154.1, 137.2, 131.6, 130.6, 128.7, 128.0, 127.4, 126.3, 125.8, 121.1, 115.9, 34.2. **FTIR (KBr):** 3418, 3028, 2925, 2852, 1660, 1624, 1595, 1496, 1455, 1234, 1169, 1098, 968, 833, 753, 737, 692 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{15}\text{H}_{13}\text{O}$ $[\text{M}-\text{H}]^+$: 209.1, found 209.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{15}\text{H}_{14}\text{O}$: C, 85.68; H, 6.71; found: C, 85.79, H, 6.83. The spectral information of the compound is matched with previous reports.

Compound 3h: 2-cinnamyl-4-methylphenol ¹⁸



Prepared 3h applying GP-A taking p-cresol (1.0 mmol), and cinnamyl alcohol (1.5 mmol) in 1 mL of optimized solvent at 80 °C for 6 h. The product was purified and separated by silica gel column chromatographic process using 100-200 mesh silica gel (taking gradient from n-hexanes/EtOAc 100:0 to 99:1 v/v). The obtained product 3h was collected as a yellow oil (89% yield). **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.38 – 7.26 (m, 4H), 7.20 (t, $J = 7.2$ Hz, 1H), 6.94 (dd, $J = 13.0, 5.0$ Hz, 2H), 6.71 (d, $J = 8.0$ Hz, 1H), 6.50 (d, $J = 15.9$ Hz, 1H), 6.37 (dt, $J = 15.8, 6.5$ Hz, 1H), 4.81 (s, 1H), 3.52 (d, $J = 6.3$ Hz, 2H), 2.26 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 151.9, 137.3, 131.5, 131.1, 130.3, 128.7, 128.4, 128.2, 127.4, 126.3, 125.6, 115.7, 34.2, 20.6. **FTIR (KBr):** 3420, 3025, 2923, 2854, 1612, 1508, 1448, 1259, 1205, 1106, 966, 812, 748, 692 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{16}\text{H}_{15}\text{O}$ $[\text{M}-\text{H}]^+$: 223.1, found 223.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{16}\text{H}_{16}\text{O}$: C, 85.68; H, 7.19; found: C, 85.78, H, 7.26. The characterization data matches with previously reported data.

Compound 3i: 2-benzyl-4-methylphenol ¹⁶

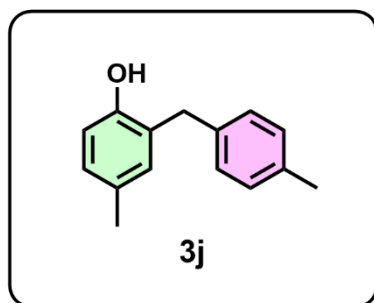


The compound 3i was synthesized by using GP-A using p-cresol (1.0 mmol) and benzyl alcohol (1.5 mmol). After completion under standard conditions, the organic crude part was separated and purified by silica gel column chromatography on 100-200 mesh silica gel (gradient from 0-1% ethyl acetate/n-hexanes solvent system) to afford 3i as a colorless oil (84% yield) $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.23 (tt, $J = 14.9, 7.2$ Hz, 5H), 6.91 (d, $J = 6.7$ Hz, 2H), 6.66 (d, $J = 8.7$ Hz, 1H), 4.91 (s, 1H), 3.95 (s, 2H), 2.24 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 151.6, 140.3, 131.6, 130.1, 128.8, 128.7,

Supporting Information

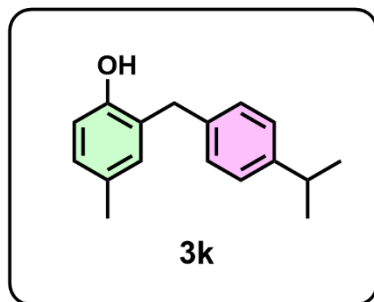
128.3, 126.9, 126.4, 36.4, 20.6. **FTIR (KBr):** 3380, 2979, 2923, 2853, 1740, 1511, 1485, 1463, 1376, 1206, 1040, 859, 806, 760 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{14}\text{H}_{13}\text{O}$ $[\text{M}-\text{H}]^+$: 197.1, found 197.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{14}\text{H}_{14}\text{O}$: C, 84.81; H, 7.12; found: C, 85.01, H, 7.17. The spectral data accordance with previously reported data.

Compound 3j: 4-methyl-2-(4-methylbenzyl)phenol



The titled compound (3j) was prepared by applying GP-A taking p-cresol (1.0 mmol) and 4-methylbenzyl alcohol (1.5 mmol) as reactant. After completion, the required organic product was isolated and purified by silica gel column chromatographic technique using 100-200 mesh silica gel (gradient from 0-2% ethyl acetate/n-hexanes solvent system) to afford 3j as a colorless oil (86%). **^1H NMR (400 MHz, CDCl_3):** δ 7.14 – 7.06 (m, 4H), 6.91 (d, $J = 7.6$ Hz, 2H), 6.67 (d, $J = 7.8$ Hz, 1H), 4.55 (s, 1H), 3.91 (s, 2H), 2.31 (s, 3H), 2.25 (s, 3H). **^{13}C NMR (151 MHz, CDCl_3):** δ 151.6, 136.9, 136.0, 131.6, 130.2, 129.5, 128.6, 128.3, 127.0, 115.8, 36.2, 21.2, 20.6. **FTIR (KBr):** 3339, 3026, 2923, 2853, 1601, 1509, 1493, 1449, 1427, 1258, 1210, 1120, 1031, 883, 832, 777, 725, 692, 623 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{15}\text{H}_{15}\text{O}$ $[\text{M}-\text{H}]^+$: 211.1, found 211.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{15}\text{H}_{16}\text{O}$: C, 84.87; H, 7.60; found: C, 85.12, H, 7.72.

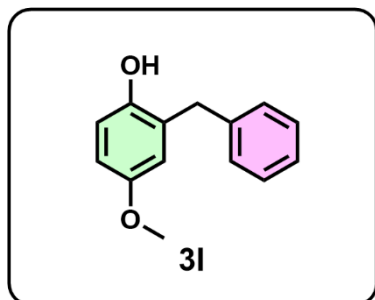
Compound 3k: 2-(4-isopropylbenzyl)-4-methylphenol



Prepared from the standard GP-A using p-cresol (1.0 mmol) and 4-isopropylbenzyl alcohol (1.5 mmol) as starting materials. After completion, the pure product was isolated from crude materials and purified by chromatographic technique using silica gel (60-120 mesh) with appropriate solvent system (1.5-5% ethyl acetate/n-hexanes) affording to 3k as colorless oil (86% yield). **NMR Analysis:** **^1H NMR (400 MHz, CDCl_3):** δ 7.14 (s, 4H), 6.95 – 6.89 (m, 2H), 6.68 (d, $J = 8.0$ Hz, 1H), 4.55 (s, 1H), 3.92 (s, 2H), 2.87 (hept, $J = 6.9$ Hz, 1H), 2.25 (s, 3H), 1.22 (d, $J = 6.9$ Hz, 6H). **^{13}C NMR (151 MHz, CDCl_3):** δ 151.7, 147.0, 137.3, 131.7, 130.2, 128.6, 128.3, 126.9, 126.9, 115.8, 36.2, 33.8, 24.1, 20.7. **FTIR (KBr):** 3435, 3011, 2959, 2924, 2868, 1613, 1510, 1462, 1418, 1382, 1259, 1187, 1106, 812, 720 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{17}\text{H}_{19}\text{O}$ $[\text{M}-\text{H}]^+$: 239.1, found 239.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{17}\text{H}_{20}\text{O}$: C, 84.96; H, 8.39; found: C, 85.12, H, 8.41.

Compound 3l: 2-benzyl-4-methoxyphenol¹⁶

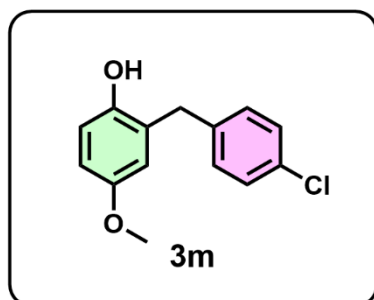
Supporting Information



Prepared the mentioned compound 3l using the standard GP-A using 4-methoxy phenol (1.0 mmol) and benzyl alcohol (1.5 mmol) as starting materials. Under standard condition, the crude product was isolated and refined by silica gel column chromatography packing with silica (60-120 mesh) with using 1.5% to 7 % ethyl acetate/n-hexanes solvent system producing 3l as colorless oil (88% yield). **NMR Analysis:** $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.29 (t, $J = 7.5$ Hz, 2H), 7.21 (dd, $J = 12.9, 7.1$ Hz, 3H), 6.73 (d, $J = 8.3$ Hz, 1H), 6.70 – 6.64 (m, 2H), 4.35 (s, 1H), 3.96 (s, 2H), 3.73 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 153.9, 147.8, 139.8, 128.8, 128.3, 126.5, 116.8, 116.6, 112.5, 55.8, 36.8. **FTIR (KBr):** 3325, 3085, 3027, 2921, 2835, 1600, 1508, 1494, 1438, 1388, 1266, 1213, 1187, 1039, 801, 726, 696 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{14}\text{H}_{13}\text{O}_2$ [M-H] $^+$: 213.1, found 213.1 (100%). **Elemental Analysis:** Anal. calcd for the $\text{C}_{14}\text{H}_{14}\text{O}_2$: C, 78.48; H, 6.59; found: C, 78.56, H, 6.53. The data are in good agreement with the previous literature reports.

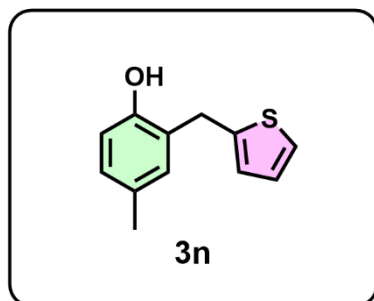
Compound 3m: 2-(4-chlorobenzyl)-4-methoxyphenol

The titled compound 3m was synthesized by applying the standard GP-A taking 4-methoxy phenol (1.0 mmol) and 4-chlorobenzyl alcohol (1.5 mmol) as starting materials. After completion, the crude product was isolated and purified by column chromatography with silica gel (60-120 mesh) with solvent gradient from 1% to 5 % ethyl acetate/n-hexanes producing 3m as colorless oil (54% yield).



$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.26 – 7.22 (m, 2H), 7.15 (d, $J = 8.3$ Hz, 2H), 6.70 (d, $J = 8.3$ Hz, 1H), 6.68 – 6.63 (m, 2H), 4.48 (s, 1H), 3.91 (s, 2H), 3.73 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 153.9, 147.6, 138.6, 132.1, 130.2, 128.7, 128.0, 116.7, 116.4, 112.5, 55.8, 35.9. **FTIR (KBr):** 3376, 2926, 2850, 1602, 1508, 1491, 1436, 1270, 1208, 1089, 1036, 840, 823, 742, 717 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{14}\text{H}_{12}\text{ClO}_2$ [M-H] $^+$: 247.0, found 247.0 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{14}\text{H}_{13}\text{ClO}_2$: C, 67.61; H, 5.27; found: C, 67.82, H, 5.35.

Compound 3n: 4-methyl-2-(thiophen-2-ylmethyl)phenol

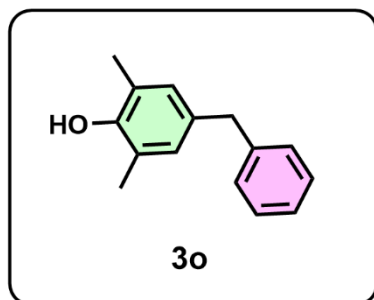


Compound 3n was produced by using the standard GP-A taking p-cresol (1.0 mmol) and 2-Thiophenemethanol (1.5 mmol) as starting reactant materials. After completion of the reaction, product was isolated and purified by silica gel column chromatography. The chromatographic method was executed by using silica gel (100-200 mesh) with solvent pair gradient from 0.5% to 5 % ethyl acetate/n-hexanes affording the required product 3n as yellow oil (79% yield). $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.15 (dd, $J = 5.1, 1.1$ Hz, 1H), 6.97 (s, 1H), 6.96 – 6.90 (m, 2H), 6.84 (dd, $J = 3.4, 1.0$ Hz, 1H), 6.69 (d, $J = 8.1$ Hz, 1H), 4.69 (s, 1H), 4.13 (s, 2H), 2.26 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 151.5, 143.3, 131.2, 130.4, 128.7, 127.0, 126.4, 125.3, 124.3, 115.9, 30.9, 20.6. **FTIR**

Supporting Information

(KBr): 3421, 2923, 2853, 1612, 1508, 1434, 1324, 1262, 1188, 1097, 1037, 850, 812, 696 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{12}\text{H}_{13}\text{OS}^+$ $[\text{M}+\text{H}]^+$: 205.1, found 205.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{12}\text{H}_{12}\text{OS}$: C, 70.55; H, 6.92; found: C, 70.69, H, 6.98.

Compound 3o: 4-benzyl-2,6-dimethylphenol¹⁹

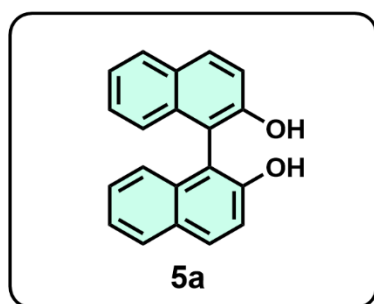


Compound 3o was synthesized via standard GP-A by using 2,6-dimethyl phenol (1.0 mmol) and benzyl alcohol (1.5 mmol) as reactant. After completion of the reaction, the final product was purified by column chromatography taking 100-200 mesh silica gel (using solvent system from 100% n-hexanes to 3 % ethyl acetate/n-hexanes affording to 3o as white solid (43% yield). **¹H NMR (400 MHz, CDCl_3):** δ 7.28 (d, J = 7.8 Hz, 2H), 7.18 (dd, J = 7.1, 5.2 Hz, 3H), 6.80 (s, 2H), 4.46 (s, 1H), 3.84 (s, 2H), 2.20 (s, 6H). **¹³C NMR (151 MHz, CDCl_3):** δ 150.6, 141.9, 132.9, 129.2, 128.9, 128.5, 41.2, 16.0. **FTIR (KBr):** 3392, 3065, 3025, 2922, 2850, 1602, 1492, 1451, 1347, 1303, 1211, 1146, 1029, 878, 779, 726, 695 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{15}\text{H}_{15}\text{O}$ $[\text{M}-\text{H}^+]$: 211.1, found 211.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{15}\text{H}_{16}\text{O}$: C, 84.87; H, 7.60; found: C, 85.01, H, 7.69. The characterization data of the synthesized compound are in accordance with the reported data.

Characterization data for oxidative coupling reaction (5a-5h)

The isolated C-C coupling products (5a-5h) were characterized by analytical tools such as ¹H-NMR, ¹³C-NMR, FT-IR, LCMS mass spectra, elemental analysis HRMS analysis.

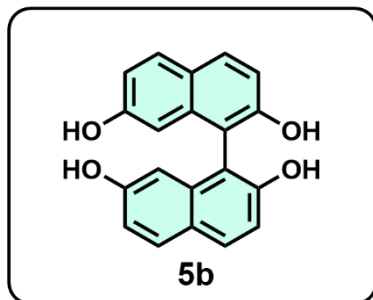
❖ Compound 5a: [1,1'-binaphthalene]-2,2'-diol¹⁰



[1,1'-binaphthalene]-2,2'-diol (5a) was synthesized by acquiring general procedure C (GP-C) taking 2-naphthol (2 mmol) as substrate. The final product was isolated and purified by using silica gel (60-120 mesh) column chromatographic technique (eluent- ethyl acetate/n-hexanes) produced 5a as gray solid (91% yield). **NMR Analysis: ¹H NMR (500 MHz, CDCl_3):** δ 7.98 (d, J = 8.9 Hz, 2H), 7.89 (d, J = 8.0 Hz, 2H), 7.37 (dd, J = 11.7, 4.8 Hz, 4H), 7.31 (t, J = 8.1 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 5.06 (s, 2H). **¹³C NMR (126 MHz, CDCl_3):** δ 152.9, 133.5, 131.6, 129.6, 128.6, 127.6, 124.3, 124.2, 117.9, 111.0. **FTIR (KBr):** 3509, 3433, 3057, 1617, 1594, 1511, 1468, 1382, 1347, 1317, 1271, 1220, 1182, 1147, 1126, 979, 962, 950, 870, 815, 748, 663, 564 cm^{-1} . **LRMS (ESI+):** m/z calculated $\text{C}_{20}\text{H}_{14}\text{O}_2$ $[\text{M}-\text{H}]^+$: 285.1, found: 285.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{14}\text{O}_2$: C, 80.90; H, 4.93; found: C, 80.78, H, 4.98. All the spectral data are according to the literature reports.

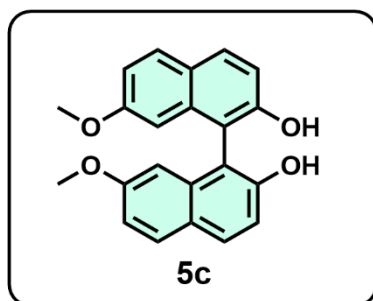
❖ Compound 5b: [1,1'-binaphthalene]-2,2',7,7'-tetraol²⁰

Supporting Information



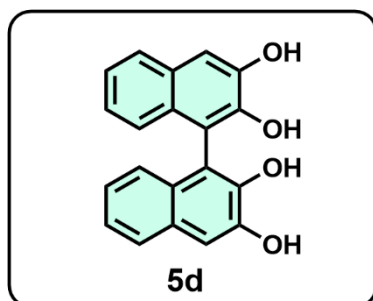
As described in GP-C 2,7-dihydroxynaphthalene (2 mmol) was taken as substrate. Compound [1,1'-binaphthalene]-2,2',7,7'-tetraol was isolated by silica gel (100-200 mesh) column chromatographic technique using the eluent ethyl acetate/n-hexanes solvent system (gradient from 5%-25%) as gray solid (94% yield). **NMR Analysis:** $^1\text{H NMR}$ (600 MHz, MeOD): δ 7.76 (d, $J = 8.8$ Hz, 2H), 7.70 (d, $J = 8.8$ Hz, 2H), 7.10 (d, $J = 8.8$ Hz, 2H), 6.86 (d, $J = 8.7$ Hz, 2H), 6.44 (s, 2H) ppm. $^{13}\text{C NMR}$ (151 MHz, MeOD): δ 156.8, 154.5, 137.4, 130.6, 130.3, 125.5, 116.2, 115.9, 114.7, 107.7 ppm. **FTIR (KBr):** 3489, 3325, 2924, 1621, 1514, 1450, 1392, 1369, 1343, 1297, 1213, 1162, 1187, 1138, 962, 880, 826, 681, 635, 569, 485 cm^{-1} . **LRMS (ESI+):** m/z calculated $\text{C}_{20}\text{H}_{13}\text{O}_4$ $[\text{M}-\text{H}]^+$: 317.1, found: 317.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{14}\text{O}_4$: C, 75.46; H, 4.43; found: C, 75.58, H, 4.53. The spectral information are good agreement with the previous report.

❖ Compound 5c: 7,7'-dimethoxy-[1,1'-binaphthalene]-2,2'-diol ²¹



The title compound 7,7'-dimethoxy-[1,1'-binaphthalene]-2,2'-diol (5c) was produced by applying the described GP-C and the compound were isolated by column chromatography taking silica gel (mesh 60-120) with eluent: ethyl acetate/n-hexanes (gradient from 5-15%). The final product was collected as pinkish-gray solid (92%). **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.85 (d, $J = 8.8$ Hz, 2H), 7.76 (d, $J = 8.9$ Hz, 2H), 7.20 (d, $J = 8.9$ Hz, 2H), 7.02 (dd, $J = 8.9, 2.5$ Hz, 2H), 6.47 (d, $J = 2.3$ Hz, 2H), 5.10 (s, 2H), 3.56 (s, 6H) ppm. $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ (ppm) 159.2, 153.4, 134.8, 131.2, 130.1, 124.9, 116.1, 115.2, 110.2, 103.3, 55.3 ppm. **FTIR (KBr):** 3367, 2996, 2923, 2852, 1711, 1628, 1516, 1464, 1430, 1382, 1337, 1270, 1221, 1186, 1019, 978, 902, 816, 775, 598, 521 cm^{-1} . **LRMS (ESI+):** m/z calculated $\text{C}_{22}\text{H}_{17}\text{O}_4$ $[\text{M}-\text{H}]^+$: 345.1, found: 345.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{22}\text{H}_{18}\text{O}_4$: C, 76.29; H, 5.24; found: C, 76.40, H, 5.31. The characterization data are matched with previous ones.

❖ Compound 5d: [1,1'-binaphthalene]-2,2',3,3'-tetraol ²⁰

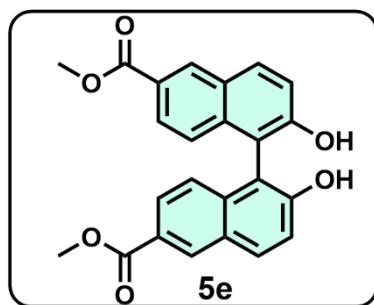


Compound named [1,1'-binaphthalene]-2,2',3,3'-tetraol (5d) was synthesized by as described the GP-C. The gray solid product was isolated by silica (60-120 mesh) gel column chromatography with solvent gradient from 15-35% ethyl acetate/n-hexanes system (88%). **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, MeOD): δ 7.67 (d, $J = 8.1$ Hz, 2H), 7.30 (s, 2H), 7.21 (t, $J = 7.4$ Hz, 2H), 7.02 (t, $J = 7.6$ Hz, 2H), 6.95 (d, $J = 8.2$ Hz, 2H) ppm. $^{13}\text{C NMR}$ (151 MHz, MeOD): δ 147.3, 145.8, 131.0, 130.3, 127.1, 125.7,

Supporting Information

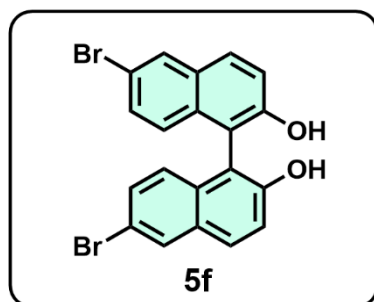
124.3, 124.2, 116.7, 110.4 ppm. **FTIR (KBr):** 3466, 3401, 2922, 2851, 2523, 1602, 1514, 1448, 1384, 1341, 1300, 1243, 1146, 1105, 921, 863, 829, 745, 699, 642, 532 cm^{-1} . **LRMS (ESI):** m/z calculated $\text{C}_{20}\text{H}_{13}\text{O}_4$ $[\text{M}-\text{H}]^+$: 317.1, found: 317.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{14}\text{O}_4$: C, 75.46; H, 4.43; found: C, 75.55, H, 4.50. All the data regarding its characterization as good agreement with literature data.

❖ Compound 5e: dimethyl 2,2'-dihydroxy-[1,1'-binaphthalene]-6,6'-dicarboxylate ²²



The title compound dimethyl 2,2'-dihydroxy-[1,1'-binaphthalene]-6,6'-dicarboxylate (5e) was produced via GP-C. The red-orange solid was collected after column chromatographic separation technique. The process used silica gel (60-120 mesh) and ethyl acetate/n-hexanes solvents system as eluent (yield: 85%). **NMR Analysis:** ^1H NMR (400 MHz, DMSO): δ 9.81 (s, 2H), 8.59 (s, 2H), 8.10 (d, $J = 9.0$ Hz, 2H), 7.69 (dd, $J = 8.9, 1.7$ Hz, 2H), 7.42 (d, $J = 8.9$ Hz, 2H), 7.01 (d, $J = 8.9$ Hz, 2H), 3.86 (s, 6H) ppm. ^{13}C NMR (151 MHz, CDCl_3): ^{13}C NMR (151 MHz, DMSO) δ 166.5, 155.6, 136.5, 131.0, 130.8, 127.1, 125.1, 124.6, 123.4, 119.5, 115.1, 52.0 ppm. **FTIR (KBr):** 3419, 2921, 2852, 1650, 1438, 1407, 1316, 1288, 1141, 1022, 953, 709 cm^{-1} . **LRMS (ESI):** m/z calculated $\text{C}_{24}\text{H}_{17}\text{O}_6$ $[\text{M}-\text{H}]^+$: 401.1, found: 401.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{24}\text{H}_{18}\text{O}_6$: C, 71.64; H, 4.51; found: C, 71.87, H, 4.62. The crystal structure of the compound was also characterized and the required data and **CCDC-2295241** number were also provided. The spectral data of the compound are in matched with previous report.

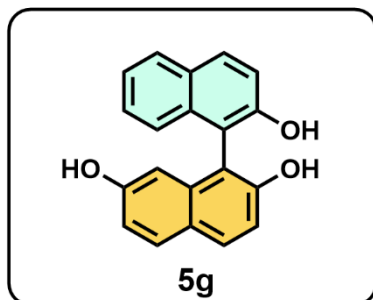
❖ Compound 5f: 6,6'-dibromo-[1,1'-binaphthalene]-2,2'-diol ²³



Compound 6,6'-dibromo-[1,1'-binaphthalene]-2,2'-diol (5f) was synthesized by using GP-C using 6-bromo-2-naphthol as starting materials. The gray solid was isolated and collected from silica column. The yield of 5f was 84%. **NMR Analysis:** ^1H NMR (400 MHz, CDCl_3): δ 8.05 (d, $J = 1.8$ Hz, 2H), 7.89 (d, $J = 8.9$ Hz, 2H), 7.43 – 7.33 (m, 4H), 6.96 (d, $J = 8.9$ Hz, 2H), 5.06 (s, 2H). ^{13}C NMR (151 MHz, CDCl_3): δ 153.1, 132.0, 131.0, 130.8, 130.7, 130.6, 126.0, 119.1, 118.1, 110.8. **FTIR (KBr):** 3401, 3062, 2923, 2852, 1710, 1588, 1497, 1464, 1379, 1337, 1265, 1211, 1078, 965, 928, 877, 812, 751, 671, 549 cm^{-1} . **LRMS (ESI):** m/z calculated $\text{C}_{20}\text{H}_{13}\text{Br}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 442.9, found: 442.9 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{12}\text{Br}_2\text{O}_2$: C, 54.09; H, 2.72; found: C, 54.18, H, 2.79. The compound 5f was characterized and the data are matched with reported data.

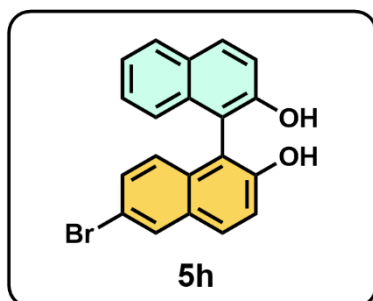
❖ Compound 5g: [1,1'-binaphthalene]-2,2',7-triol ²⁴

Supporting Information



The cross product of 2-naphthol and 2,7-dihydroxynaphthalene, compound (5g) [1,1'-binaphthalene]-2,2',7-triol was synthesized by applying GP-C. The final product was collected from column chromatography using silica gel (60-120 mesh), with 7-11% ethyl acetate/n-hexanes solvent system. The product was collected as gray solid with 81% yield. **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.97 (d, $J = 8.9$ Hz, 1H), 7.92 – 7.86 (m, 2H), 7.79 (d, $J = 8.8$ Hz, 1H), 7.41 – 7.35 (m, 2H), 7.32 (t, $J = 6.9$ Hz, 1H), 7.22 (d, $J = 8.9$ Hz, 1H), 7.17 (d, $J = 8.3$ Hz, 1H), 6.97 (dd, $J = 8.8, 2.5$ Hz, 1H), 6.41 (s, 1H), 5.21 (d, $J = 118.6$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 155.2, 153.6, 152.9, 135.1, 133.4, 131.6, 131.4, 130.6, 129.6, 128.6, 127.7, 124.9, 124.3, 124.2, 117.9, 115.7, 115.4, 111.0, 109.5, 106.5. **FTIR (KBr):** 3402, 2922, 2851, 1620, 1515, 1463, 1378, 1184, 972, 820, 748 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{20}\text{H}_{13}\text{O}_3$ $[\text{M}-\text{H}]^+$: 301.1, found: 301.1 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{14}\text{O}_3$: C, 79.46; H, 4.67; found: C, 79.59, H, 4.63. The spectral data are in according to the previous one.

❖ Compound 5h: 6-bromo-[1,1'-binaphthalene]-2,2'-diol ²⁴

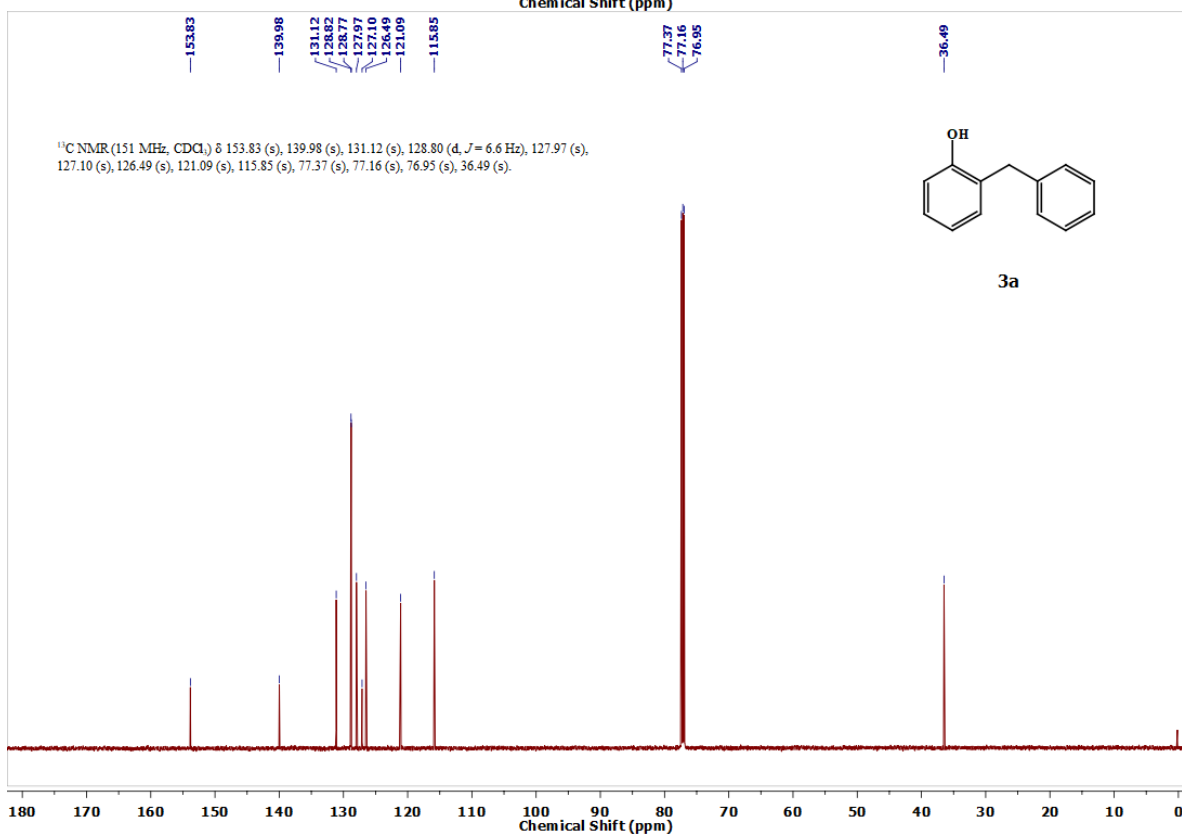
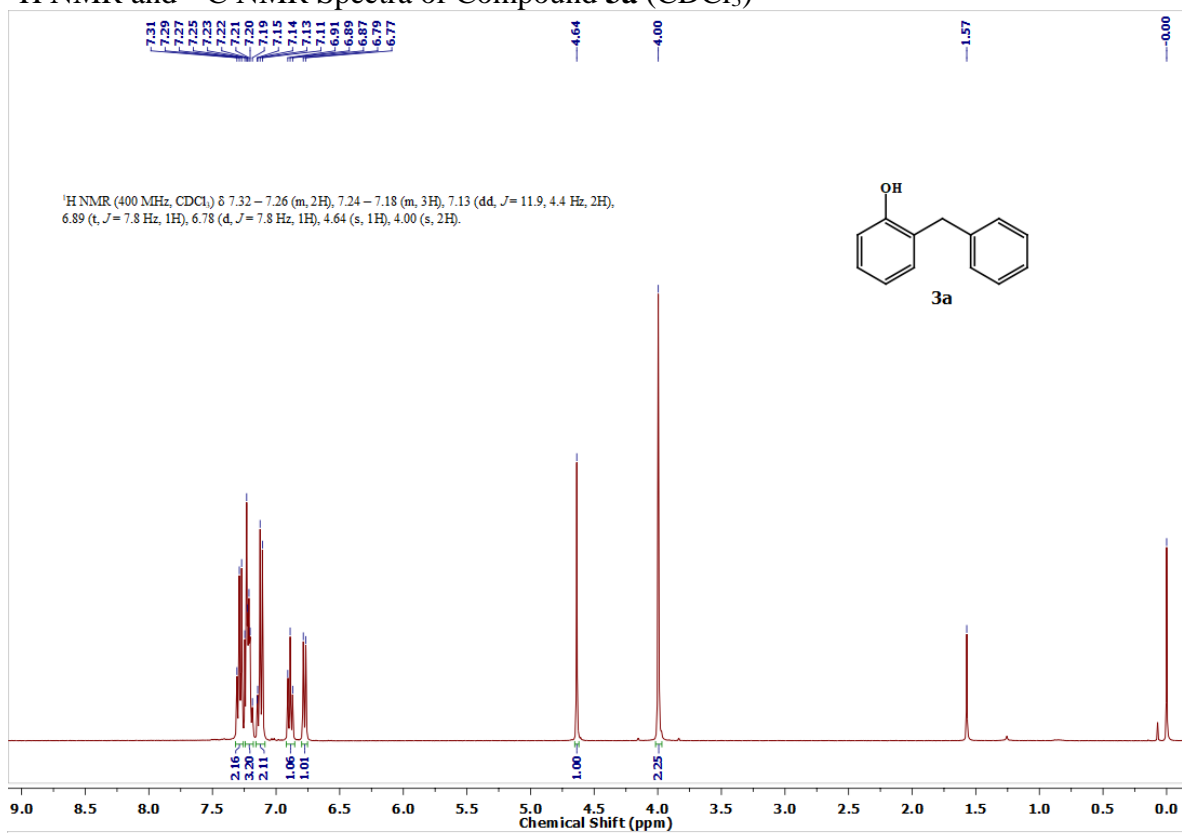


The cross product of 2-naphthol and 6-bromo-2-naphthol, compound (5h) 6-bromo-[1,1'-binaphthalene]-2,2'-diol was produced by using GP-C. The final product was isolated and collected from silica gel (60-120 mesh) column chromatography using appropriate solvents system (2-4% ethyl acetate/n-hexanes). The product was collected as white solid as 70% **NMR Analysis:** $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.03 (d, $J = 1.9$ Hz, 1H), 7.96 (d, $J = 8.9$ Hz, 1H), 7.87 (t, $J = 8.4$ Hz, 2H), 7.41 – 7.28 (m, 5H), 7.08 (d, $J = 8.4$ Hz, 1H), 7.00 (d, $J = 8.9$ Hz, 1H), 5.05 (d, $J = 36.7$ Hz, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 153.1, 152.8, 133.4, 132.1, 131.8, 130.8, 130.7, 130.5, 130.5, 129.6, 128.6, 127.8, 126.2, 124.3, 124.1, 119.1, 118.0, 117.9, 111.4, 110.4. **FTIR (KBr):** 3421, 2924, 2853, 2347, 1594, 1460, 1377, 1176, 817, 747 cm^{-1} . **LRMS (ESI):** m/z calculated for $\text{C}_{20}\text{H}_{14}\text{BrO}_2$ $[\text{M}+\text{H}]^+$: 365.0, found 365.0 (100%). **Elemental Analysis:** Anal. calcd for $\text{C}_{20}\text{H}_{13}\text{BrO}_2$: C, 65.77; H, 3.59; found: C, 65.91, H, 3.53. The spectral information of compound 5h is in good agreement with previous report.

Supporting Information

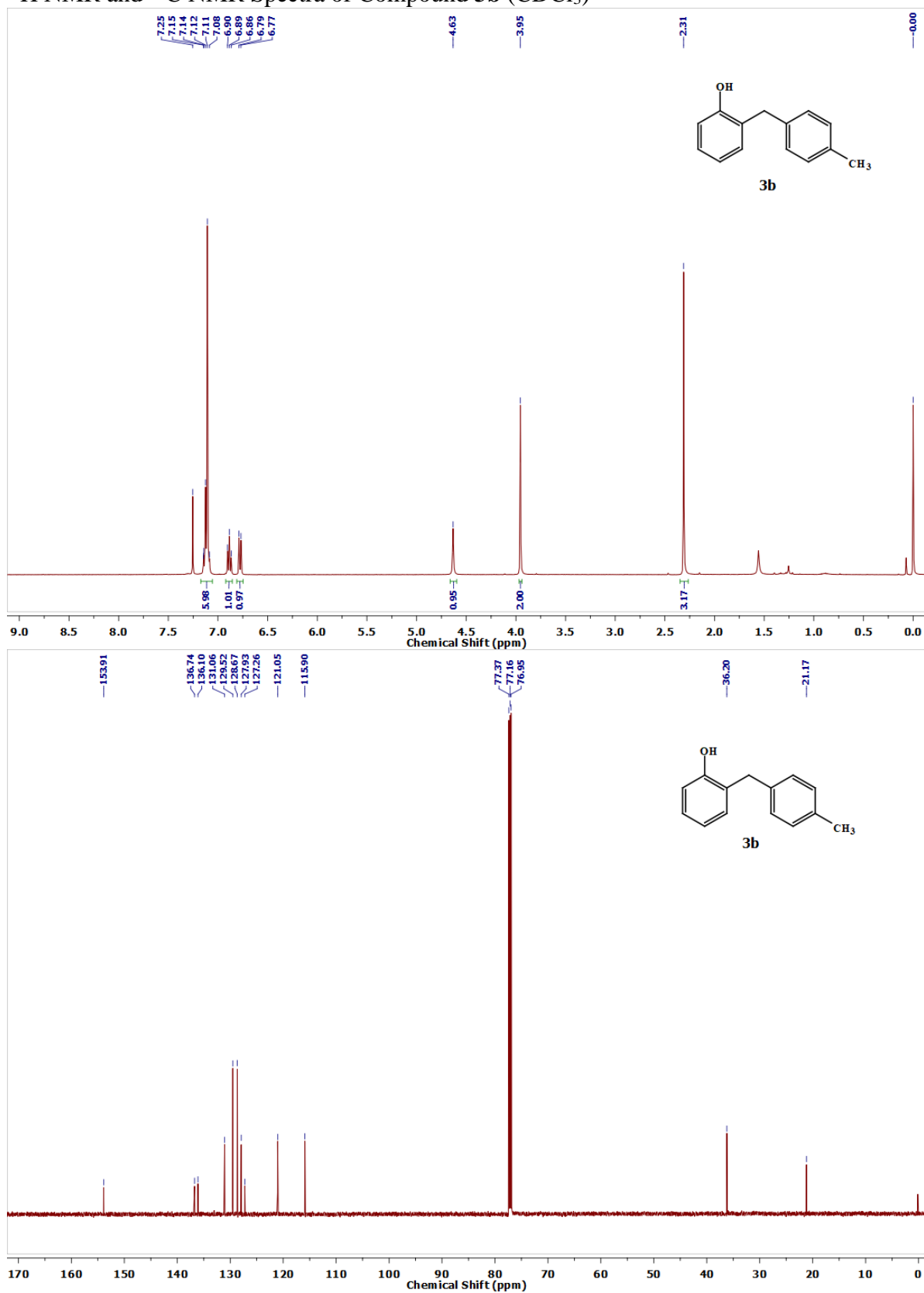
❖ NMR Spectra of all synthesized products, Compound 3a-3o

• ^1H NMR and ^{13}C NMR Spectra of Compound 3a (CDCl_3)



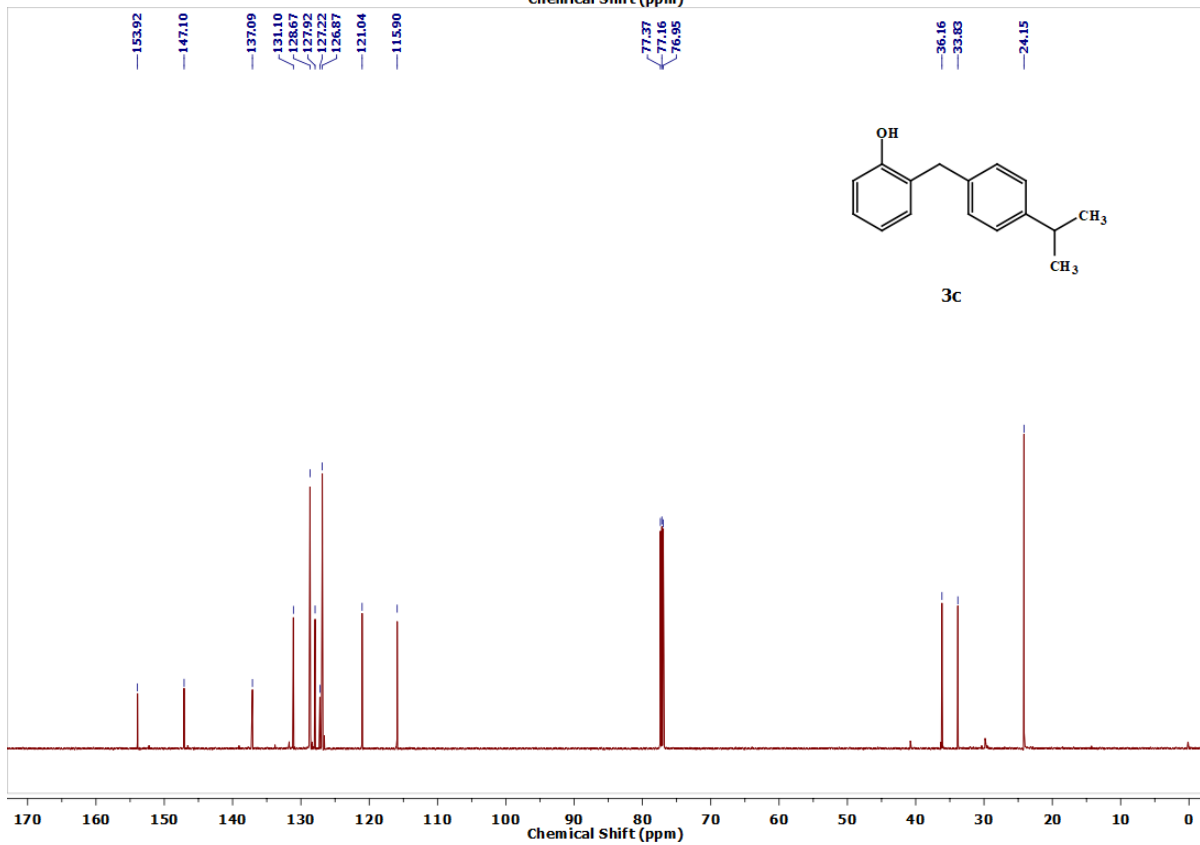
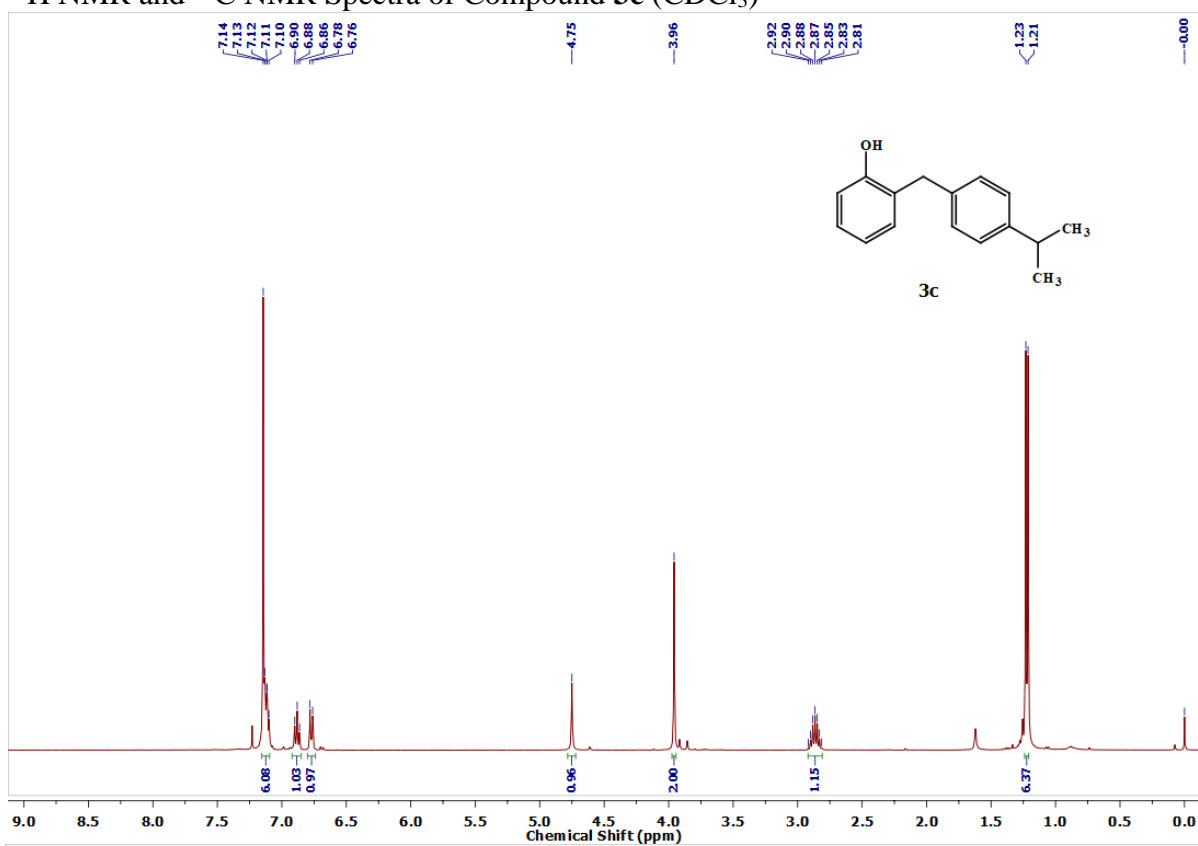
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3b** (CDCl_3)



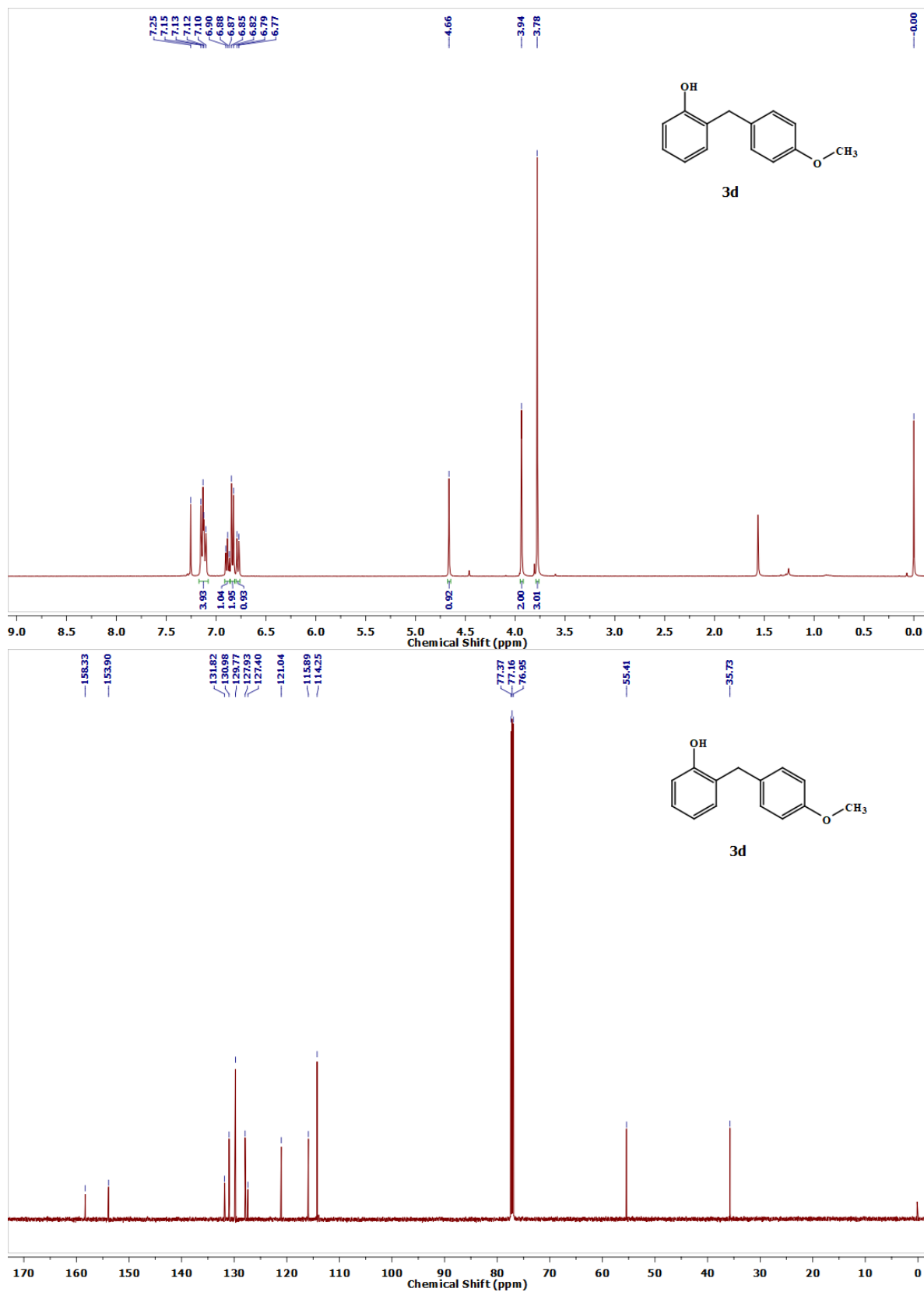
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3c** (CDCl_3)



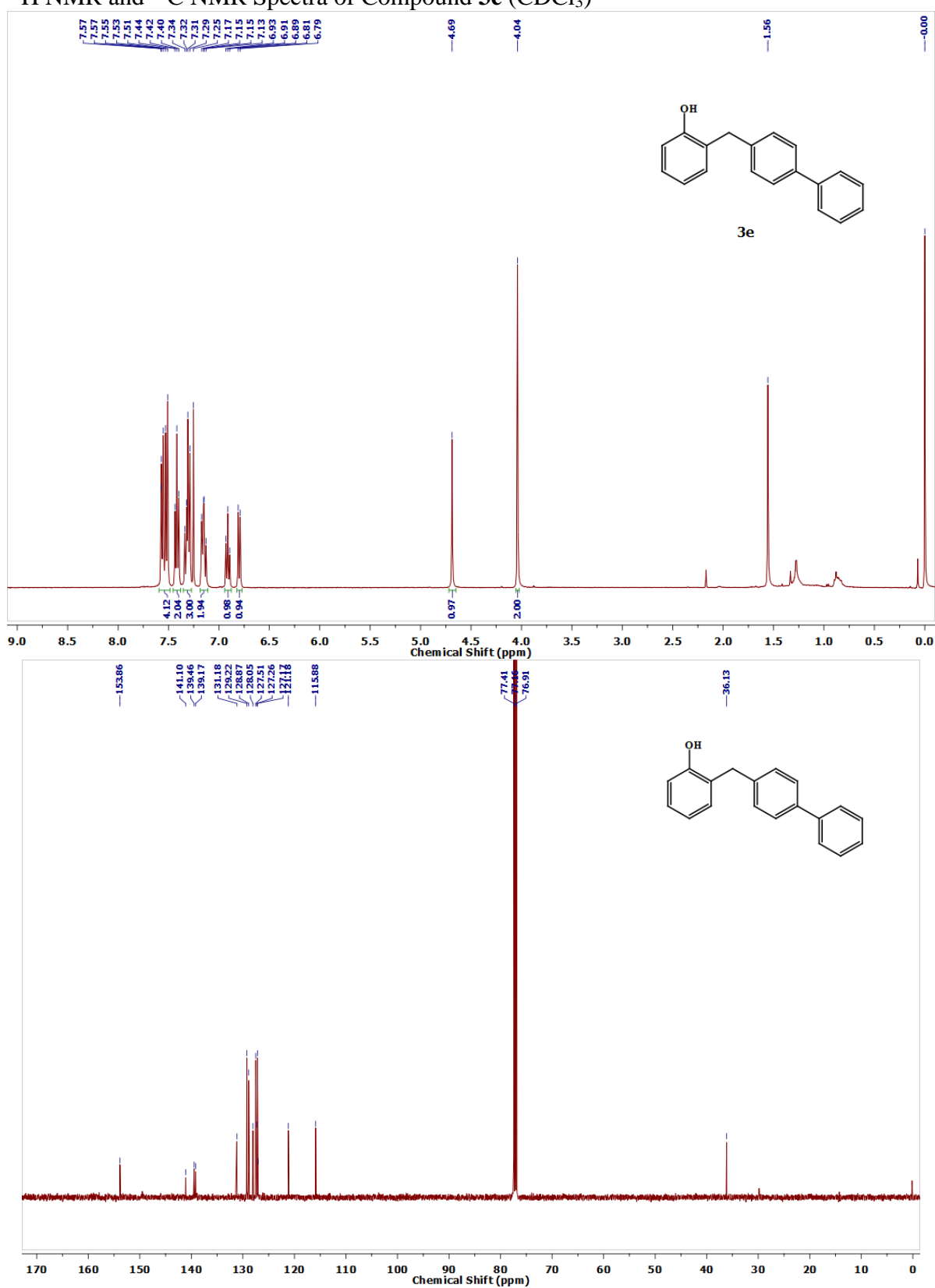
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3d** (CDCl_3)



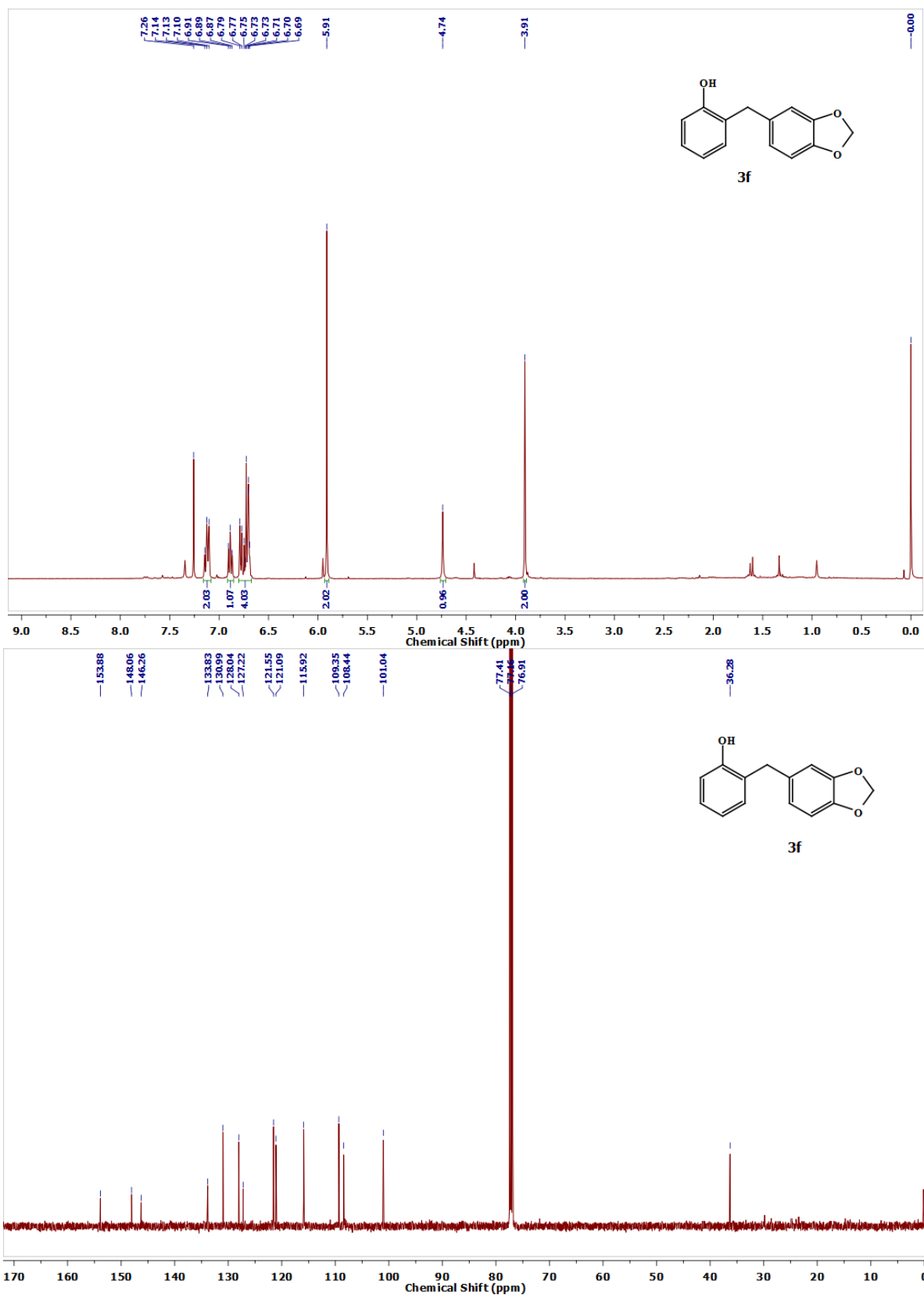
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3e** (CDCl_3)



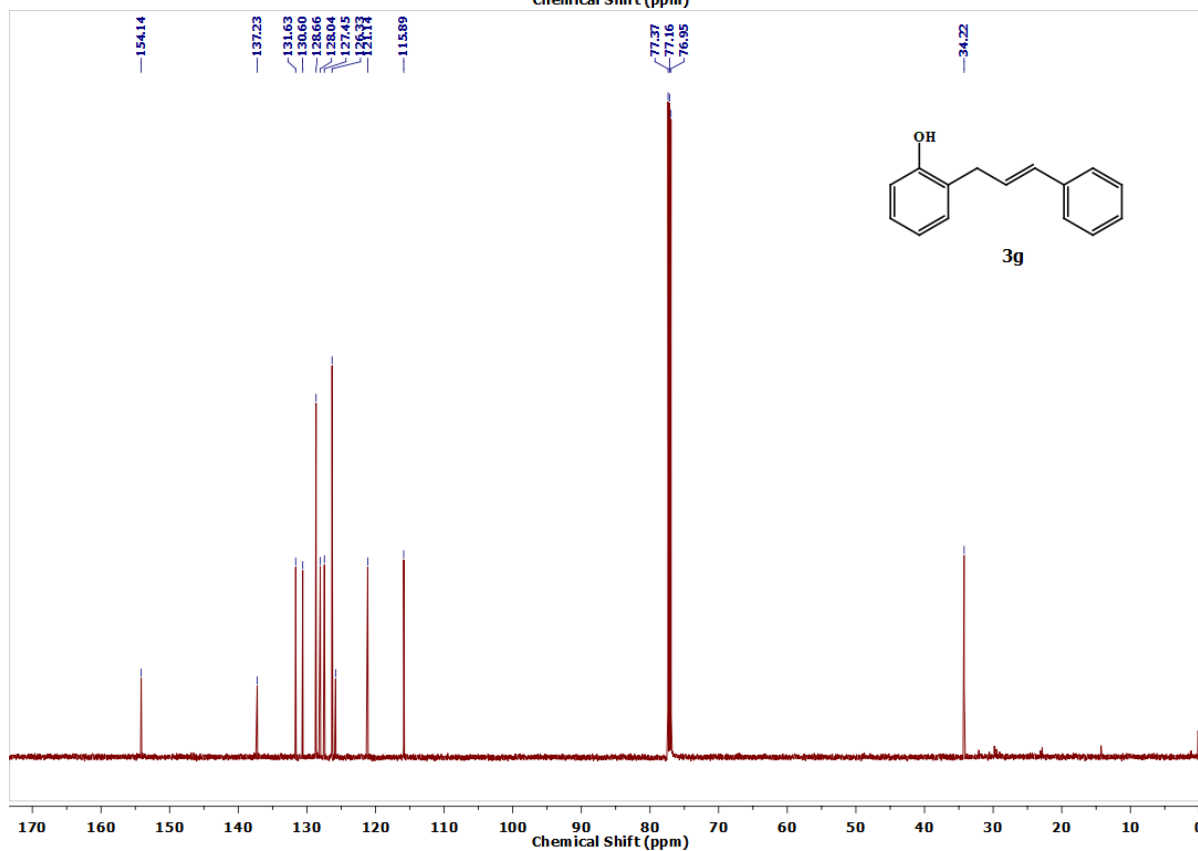
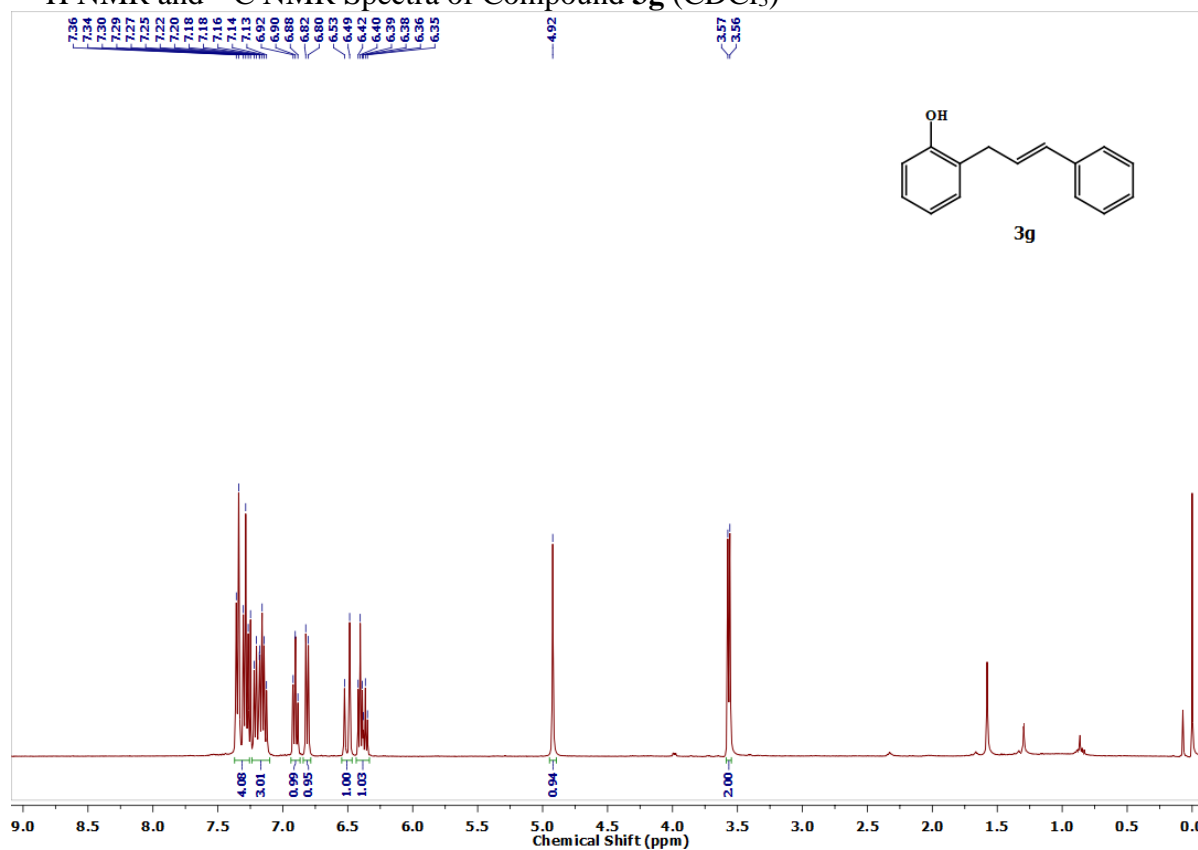
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3f** (CDCl_3)



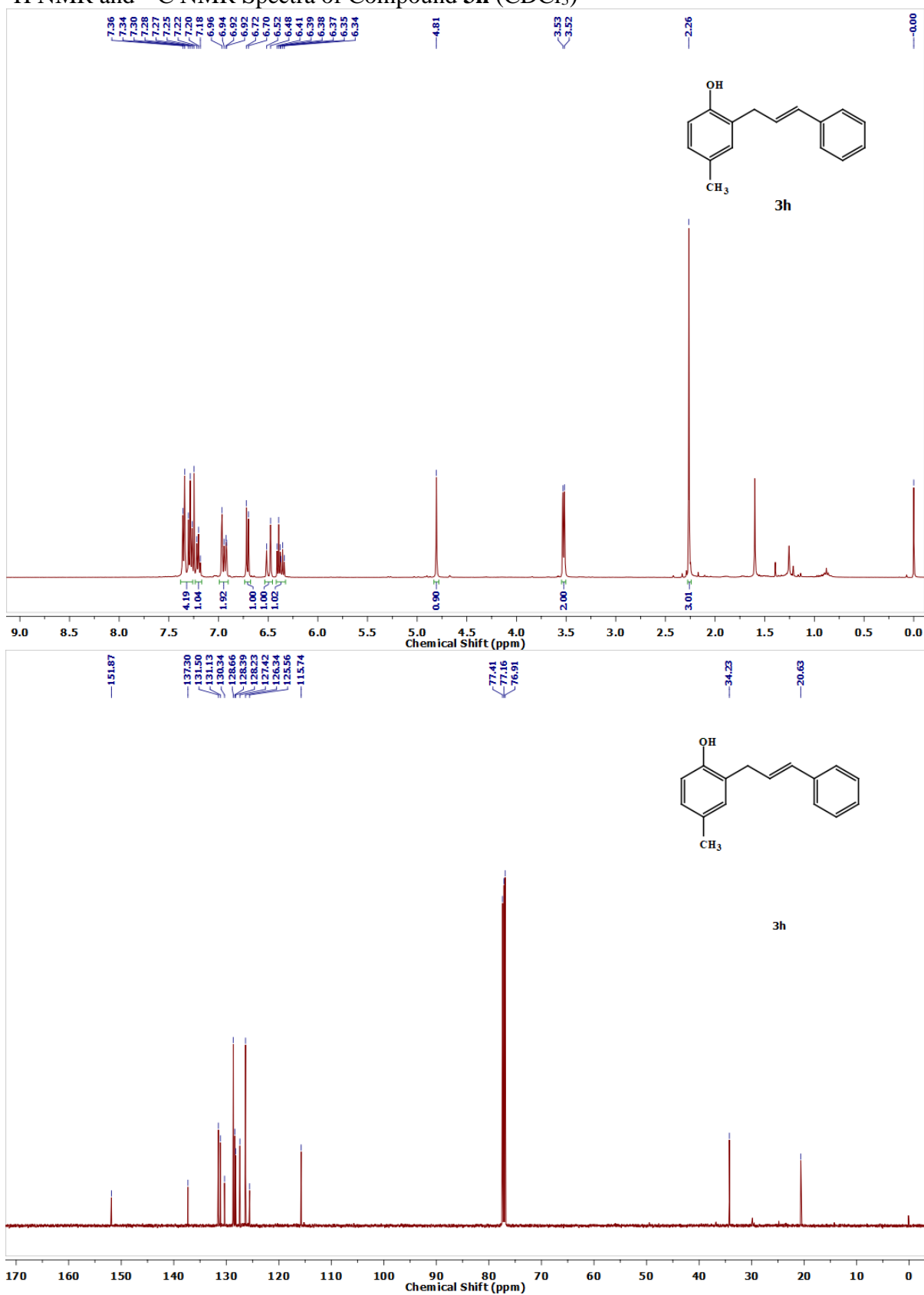
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3g** (CDCl_3)



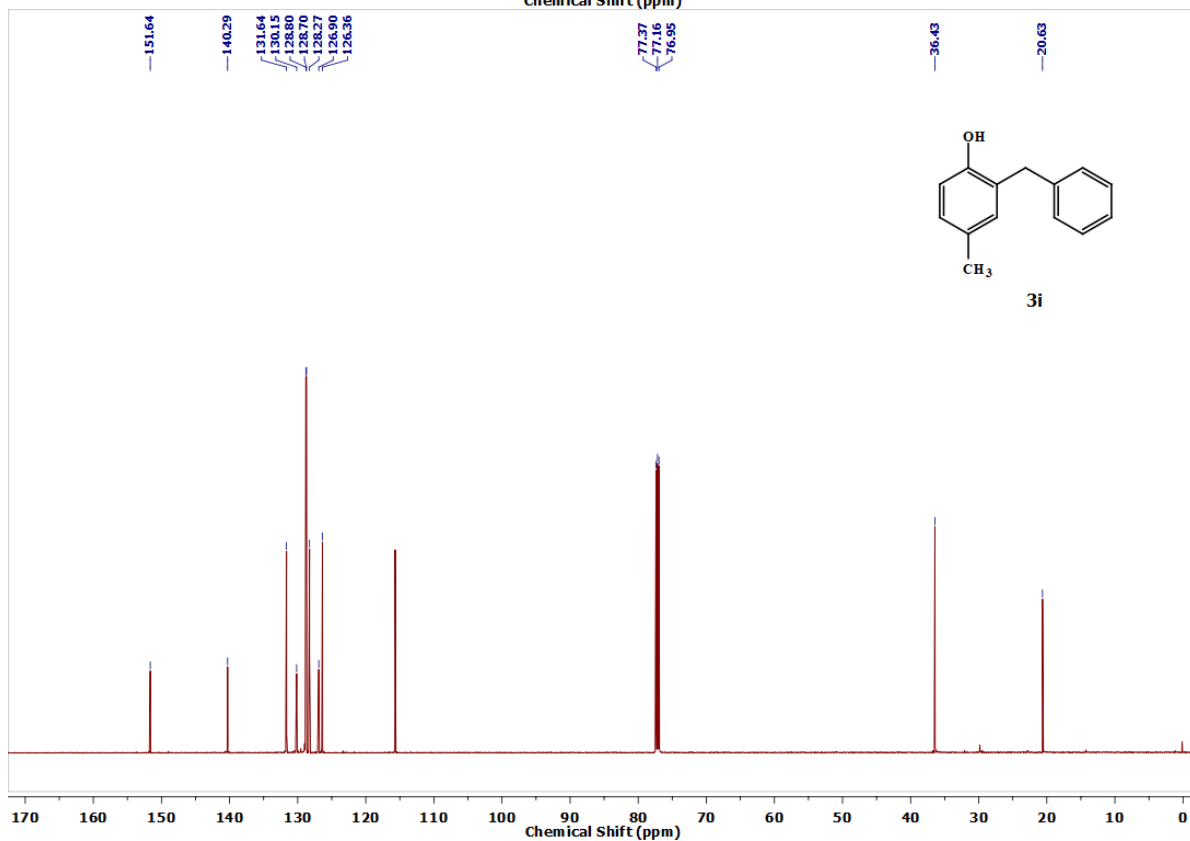
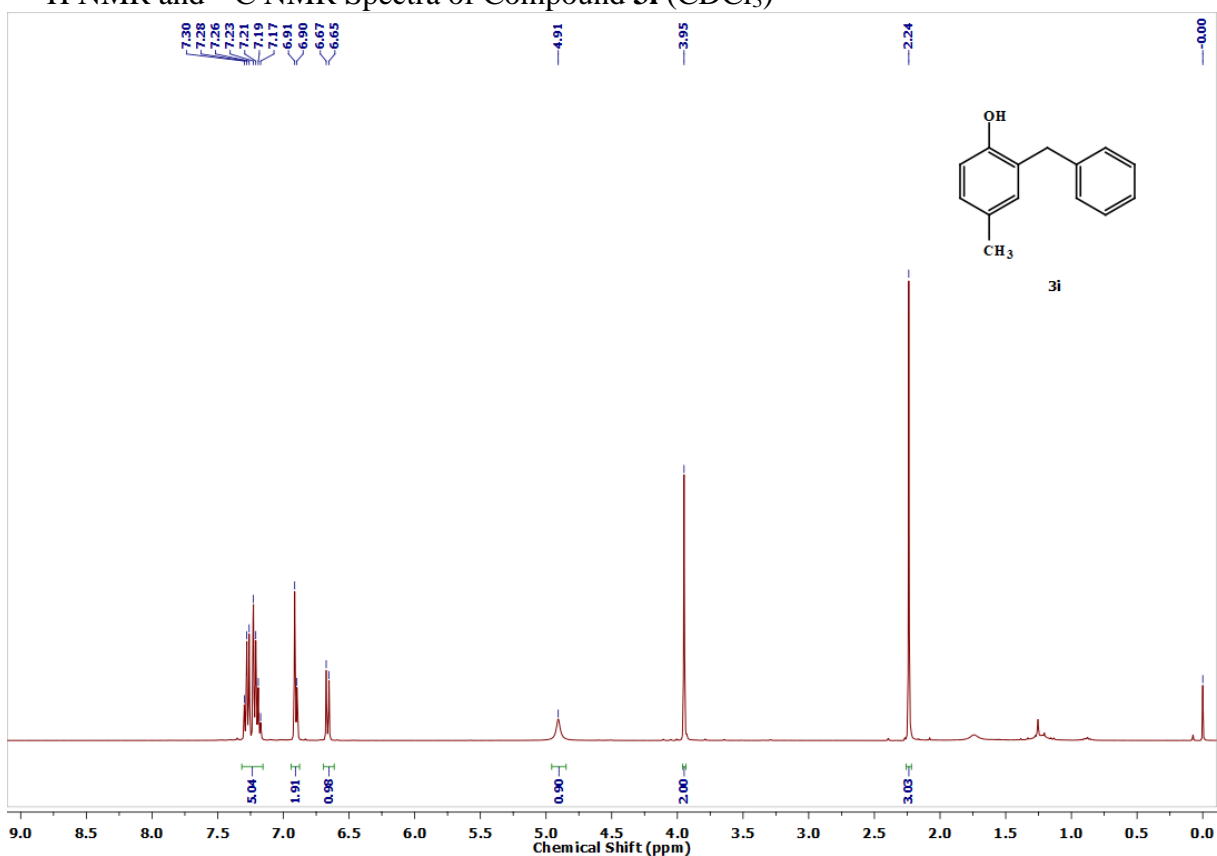
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3h** (CDCl_3)



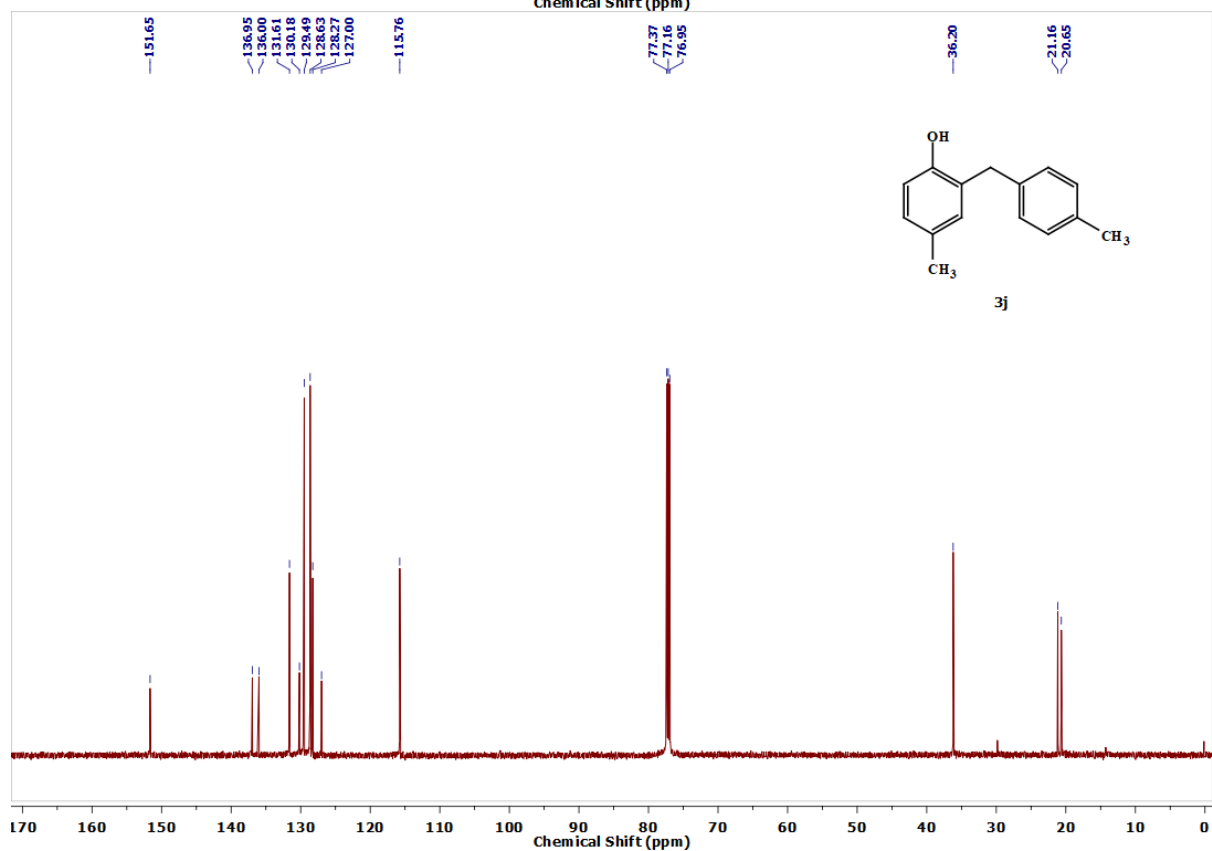
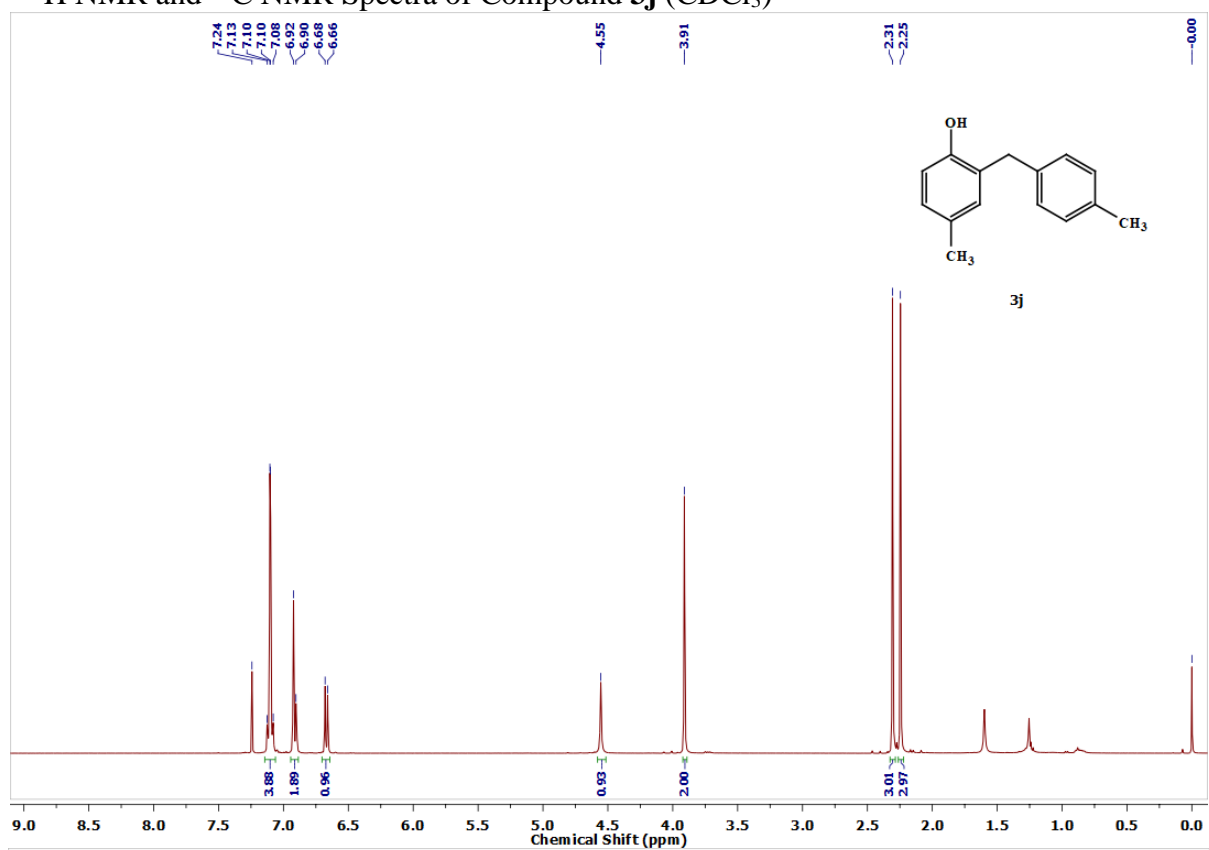
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3i** (CDCl_3)



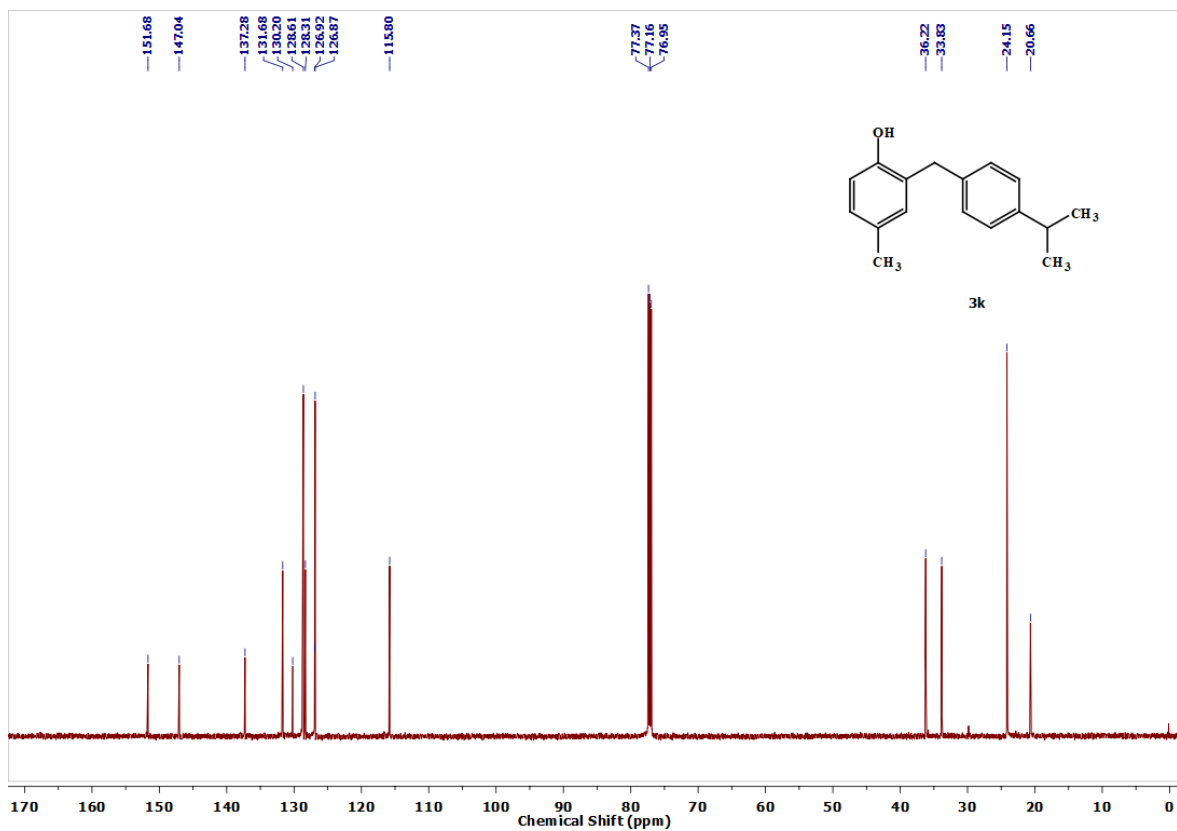
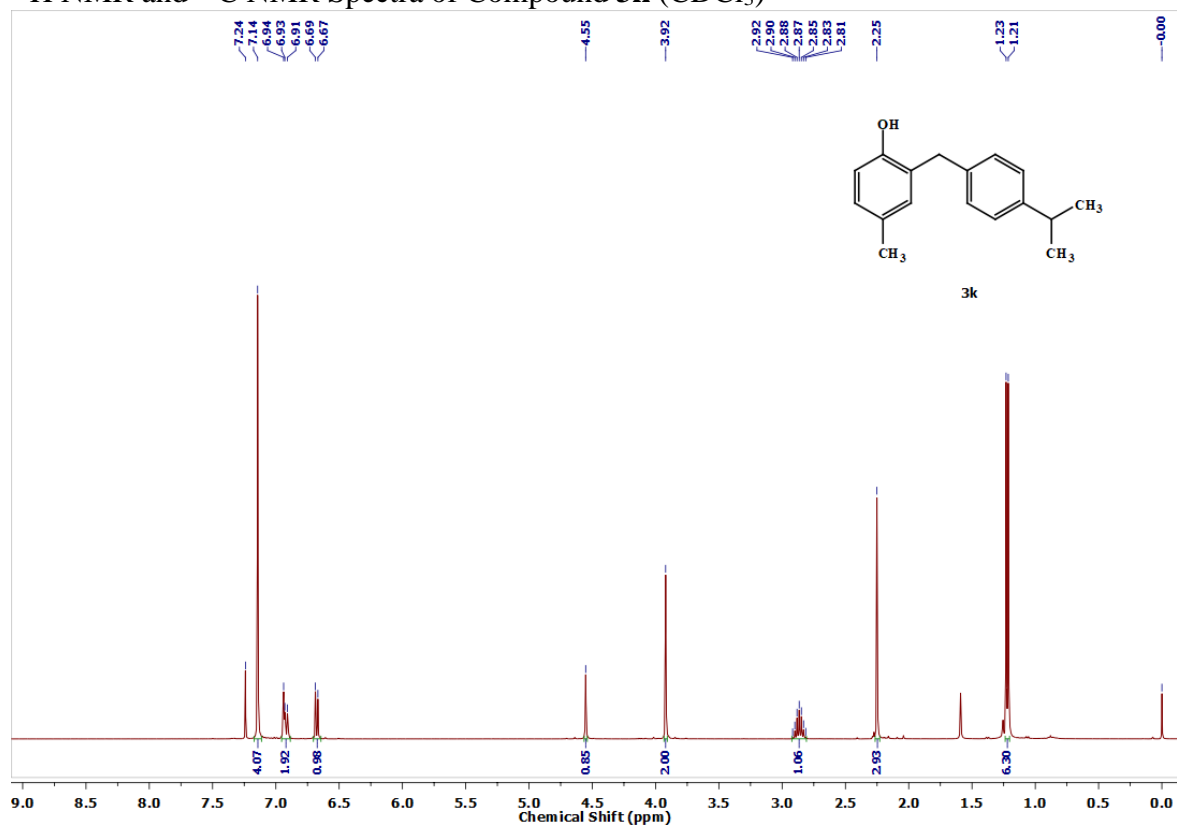
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3j** (CDCl_3)



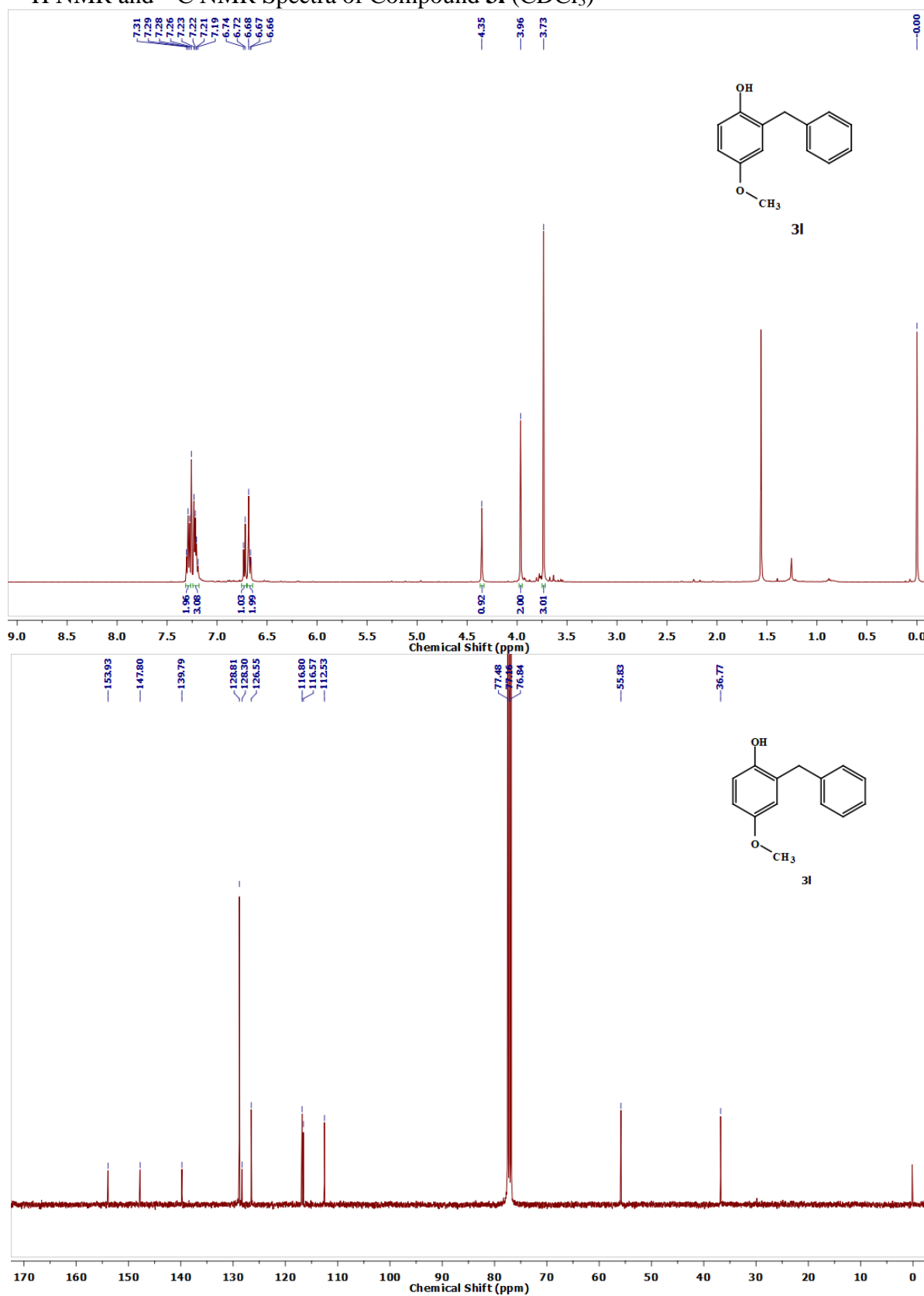
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3k** (CDCl_3)



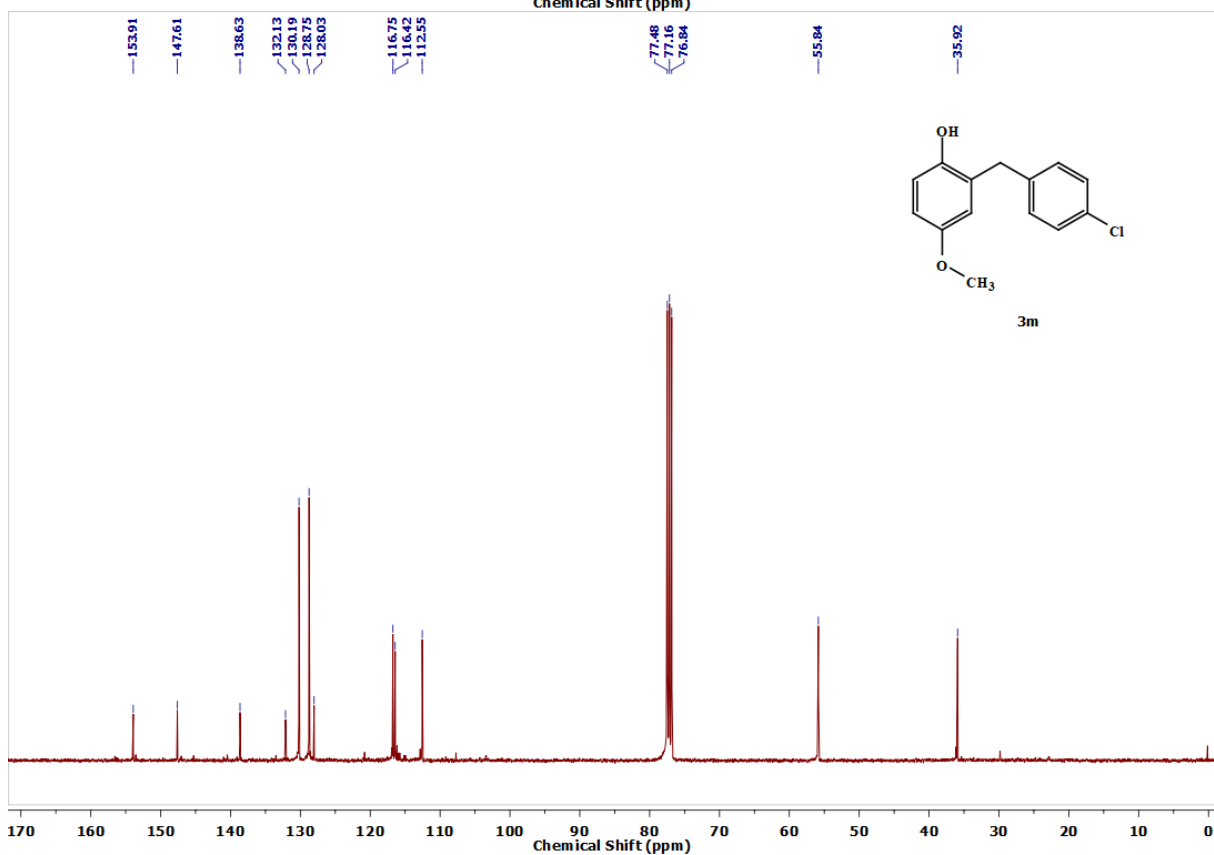
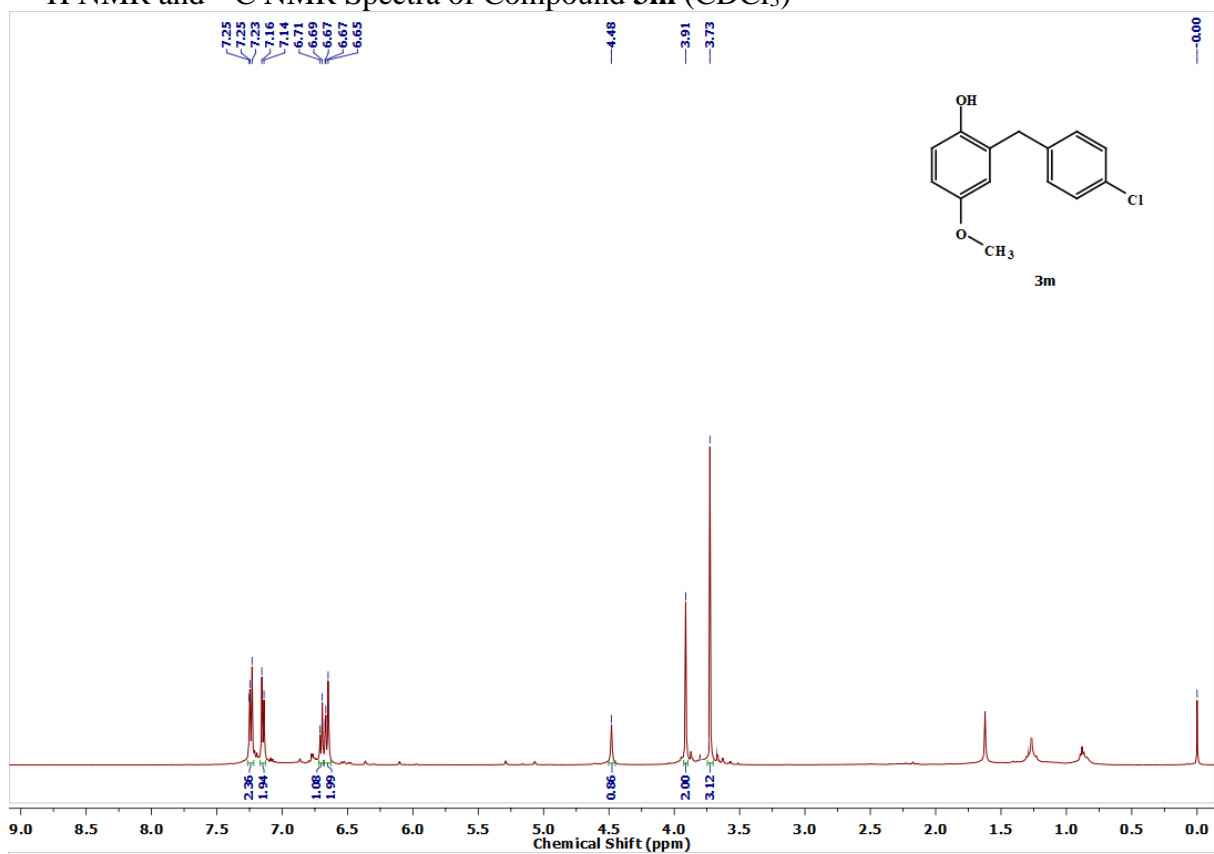
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **31** (CDCl_3)



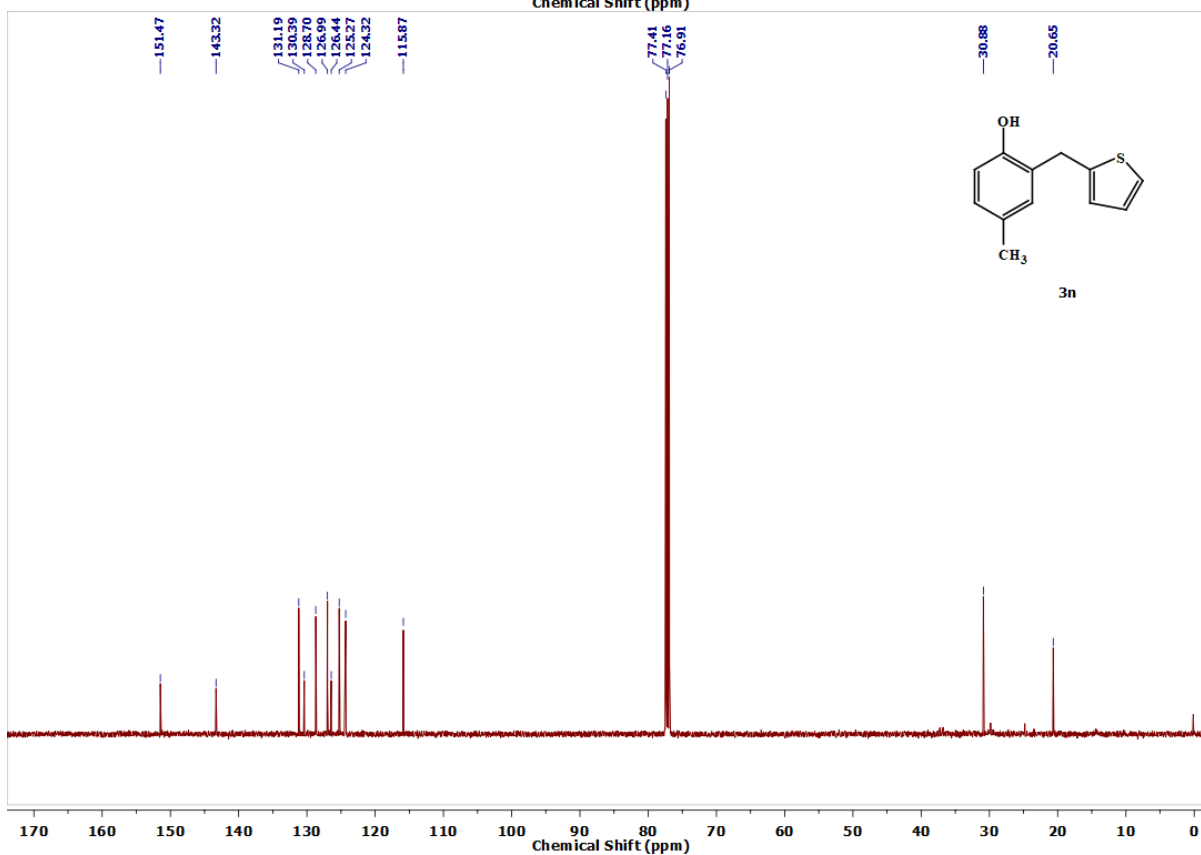
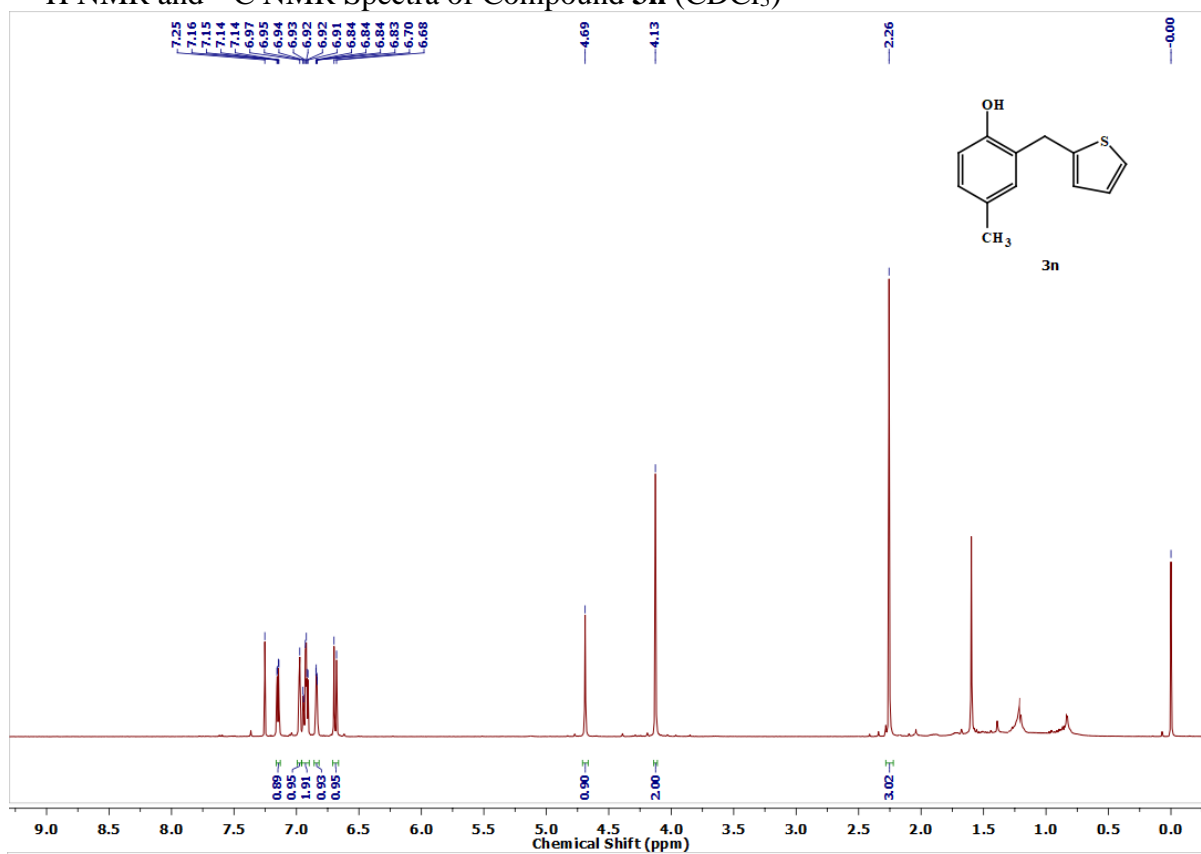
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3m** (CDCl_3)



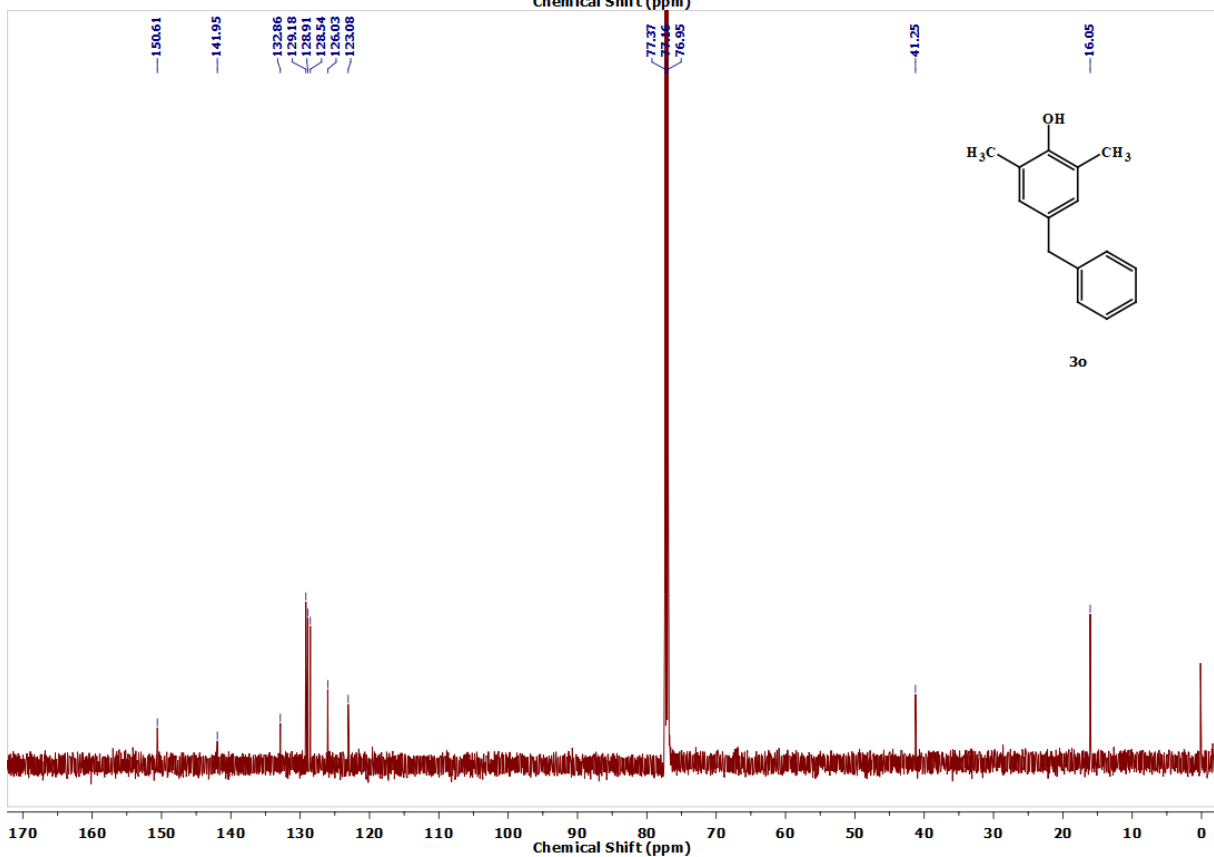
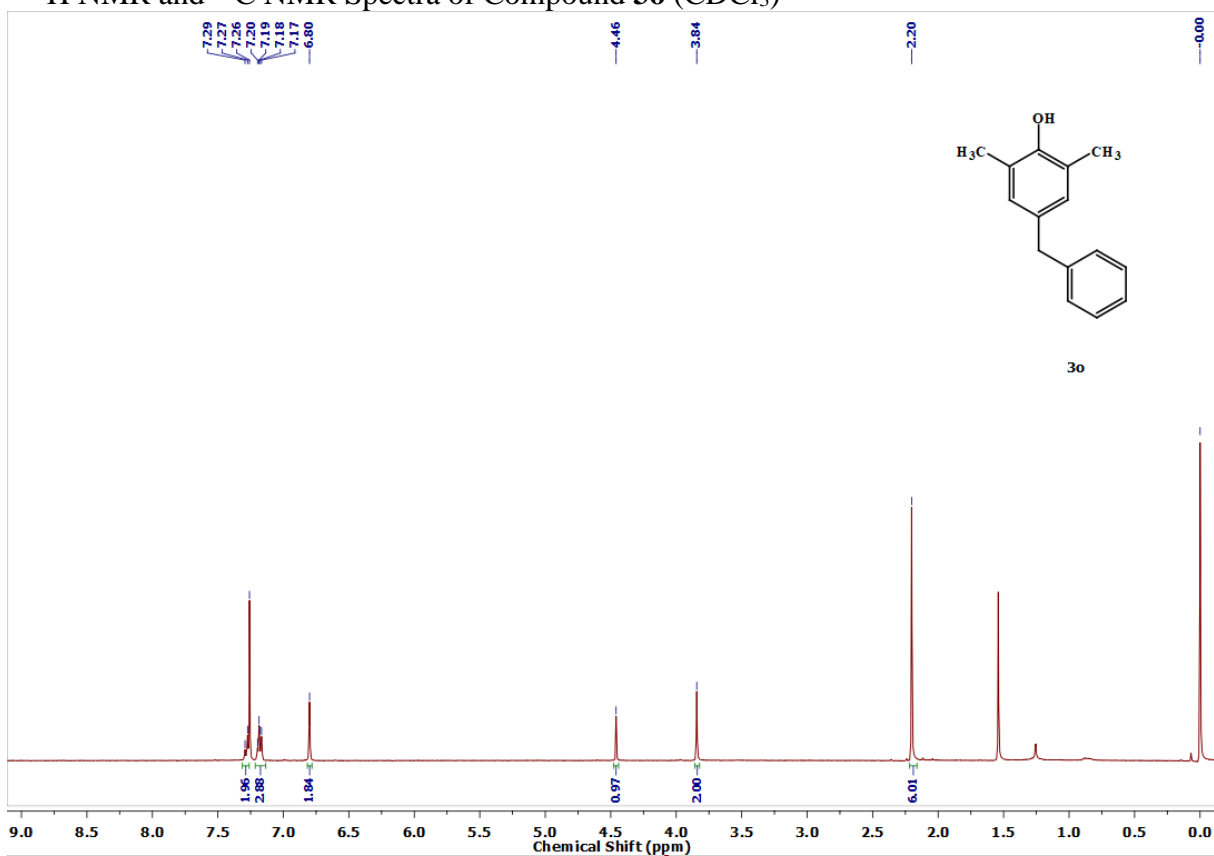
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **3n** (CDCl_3)



Supporting Information

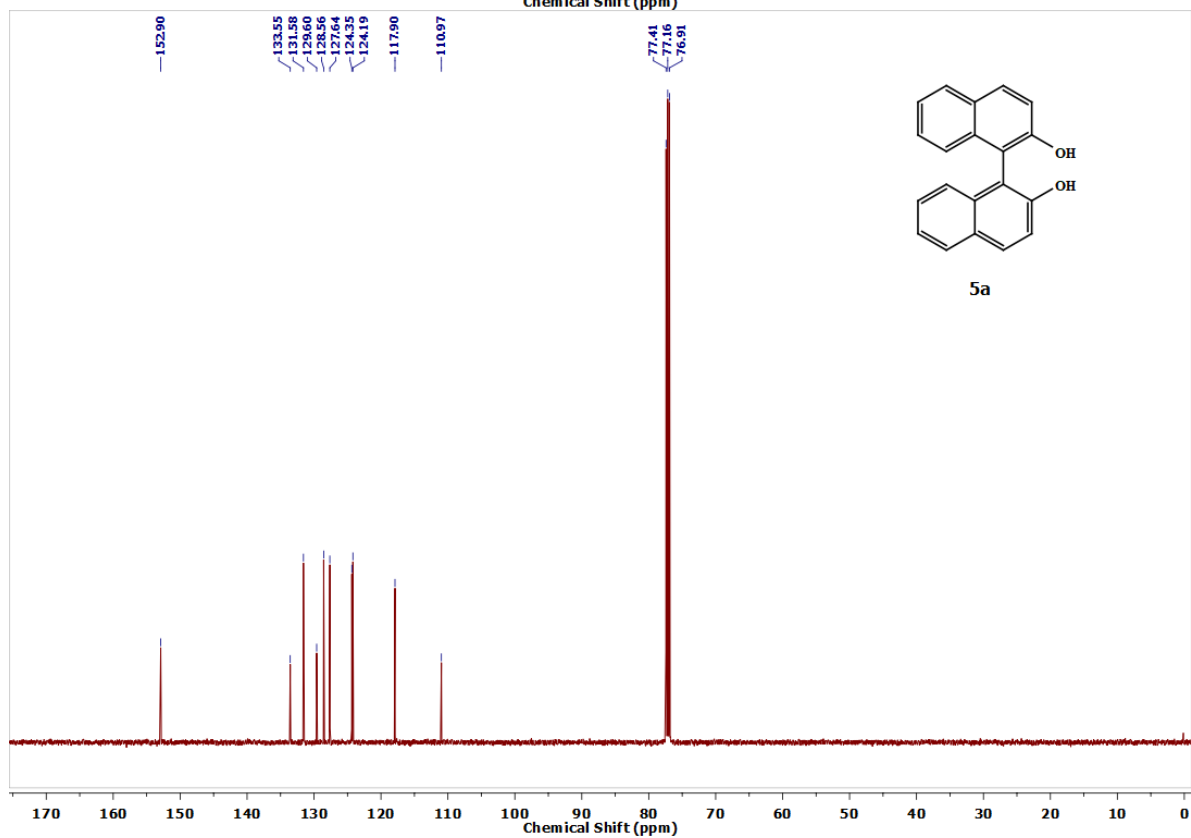
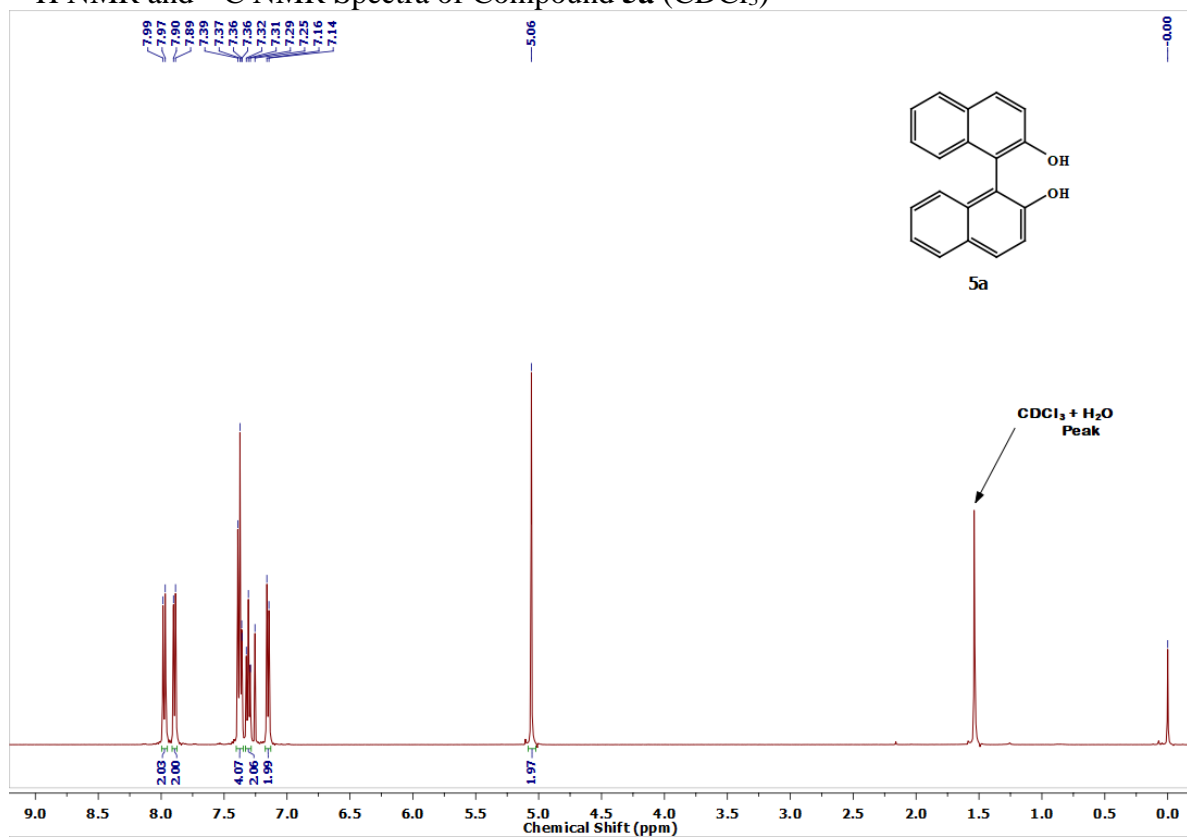
- ^1H NMR and ^{13}C NMR Spectra of Compound **3o** (CDCl_3)



Supporting Information

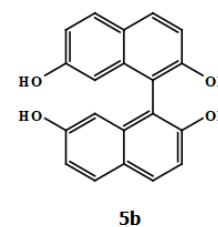
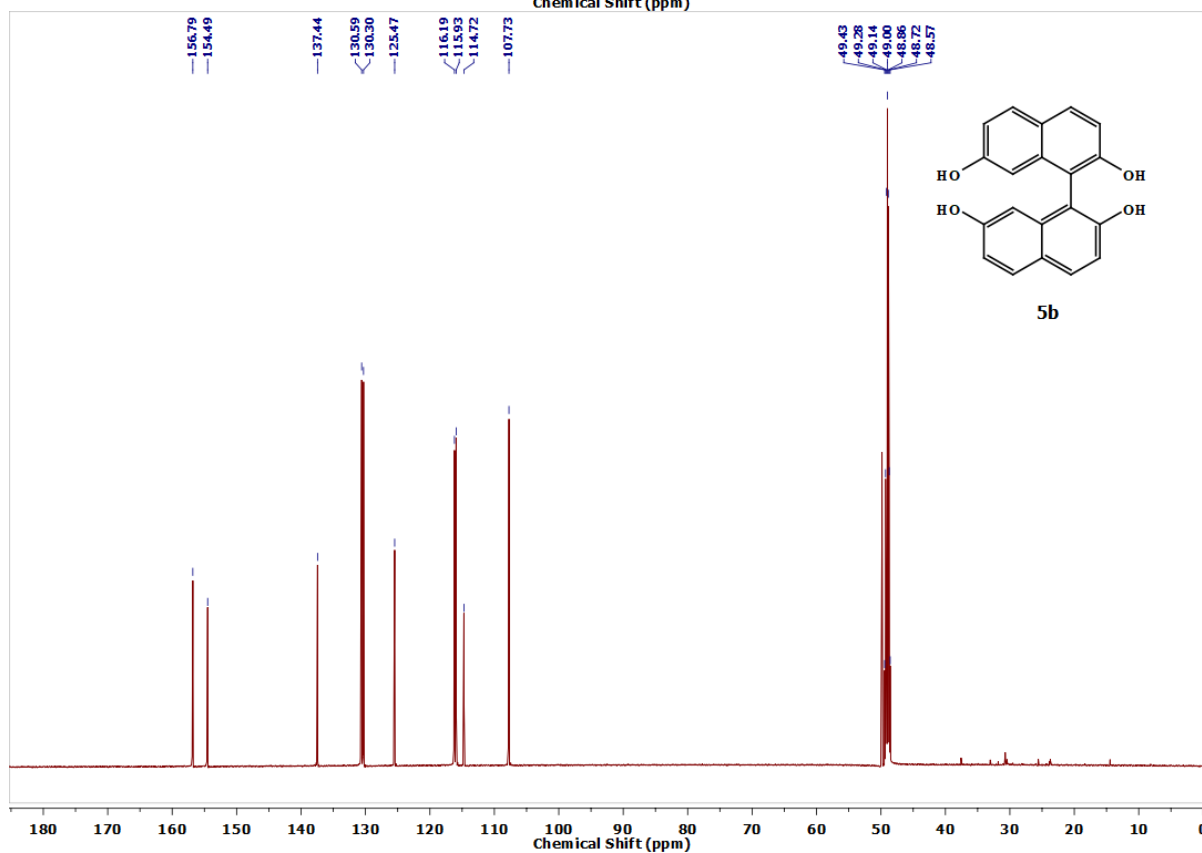
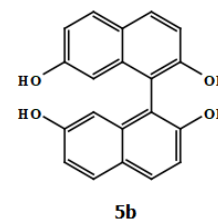
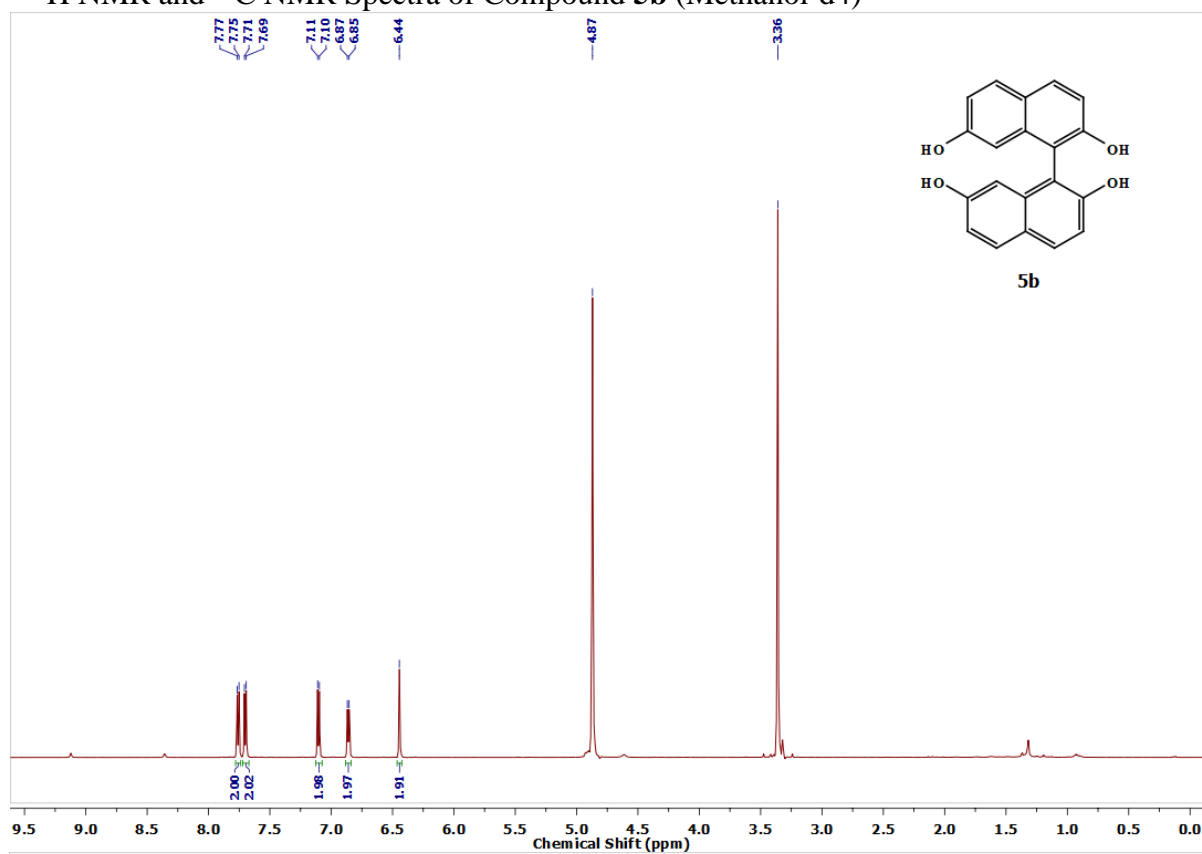
NMR Spectra of the products, Compound 5a-5h

❖ ^1H NMR and ^{13}C NMR Spectra of Compound 5a (CDCl_3)



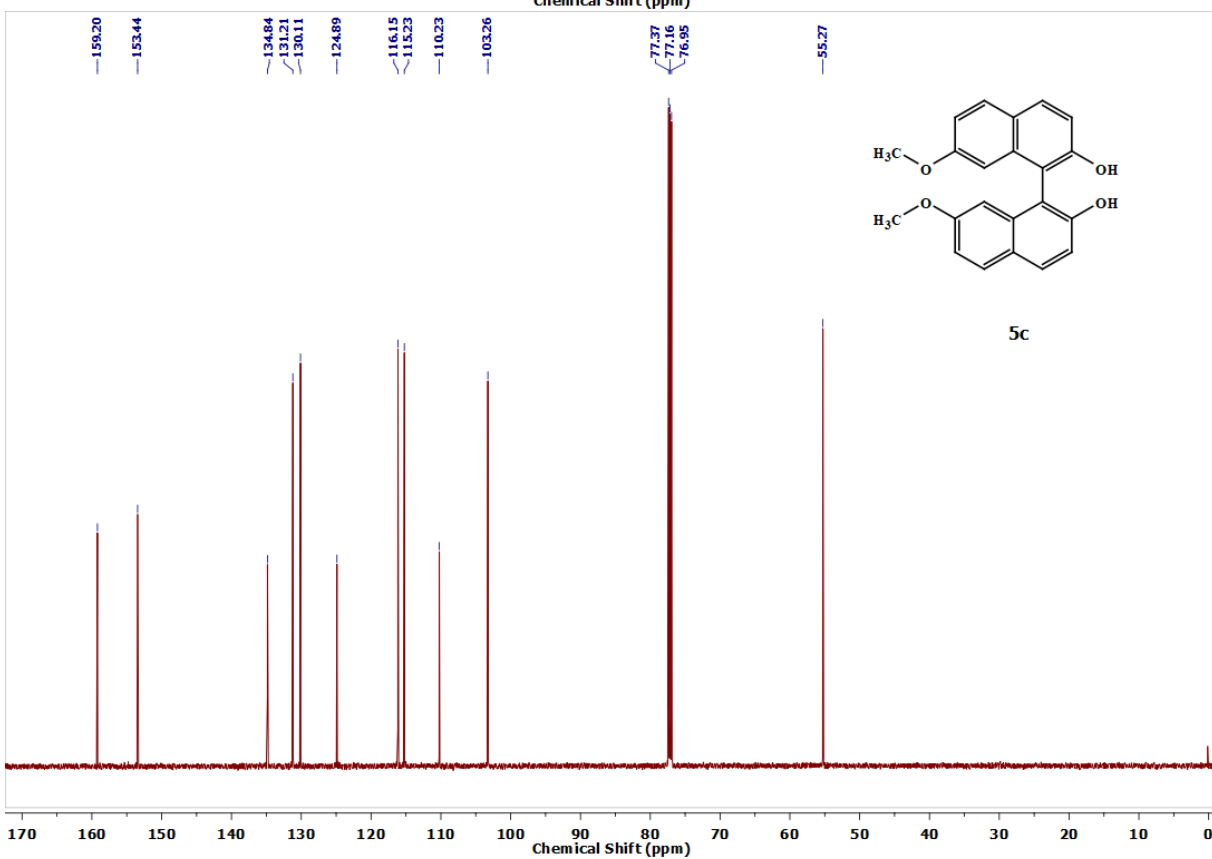
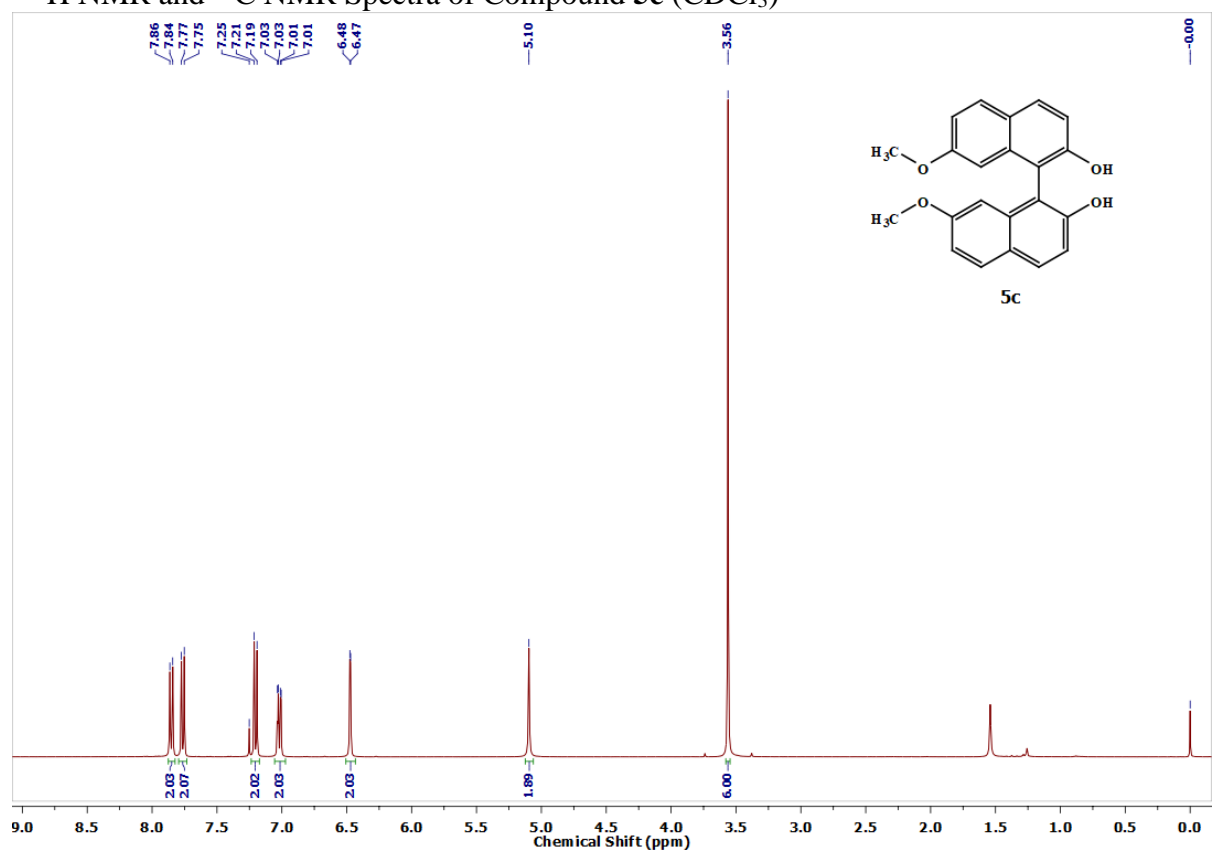
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5b** (Methanol- d_4)



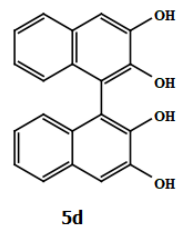
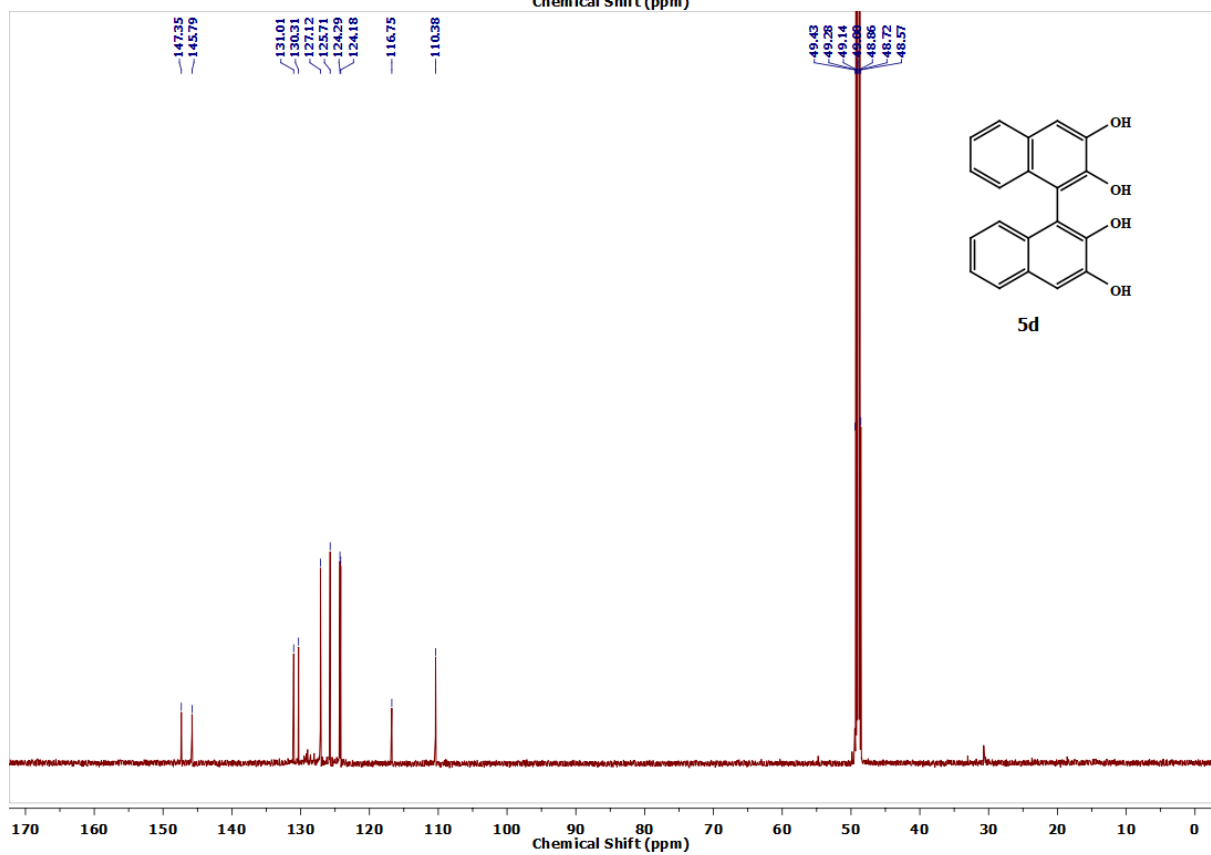
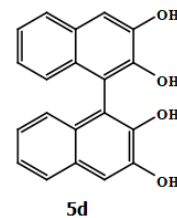
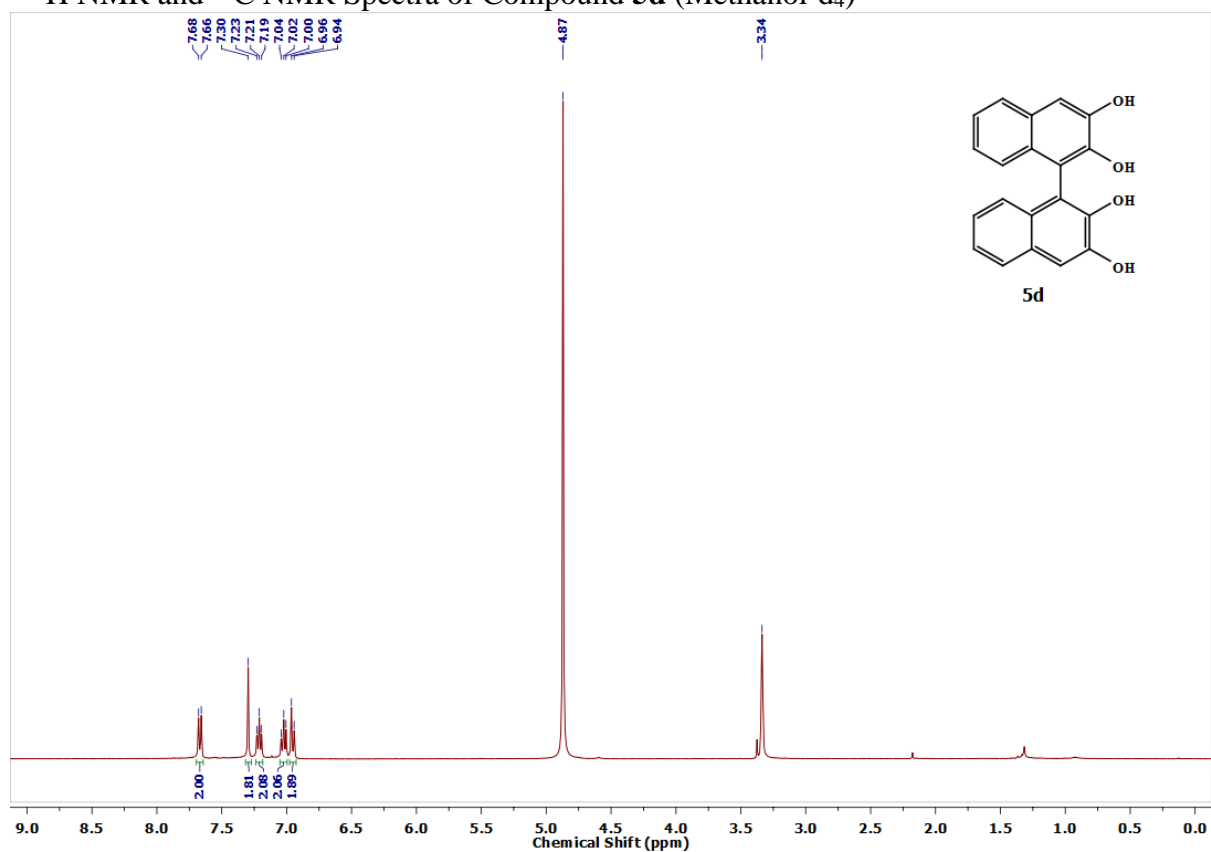
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5c** (CDCl_3)



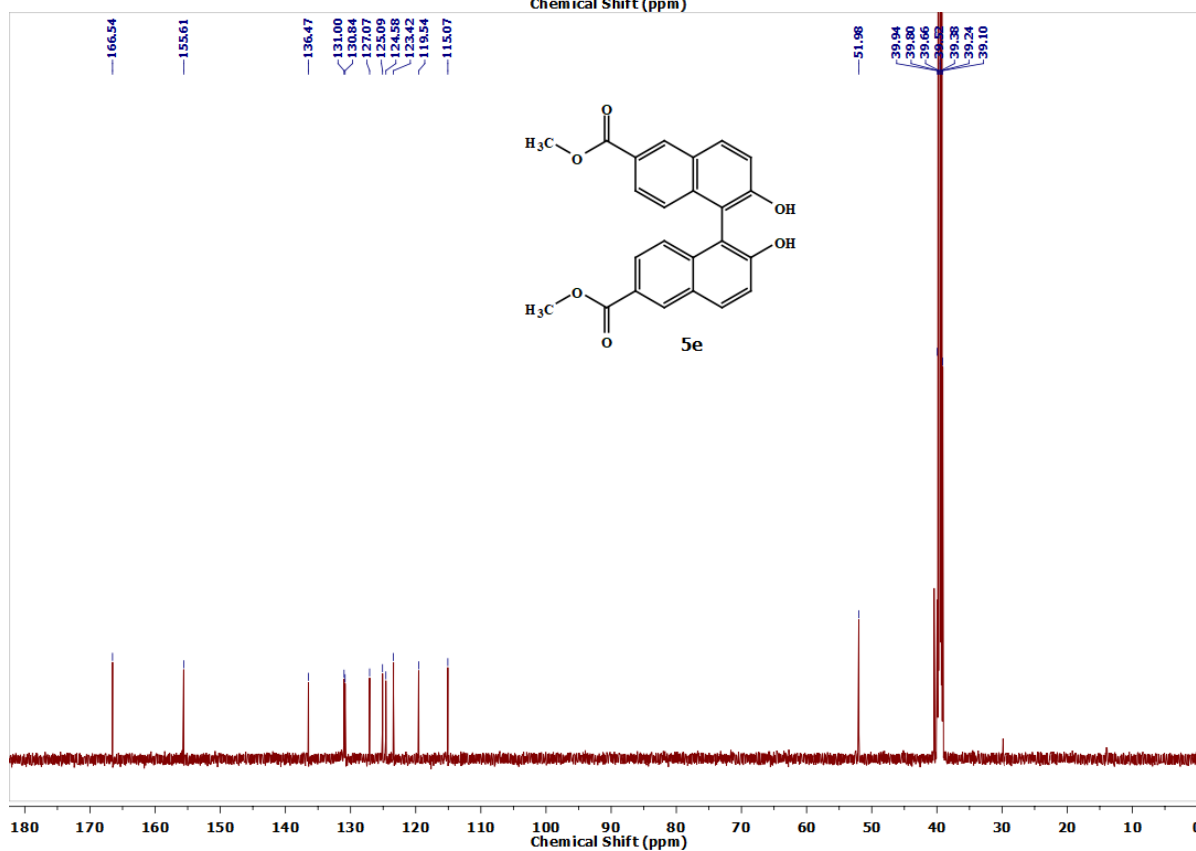
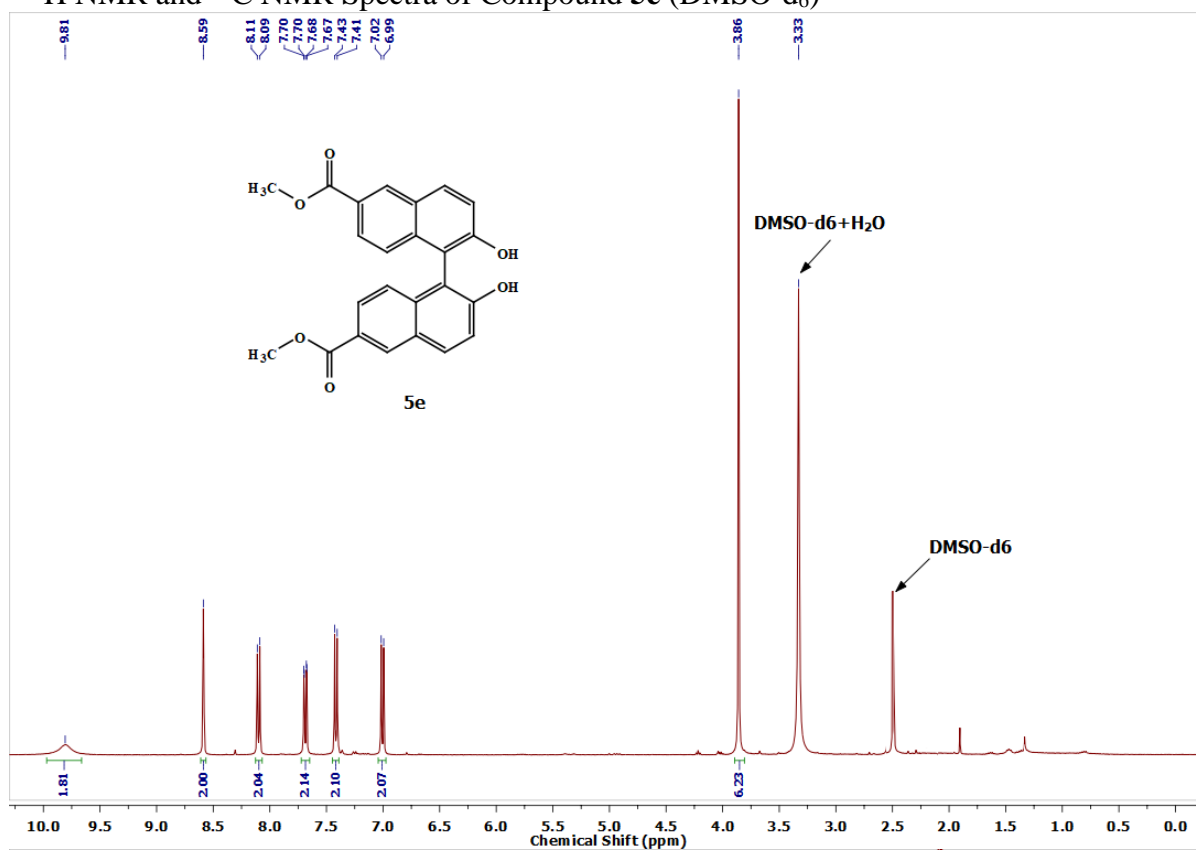
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5d** (Methanol- d_4)



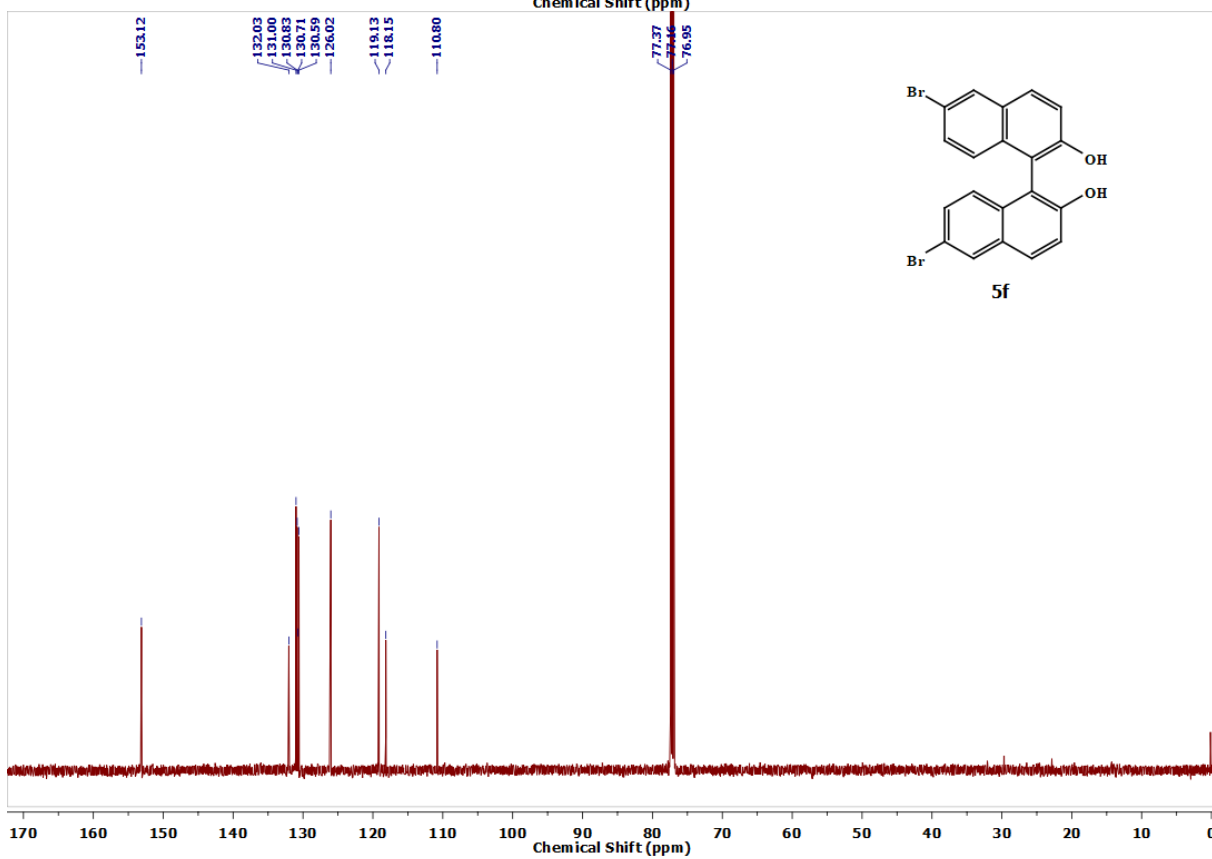
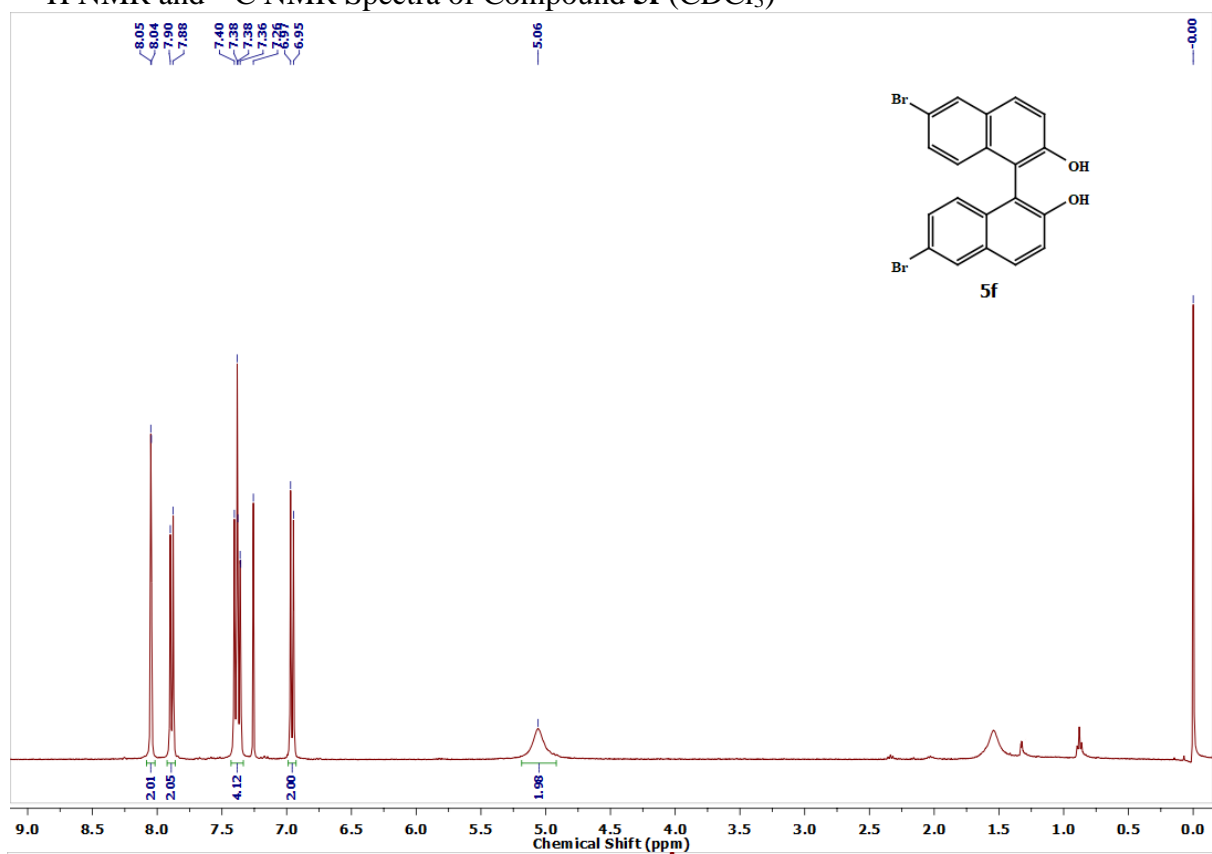
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5e** (DMSO-d_6)



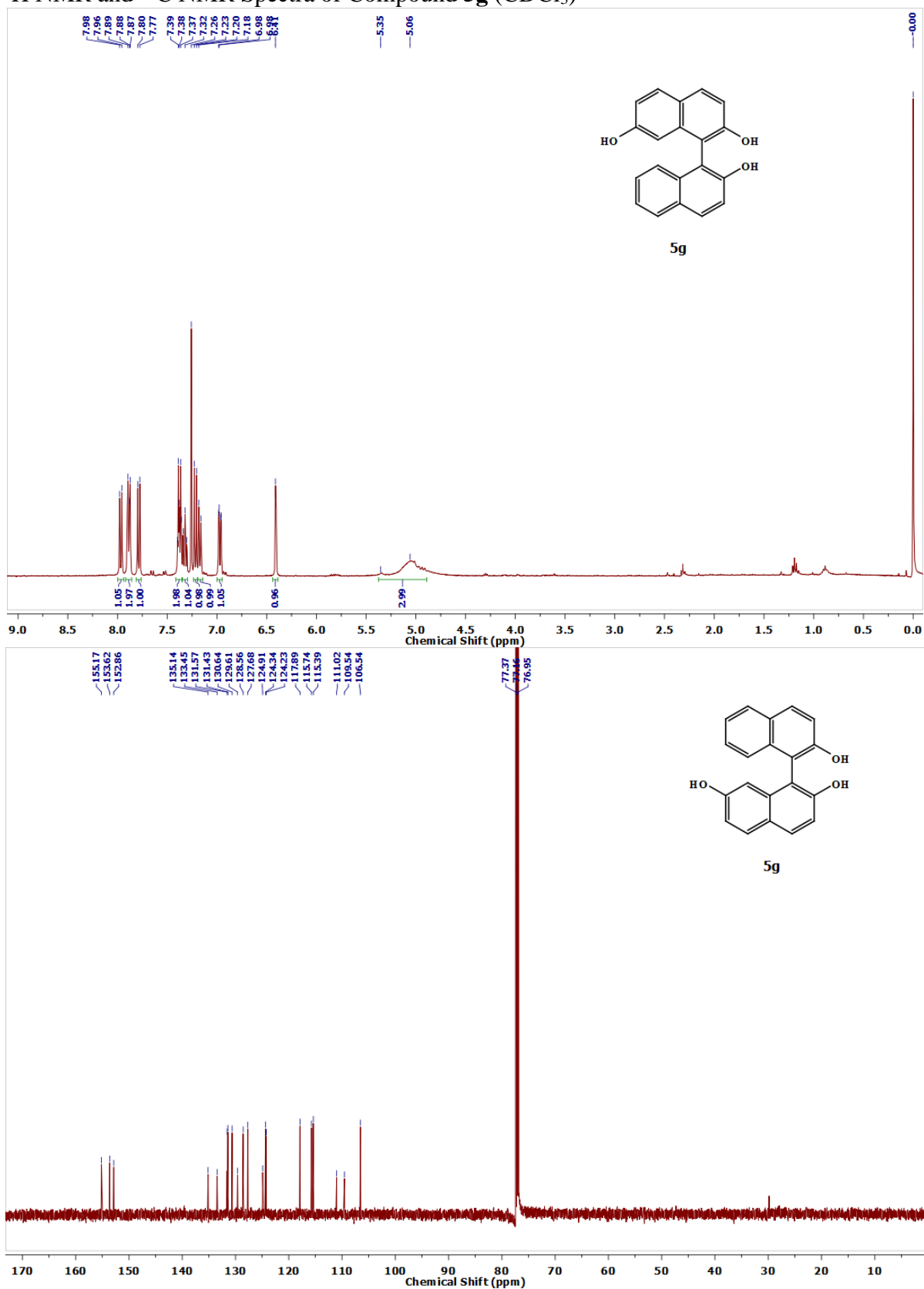
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5f** (CDCl_3)



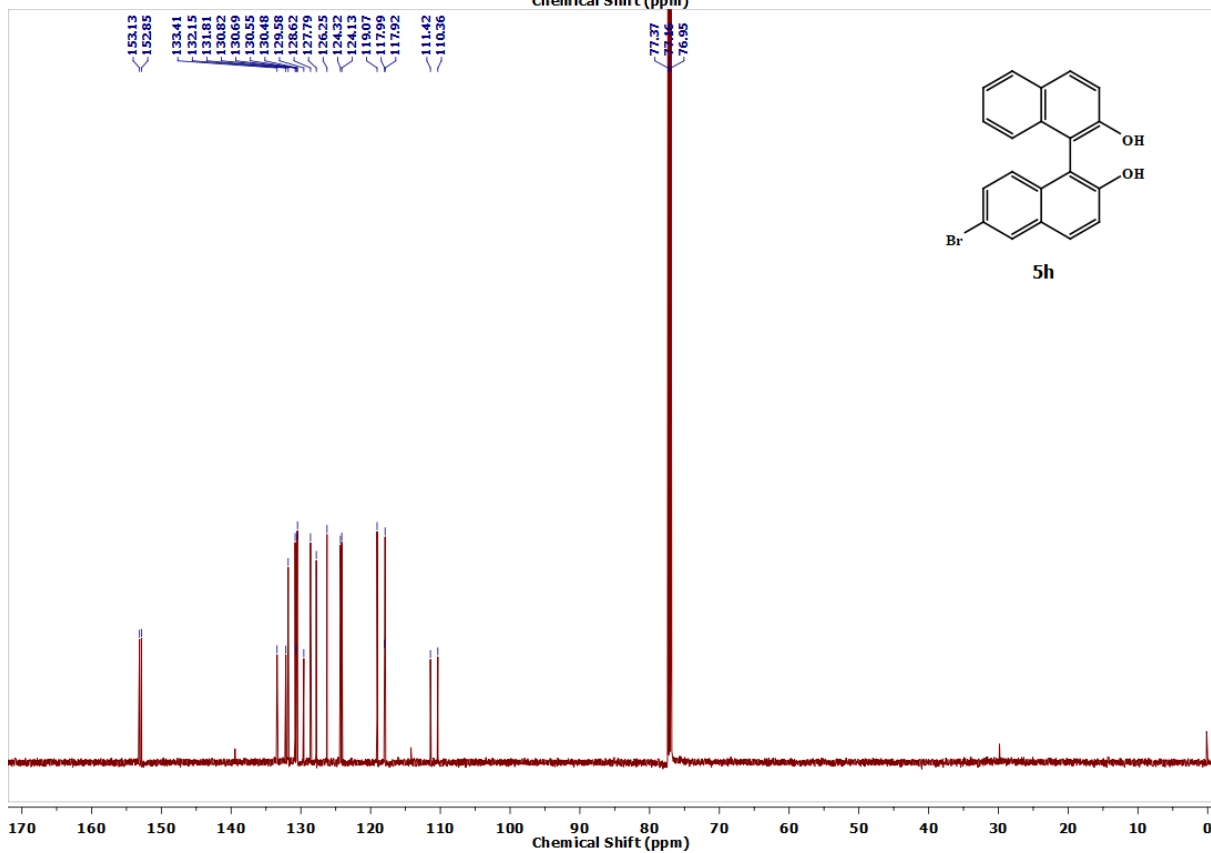
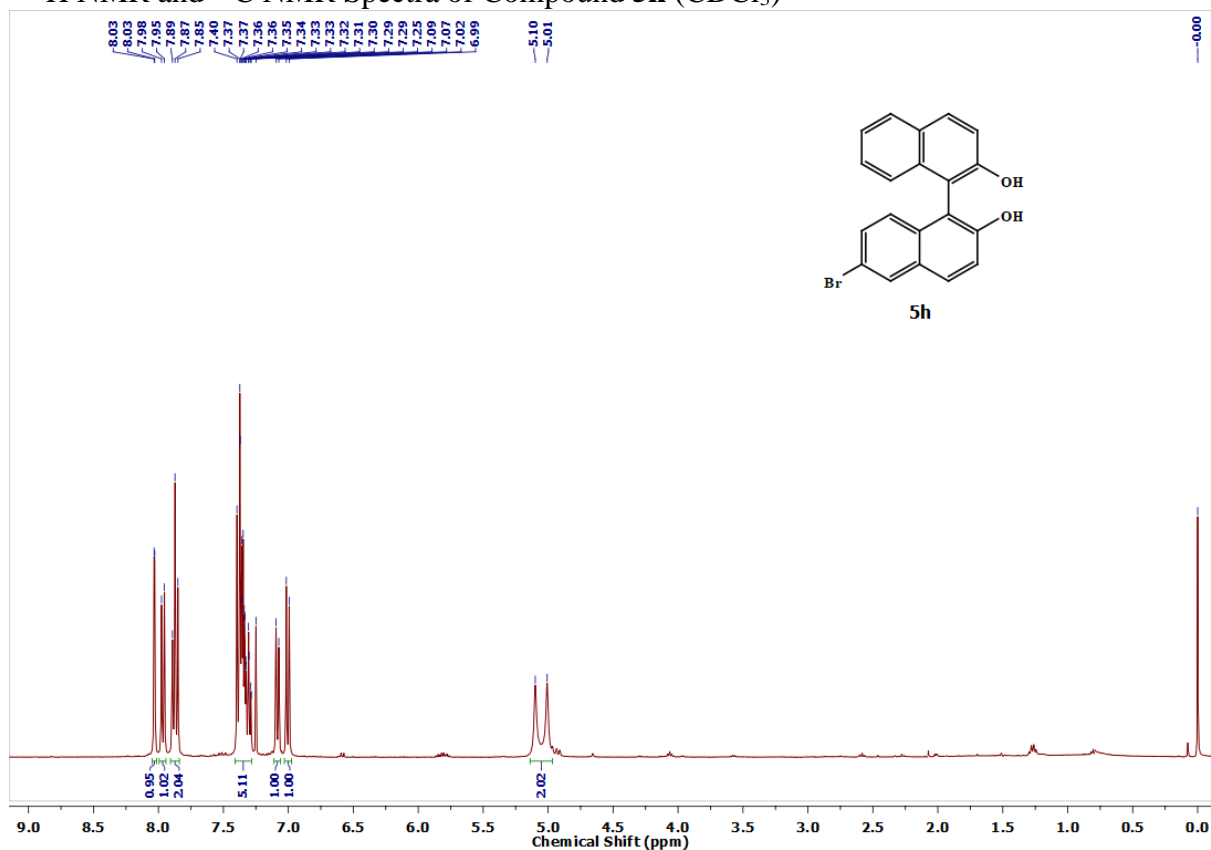
Supporting Information

- ^1H NMR and ^{13}C NMR Spectra of Compound **5g** (CDCl_3)



Supporting Information

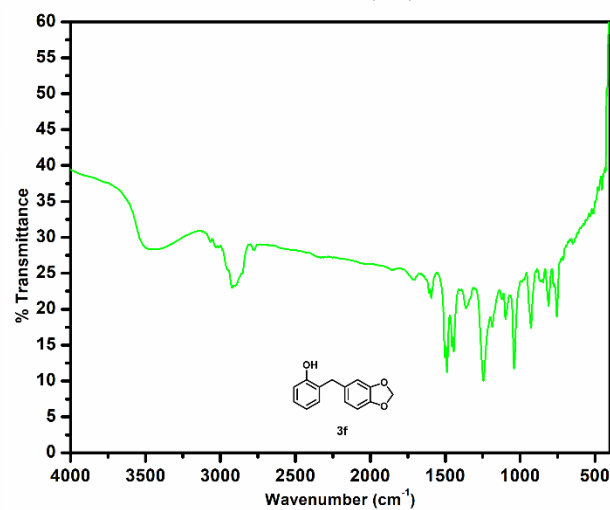
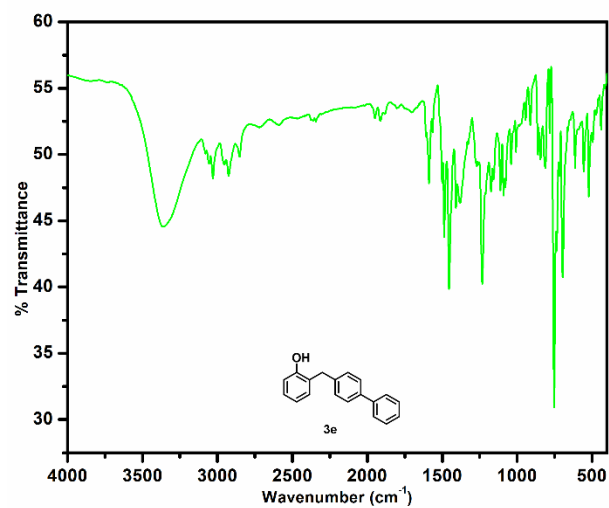
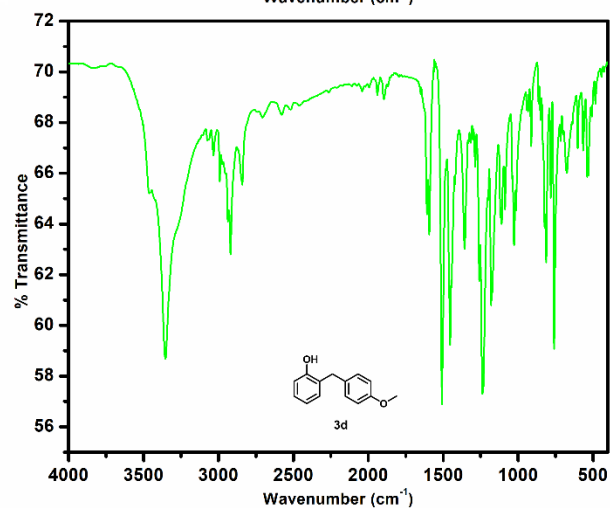
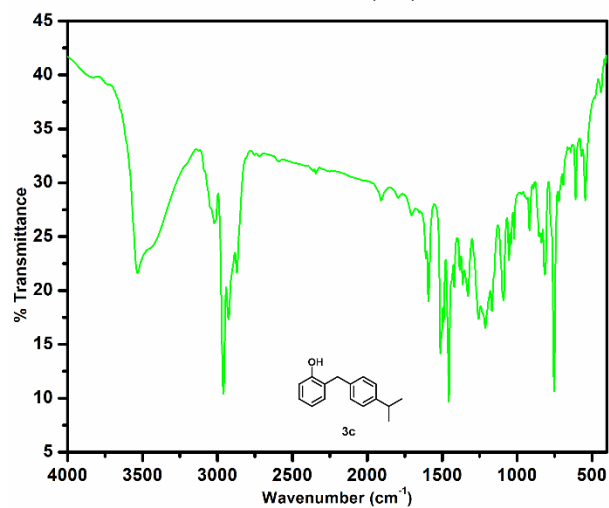
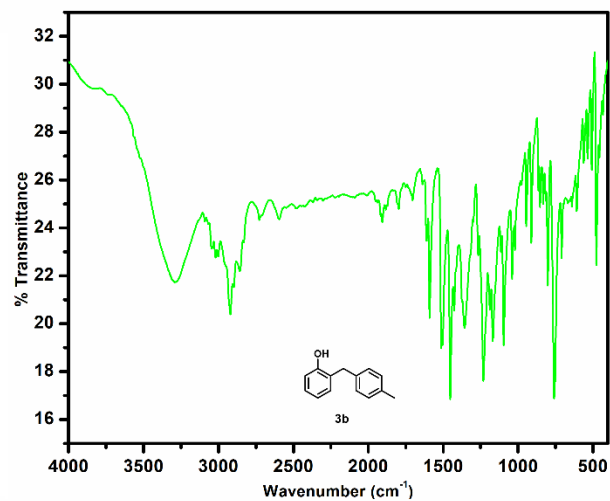
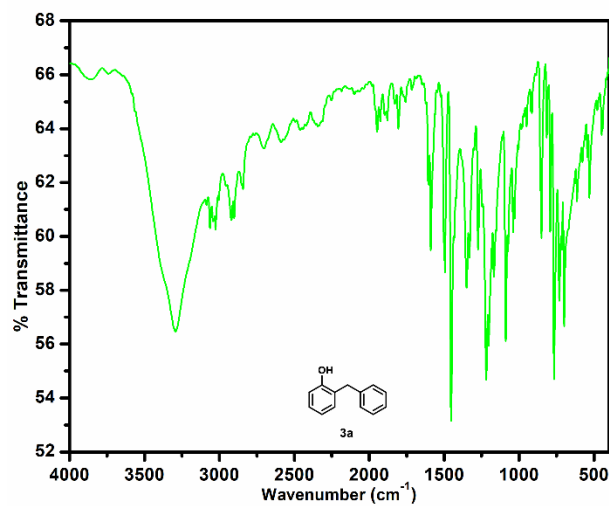
- ^1H NMR and ^{13}C NMR Spectra of Compound **5h** (CDCl_3)



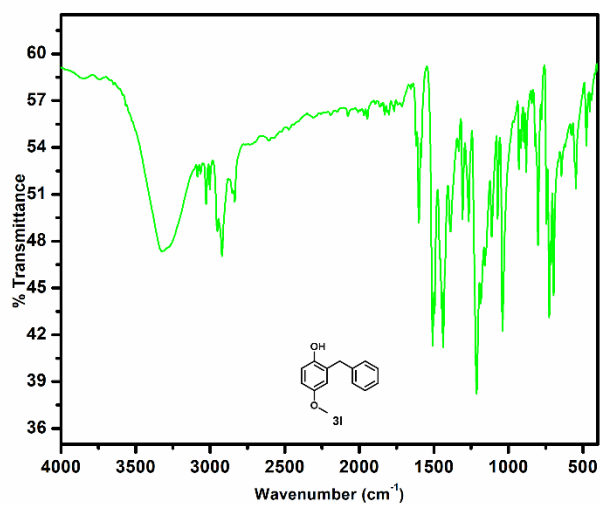
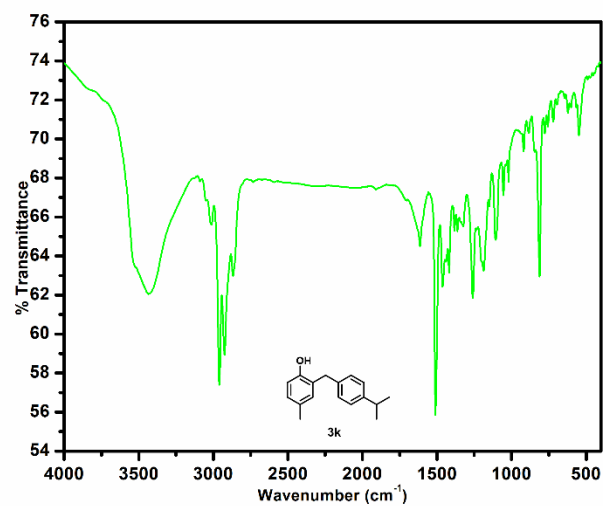
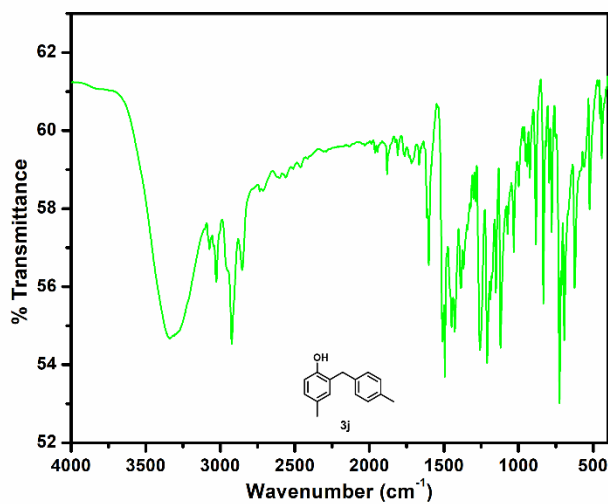
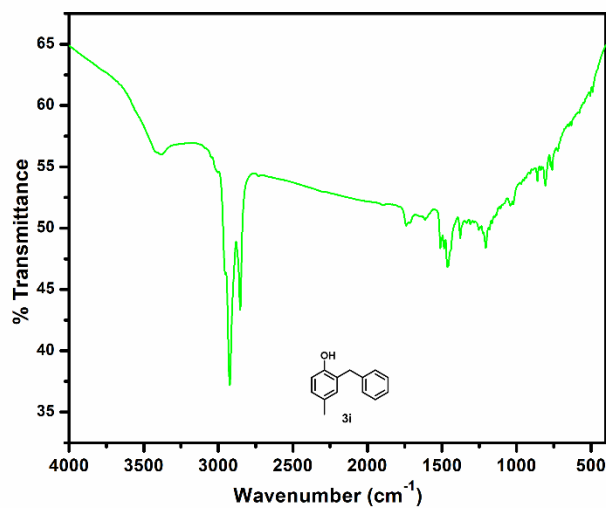
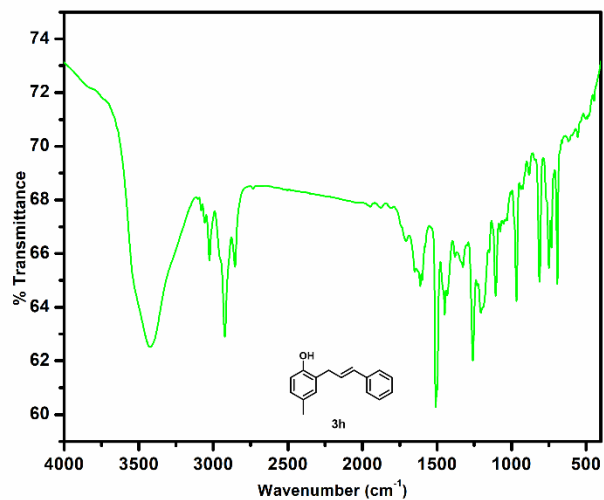
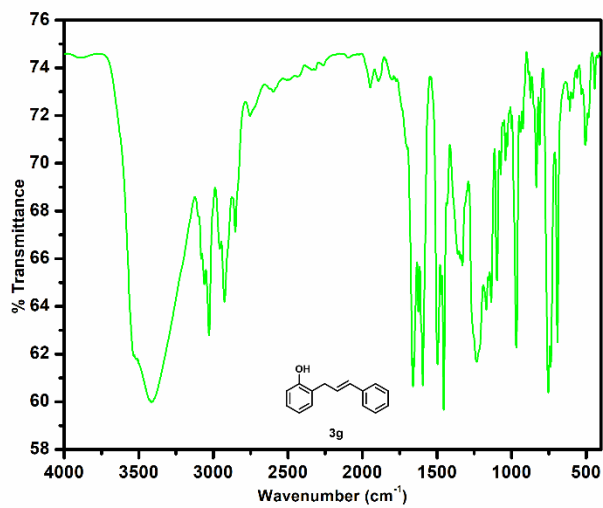
Supporting Information

FT-IR Spectra of all synthesized compound

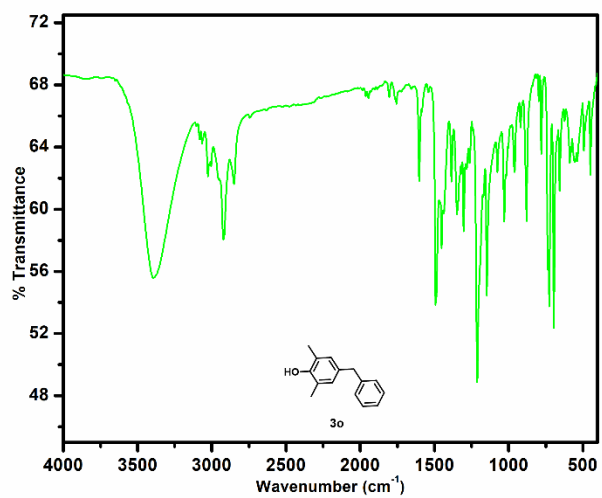
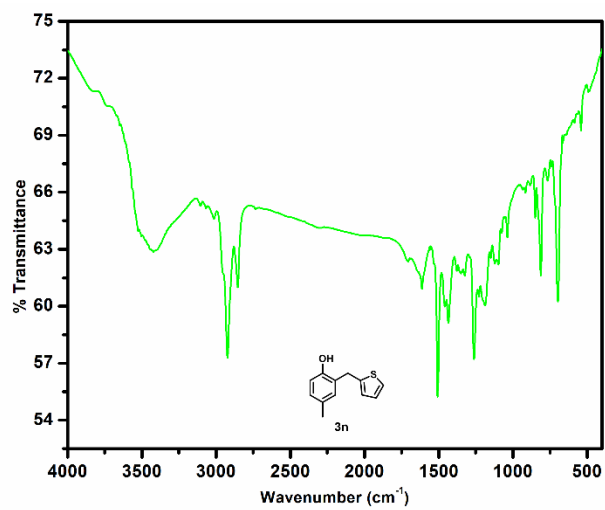
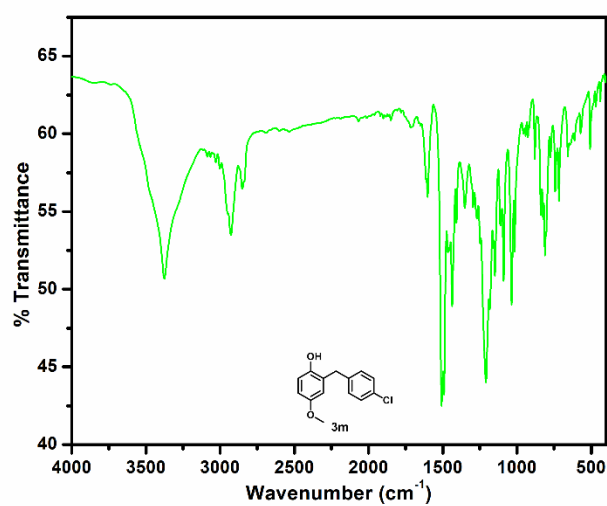
FT-IR Spectra of compound 3a-3o



Supporting Information

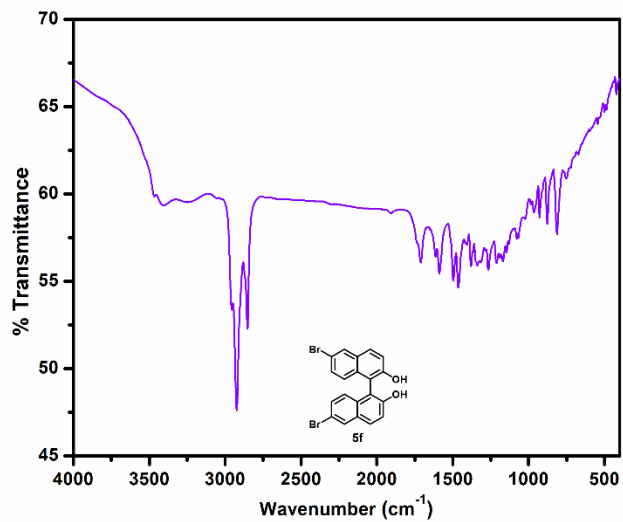
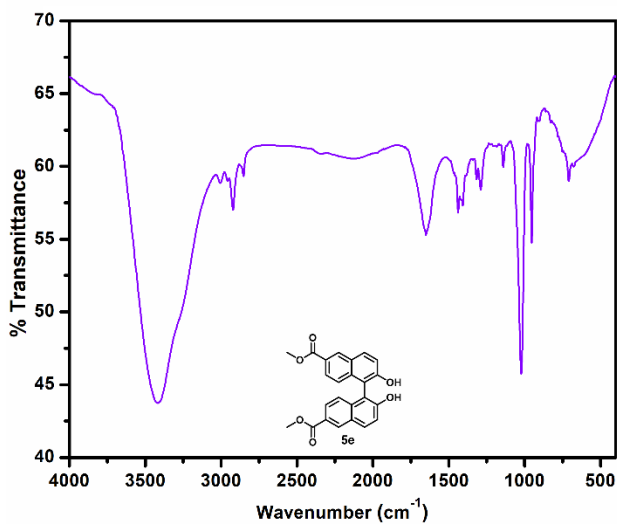
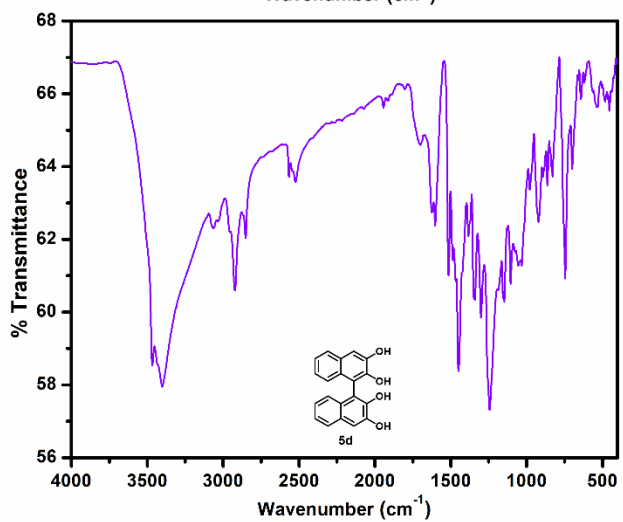
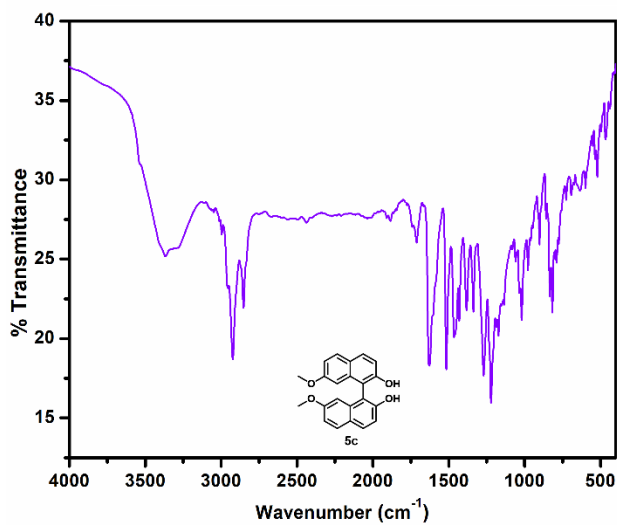
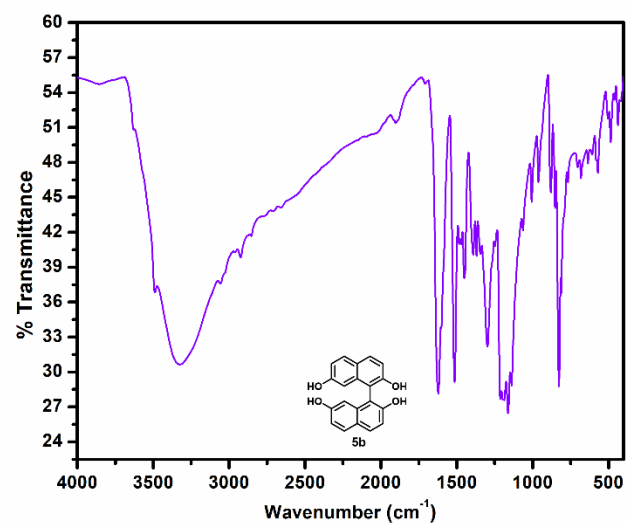
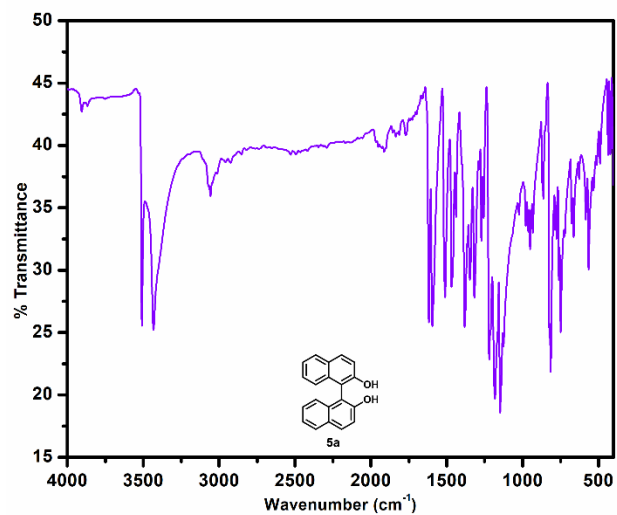


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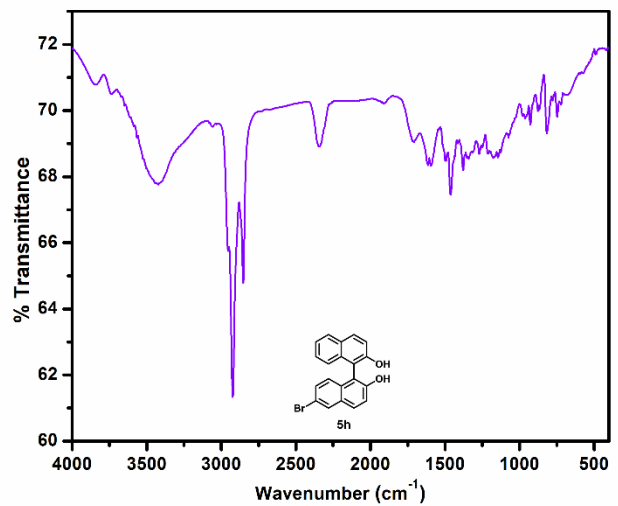
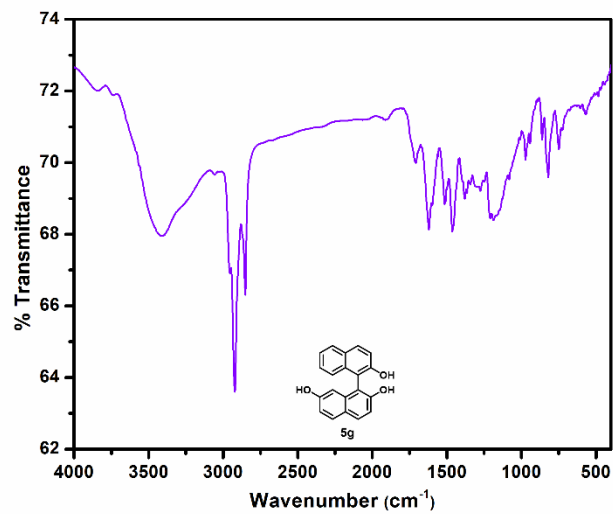


Supporting Information

FT-IR Spectra of compound 5a-5h



Supporting Information



Supporting Information

Cartesian Coordinates of all the optimized geometries at B3LYP/6-311+G(d,p)/SDD level of theory

Species	Atomic No. (Z)	Cartesian Coordinates (in Å)		
		X	Y	Z
C₆H₅CH₂⁺	6	0.000001000	-1.126777000	1.202201000
	6	0.000001000	0.262009000	1.232929000
	6	0.000001000	0.962225000	0.000000000
	6	0.000001000	0.262009000	-1.232929000
	6	0.000001000	-1.126777000	-1.202201000
	6	0.000001000	-1.826630000	0.000000000
	1	0.000003000	-1.656865000	2.148620000
	1	0.000001000	0.794913000	2.173769000
	1	0.000001000	0.794913000	-2.173769000
	1	0.000003000	-1.656865000	-2.148620000
	1	0.000001000	-2.909086000	0.000000000
	6	-0.000006000	2.379194000	0.000000000
	1	0.928979000	2.960741000	0.000000000
	1	-0.928997000	2.960731000	0.000000000
C₆H₅CH₃CH₂⁺	6	-0.639392000	1.227224000	-0.010157000
	6	0.731444000	1.239836000	-0.002465000
	6	1.439273000	-0.000003000	0.001161000
	6	0.731433000	-1.239837000	-0.002526000
	6	-0.639401000	-1.227212000	-0.010217000
	6	-1.353031000	0.000011000	-0.012748000
	1	-1.192671000	2.158692000	-0.016800000
	1	1.280491000	2.173890000	-0.001729000
	1	1.280472000	-2.173896000	-0.001837000
	1	-1.192689000	-2.158674000	-0.016907000
	6	2.984052000	-0.000008000	0.009179000
	1	3.525242000	0.939202000	0.012687000

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	1	3.525238000	-0.939220000	0.012641000
	6	-2.842468000	0.000002000	0.008128000
	1	-3.183079000	-0.000383000	1.053824000
	1	-3.257248000	0.892964000	-0.461694000
	1	-3.257220000	-0.892658000	-0.462303000
C₆H₅NO₂CH₂⁺	6	-0.000781000	1.228558000	-0.161249000
	6	-1.377911000	1.232100000	-0.170603000
	6	-2.074422000	0.000000000	0.000000000
	6	-1.377911000	-1.232100000	0.170603000
	6	-0.000781000	-1.228559000	0.161249000
	6	0.652381000	0.000000000	0.000000000
	1	0.579041000	2.136669000	-0.264284000
	1	-1.928405000	2.156087000	-0.299745000
	1	-1.928405000	-2.156087000	0.299745000
	1	0.579041000	-2.136670000	0.264284000
	6	-3.624022000	0.000000000	0.000000000
	1	-4.166277000	0.931927000	-0.124503000
	1	-4.166277000	-0.931927000	0.124504000
	7	2.142663000	0.000000000	0.000000000
	8	2.678333000	0.979691000	0.481888000
8	2.678333000	-0.979691000	-0.481888000	
	14	2.452232000	1.671559000	0.000044000
	8	2.319587000	-0.000104000	-0.000095000
	14	-0.776240000	-2.803102000	-0.000171000
	8	0.724168000	-1.905064000	0.000244000
	8	-1.651761000	-1.318116000	0.000184000
	13	-3.228289000	0.000150000	0.000011000
	14	-0.775963000	2.803179000	-0.000249000
	8	0.724361000	1.904972000	0.000276000

Supporting Information

Ru(III)- Zeolite	8	-1.651713000	1.318308000	0.000016000
	1	-3.753330000	-0.000186000	-1.465695000
	1	-0.933566000	-3.514943000	1.270115000
	1	-0.933270000	-3.514264000	-1.270879000
	1	2.991663000	-2.175356000	-1.265180000
	1	2.992195000	-2.175458000	1.264699000
	1	2.992303000	2.175088000	1.264937000
	1	2.991989000	2.175198000	-1.264943000
	1	-0.932834000	3.514359000	-1.270966000
	1	-0.933283000	3.515034000	1.270030000
	1	-3.753569000	0.000290000	1.465599000
	14	2.452058000	-1.671778000	-0.000105000
	44	-0.213793000	0.000007000	0.000088000
	IM1	14	-1.715520000	2.625204000
8		-2.110573000	2.128383000	-0.574151000
14		-2.436690000	-1.894454000	-0.697215000
8		-1.813132000	-0.399502000	-1.333387000
8		-1.178097000	-2.013366000	0.431088000
13		-0.096933000	-2.524764000	1.959978000
14		0.346455000	0.717266000	2.622804000
8		-0.589974000	1.453189000	1.441053000
8		0.630907000	-0.741049000	1.772263000
1		-0.949234000	-2.637302000	3.263067000
1		-2.352725000	-2.944947000	-1.715854000
1		-3.740129000	-1.657771000	-0.063171000
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1		-1.910184000	1.515727000	-3.040384000
1		-1.040387000	3.926834000	0.876305000
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Supporting Information

	1	1.613710000	1.439160000	2.795954000
	1	0.982663000	-3.473608000	1.299294000
	14	-2.551473000	1.123244000	-1.780815000
	44	0.015881000	-0.482309000	-0.166706000
	6	1.609321000	0.588858000	-1.517293000
	6	2.731008000	-0.230165000	-1.161977000
	6	3.772550000	0.322547000	-0.435452000
	6	3.734771000	1.677372000	-0.074433000
	6	2.644820000	2.490120000	-0.408255000
	6	1.595502000	1.959606000	-1.144368000
	1	1.004776000	0.287197000	-2.375599000
	1	4.625099000	-0.284514000	-0.152644000
	1	4.568327000	2.101621000	0.474575000
	1	2.646399000	3.538028000	-0.133978000
	1	0.787509000	2.597759000	-1.482436000
	6	2.679733000	-1.687628000	-1.540537000
	1	2.775018000	-1.833623000	-2.619179000
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	1	1.356158000	-2.163514000	-1.145070000
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	14	-2.041284000	-1.109116000	-2.438024000
	8	-1.900879000	-2.277503000	-1.302444000
	14	-0.412293000	-1.644888000	2.718519000
	8	-0.964334000	-1.832233000	1.107448000
	8	-0.445782000	0.069420000	2.593745000
	13	-1.221816000	3.692905000	1.133559000
	14	-1.939624000	2.021534000	-1.569108000
	8	-1.725291000	0.328750000	-1.511326000
	8	-1.401109000	2.246048000	0.039840000

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IM2	1	-1.738859000	4.982813000	0.427696000
	1	0.958302000	-2.138549000	2.895009000
	1	-1.434948000	-2.112728000	3.658473000
	1	-2.429391000	-3.897627000	0.621925000
	1	-0.105845000	-3.824499000	-0.293338000
	1	-0.977989000	-1.202156000	-3.447223000
	1	-3.414945000	-0.990179000	-2.940133000
	1	-3.358833000	2.369313000	-1.715481000
	1	-1.008059000	2.634625000	-2.524410000
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	14	-1.359253000	-3.114694000	-0.005906000
	44	-0.941691000	0.235732000	0.503106000
	6	3.593402000	-0.975103000	-1.049268000
	6	4.940506000	-1.235526000	-0.822583000
	6	5.762744000	-0.238867000	-0.293564000
	6	5.239238000	1.020969000	0.003473000
	6	3.892740000	1.283497000	-0.224054000
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	1	3.493094000	2.269157000	-0.008581000
	6	1.612213000	0.569744000	-1.002876000
	1	1.434046000	1.625547000	-1.231444000
	1	1.205201000	-0.049271000	-1.807130000
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Supporting Information

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	8	-3.419682000	-0.613257000	-0.205355000
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	13	0.156863000	3.467394000	-0.142328000
	14	1.450430000	0.399263000	-0.144086000
	8	0.108679000	-0.738823000	-0.109779000
	8	0.113940000	1.669092000	-0.202168000
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	1	-5.306386000	0.709007000	-1.457558000
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	1	-3.912297000	-2.714023000	1.217563000
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	1	0.593436000	-3.092952000	-1.065660000
	1	2.025358000	0.733341000	-1.454314000
	1	1.996285000	0.802636000	1.158359000
	1	-1.306631000	4.029161000	-0.083129000
	14	-3.365024000	-2.345333000	-0.094197000
	44	-1.538402000	0.547163000	0.066498000
	6	4.890982000	-0.473243000	1.203443000
	6	6.153602000	0.074543000	1.238664000
	6	6.831350000	0.353245000	0.036902000
	6	6.232099000	0.076136000	-1.206213000
	6	4.969923000	-0.471965000	-1.252879000
	6	4.265322000	-0.779395000	-0.046265000
	1	4.370293000	-0.703876000	2.126272000
	1	6.632868000	0.283645000	2.187182000
	1	7.826181000	0.782183000	0.069106000
	1	6.771413000	0.286174000	-2.121712000
	1	4.510192000	-0.702916000	-2.207418000
6	2.978358000	-1.377525000	-0.088730000	

Supporting Information

	1	2.699589000	-1.864771000	-1.019805000
	1	2.644983000	-1.864372000	0.826081000
	8	-1.687292000	0.501961000	1.790135000
	1	-3.271198000	2.754387000	-0.081761000
IM4	14	-2.575525000	0.992661000	-2.710498000
	8	-2.739295000	-0.623056000	-2.521829000
	14	-1.916791000	-2.708633000	1.103358000
	8	-2.447434000	-2.072724000	-0.325964000
	8	-1.710132000	-1.201895000	1.922041000
	13	-4.902428000	1.022307000	2.593591000
	14	-4.114057000	2.275069000	-0.259820000
	8	-2.792879000	1.642944000	-1.126872000
	8	-3.957429000	1.268528000	1.089769000
	1	-6.205845000	1.879388000	2.657350000
	1	-0.615125000	-3.381166000	0.980125000
	1	-2.957768000	-3.474361000	1.803024000
	1	-3.896346000	-2.879108000	-2.278981000
	1	-1.430883000	-2.826021000	-2.557472000
	1	-1.216287000	1.358898000	-3.124353000
	1	-3.666070000	1.539809000	-3.530737000
	1	-5.365413000	2.028502000	-0.993137000
	1	-3.848166000	3.673943000	0.100605000
	1	-4.203576000	-0.008100000	3.539674000
	14	-2.633364000	-2.181962000	-2.003904000
	44	-1.916502000	0.397180000	0.480946000
	6	5.503564000	2.256886000	0.915047000
	6	6.869450000	2.061133000	0.927971000
	6	7.489794000	1.434259000	-0.162926000
6	6.750401000	0.998441000	-1.270108000	
6	5.383166000	1.192914000	-1.296197000	

Supporting Information

	6	4.732507000	1.836291000	-0.205973000
	1	5.009620000	2.747799000	1.746131000
	1	7.464030000	2.394039000	1.769548000
	1	8.564331000	1.289226000	-0.151014000
	1	7.252762000	0.520642000	-2.101806000
	1	4.799110000	0.873859000	-2.151726000
	6	3.356267000	2.079075000	-0.247082000
	1	2.802614000	1.918377000	-1.163110000
	1	2.885260000	2.689841000	0.511539000
	8	-0.253196000	0.328587000	-0.085986000
	1	-1.411186000	-1.131630000	2.836543000
	6	3.969438000	-1.226445000	1.398347000
	6	3.007772000	-0.853184000	0.461298000
	6	2.709771000	-1.665837000	-0.634033000
	6	3.372241000	-2.883389000	-0.772302000
	6	4.333512000	-3.272915000	0.161595000
	6	4.630562000	-2.443004000	1.242186000
	1	4.172638000	-0.580089000	2.243234000
	1	1.969107000	-1.350310000	-1.360842000
	1	3.144353000	-3.524975000	-1.615373000
	1	4.848604000	-4.218739000	0.046270000
	1	5.372570000	-2.745717000	1.971355000
	8	2.380680000	0.373308000	0.639642000
	1	1.452460000	0.349207000	0.303563000
	14	1.869416000	1.810435000	-2.059352000
	8	2.280419000	2.751639000	-0.801605000
	14	4.517502000	0.787304000	1.454040000
	8	3.999779000	2.294252000	1.163921000
	8	3.098532000	-0.228154000	1.567689000
	13	2.390140000	-4.019480000	-0.580551000

Supporting Information

IM5	14	2.499585000	-1.267632000	-2.277916000
	8	2.038183000	0.184687000	-1.506181000
	8	2.211560000	-2.290447000	-0.990352000
	1	3.035426000	-4.876284000	-1.717017000
	1	5.158915000	0.653978000	2.767874000
	1	5.254872000	0.232993000	0.307456000
	1	4.371675000	4.203534000	-0.496439000
	1	2.515568000	4.359689000	1.147644000
	1	0.451707000	2.003563000	-2.394491000
	1	2.790037000	1.922201000	-3.205891000
	1	3.927043000	-1.202440000	-2.628849000
	1	1.601585000	-1.536590000	-3.412949000
	1	1.838099000	-4.329777000	0.848753000
	14	3.318401000	3.509482000	0.260394000
	44	1.306659000	-0.570763000	0.473433000
	6	-5.876383000	0.284401000	-1.436910000
	6	-7.171781000	0.557244000	-1.060486000
	6	-7.412758000	1.453524000	-0.004625000
	6	-6.361098000	2.075750000	0.685496000
	6	-5.058578000	1.811282000	0.320373000
	6	-4.781999000	0.920535000	-0.766239000
	1	-5.671332000	-0.395251000	-2.256236000
	1	-8.004413000	0.094191000	-1.575109000
	1	-8.436097000	1.670400000	0.281906000
	1	-6.578227000	2.763328000	1.493313000
	1	-4.232941000	2.291418000	0.832173000
	6	-3.483555000	0.729085000	-1.204610000
	1	-2.659785000	1.290221000	-0.785922000
	1	-3.275919000	0.139549000	-2.088494000
	8	0.824563000	-1.245804000	2.192482000
1	2.893028000	-0.602067000	2.442136000	

Supporting Information

	6	-2.628647000	-1.767090000	-0.272564000
	6	-1.794977000	-0.807064000	0.352904000
	6	-2.168022000	-0.298577000	1.617314000
	6	-3.327065000	-0.750576000	2.230739000
	6	-4.135083000	-1.719798000	1.615400000
	6	-3.776639000	-2.227947000	0.371356000
	1	-2.317795000	-2.180107000	-1.225417000
	1	-1.535725000	0.437407000	2.100210000
	1	-3.600934000	-0.362668000	3.205259000
	1	-5.022192000	-2.083494000	2.119320000
	1	-4.384651000	-2.990311000	-0.101729000
	8	-0.672654000	-0.417662000	-0.270403000
	1	0.065035000	-1.843618000	2.244987000
	14	3.784320000	-1.843665000	-0.567712000
	8	2.976571000	-0.575962000	-1.355807000
	14	1.892856000	2.961976000	-0.922552000
	8	2.411482000	1.901556000	-2.083487000
	8	1.601026000	2.007176000	0.435961000
	13	1.933831000	1.966997000	2.228300000
	14	2.943789000	-1.228433000	2.471333000
	8	2.927785000	-1.812475000	0.873837000
	8	2.032415000	0.147831000	2.233703000
	1	3.317461000	2.683168000	2.647245000
	1	0.622761000	3.549453000	-1.379475000
	1	2.941103000	3.945374000	-0.600998000
	1	4.718430000	0.843091000	-2.598814000
	1	2.703486000	0.077102000	-3.831696000
	1	3.521088000	-3.111079000	-1.259604000
	1	5.200611000	-1.498804000	-0.365331000
	1	4.322355000	-0.917797000	2.882779000

Supporting Information

IM6	1	2.229221000	-2.201697000	3.307174000
	1	0.664557000	2.493587000	3.079889000
	14	3.266347000	0.598313000	-2.578848000
	44	1.172789000	-0.201874000	0.148560000
	6	-5.689726000	1.035405000	-0.821090000
	6	-6.562633000	1.502634000	0.140480000
	6	-6.092247000	1.765824000	1.444637000
	6	-4.734208000	1.558968000	1.767052000
	6	-3.865388000	1.092728000	0.803210000
	6	-4.324481000	0.815095000	-0.512004000
	1	-6.045396000	0.847877000	-1.827899000
	1	-7.604421000	1.675243000	-0.100448000
	1	-6.775783000	2.136670000	2.199594000
	1	-4.381810000	1.779503000	2.767146000
	1	-2.817252000	0.957412000	1.043248000
	6	-3.379061000	0.329495000	-1.579704000
	1	-3.854117000	0.429579000	-2.556662000
	1	-2.476381000	0.946529000	-1.588978000
	6	-2.911446000	-1.164600000	-1.435501000
	6	-1.773813000	-1.369054000	-0.458117000
	6	-1.813614000	-2.469338000	0.433704000
	6	-2.895176000	-3.314699000	0.441822000
	6	-4.021312000	-3.155291000	-0.433346000
	6	-4.042059000	-2.132227000	-1.311845000
	1	-2.439485000	-1.393579000	-2.409229000
	1	-0.983580000	-2.624030000	1.113592000
	1	-2.901172000	-4.145724000	1.140272000
	1	-4.838689000	-3.863063000	-0.376473000
	1	-4.878885000	-2.000838000	-1.989801000
	8	-0.796528000	-0.555723000	-0.517575000

Supporting Information

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