Supplementary Information

Ruthenium/Yb(OTf)₃-CocatalyzedDehydrogenativeSynthesis of 14-substituted-14-H-dibenzo[a,j]xanthenes from β -Naphthol and Alcohols

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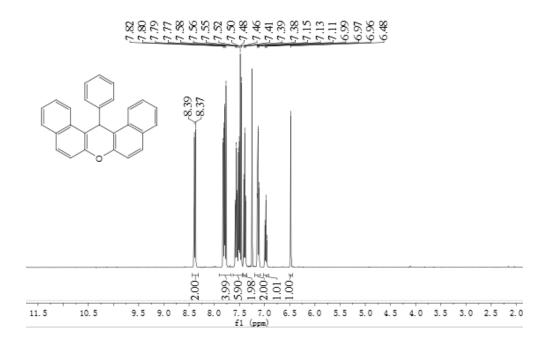
General information

All the obtained products were characterized by melting points (m.p), ¹H-NMR, ¹³C-NMR infrared spectra (IR), the ¹H-NMR spectra of the known compounds were found to be identical with the ones reported in the literatures. Additionally, the new products were further determined by high resolution mass spectra (HR-MS). Melting points were measured on an Electrothemal SGW-X4 microscopy digital melting point apparatus and are uncorrected; IR spectra were recorded on a FTLA2000 spectrometer; ¹H-NMR and ¹³C-NMR spectra were obtained on Bruker-400. Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), multiplet (m); High-resolution mass spectra (HRMS) were recorded on a JEOL JMS-600 spectrometer. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF254), and visualization was effected at 254 nm; All the reagents were purchased from commercial sources (J&KChemic, TCI, Fluka, Acros, SCRC), and used without further purification.

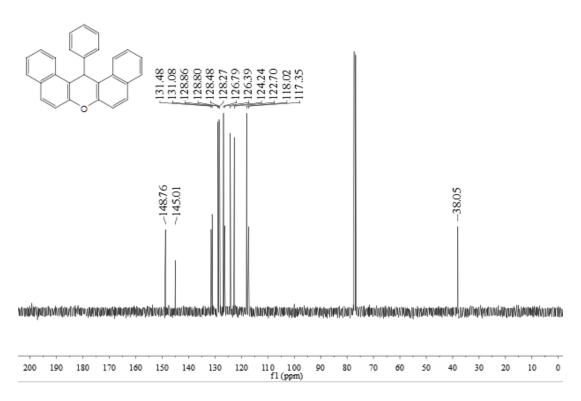
Typical procedure for the synthesis of 3a

In a schlenk tube equipped with a magnetic stirrer bar, benzyl alcohol **1a** (1.5 mmol, 162.2 mg), β -naphthol **2a** (1 mmol, 144.2 mg), [P^O]₂Cl₂Ru (Cat 5, 0.005 mmol, 3.8 mg) and Yb(OTf)₃ (0.05 mmol, 31.0 mg) and toluene (1 mL) were introduced successively. The resulting mixture was stirred at 110 °C for 16 h without insert any gas protection. After cooling down to room temperature, the reaction solvent was removed under vacuum, the residue was directly purified by flash chromatography on silica gel eluting with petroleum ether : ethyl acetate (30 : 1) to give 14-phenyl-14-*H*-dibenzo[*a,j*]xanthene **3a** as a white solid (148 mg, 83%).

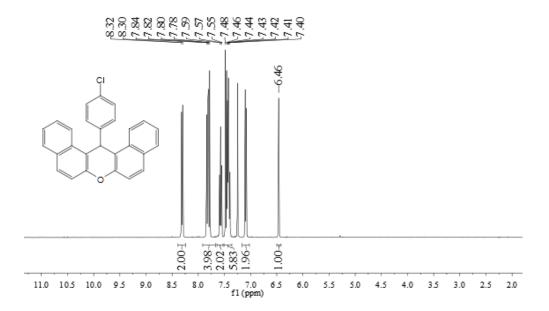
NMR spectra of the obtained compounds ¹H-NMR of 3a



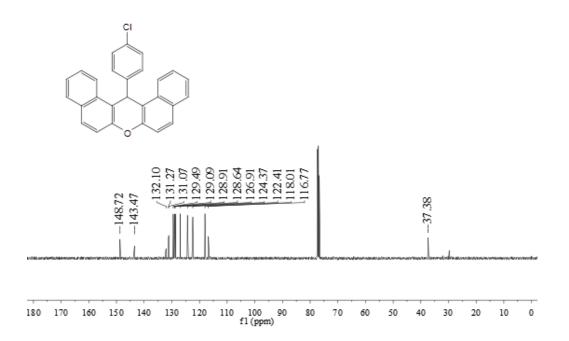
¹³C-NMR of 3a

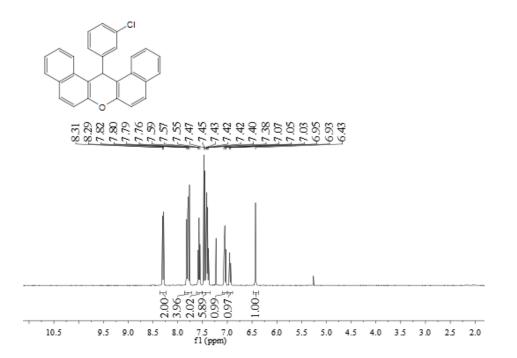


¹H-NMR of 3b

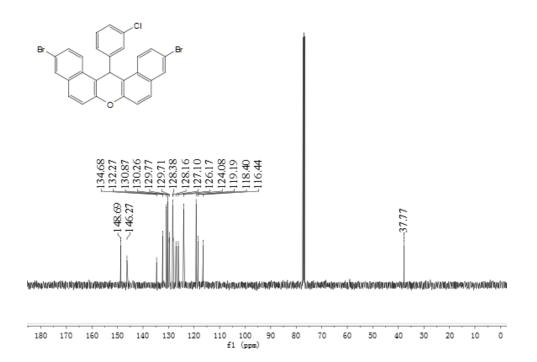


¹³C-NMR of 3b

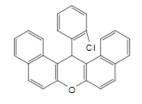


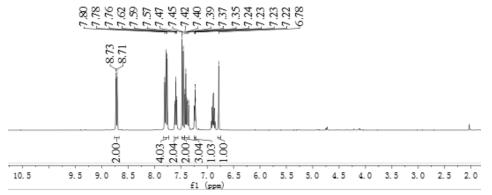


¹³C-NMR of 3c

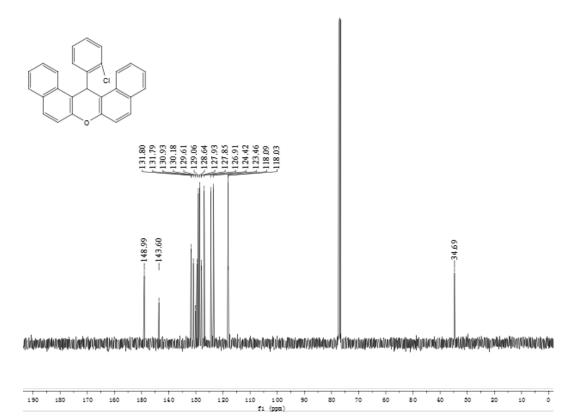


¹H-NMR of 3d

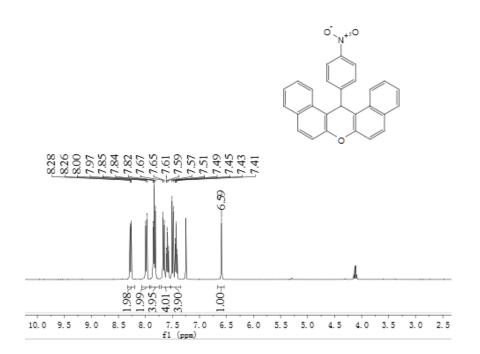




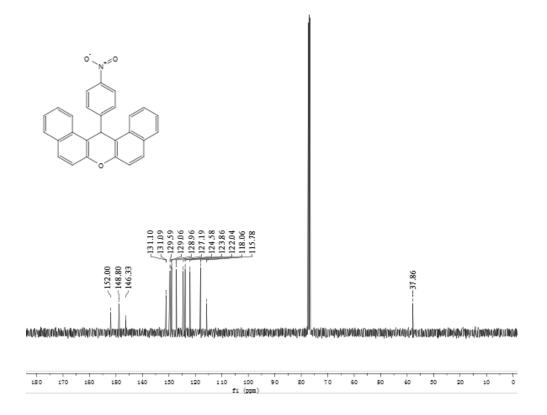
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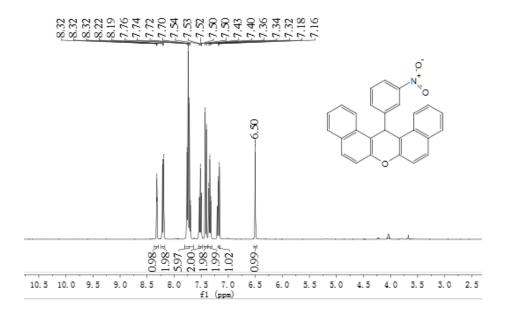
¹H-NMR of 3e



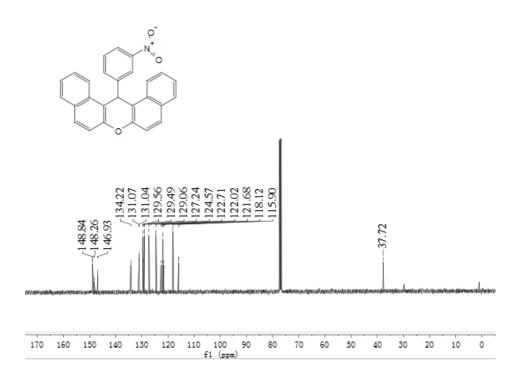


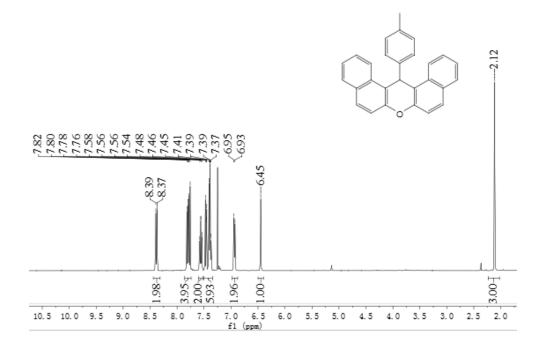




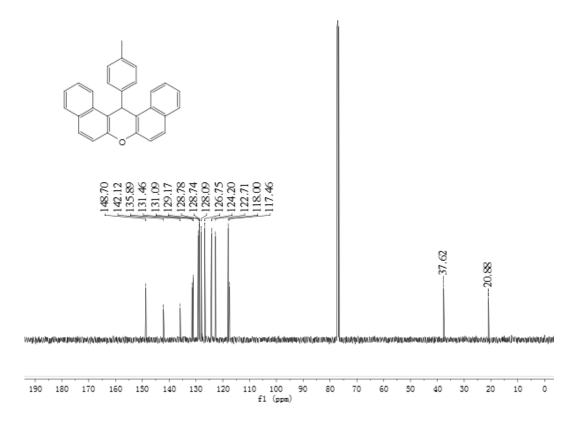




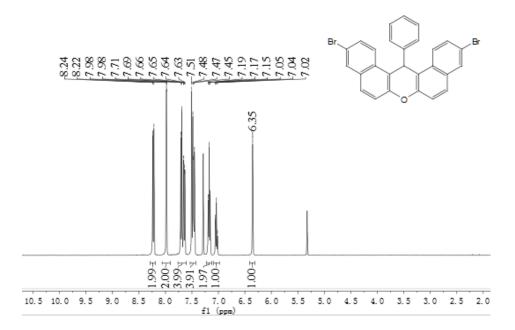


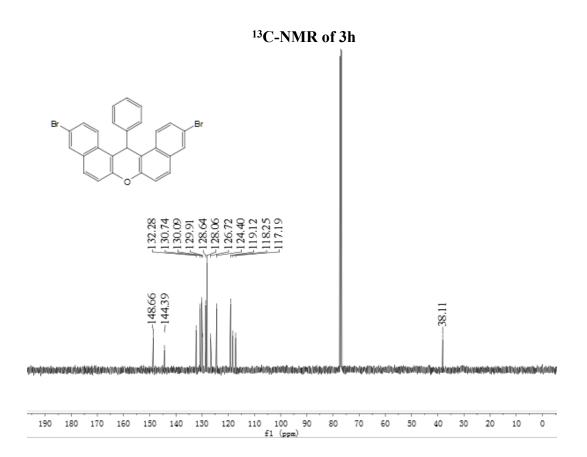


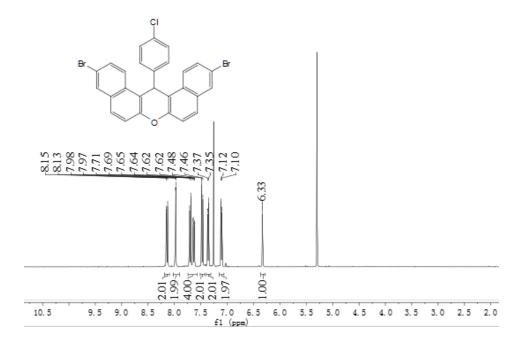
¹³C-NMR of 3g



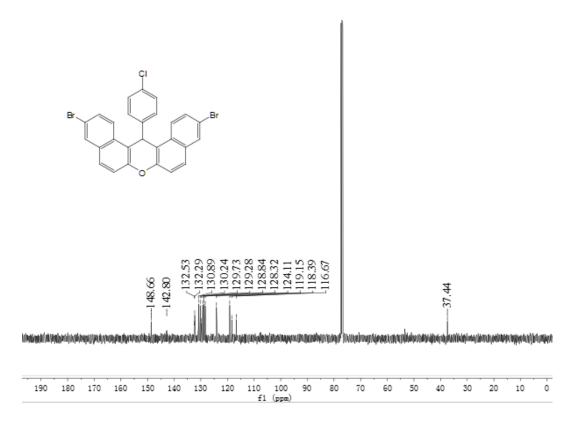


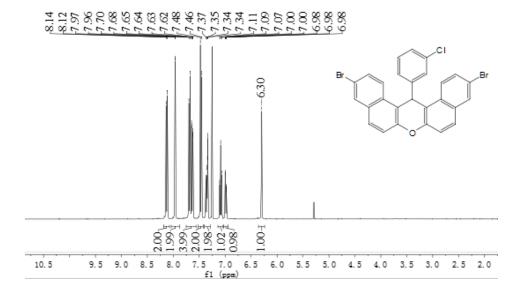




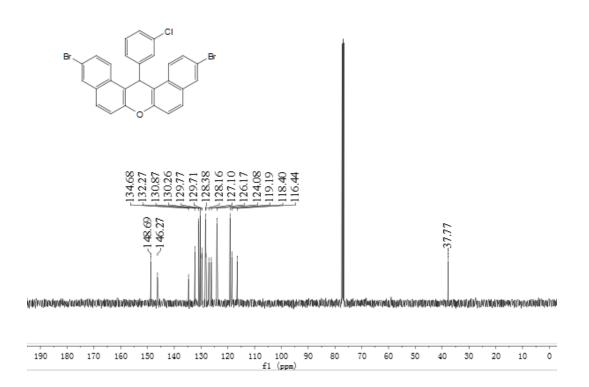


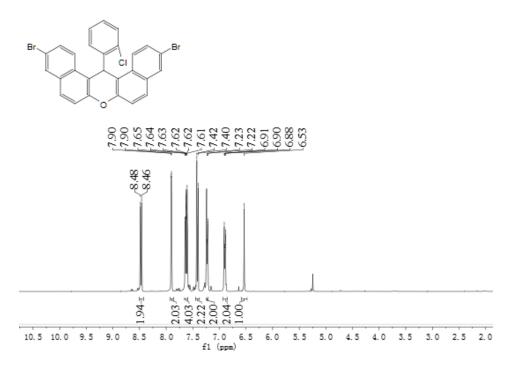
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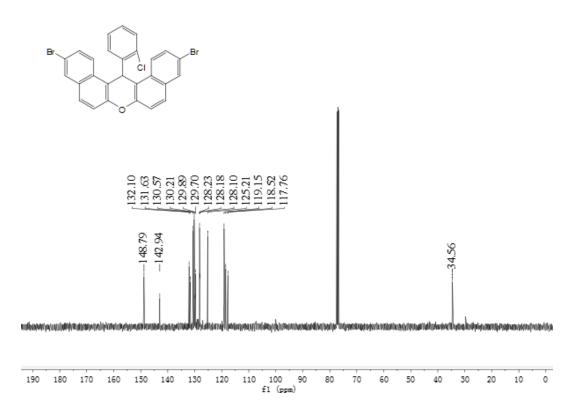


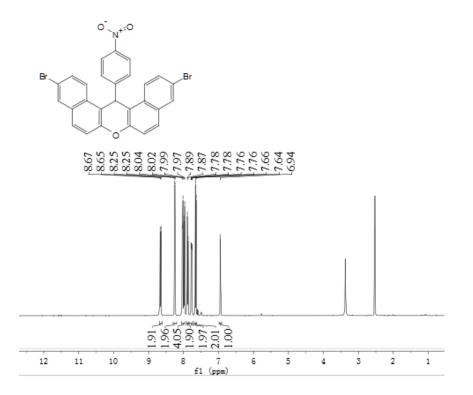
¹³C-NMR of 3j



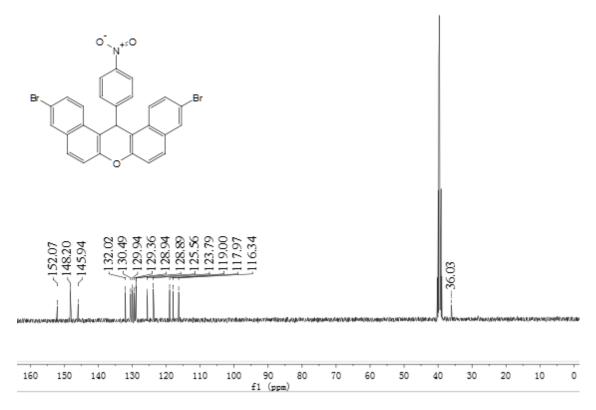


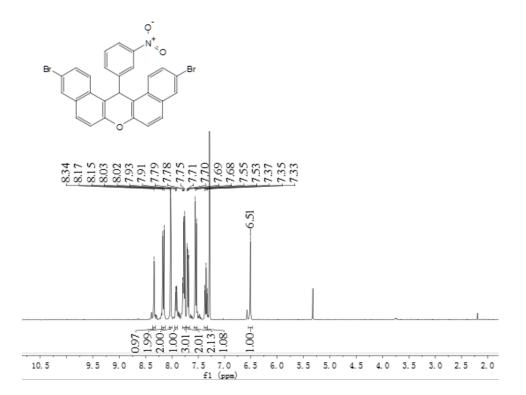




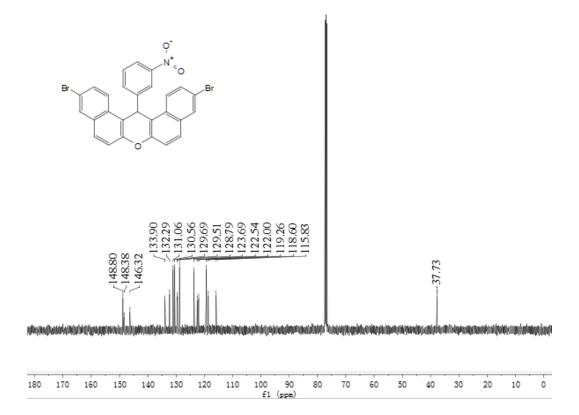


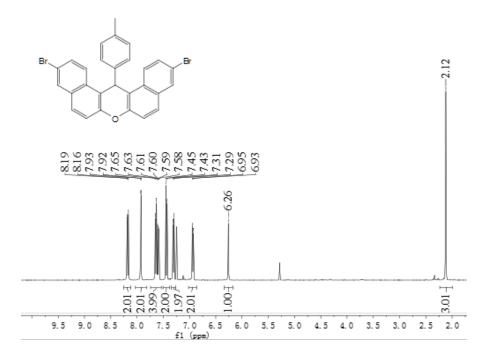
¹³C-NMR of 31



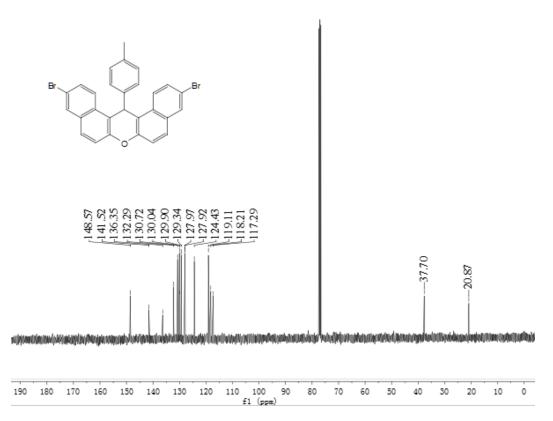


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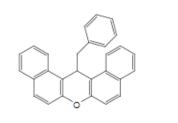


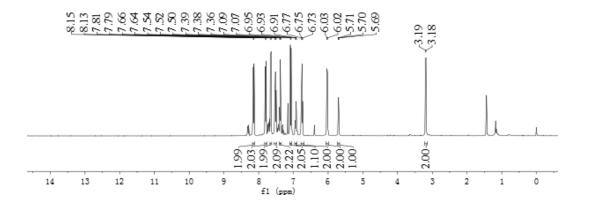


¹³C-NMR of 3n

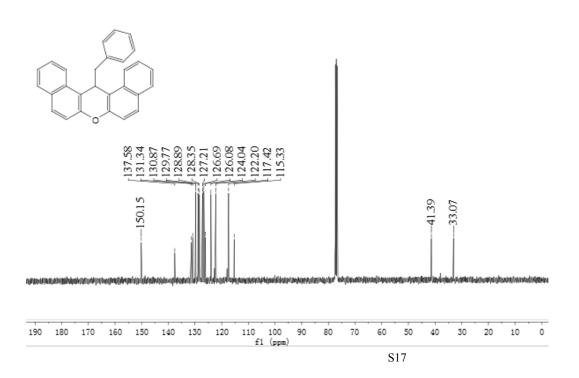




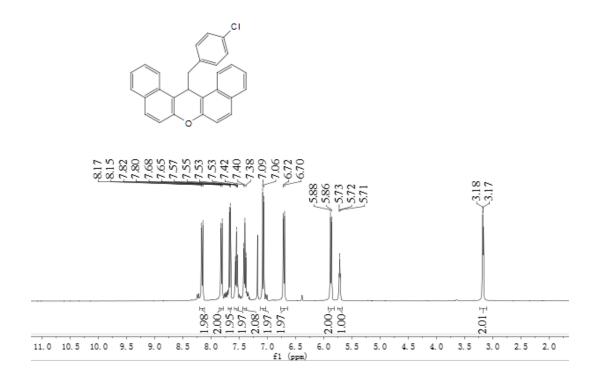




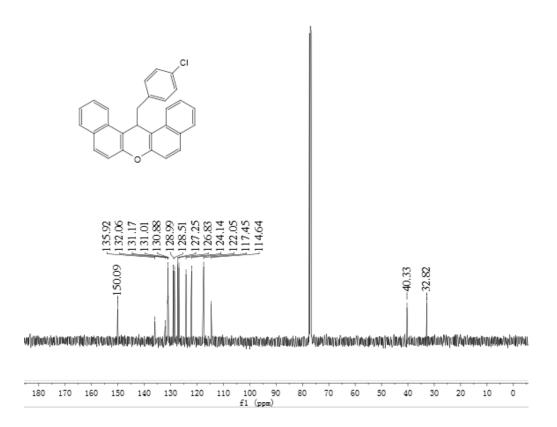


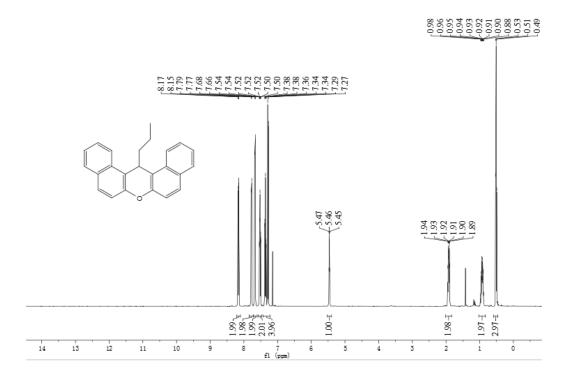


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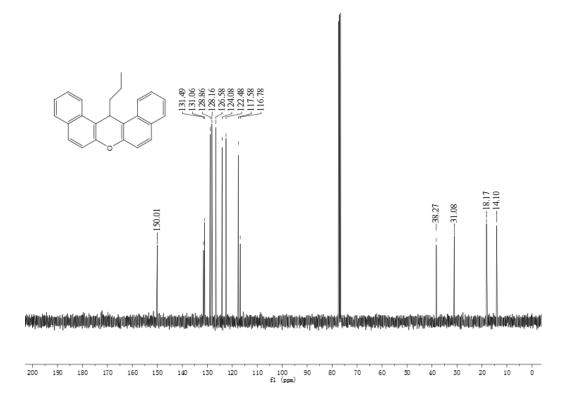


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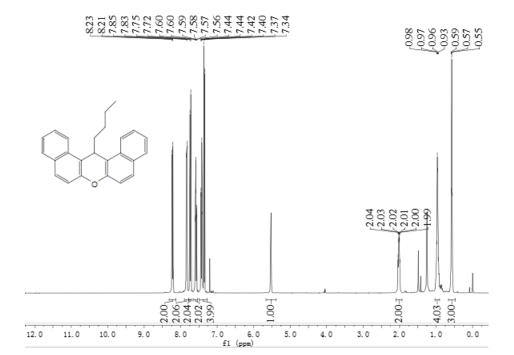




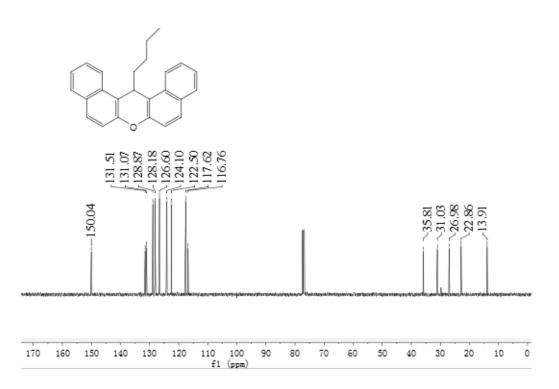




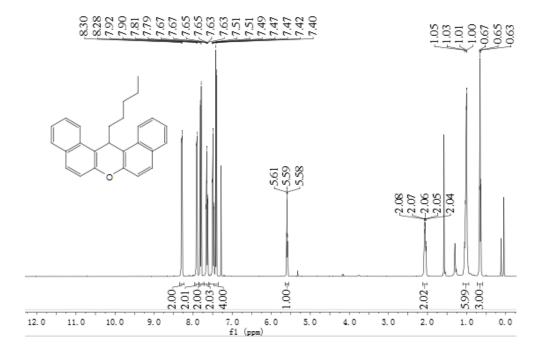
¹H-NMR of 3r



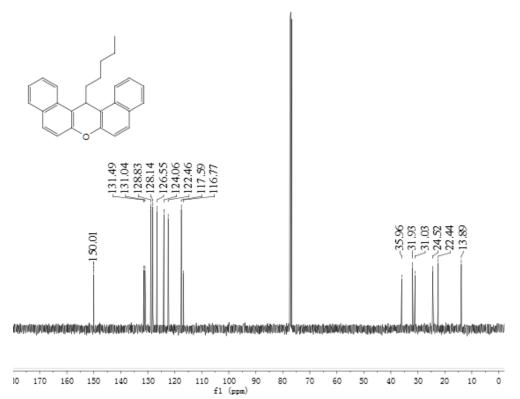
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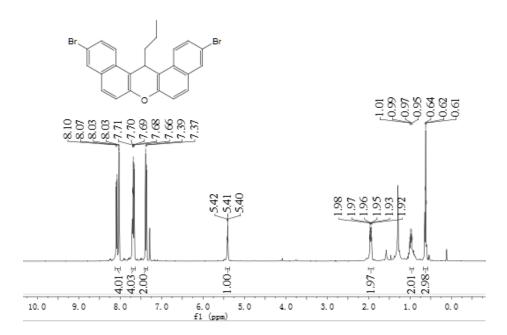
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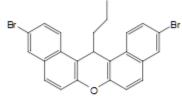
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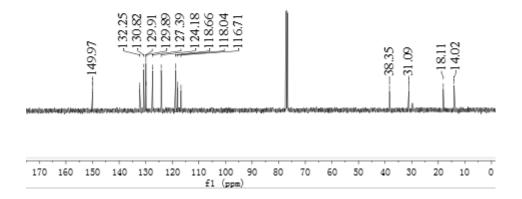




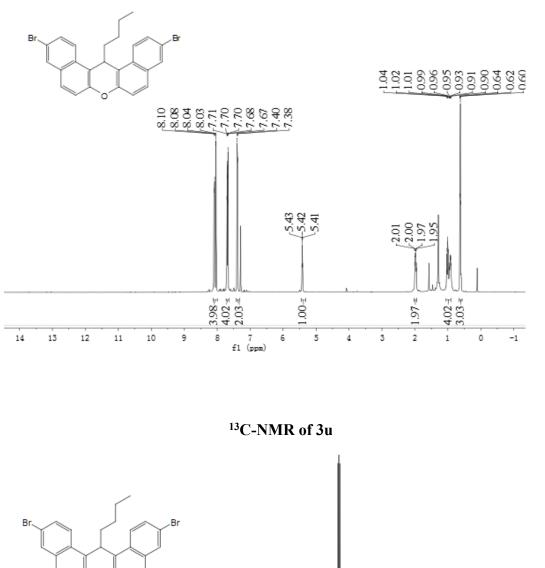


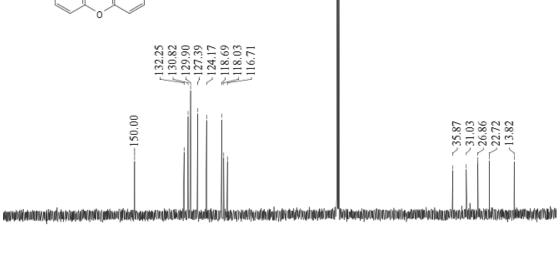
¹³C-NMR of 3t





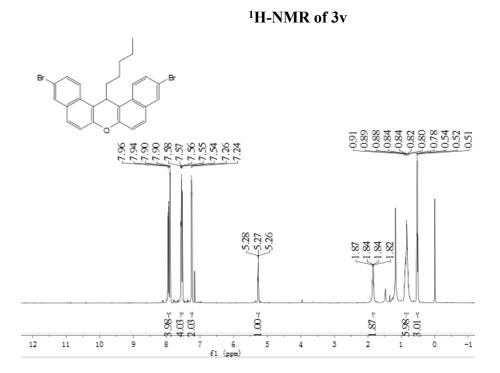






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¹³C-NMR of 3v

