

SUPPLEMENTARY MATERIAL

Recognition of flavin analogue by novel bile acid-based receptors: Effects of hydrogen bonding and aromatic π -stacking interactions

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NMR and Mass spectra

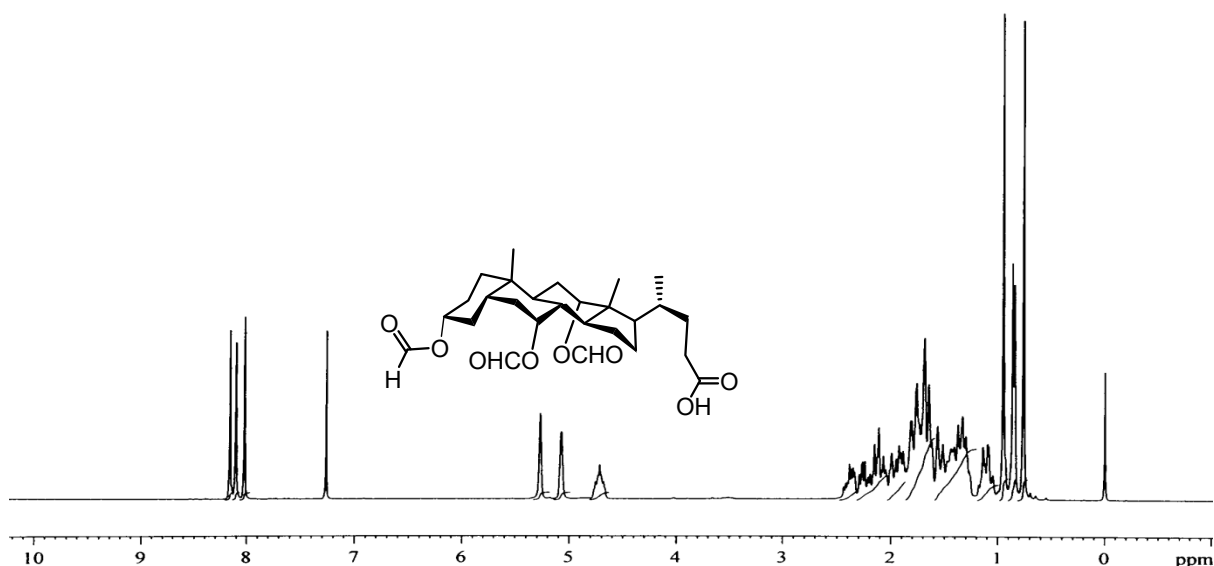


Figure S1: ¹H NMR spectrum of **2**

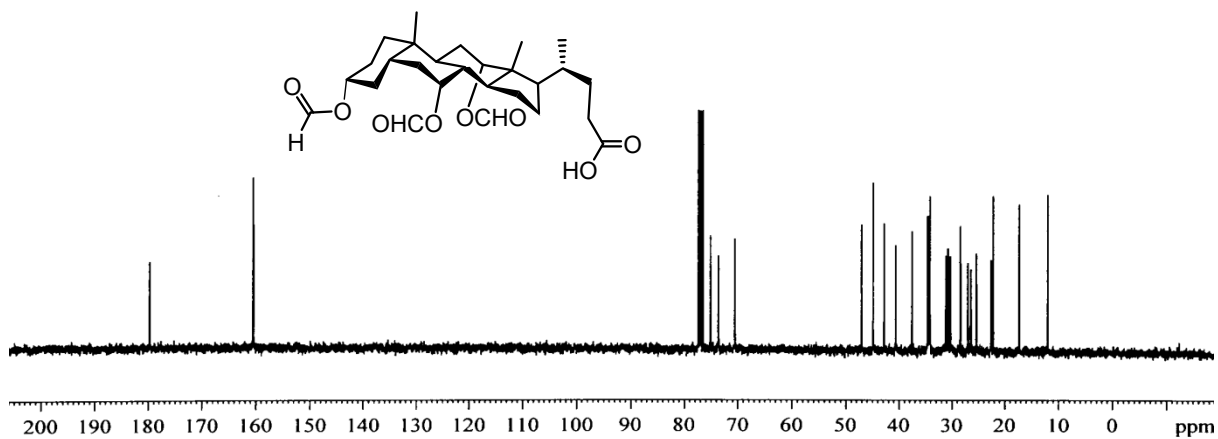


Figure S2: ^{13}C NMR spectrum of **2**

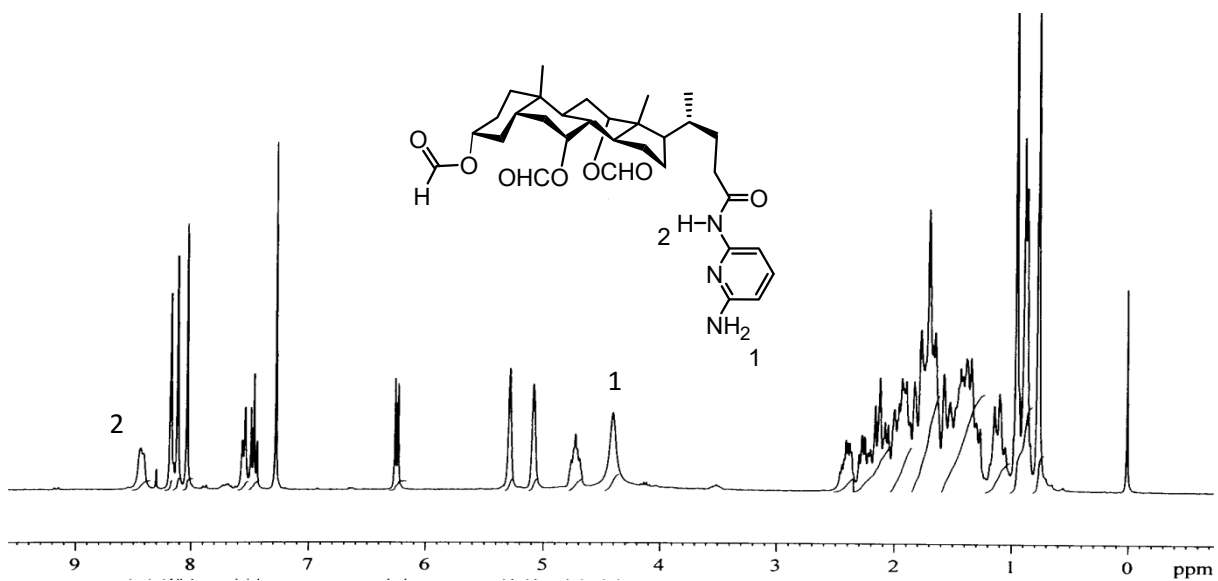


Figure S3: ^1H NMR spectrum of **3**

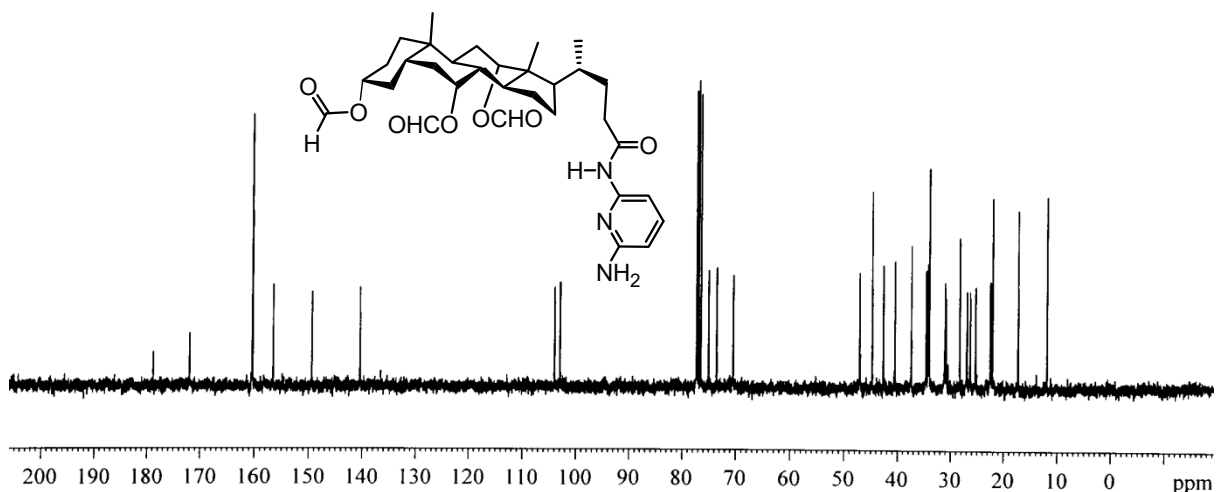


Figure S4: ^{13}C NMR spectrum of **3**

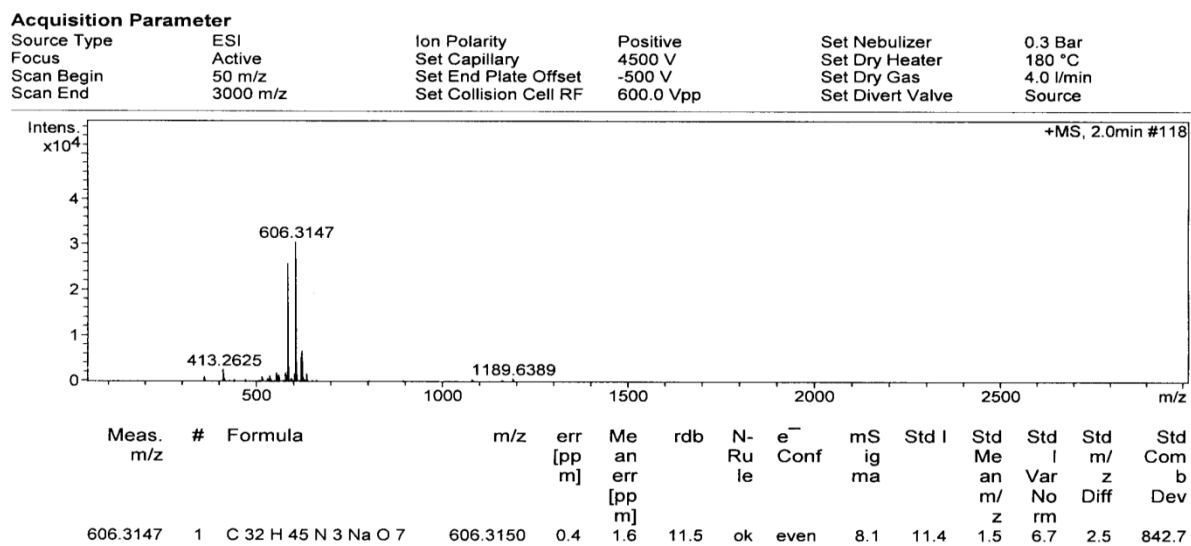


Figure S5: HRMS (ES^+) spectrum of **3**

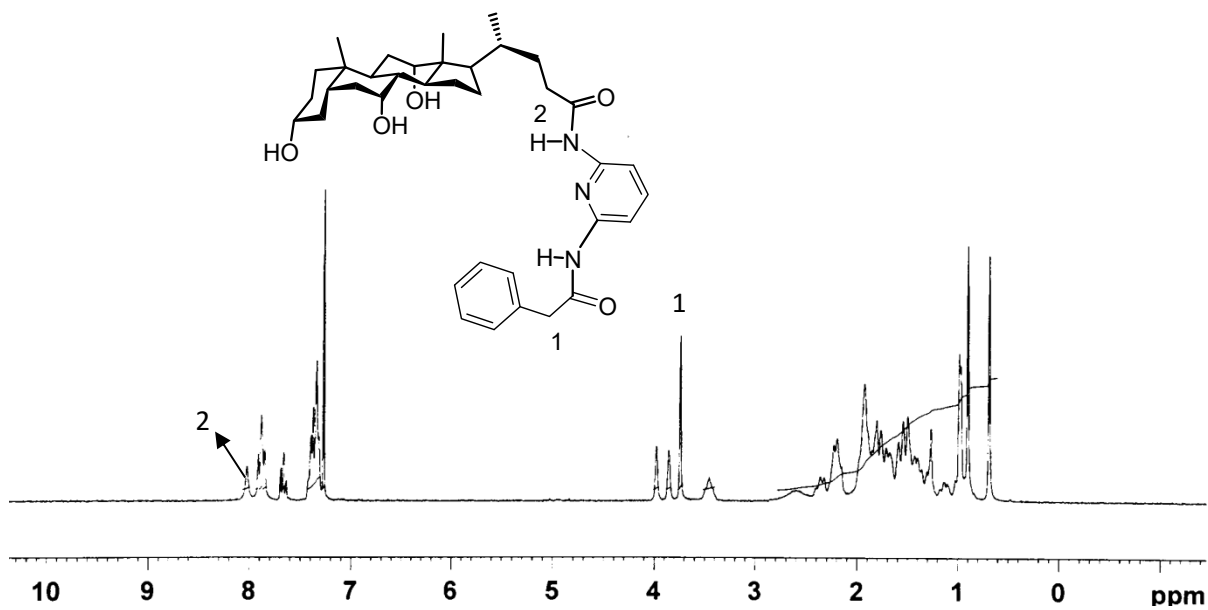


Figure S6: ^1H NMR spectrum of **4a**

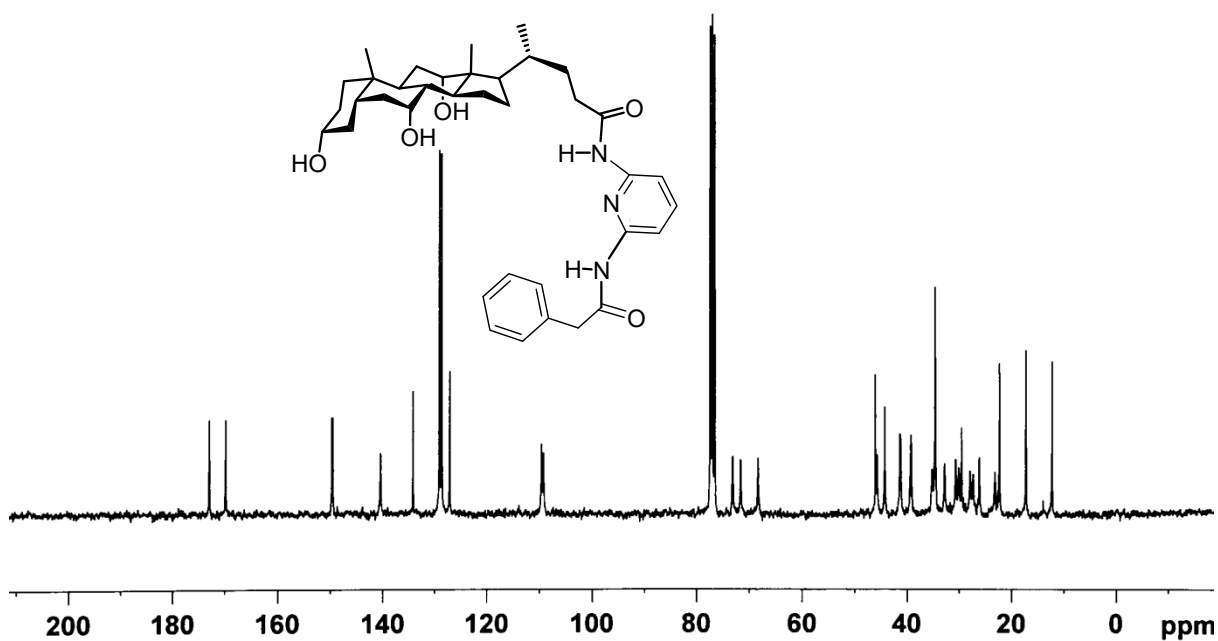


Figure S7: ^{13}C NMR spectrum of **4a**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source

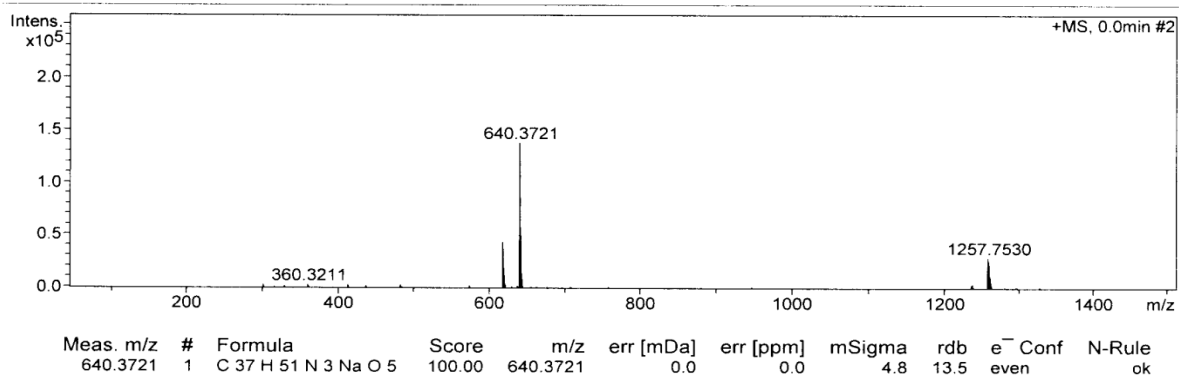


Figure S8: HRMS (ES⁺) spectrum of 4a

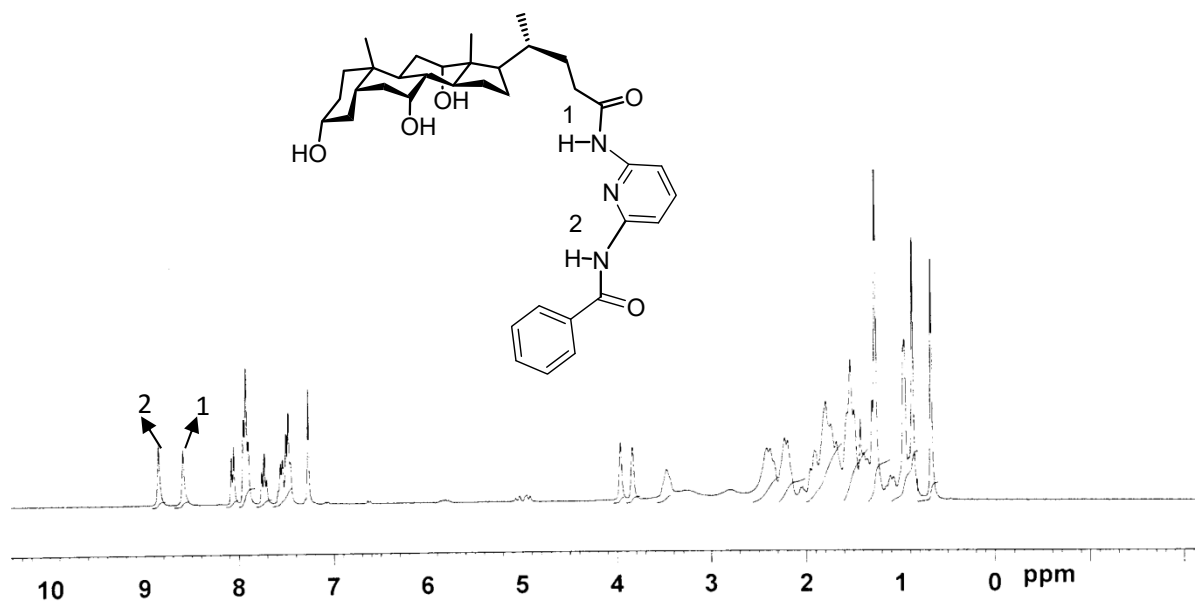


Figure S9: ¹H NMR spectrum of 4b

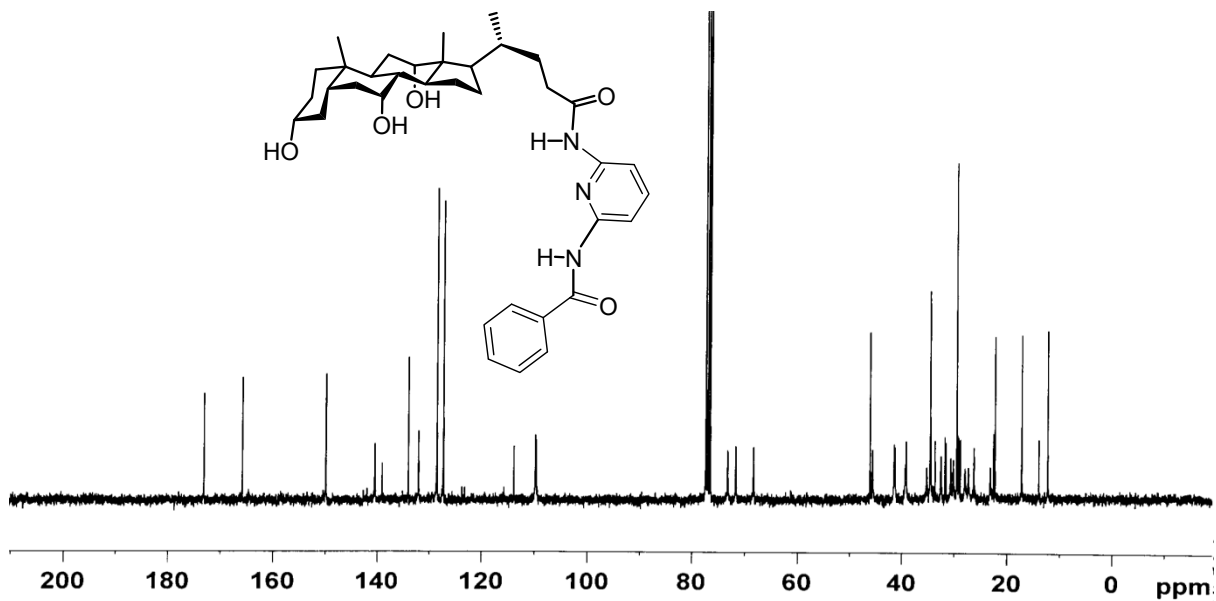
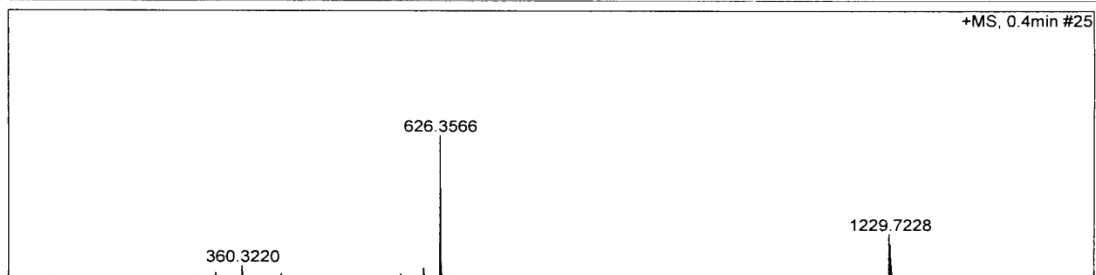


Figure S10: ^{13}C NMR spectrum of **4b**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-R rule
626.3566	1	C ₃₆ H ₄₉ N ₃ NaO ₅	100.00	626.3564	-0.2	-0.0	8.7	13.5	even	ok

Figure S11: HRMS (ES^+) spectrum of **4b**

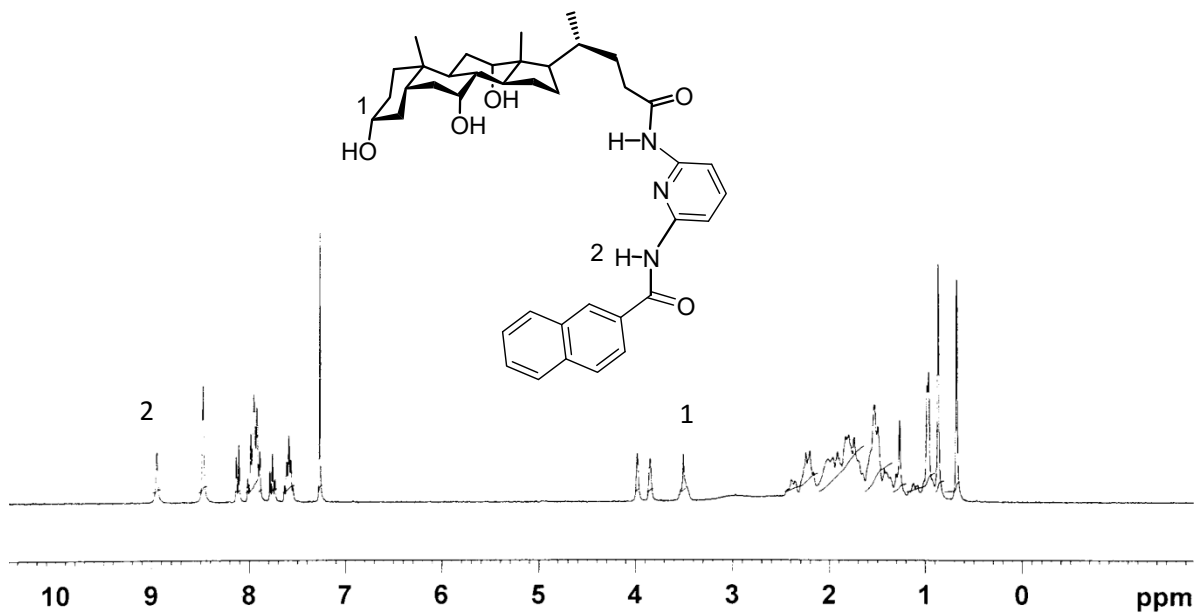


Figure S12: ¹H NMR spectrum of 4c

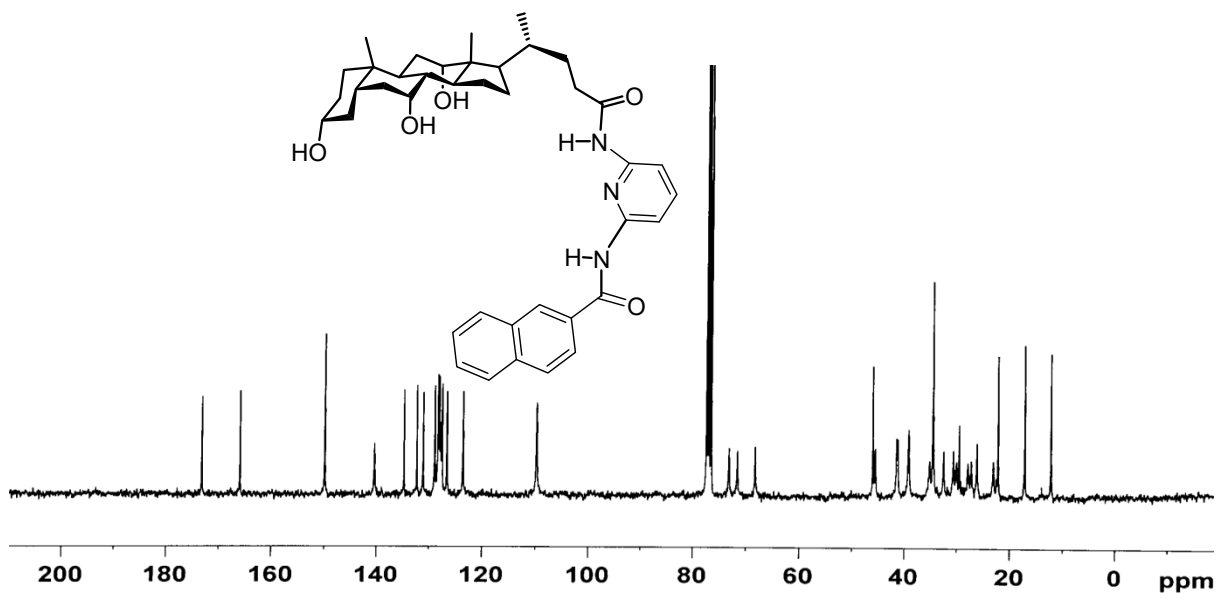


Figure S13: ¹³C NMR spectrum of 4c

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source

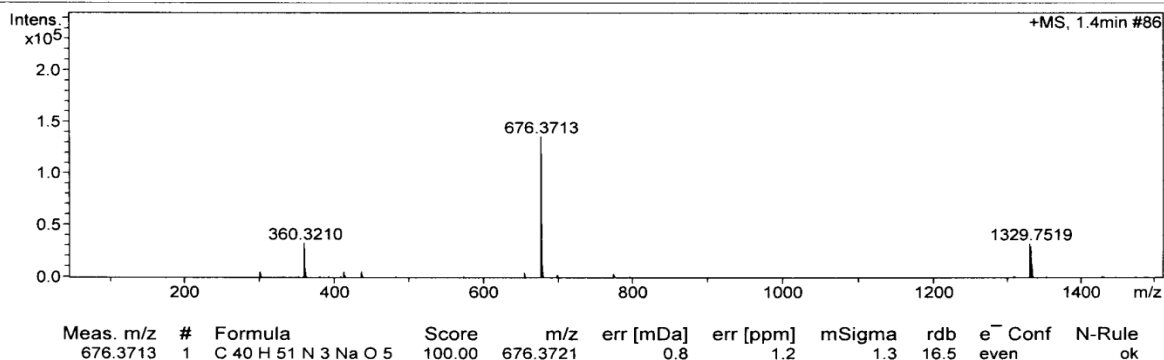


Figure S14: HRMS (ES⁺) spectrum of 4c

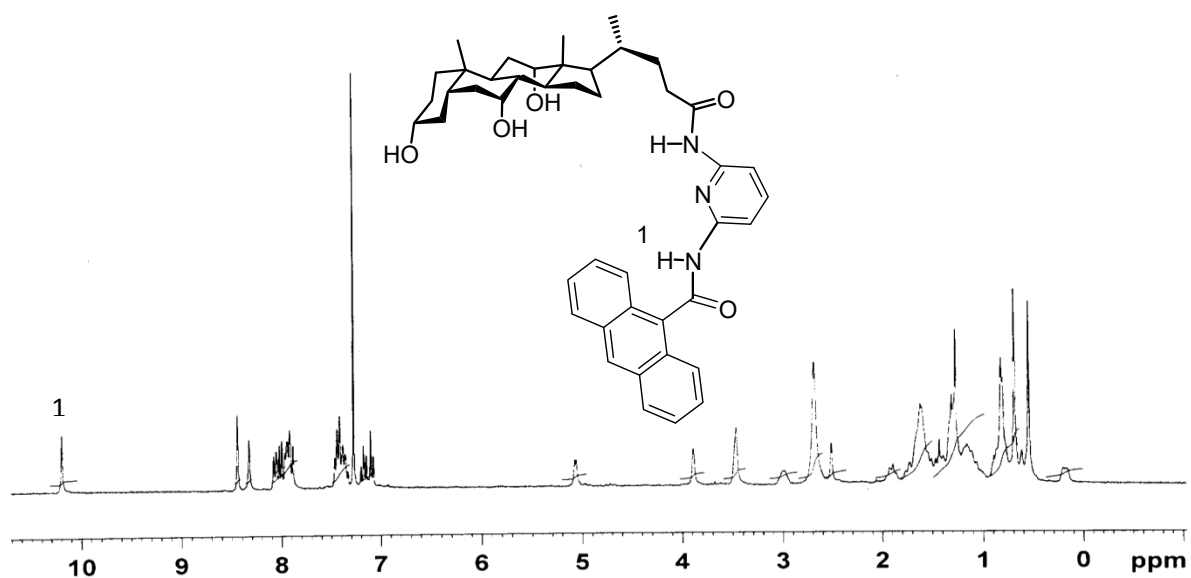


Figure S15: ¹H NMR spectrum of 4d

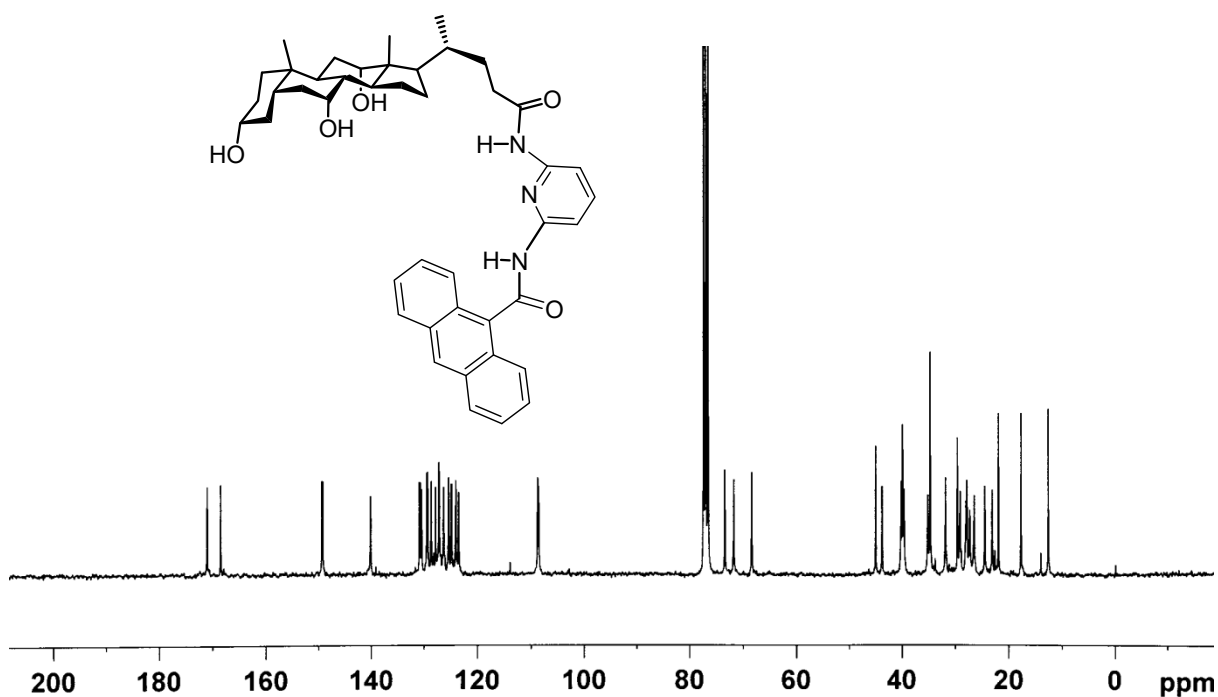


Figure S16: ^{13}C NMR spectrum of **4d**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source

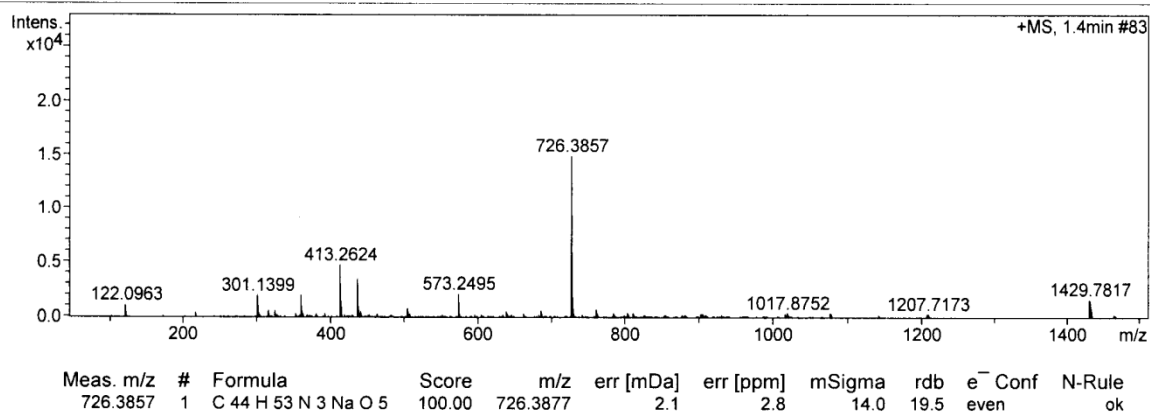
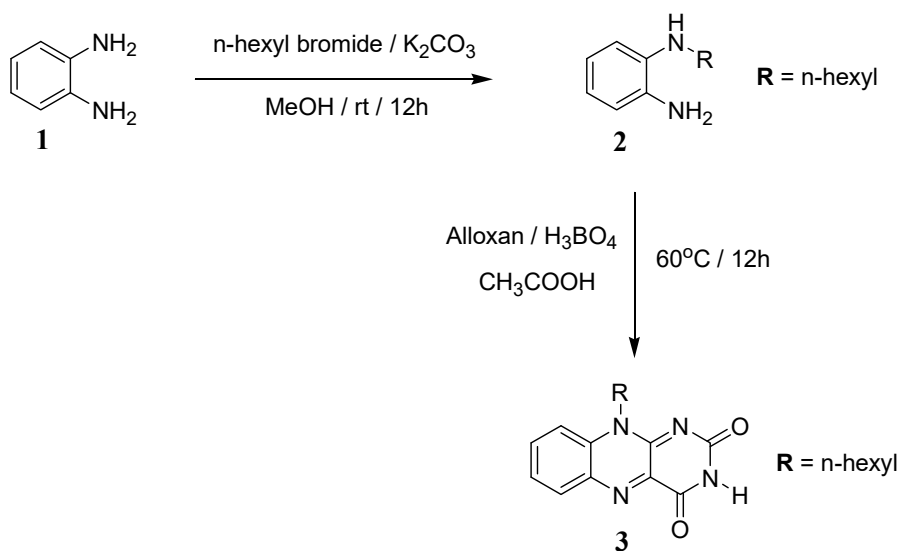


Figure S17: HRMS (ES^+) spectrum of **4d**

Synthesis of *N*(10)-hexylflavin

N(10)-hexylflavin was synthesized from *ortho*-phenylenediamine, by following the reaction sequence.



Chattopadhyay, P.; Rai, R.; Pandey, P. S. *Synth. Commu.*, **2006**, *36*, 1857.