

NIR Organic Dyes based on Phenazine-cyanine for Photoacoustic Imaging-guided Photothermal Therapy

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Supporting Information

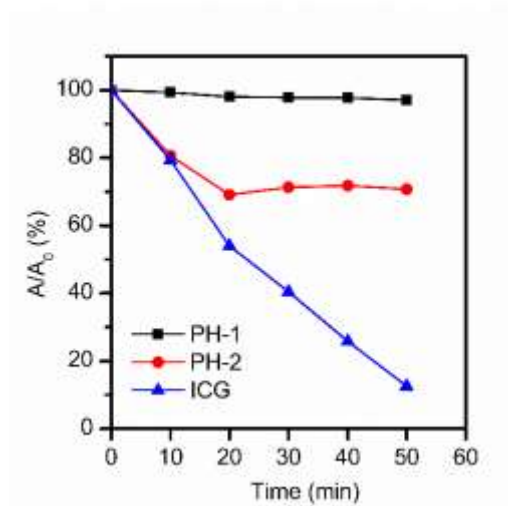


Fig. S1 A/A_0 of **PH-1**, **PH-2** and ICG exposed to white light for different time.

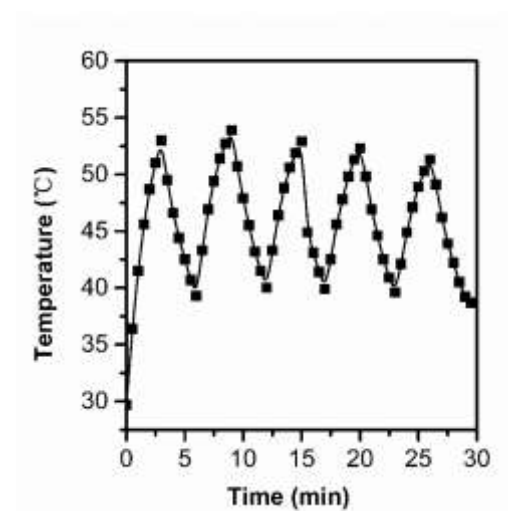


Fig. S2 Photothermal stability of **PH-1@HSA** in PBS buffer (pH = 7.4).

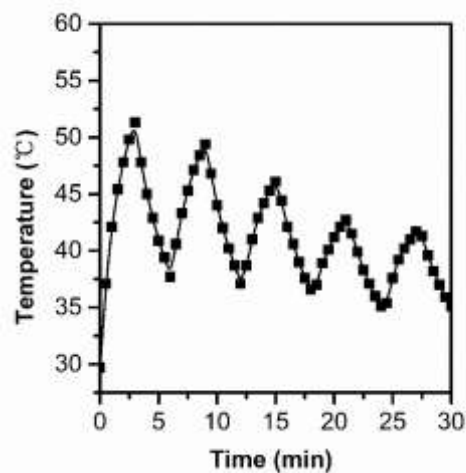


Fig. S3 Photothermal stability of **PH-2@HSA** in PBS buffer (pH = 7.4).

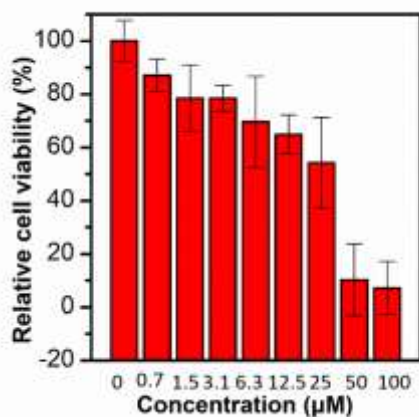


Fig. S4 Relative cell viability of **PH-1@HSA** (inhabited for 48 h with different concentration).

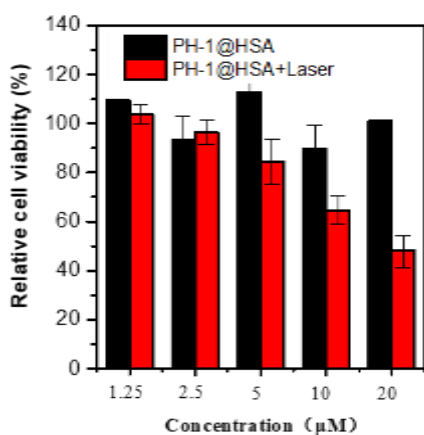


Fig. S5 Relative cell viability of **PH-1@HSA** with or without laser (the black is NPs only, the red is NPs with 808 nm laser).

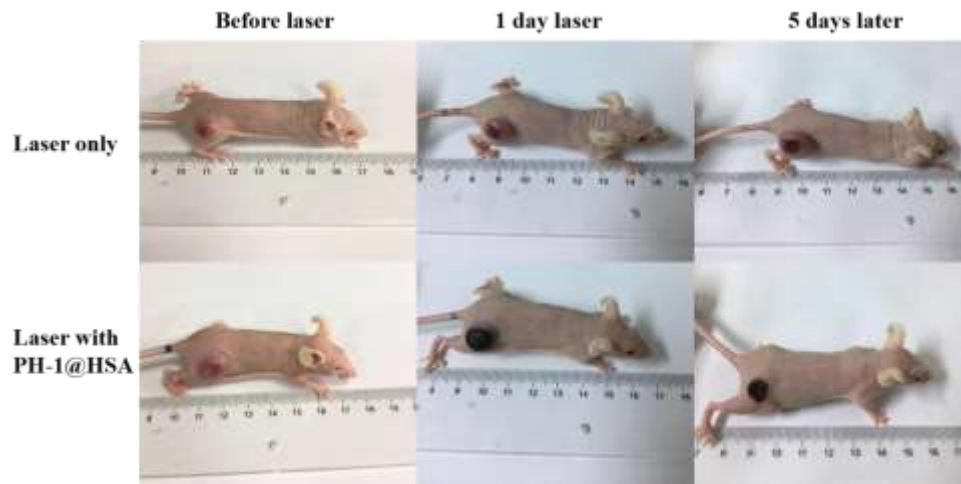


Fig. S6 The daylight images of mice before and after PTT.

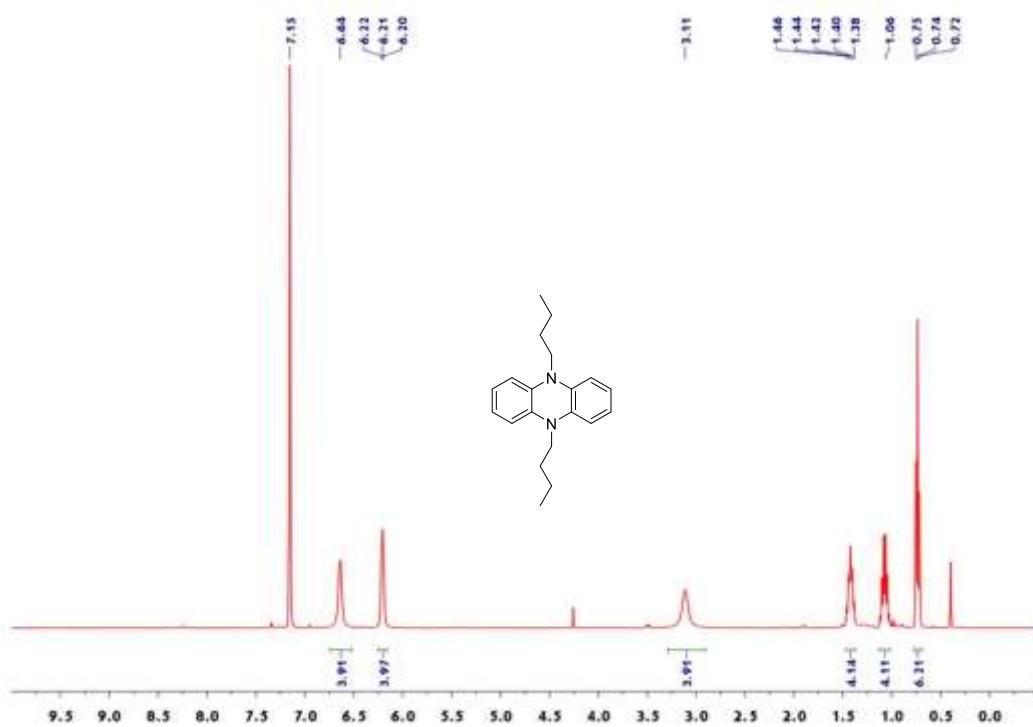


Fig. S7 ^1H NMR spectrum of compound 2 in chloroform-*d*

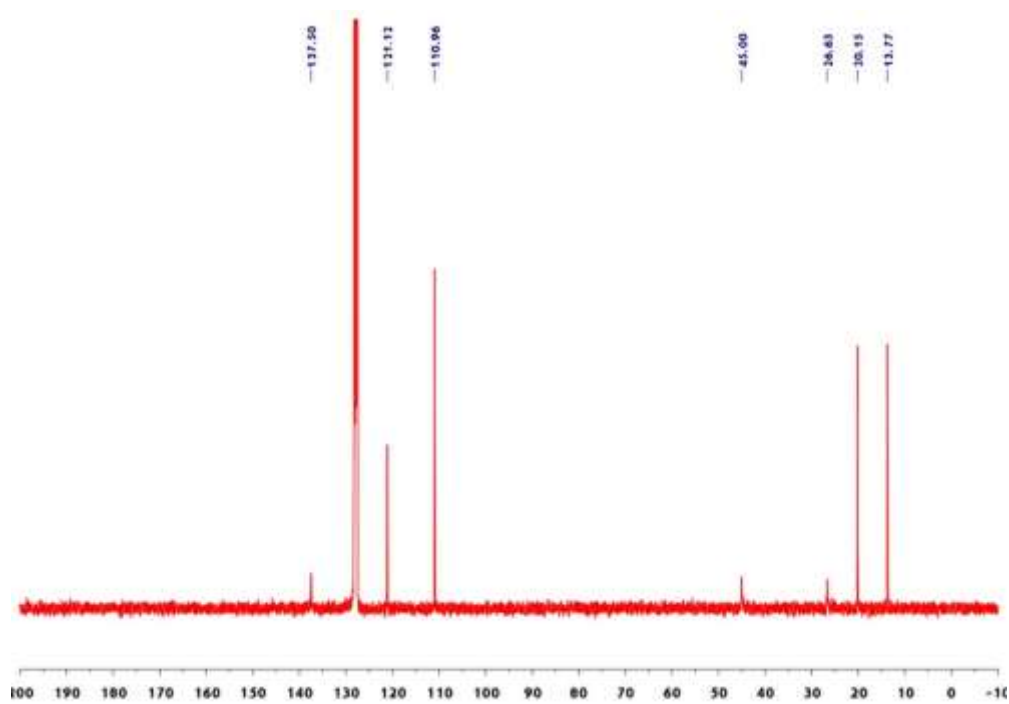


Fig. S8 ^{13}C NMR spectrum of compound 2 in chloroform-*d*

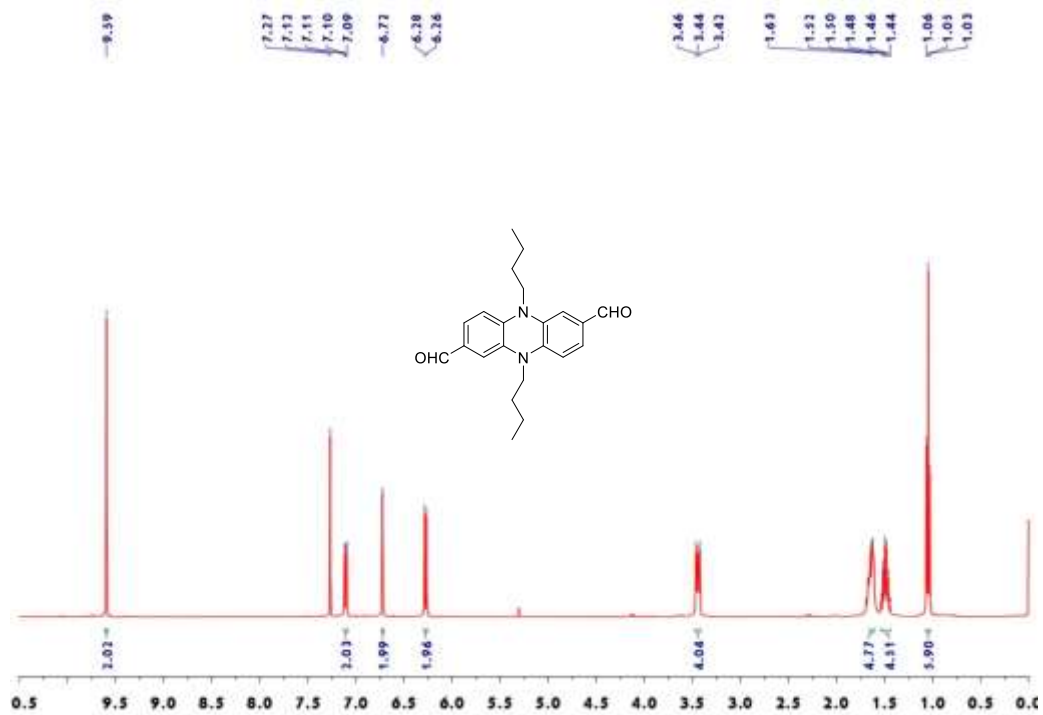


Fig. S9 ^1H NMR spectrum of **PH-CHO** in chloroform-*d*

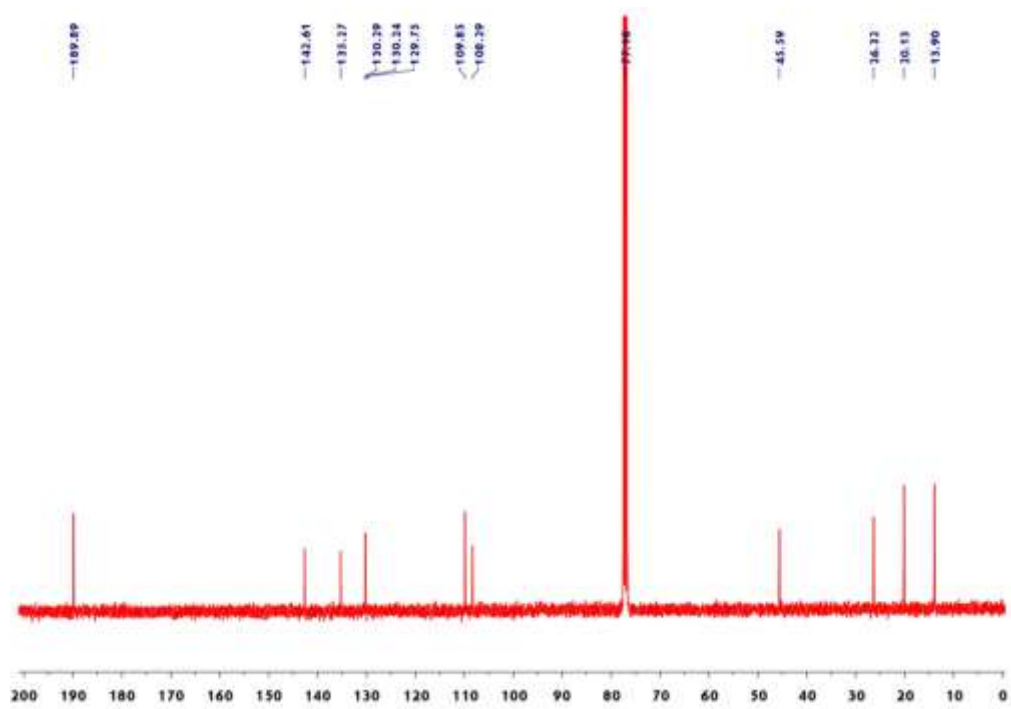


Fig. S10 ^{13}C NMR spectrum of **PH-CHO** in chloroform-*d*

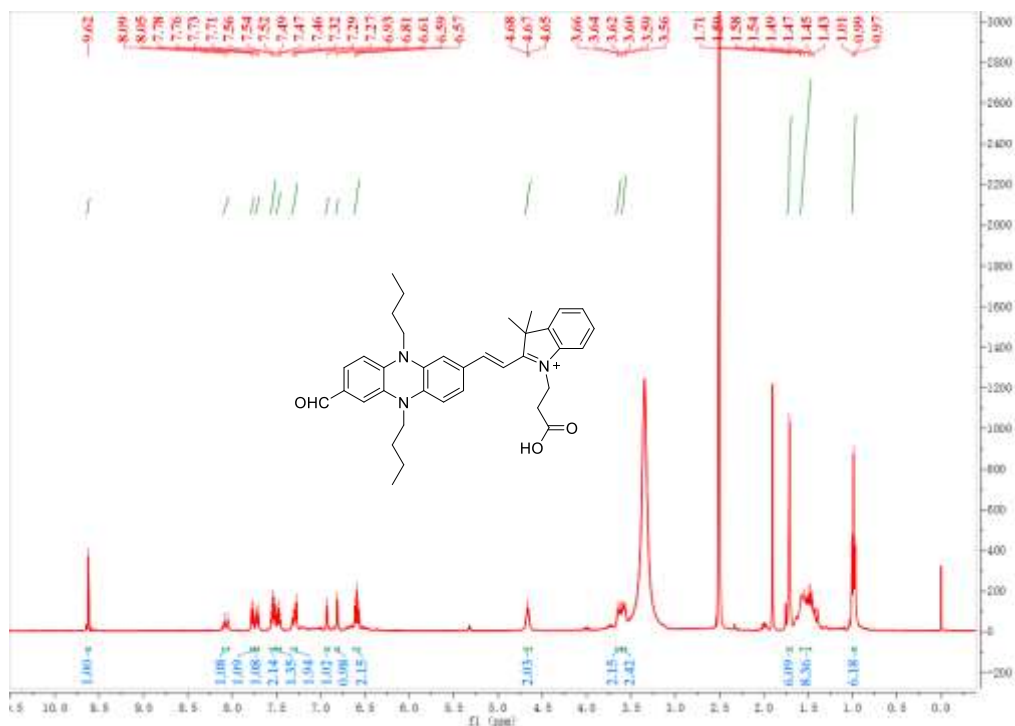


Fig. S11 ^1H NMR spectrum of **PH-1** in $\text{DMSO-}d_6$

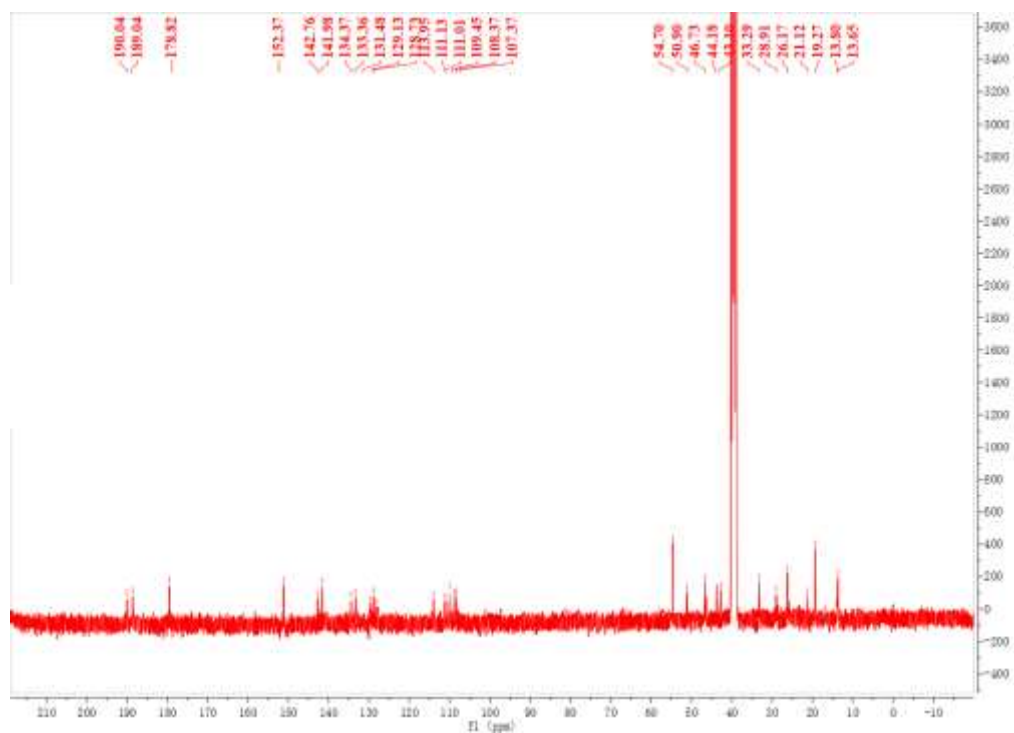


Fig. S12 ^{13}C NMR spectrum of **PH-1** in $\text{DMSO-}d_6$

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-36 H: 0-42 N: 0-3 O: 0-3 Na: 0-1

JL-HUA

HL-YYC-003 185 (2.112) Cm (185)



Fig. S13 High resolution mass spectrum of **PH-1**

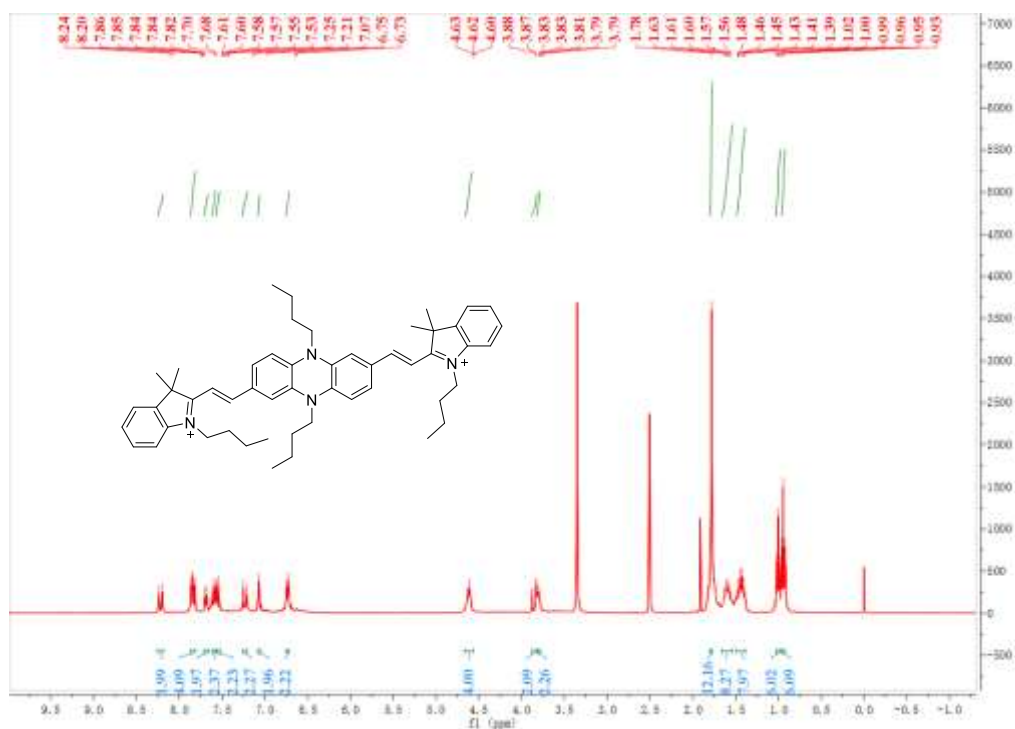


Fig. S14 ¹H NMR spectrum of **PH-2** in DMSO-*d*₆

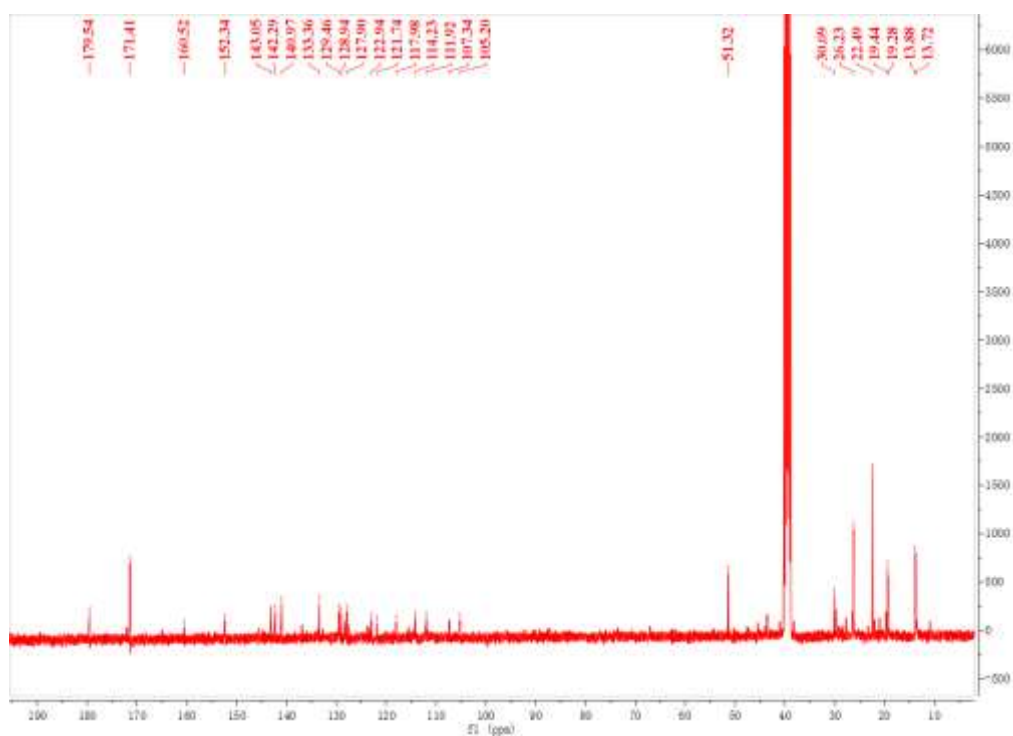


Fig. S15 ^{13}C NMR spectrum of **PH-2** in $\text{DMSO-}d_6$

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

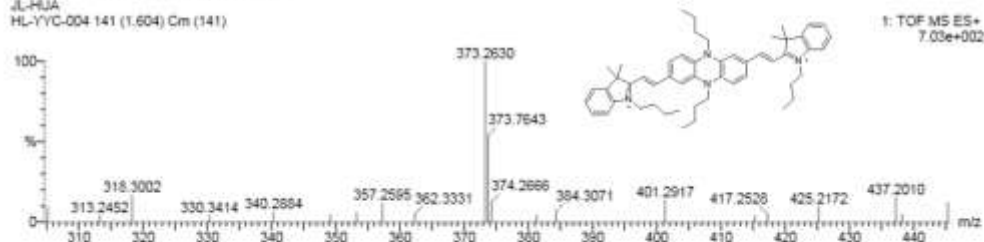
4 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-26 H: 0-33 N: 0-2 Na: 0-1

JL-HJA

HL-YYC-004 141 (1.604) Cm (141)



Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
373.2630	373.2644	-1.4	-3.8	11.5	29.6	0.0	C ₂₆ H ₃₃ N ₂

Fig. S16 High resolution mass spectrum of **PH-2**