Naphthyl-naphthalimides as high performance visible light photoinitiators for 3D printing and photocomposites synthesis

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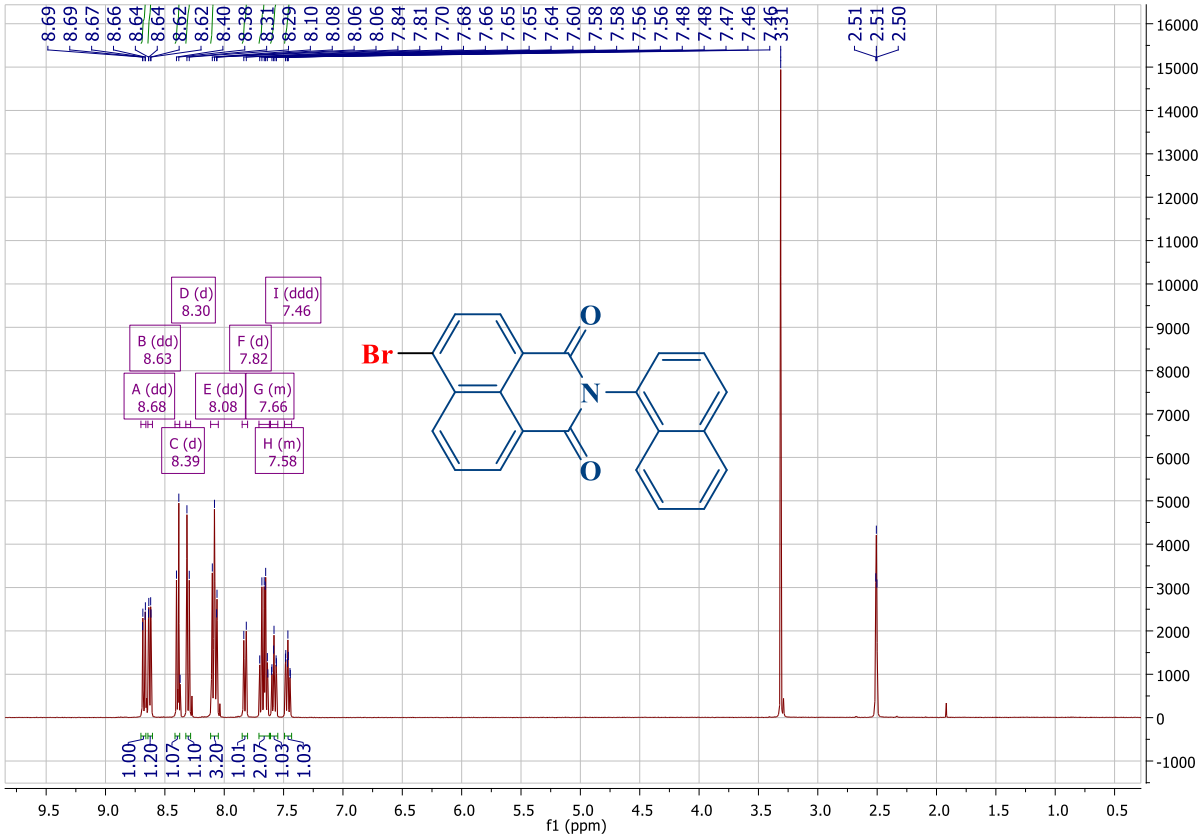
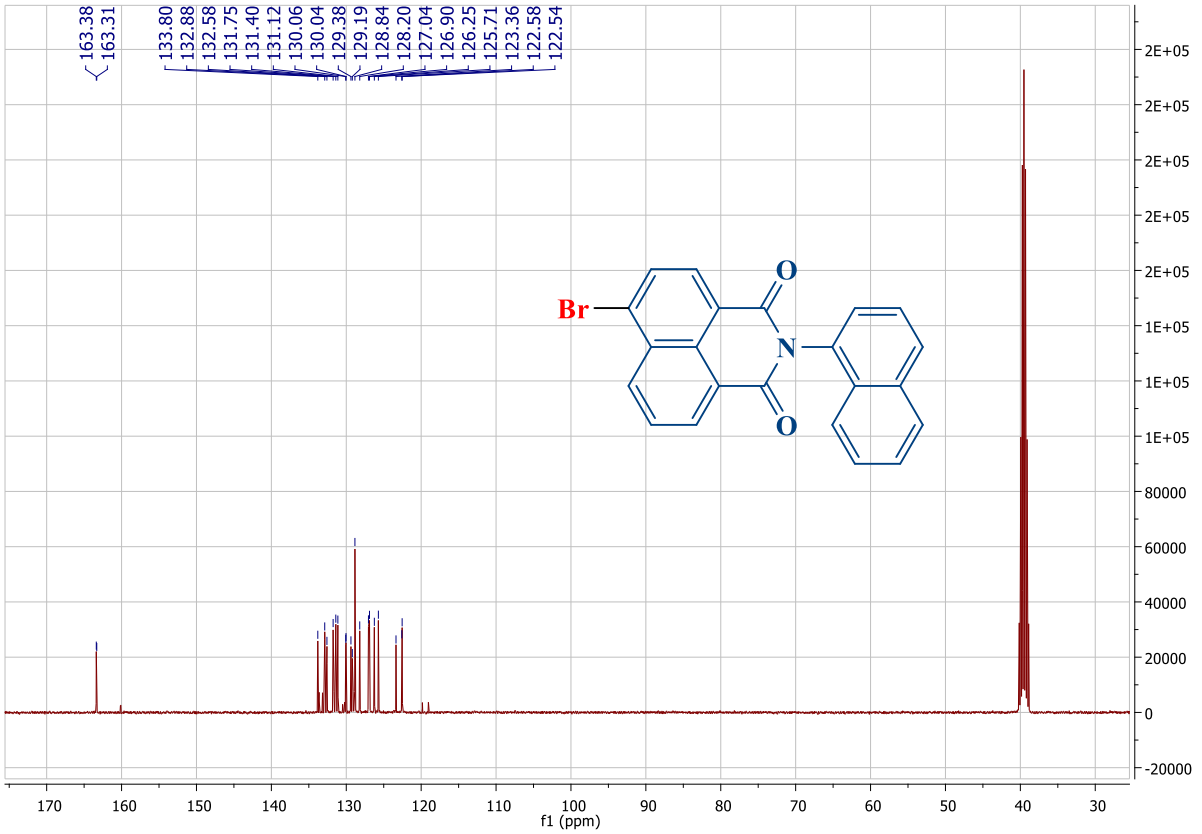
All reagents and solvents were purchased from Aldrich or Alfa Aesar and used as received without further purification. Mass spectroscopy was performed by the Spectropole of Aix-Marseille University. ESI mass spectral analyses were recorded with a 3200 QTRAP (Applied Biosystems SCIEX) mass spectrometer. The HRMS mass spectral analysis was performed with a QStar Elite (Applied Biosystems SCIEX) mass spectrometer. Elemental analyses were recorded with a Thermo Finnigan EA 1112 elemental analysis apparatus driven by the Eager 300 software. ^{1}H and ^{13}C NMR spectra were determined at room temperature in 5 mm o.d. tubes on a Bruker Avance 400 or a Bruker Avance 300 spectrometer of the Spectropole: ^{1}H (400 MHz), ^{1}H (300 MHz), ^{13}C (100 MHz), and ^{13}C (75 MHz). All ^{1}H chemical shifts were referenced to the solvent peak $CDCl_3$ (7.26 ppm), DMSO-d_6 (2.49 ppm) and the ^{13}C chemical shifts were referenced to the solvent peak $CDCl_3$ (77.0 ppm). All photoinitiators were prepared with analytical purity up to accepted standards for new organic compounds (>98%) which was checked by high field NMR analysis.

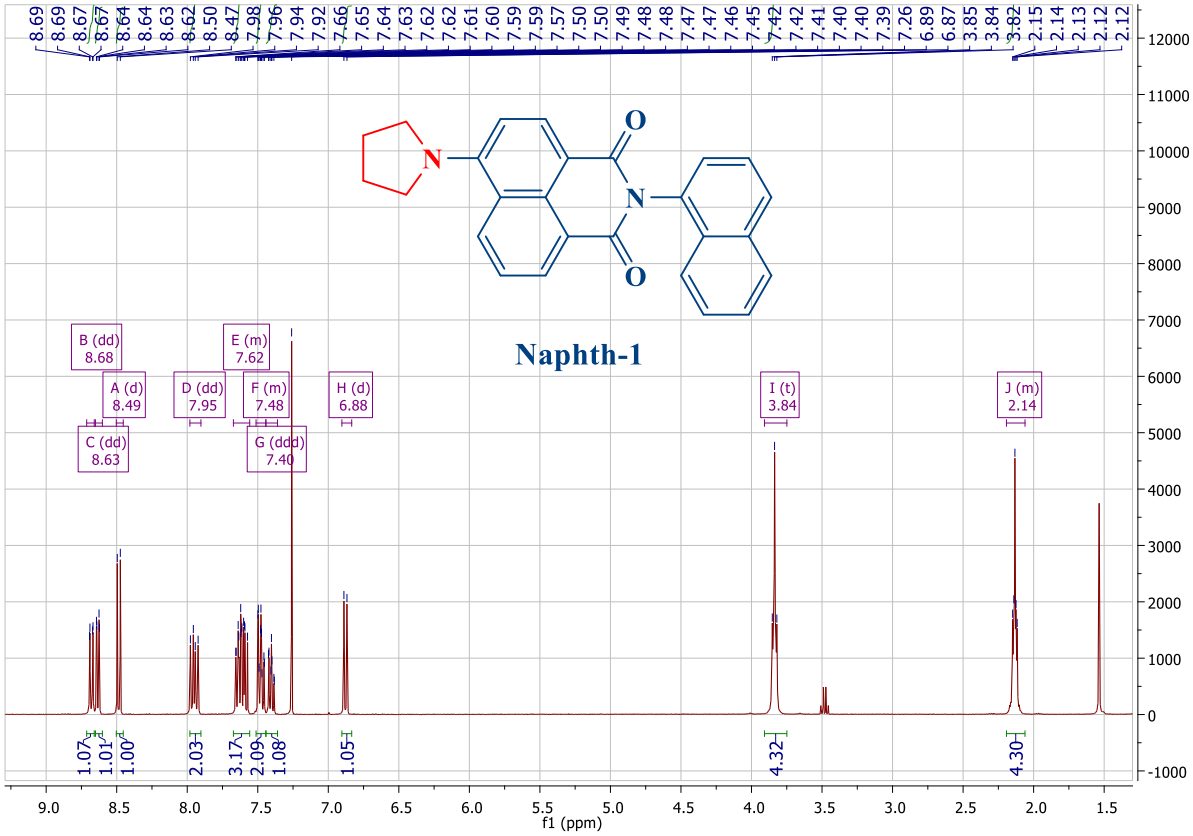
^{1}H NMR spectrum of 6-bromo-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione



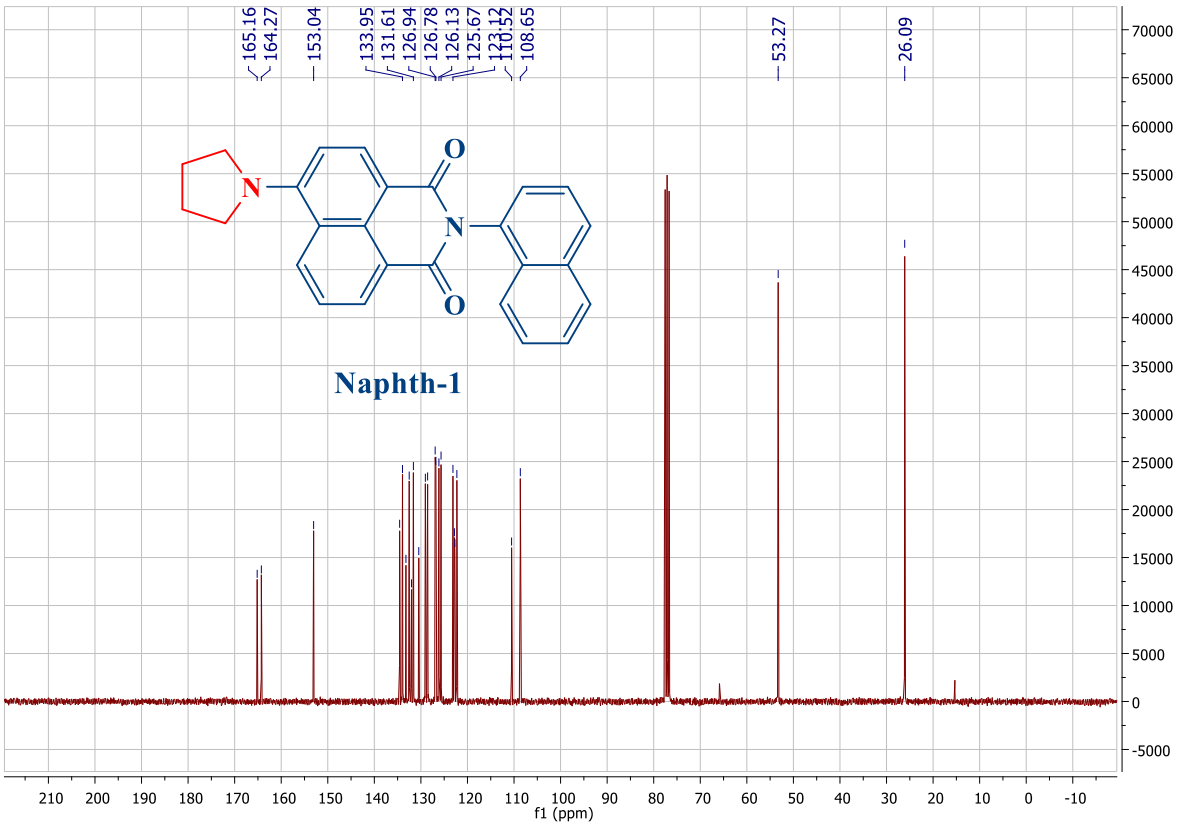
^{13}C NMR spectrum of 6-bromo-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione



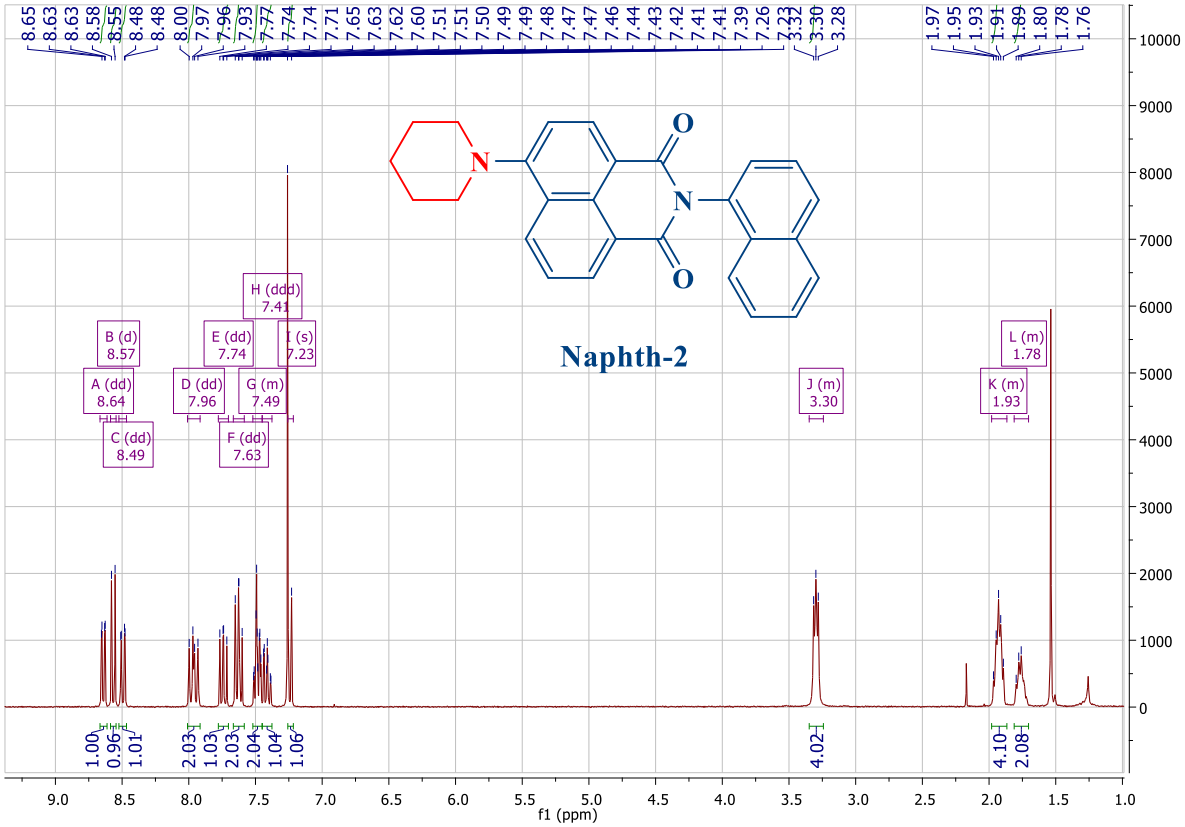
^{1}H NMR spectrum of 2-(naphthalen-1-yl)-6-(pyrrolidin-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-1)



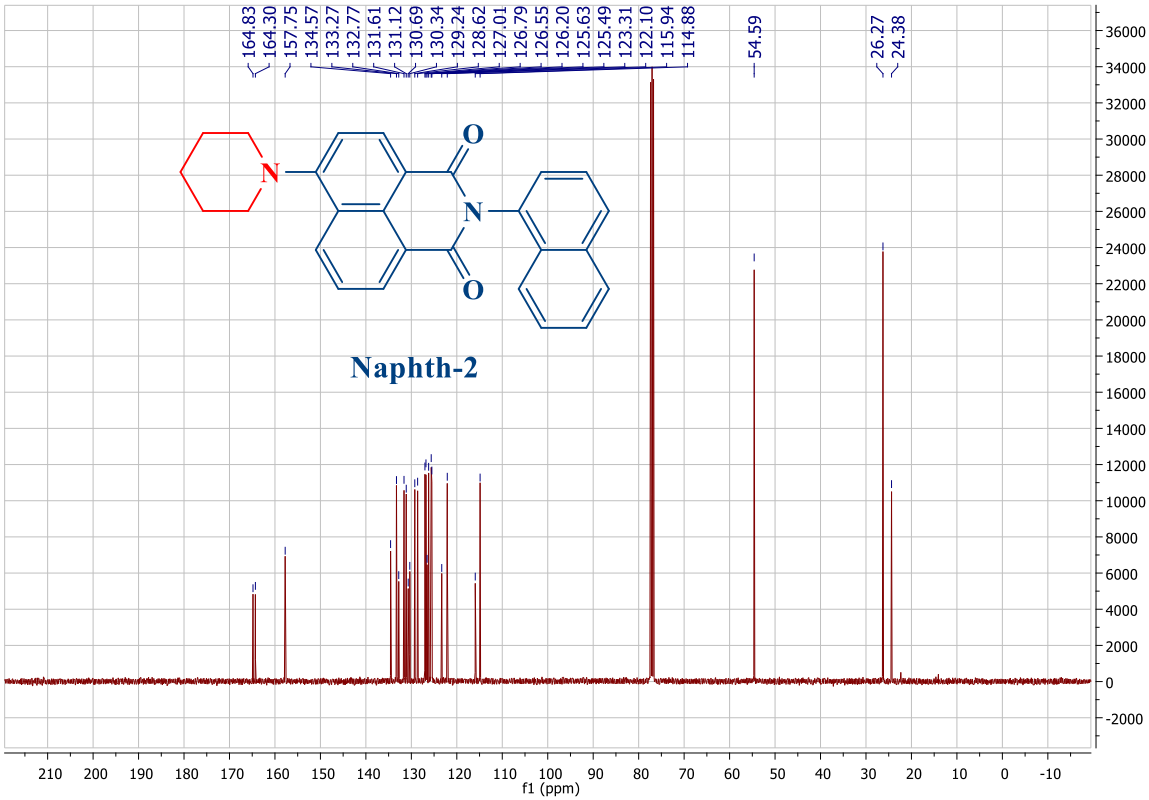
^{13}C NMR spectrum of 2-(naphthalen-1-yl)-6-(pyrrolidin-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-1)



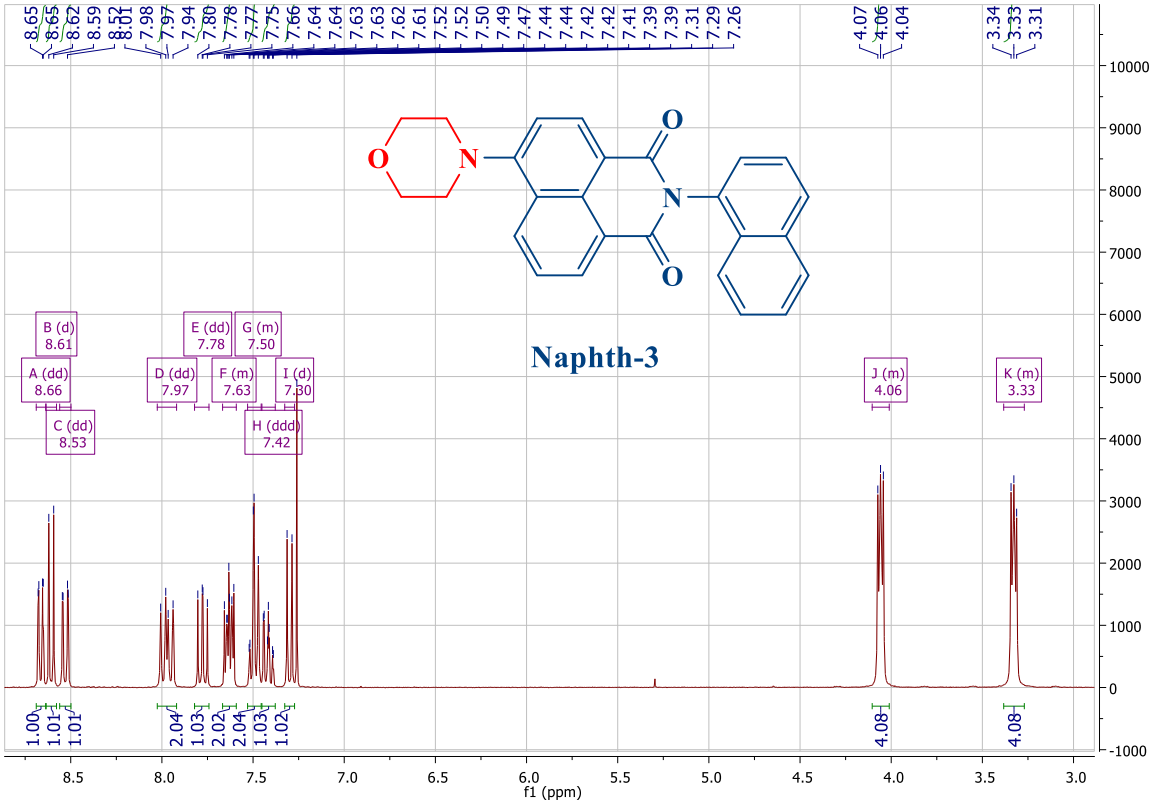
^{1}H NMR spectrum of 2-(naphthalen-1-yl)-6-(piperidin-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-2)



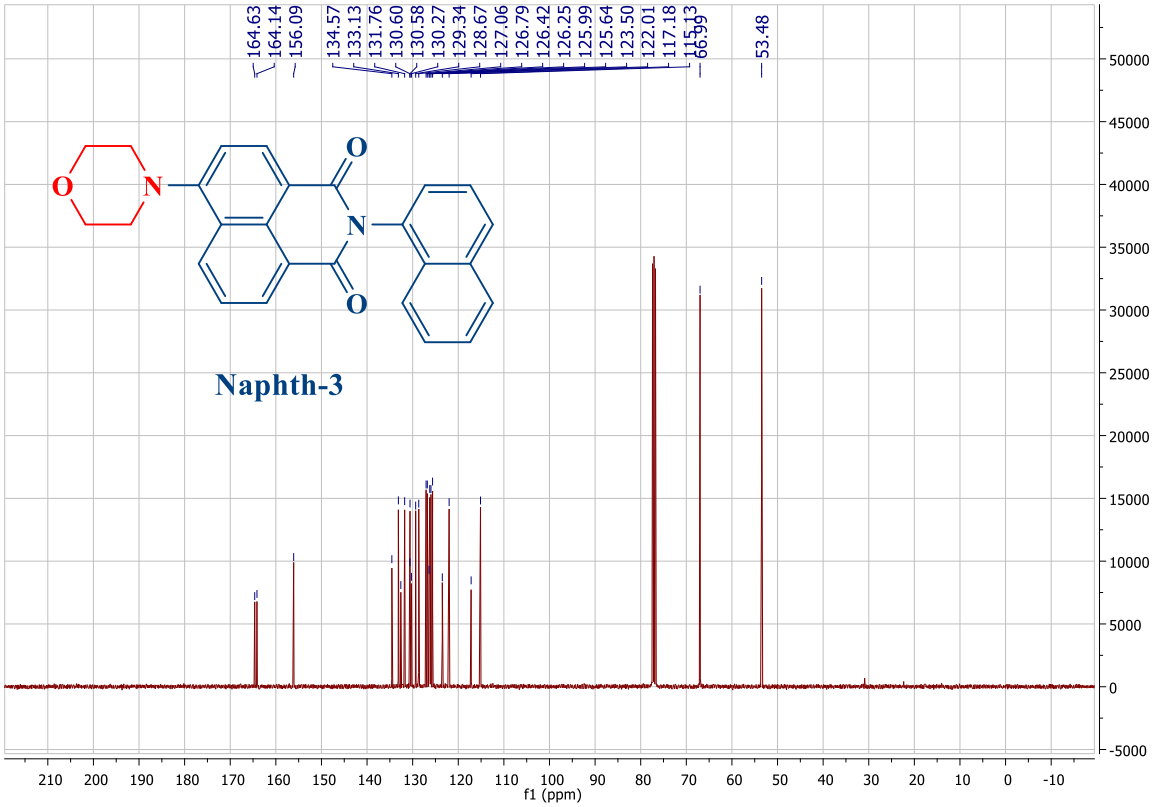
^{13}C NMR spectrum of 2-(naphthalen-1-yl)-6-(piperidin-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-2)



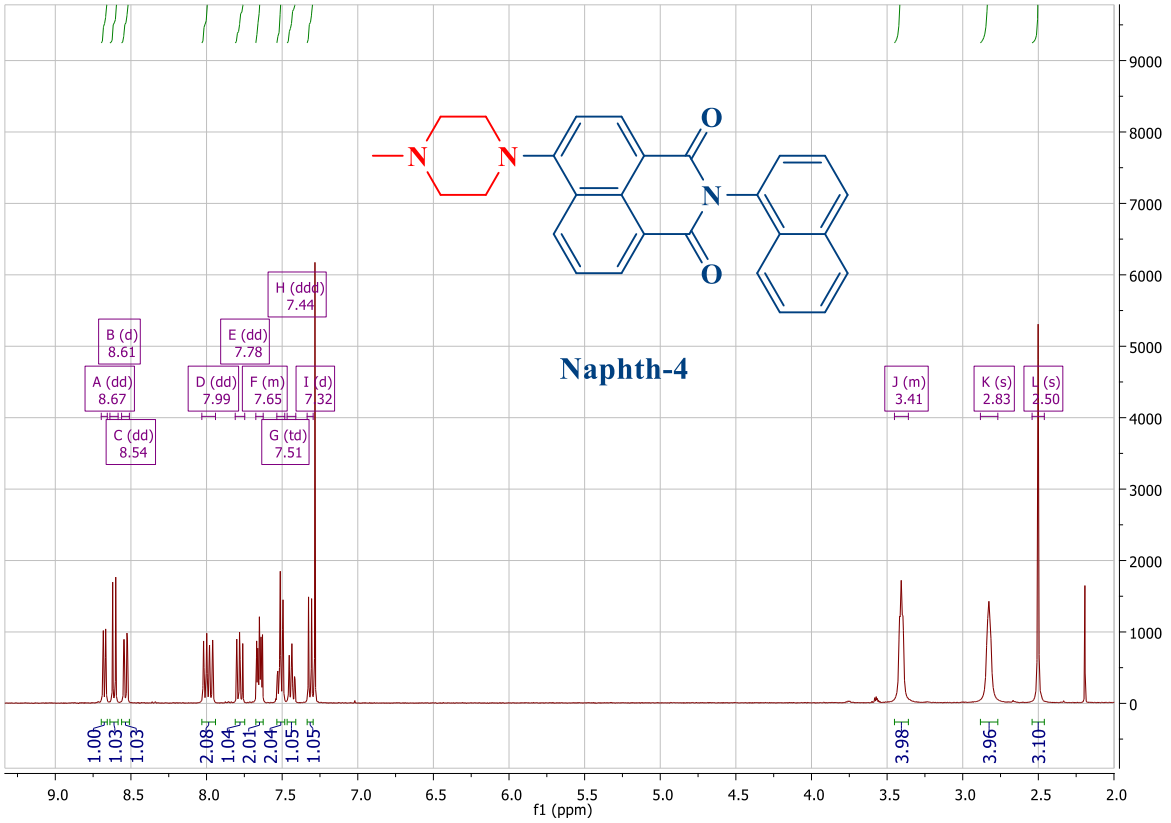
^{1}H NMR spectrum of 6-morpholino-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-3)



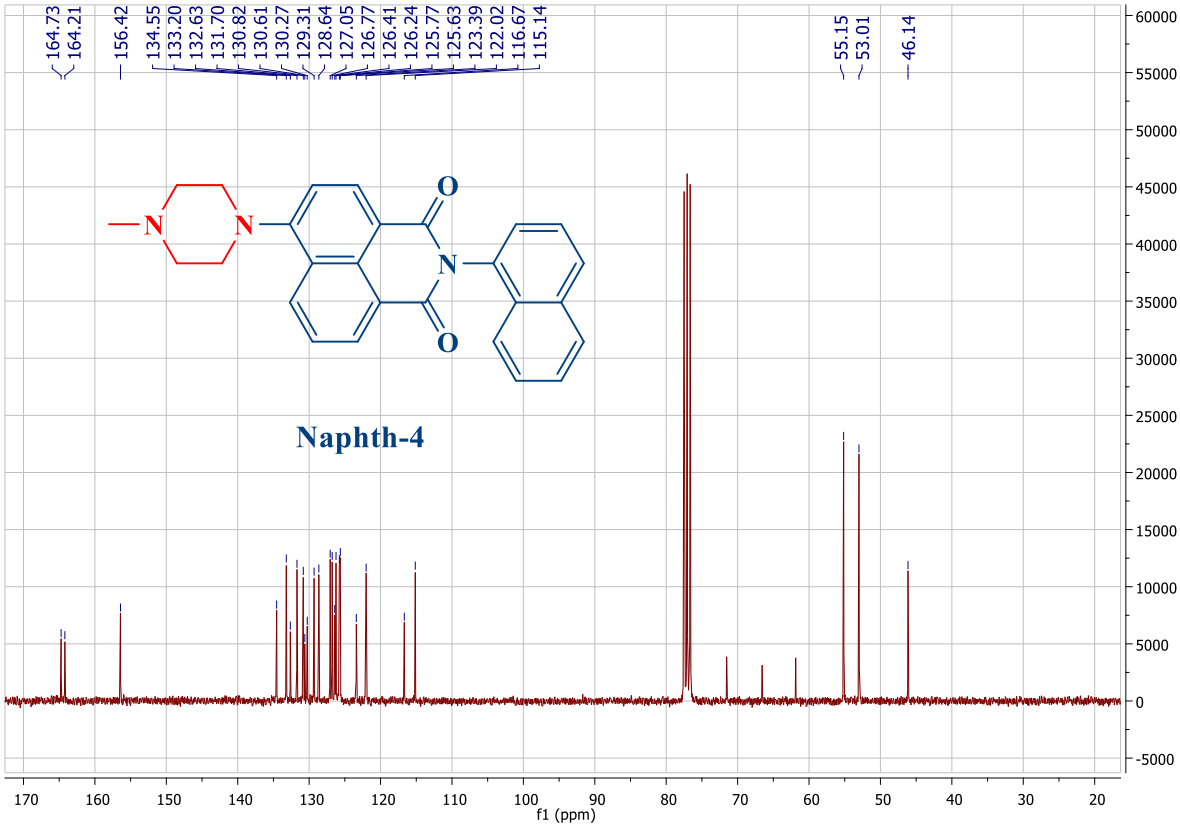
^{13}C NMR spectrum of 6-morpholino-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-3)



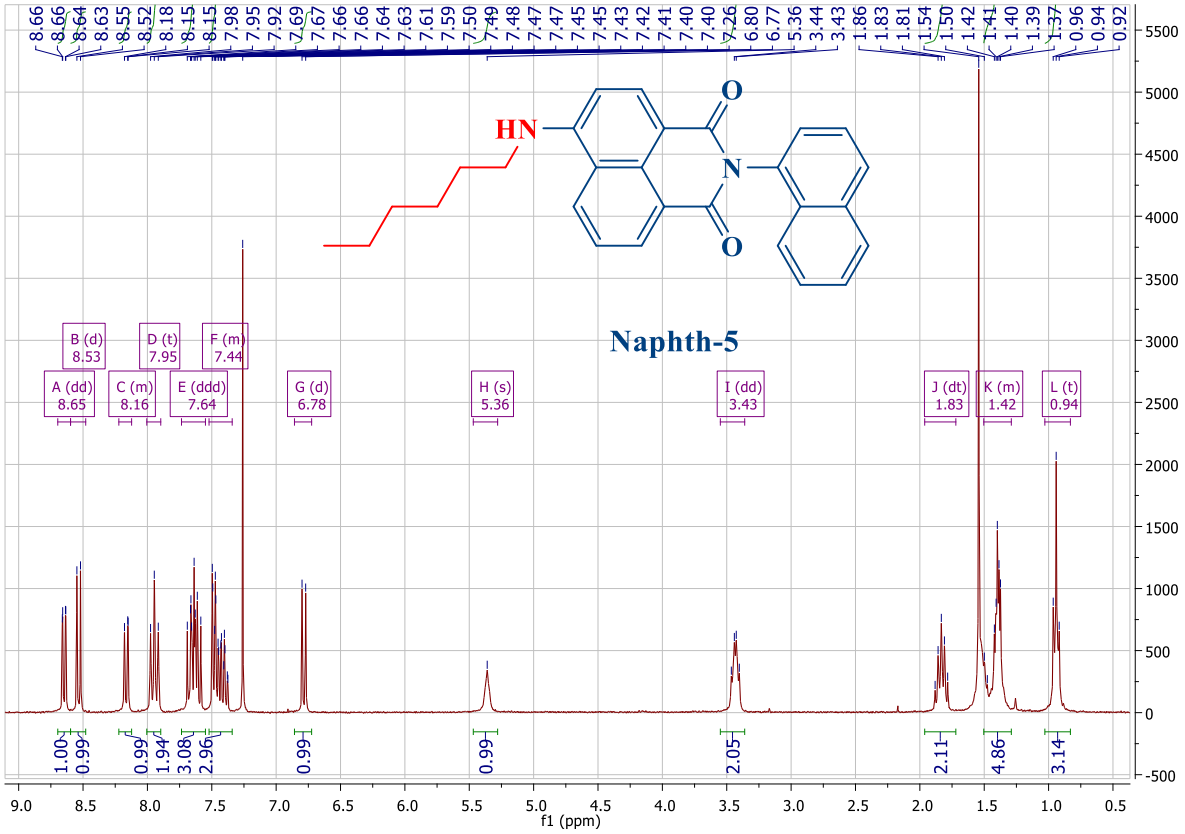
^{1}H NMR spectrum of 6-(4-Methylpiperazin-1-yl)-2-(naphthalen-1-yl)-1H-benzo[de] isoquinoline-1,3(2H)-dione (Naphth-4)



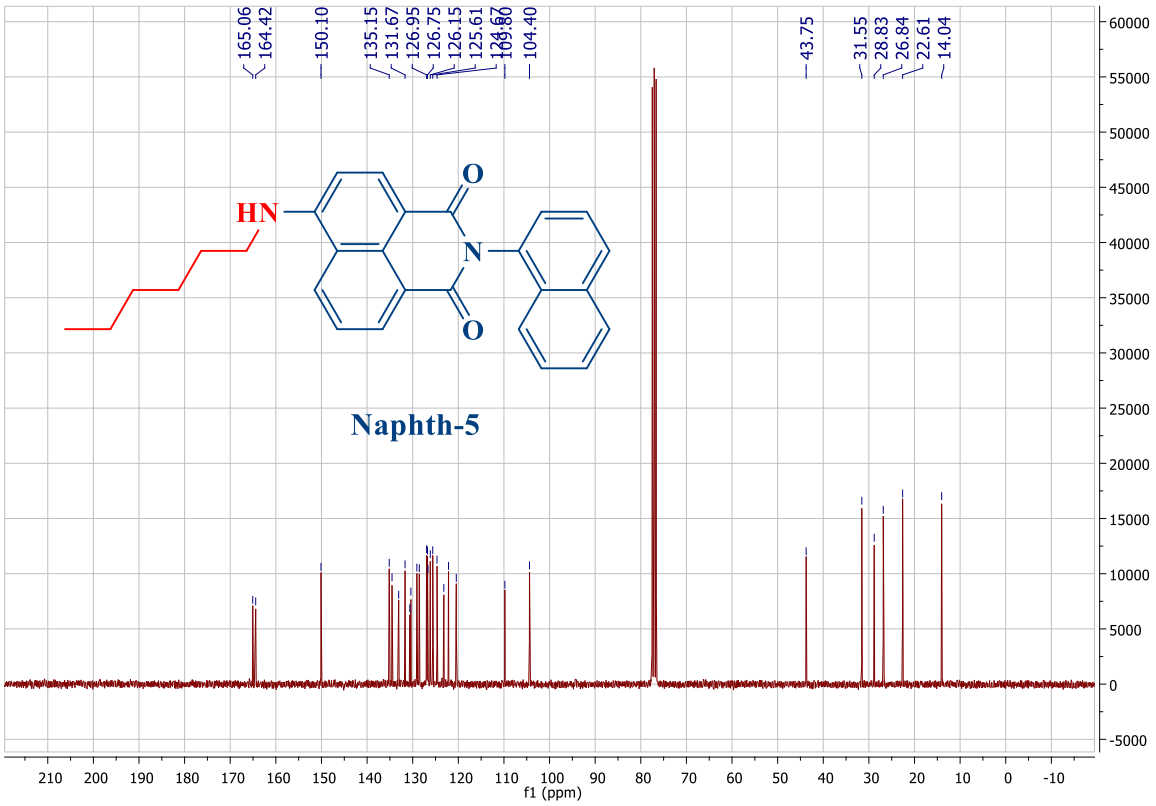
^{13}C NMR spectrum of 6-(4-Methylpiperazin-1-yl)-2-(naphthalen-1-yl)-1H-benzo[de] isoquinoline-1,3(2H)-dione (Naphth-4)



^{1}H NMR spectrum of 6-(hexylamino)-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-5)



^{13}C NMR spectrum of 6-(hexylamino)-2-(naphthalen-1-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (Naphth-5)



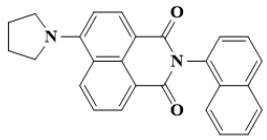
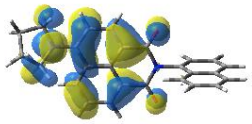
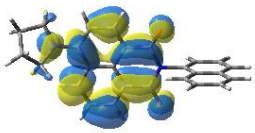
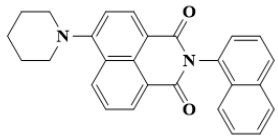
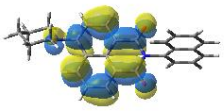
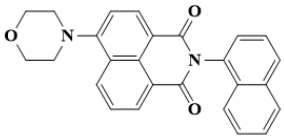
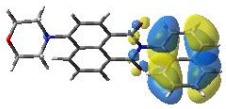
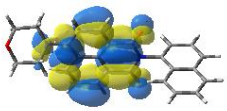
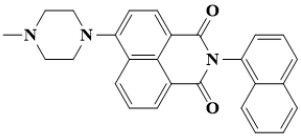
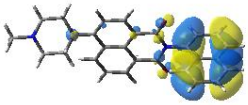
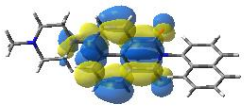
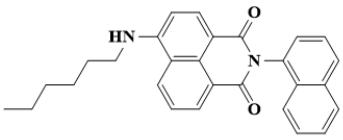
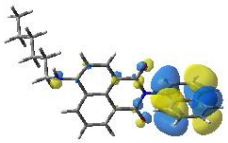
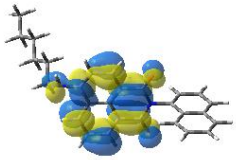
	HOMO	LUMO
(Napht-1) 		
(Napht-2) 		
(Napht-3) 		
(Napht-4) 		
(Napht-5) 		

Figure S1. Contour plots of HOMOs and LUMOs for Napht-1 to Napht-5; structures optimized at the B3LYP/6-31G* level of theory.