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Selective Fluorescence Sensing of Salicylic Acids Using a Simple Pyrenesulfonamide Receptor

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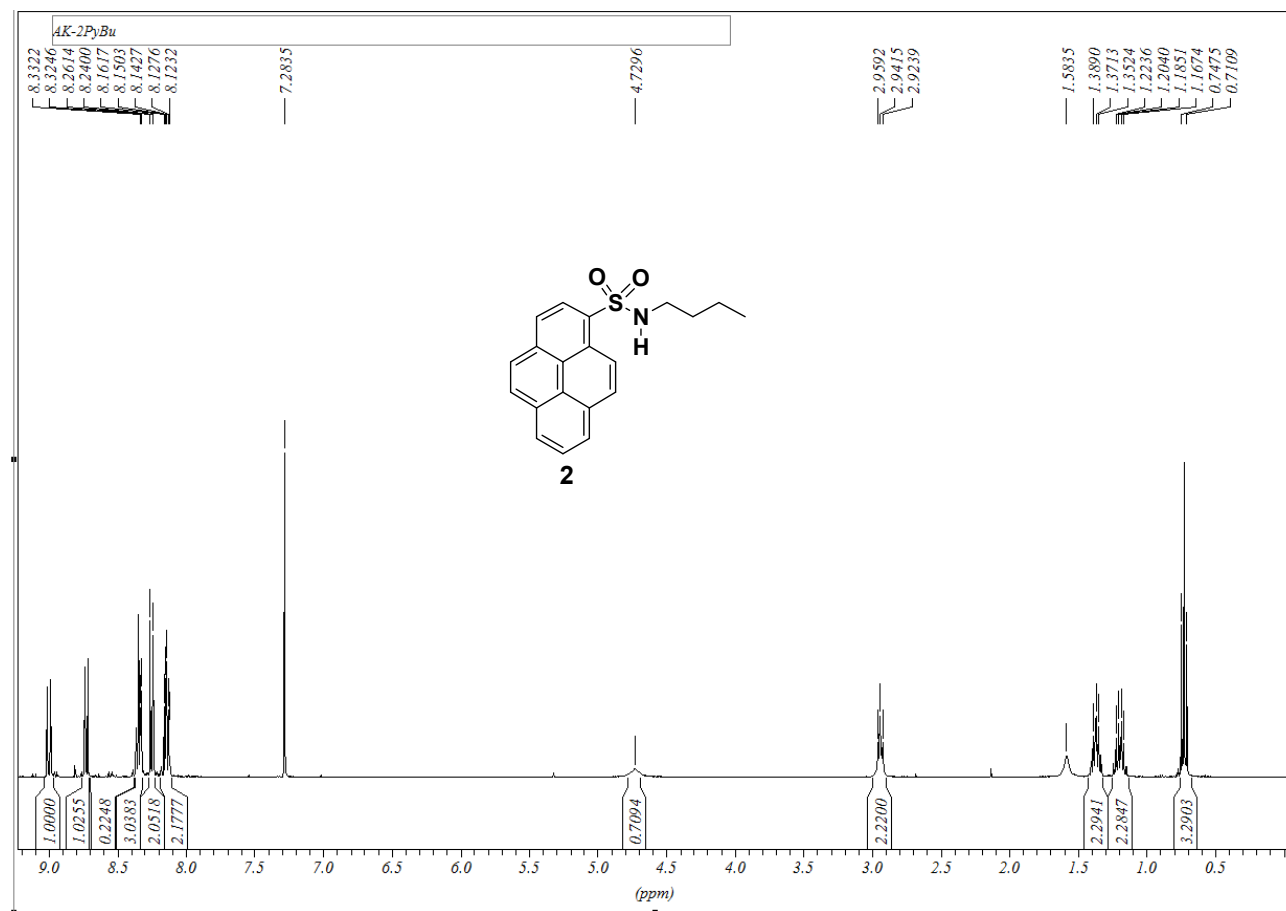
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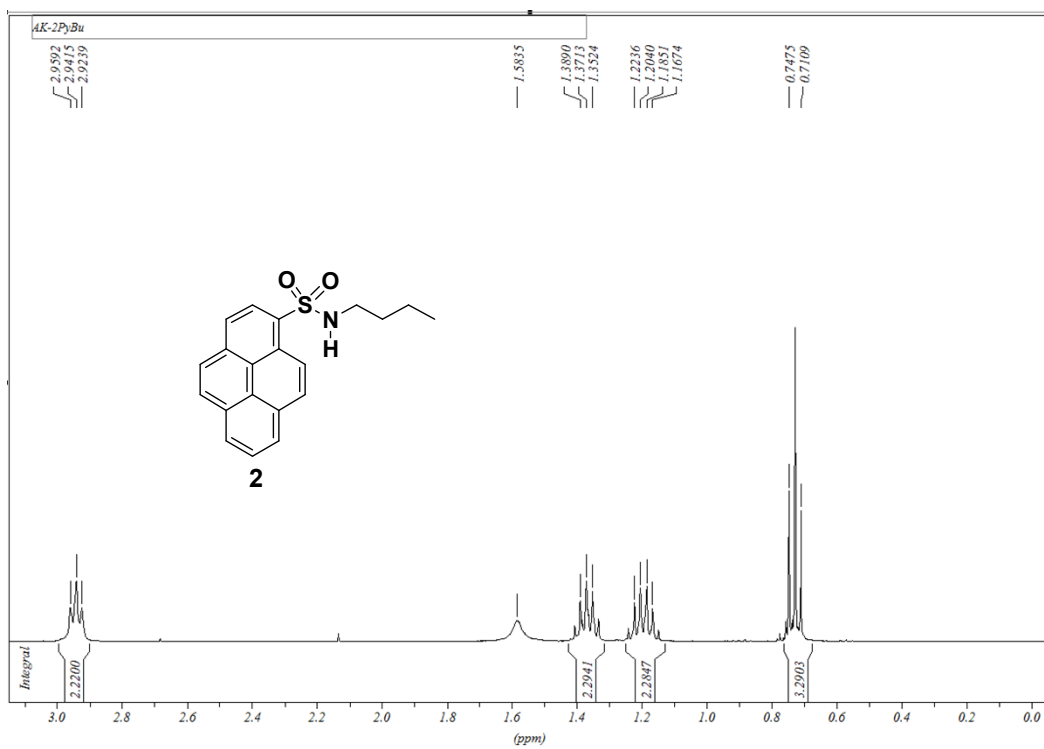
and probe **3** + 3,5-DNSA.

26. Fig. SI 21: Fluorescence emission spectra of probe **3** and its complexes with 3,5-DNSA and 5-NSA, obtained by using B3LYP/6-31G*.

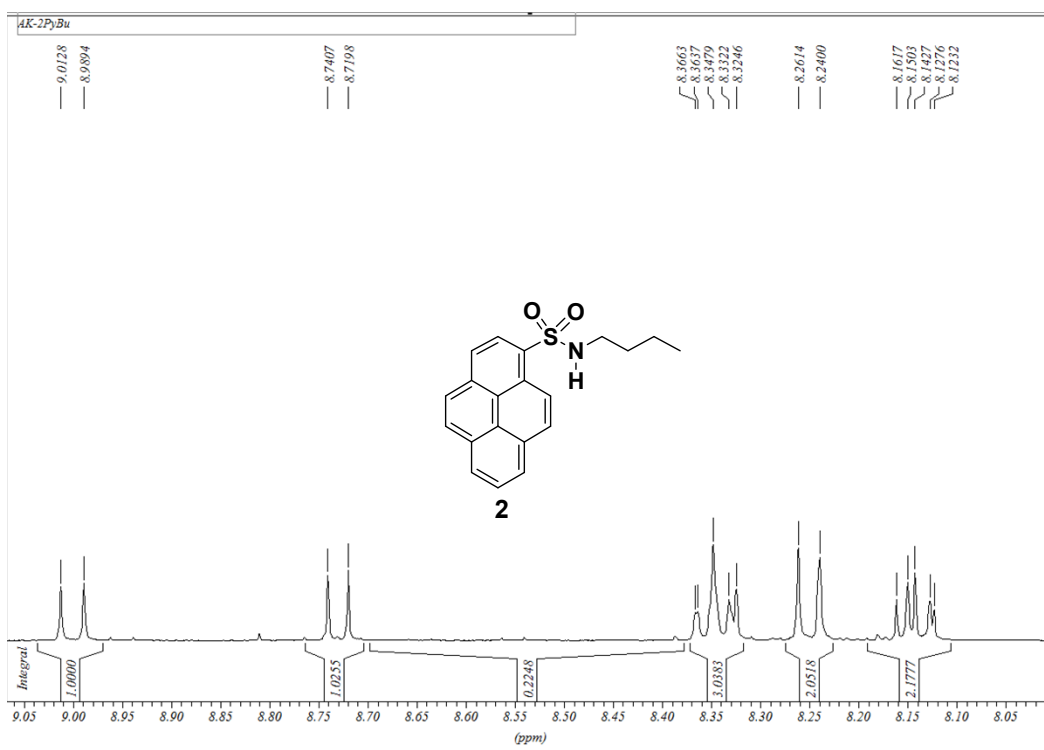
Fig. SI 22: Fluorescence intensity at λ_{max} of probe **3** and [**3**•3,5-DNSA] (1 μ M, EtOH-H₂O 10%) vs pH, λ_{ex} = 336 nm, slit width 3,3.



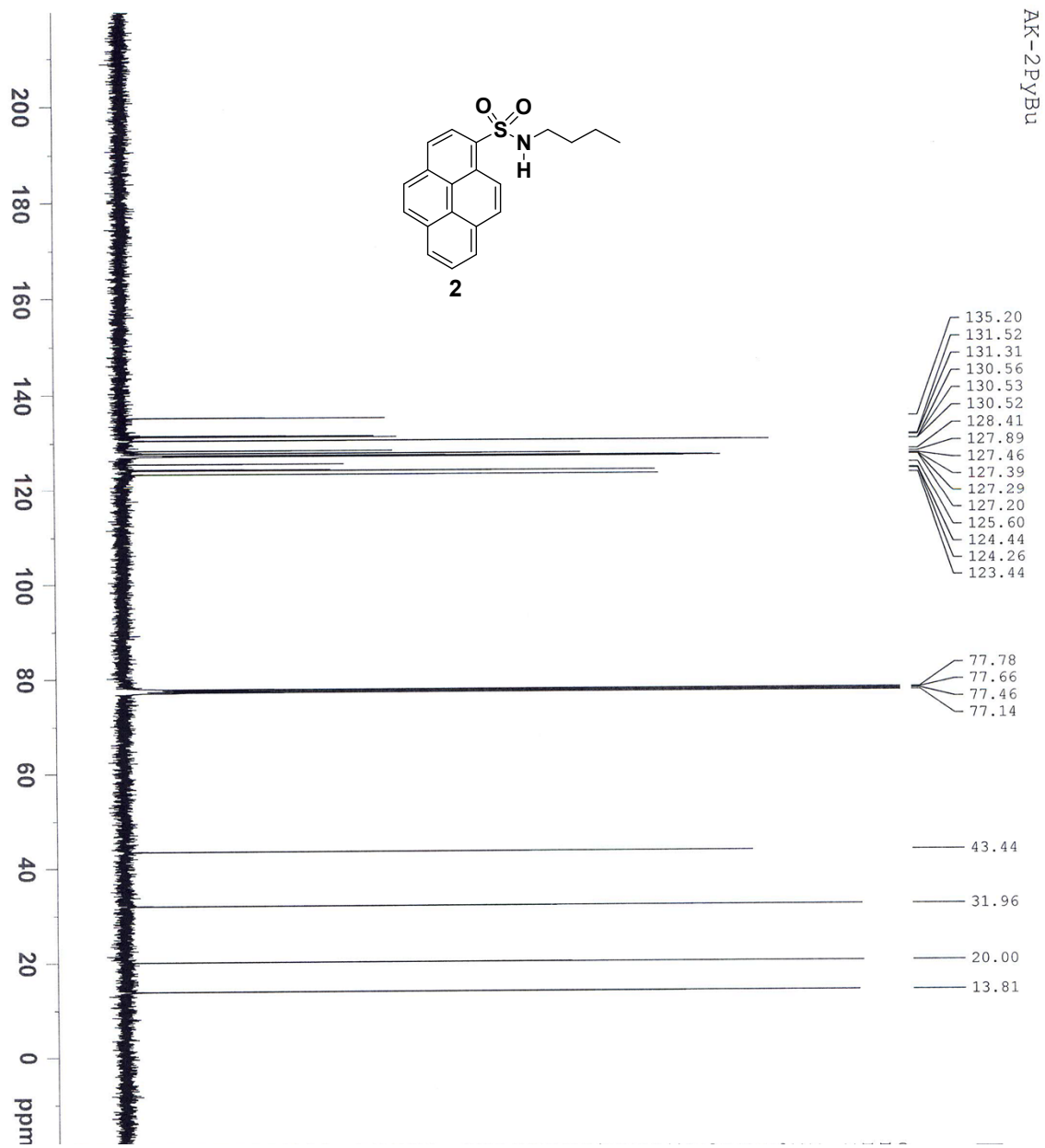
¹H NMR of probe **2** CDCl₃.



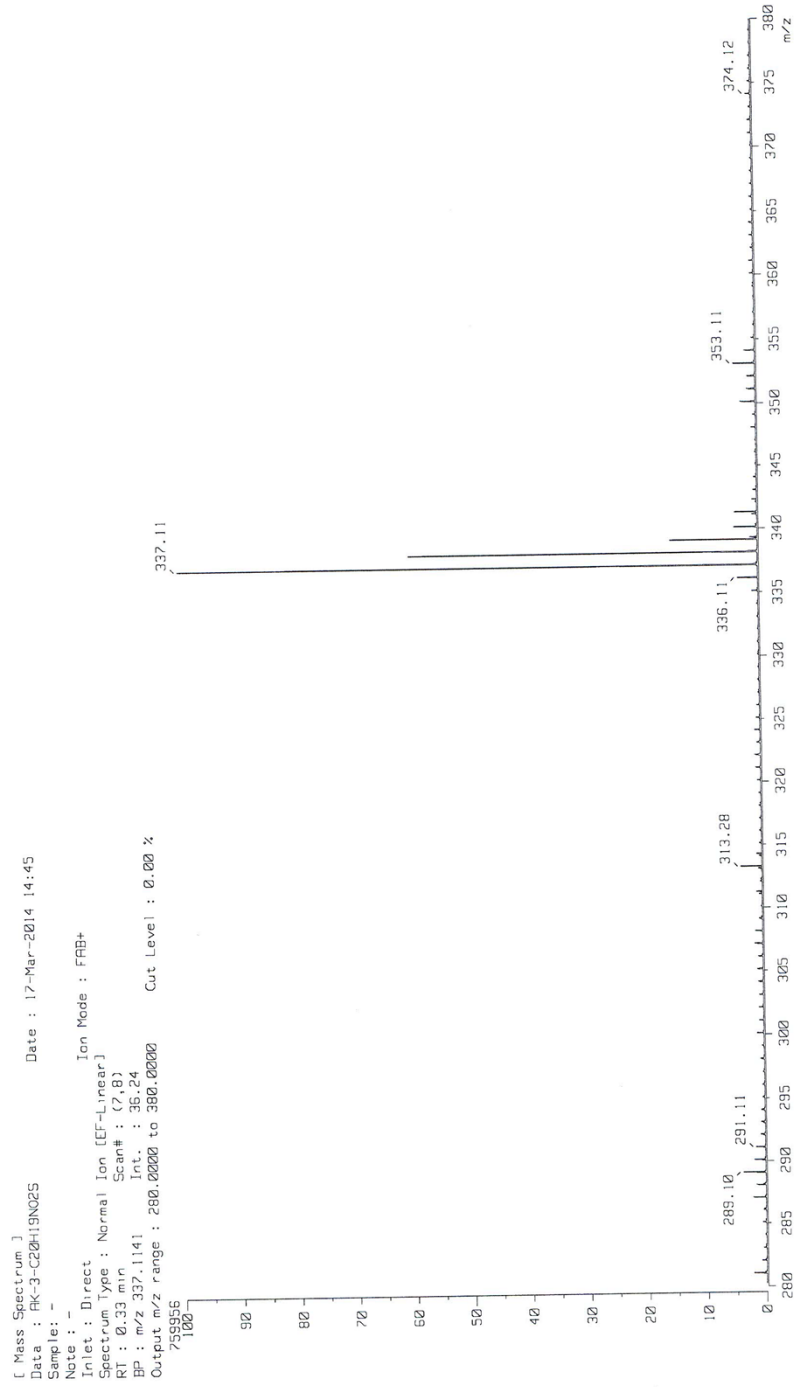
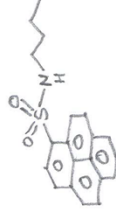
¹H NMR of probe **2** aliphatic region in CDCl₃



¹H NMR of probe **2** aromatic region in CDCl₃

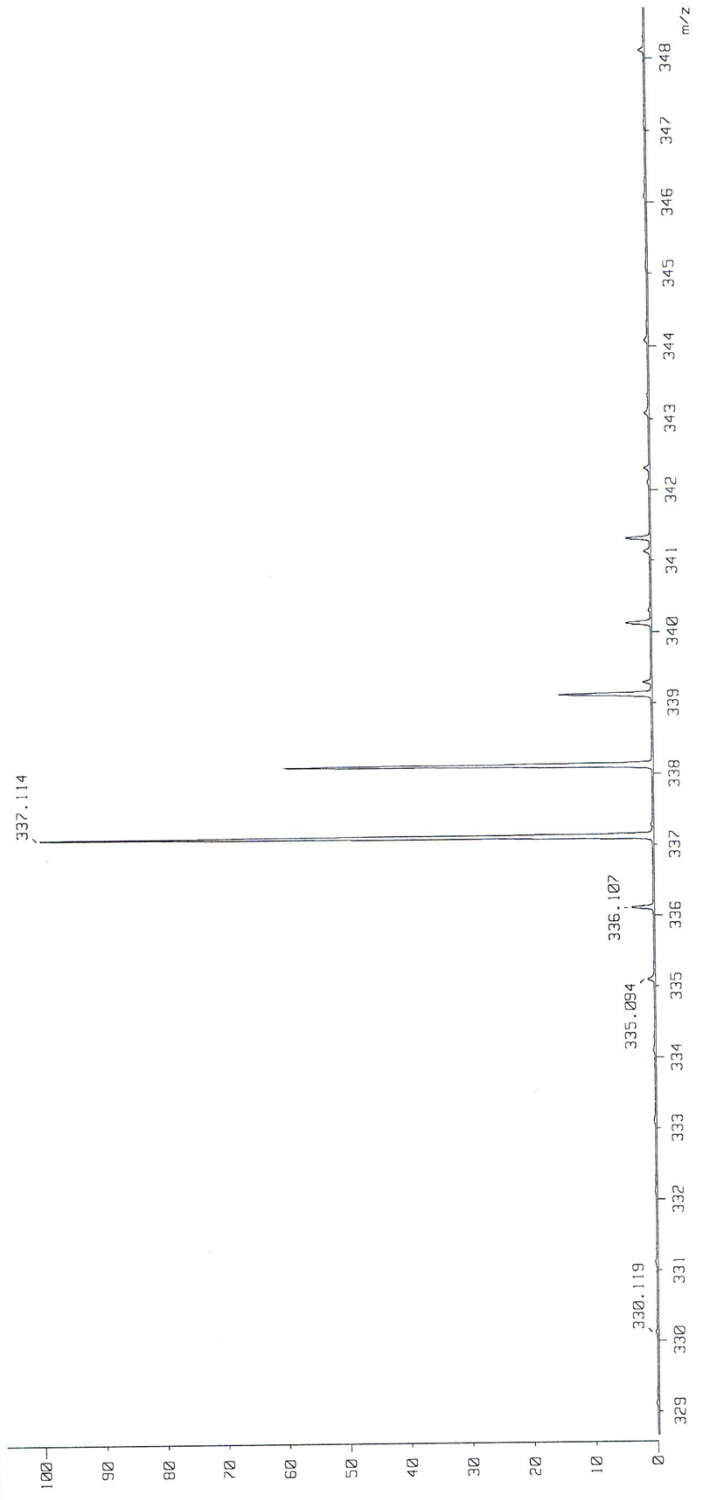


^{13}C NMR of probe **2** in CDCl_3

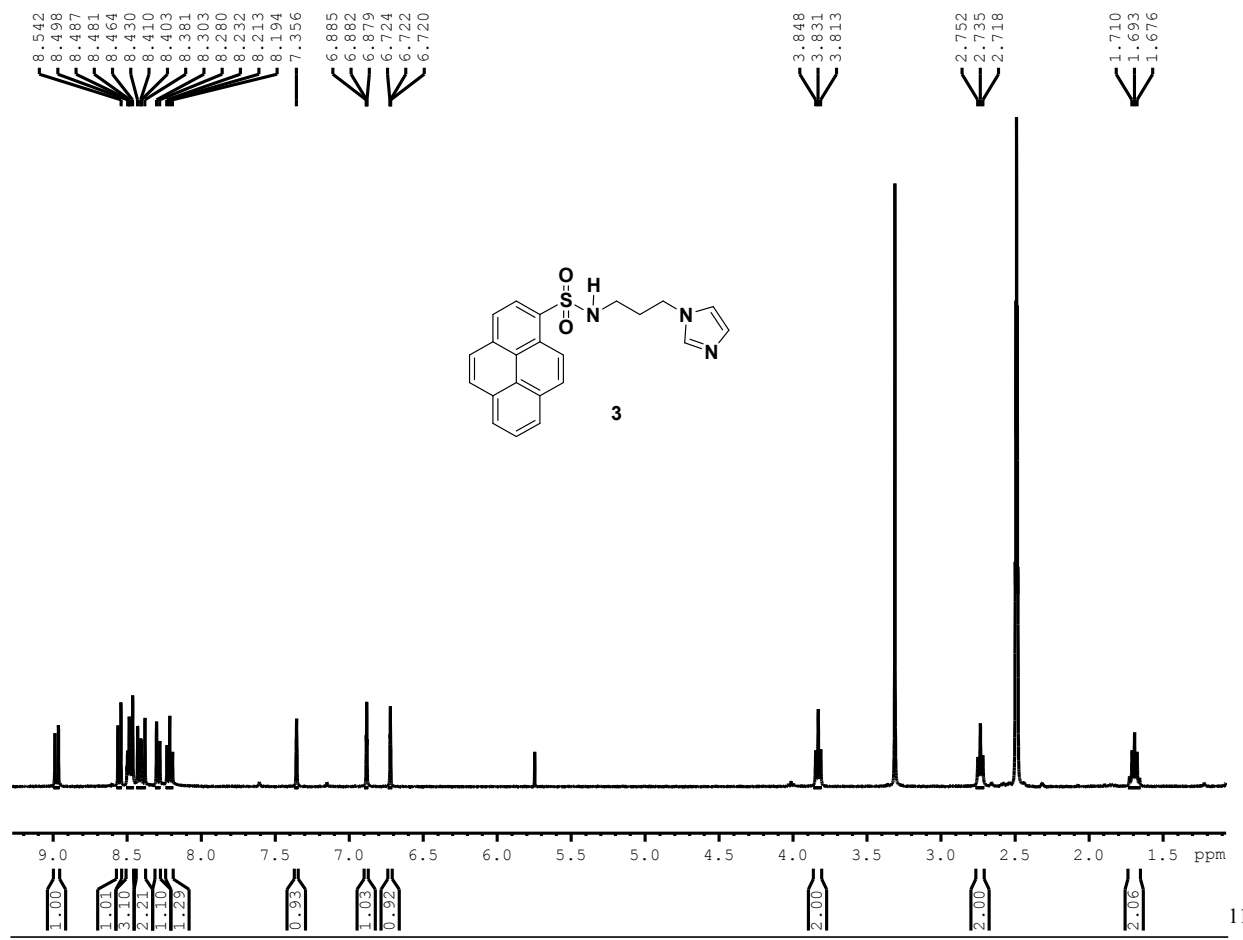


HRMS of probe 2

[Mass Spectrum]
Date : 17-Mar-2014 14:45
Sample : -
Note : -
Inlet : Direct Ion Mode : FFB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.33 min Scan# : (7,8)
BP : m/z 337.114 Int. : 36.24
Output m/z range : 328.6647 to 348.6944 Cut Level : 0.00 %
807915

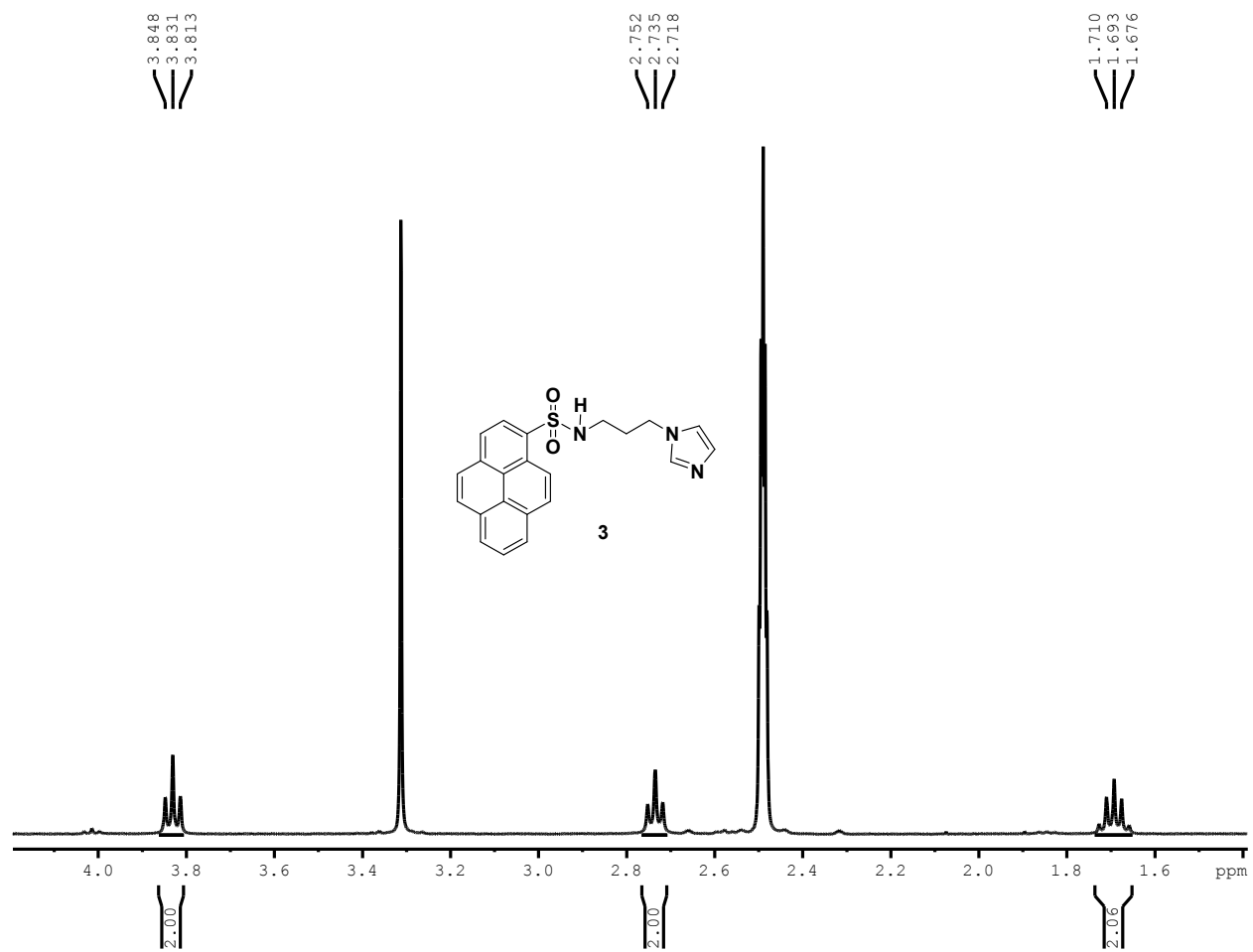


HRMS of probe 2

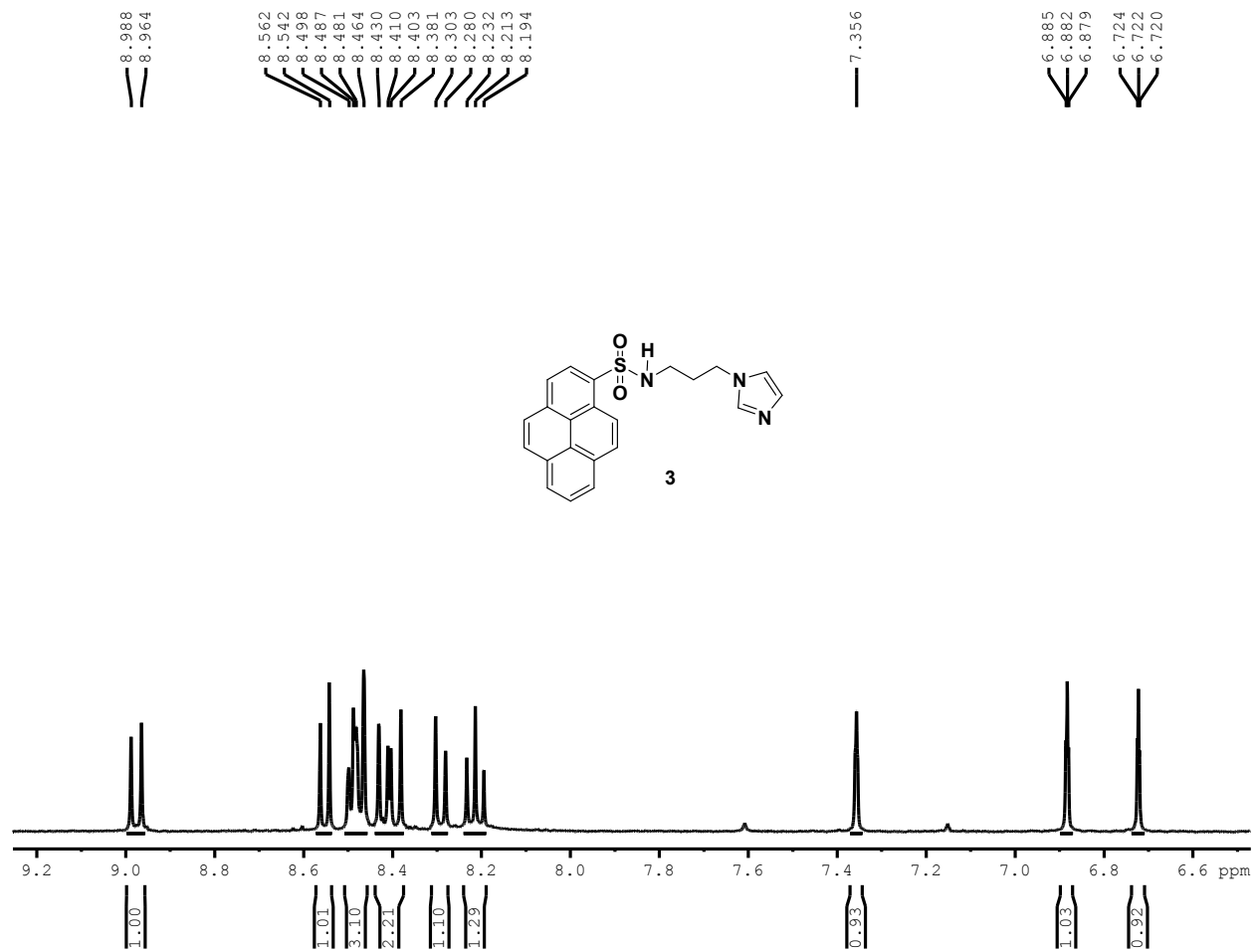


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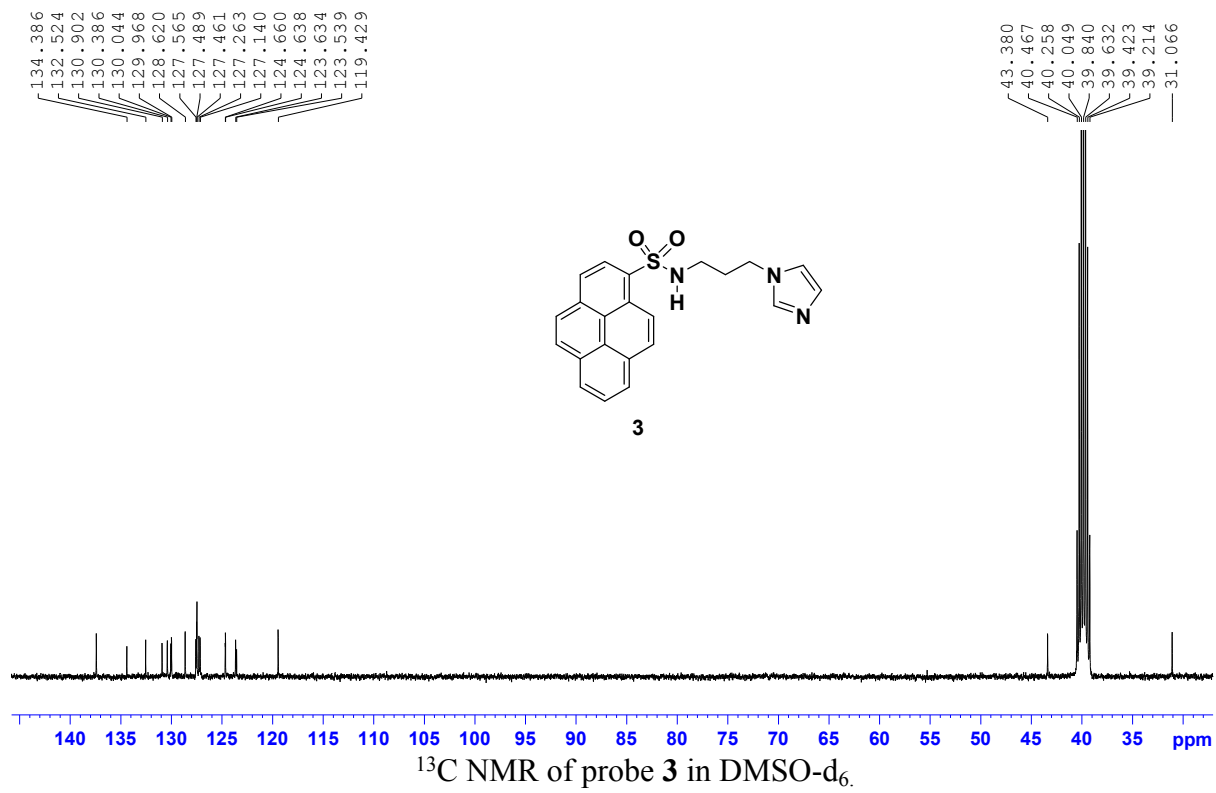
¹H NMR of probe 3 in DMSO-d₆.

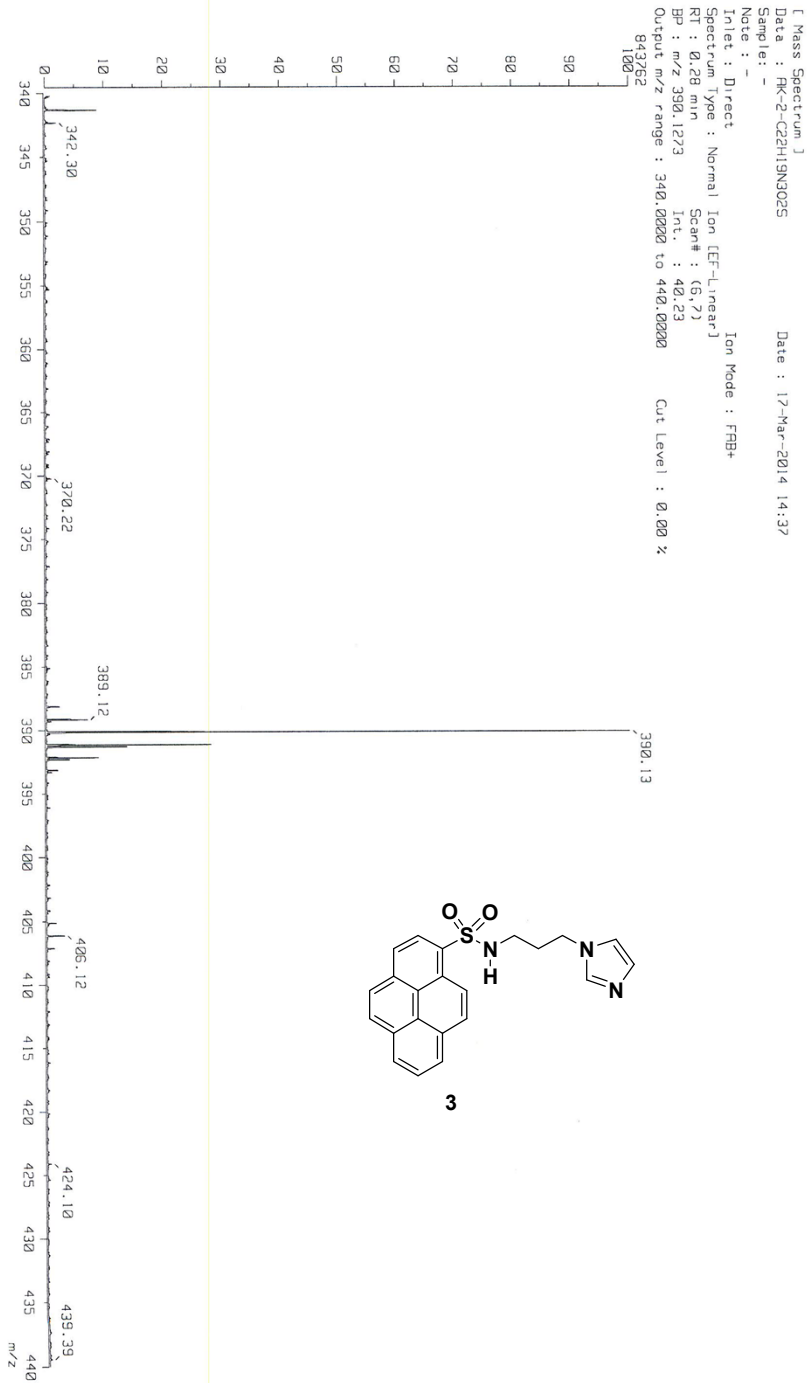


^1H NMR of probe **3** aliphatic region in DMSO-d_6 .

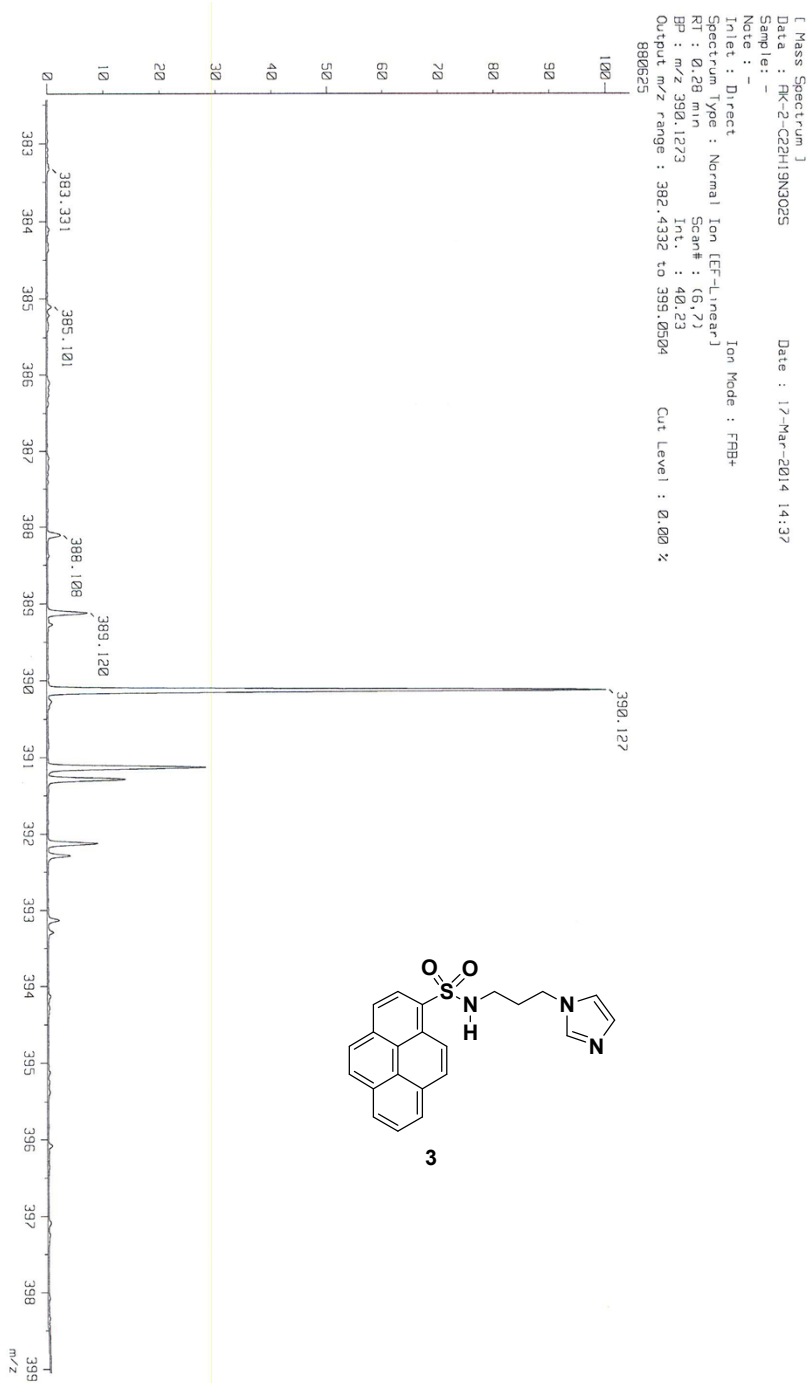


¹H NMR of probe **3** aromatic region in DMSO-d₆

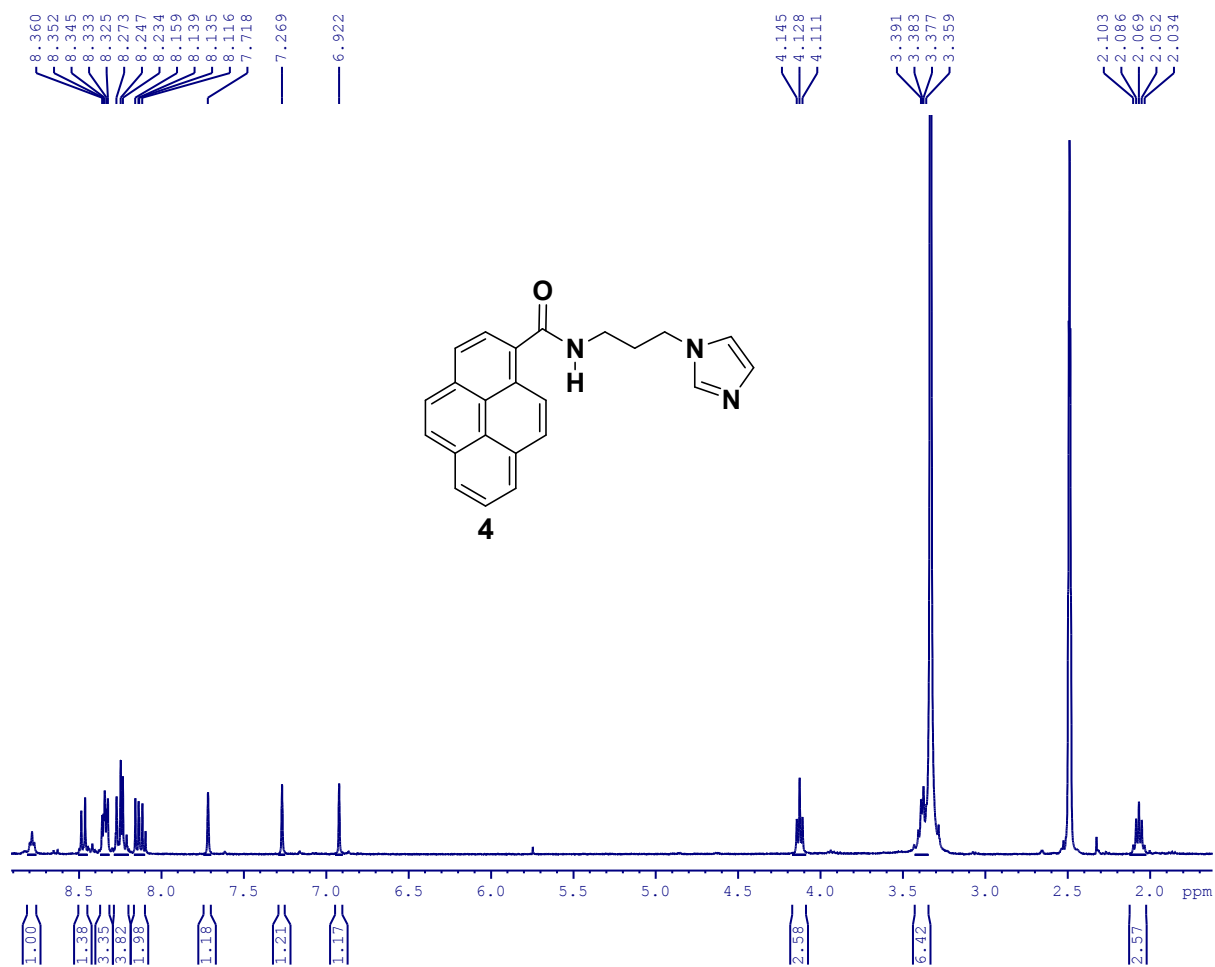




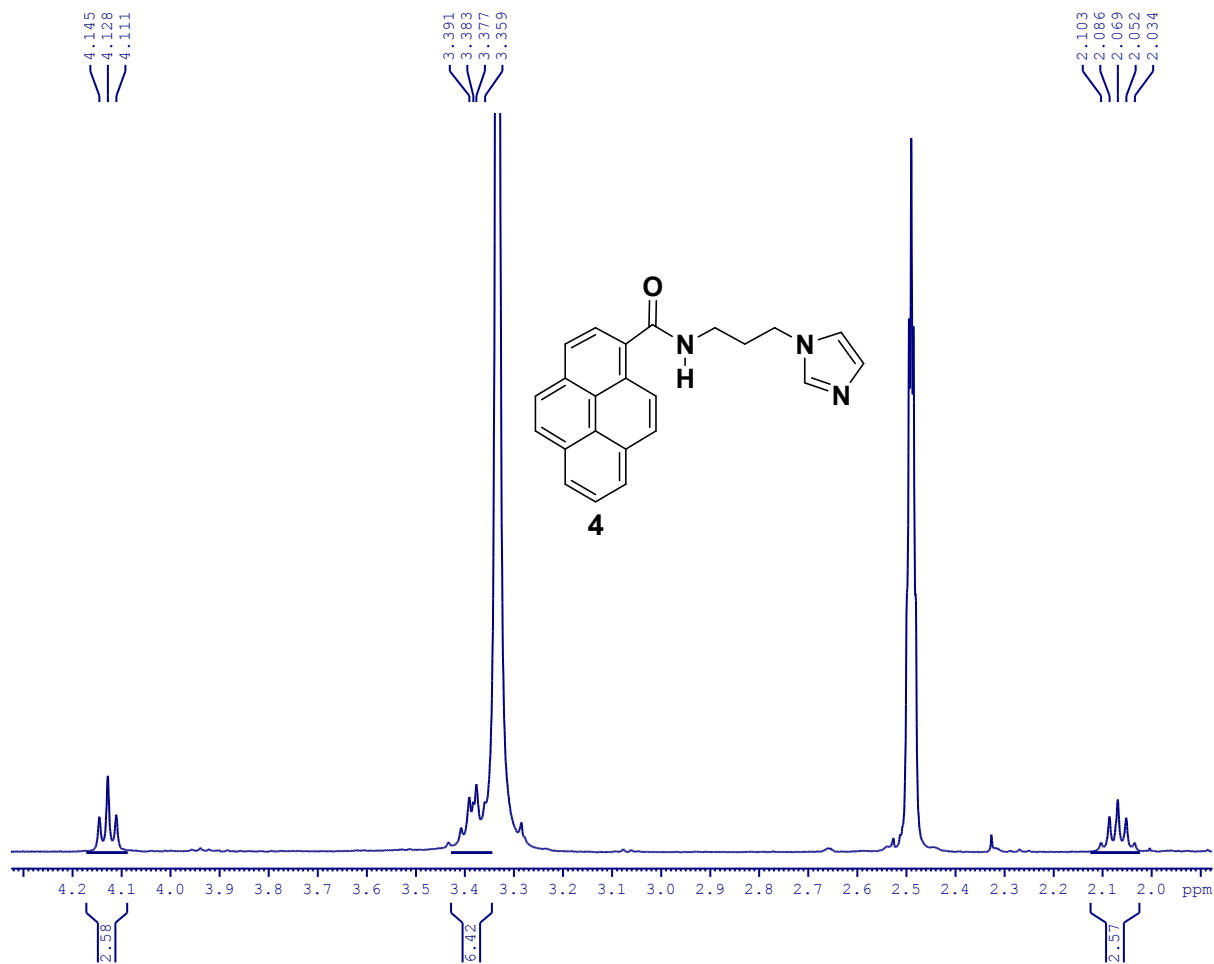
HRMS of probe 3



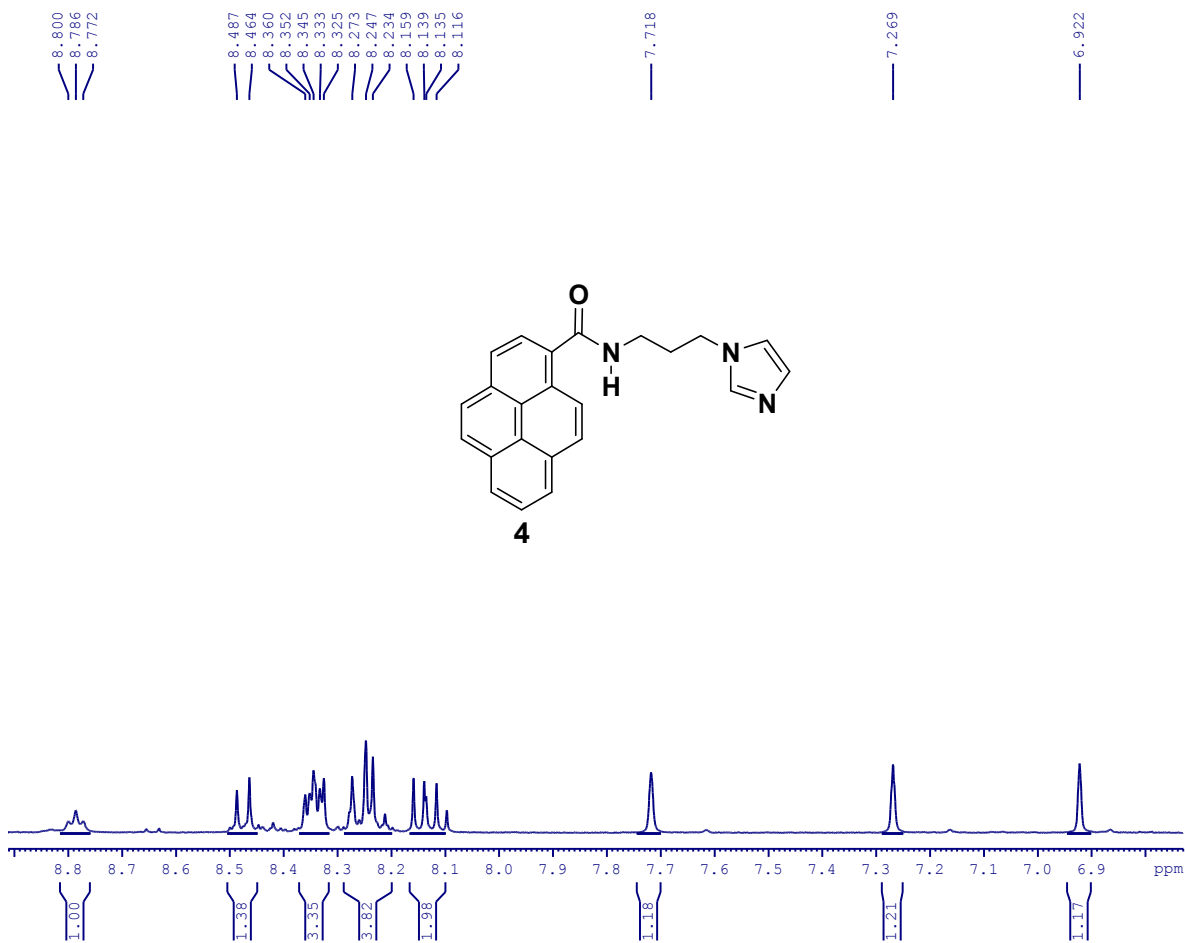
HRMS of probe 3



¹H NMR of probe 4 in DMSO-d₆.

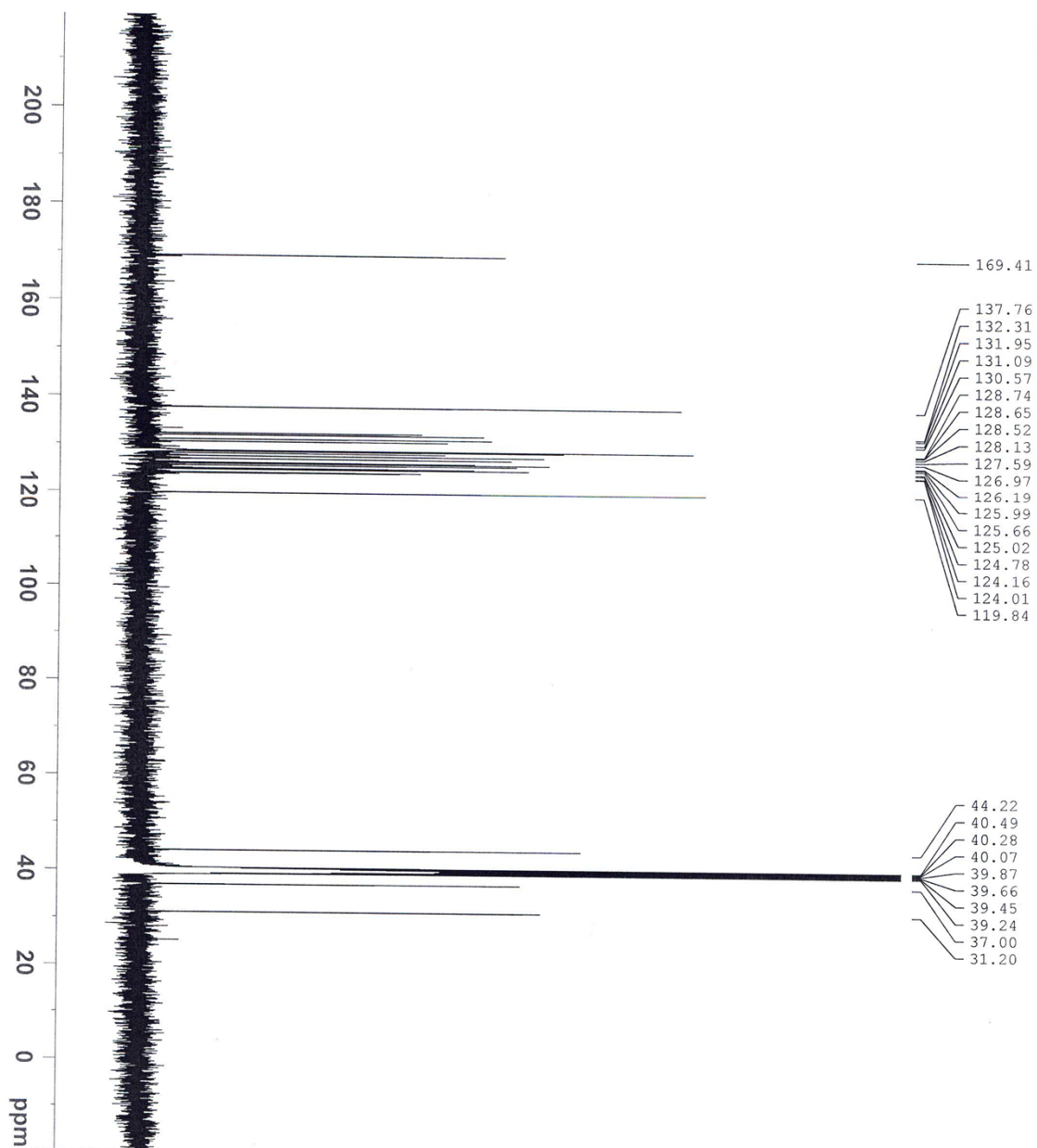


¹H NMR of probe 4 aliphatic region in DMSO-d₆.

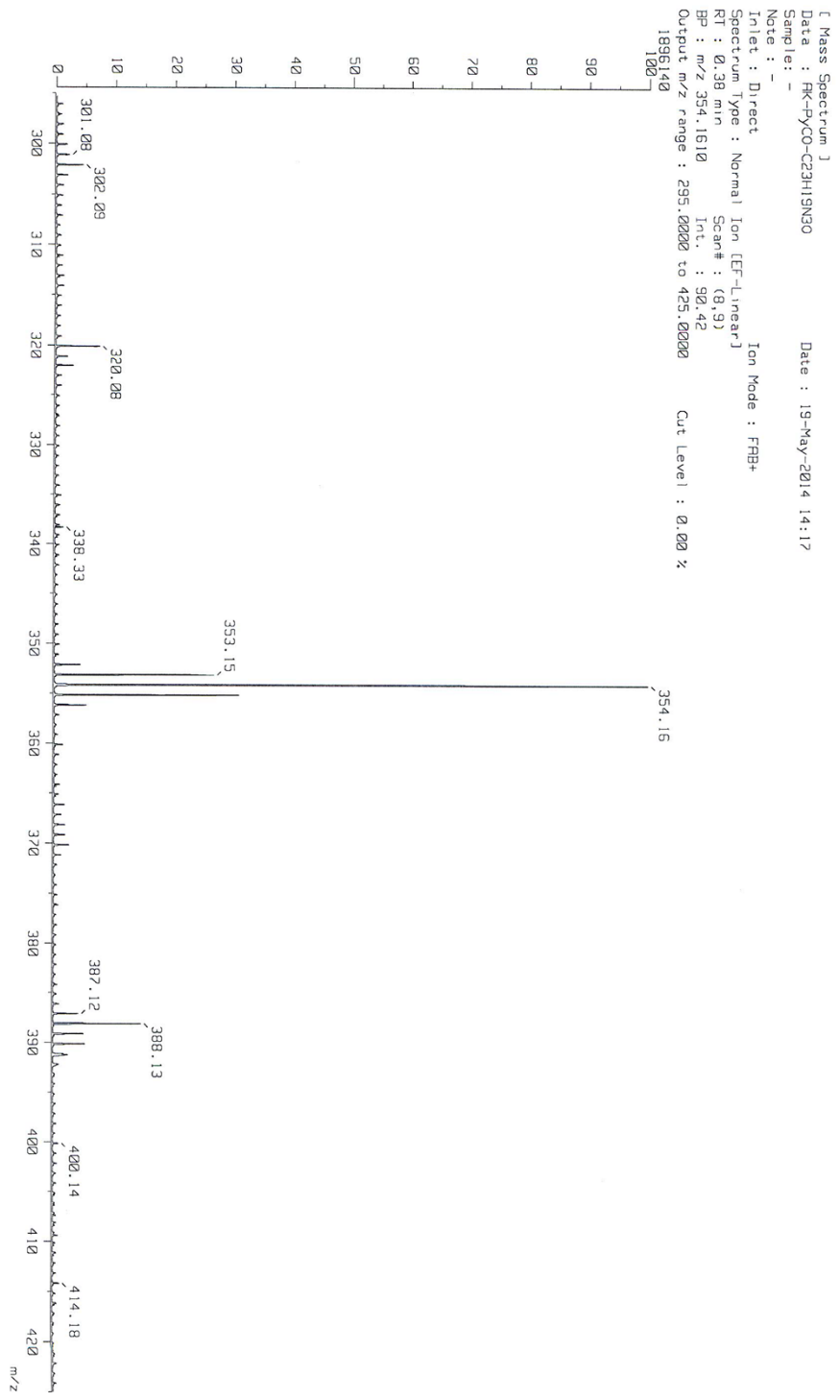


¹H NMR of probe 4 aromatic region in DMSO-d₆

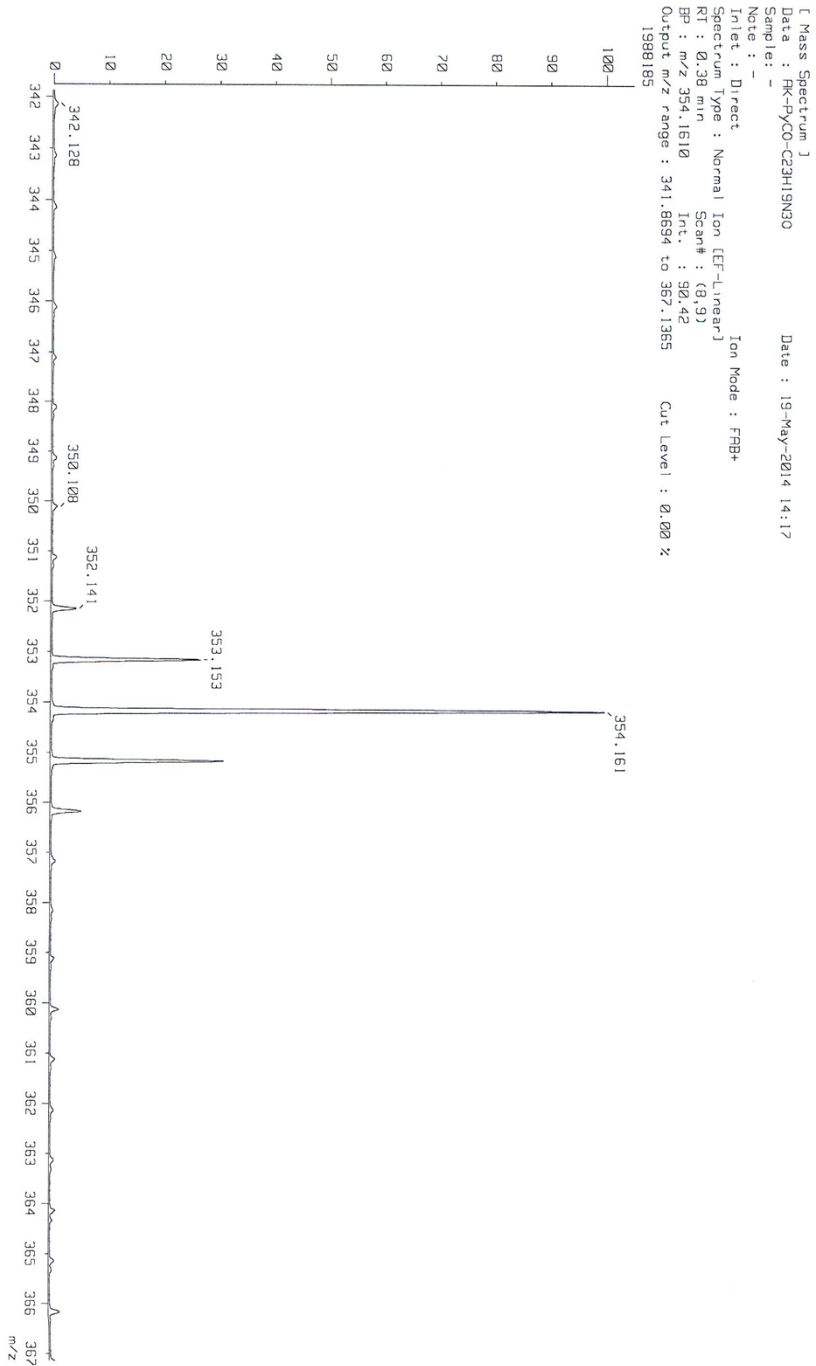
AK-8



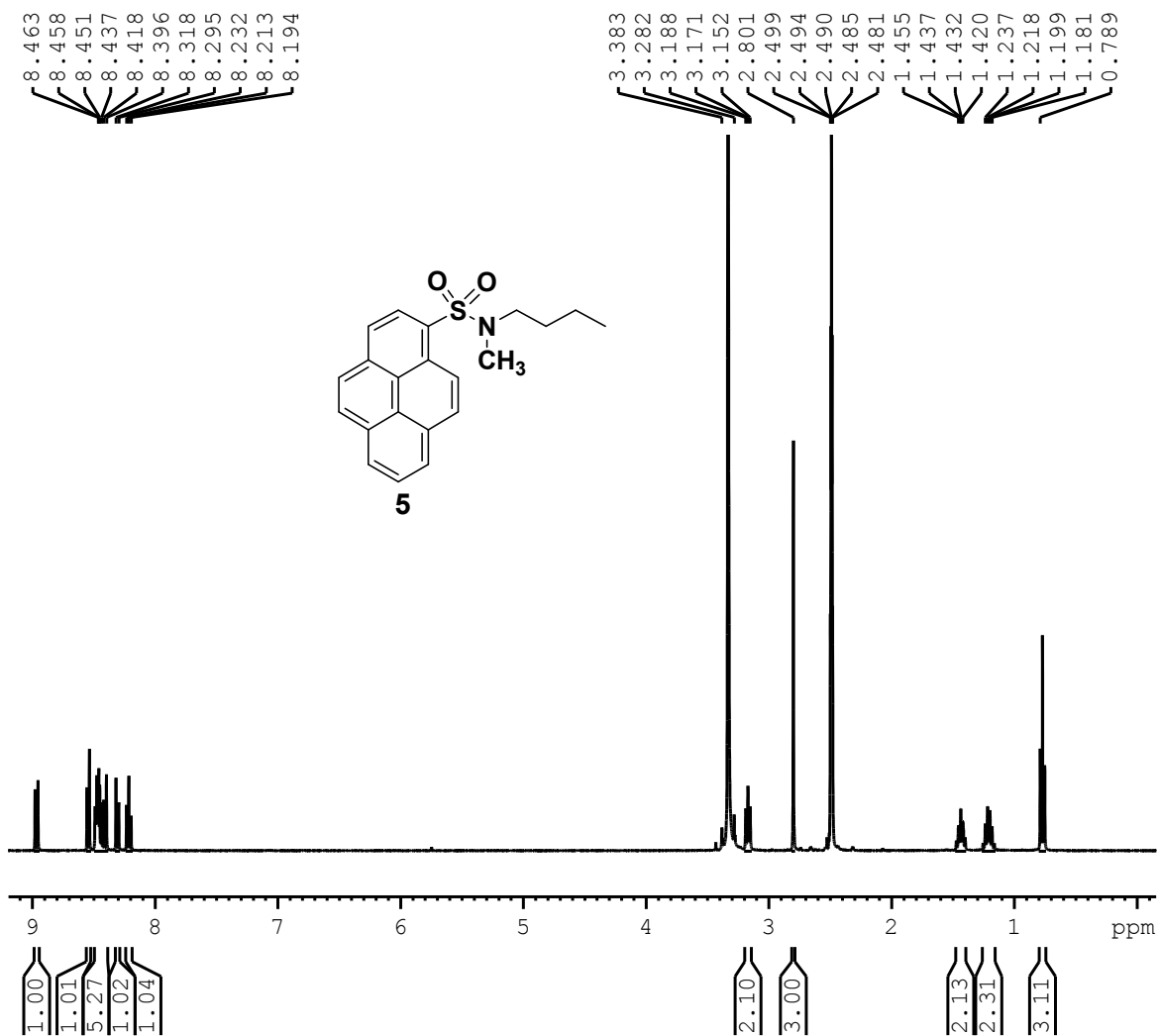
¹³C NMR of probe 4 in DMSO-d₆.



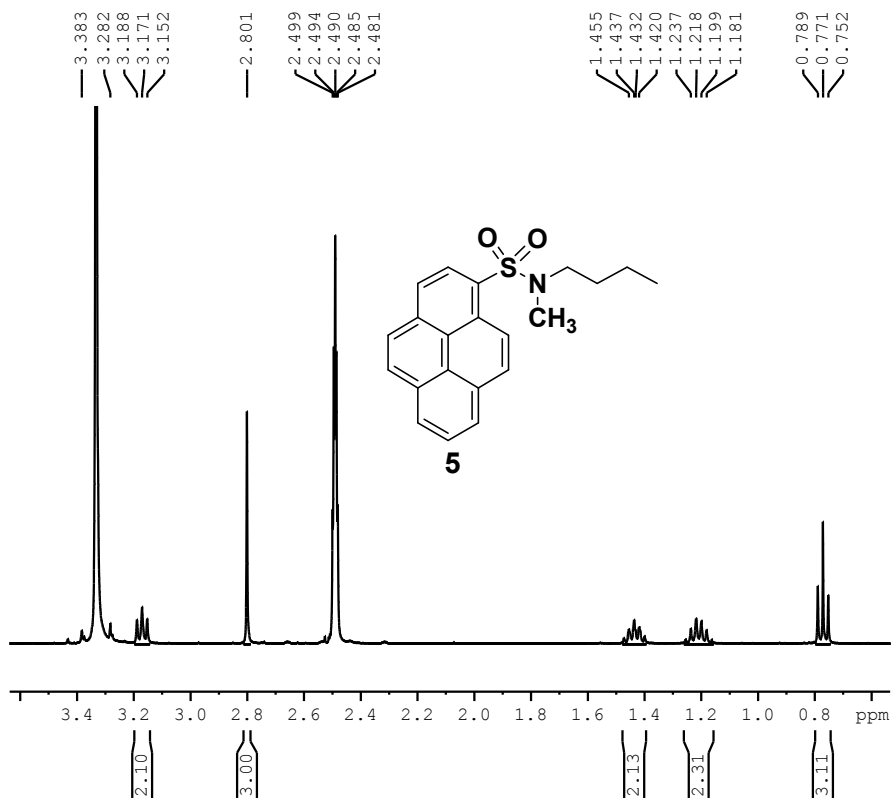
HRMS of probe 4



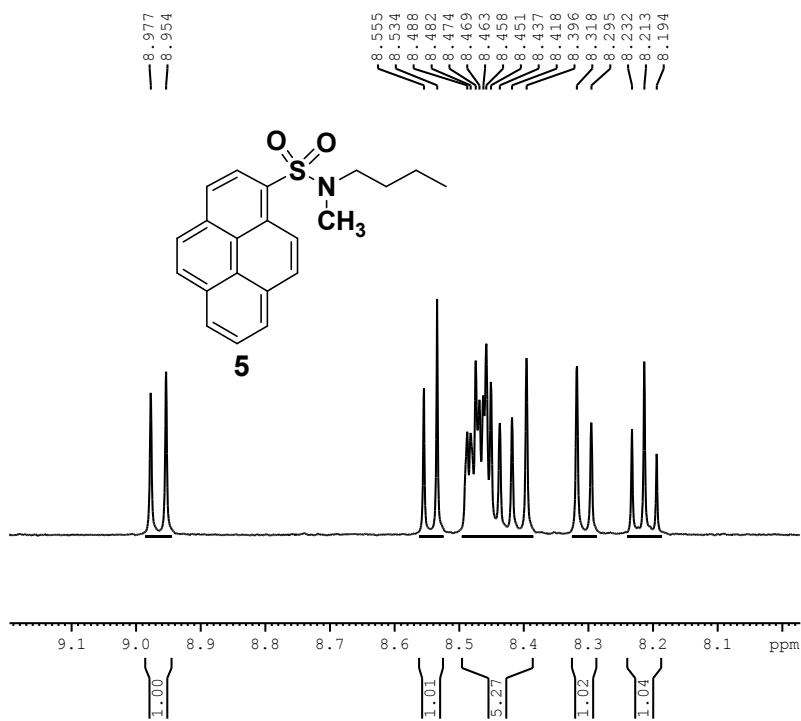
HRMS of probe 4



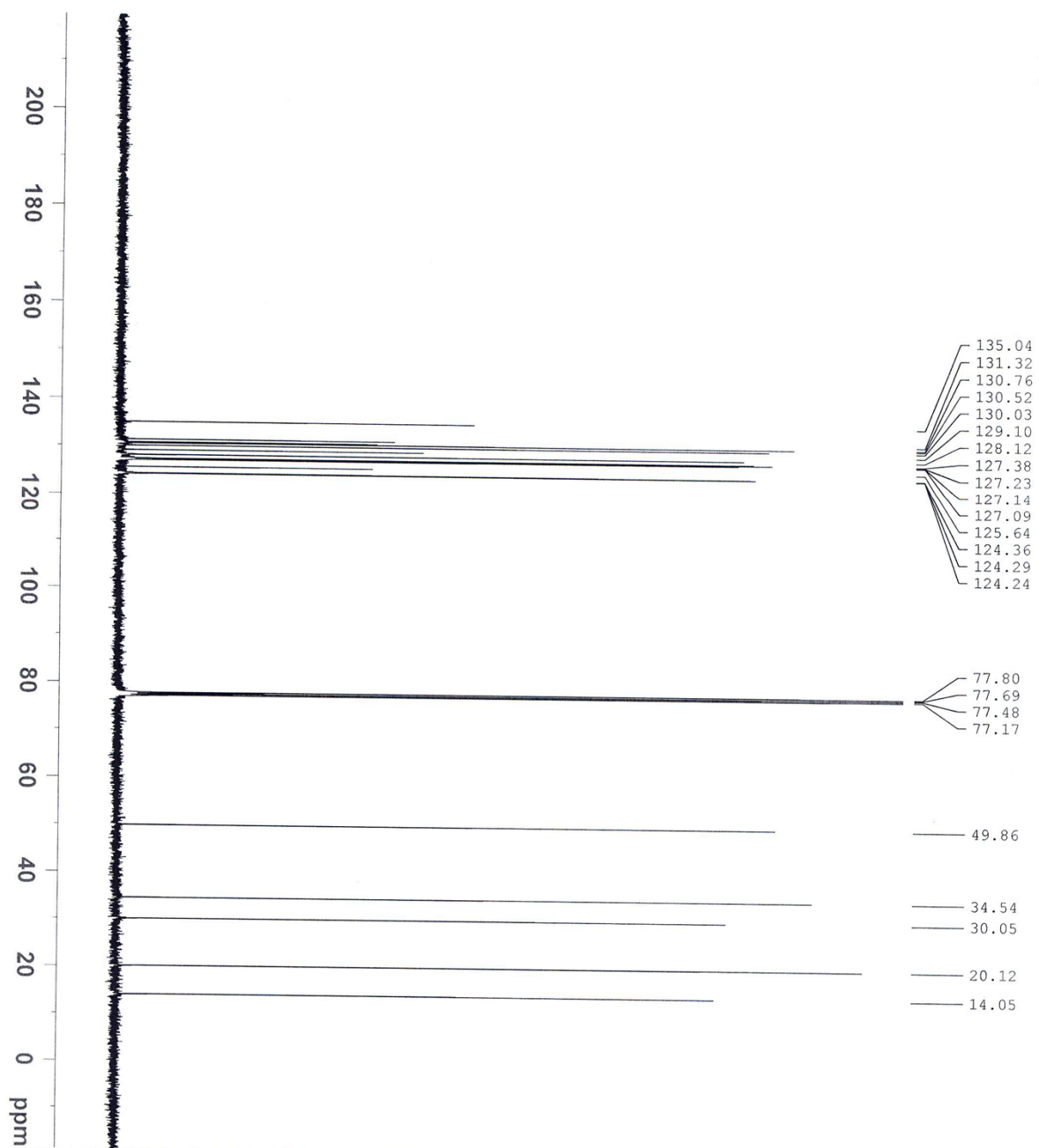
¹H NMR of probe **5** in CDCl₃.



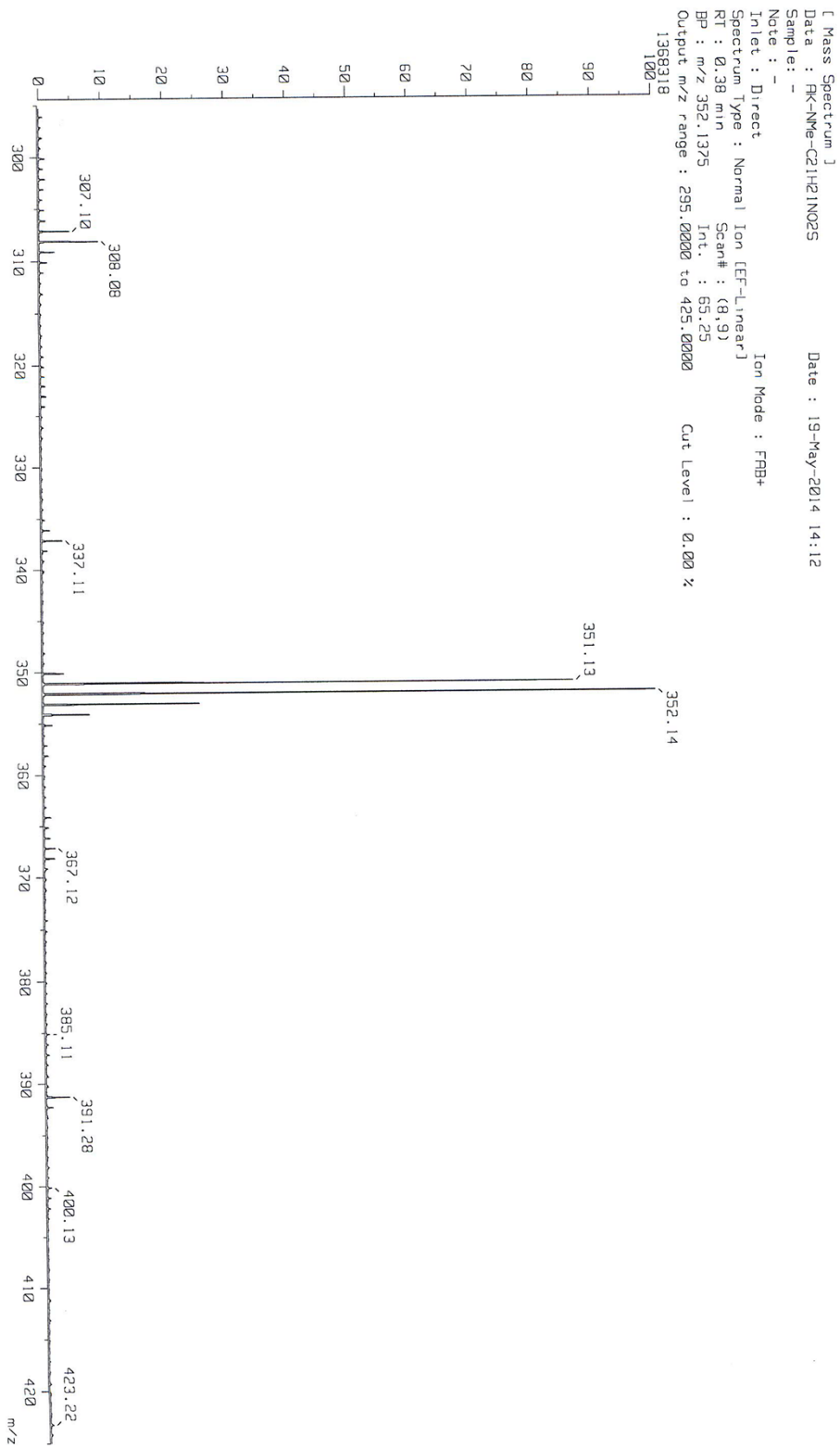
¹H NMR of probe **5** aliphatic region in CDCl₃.



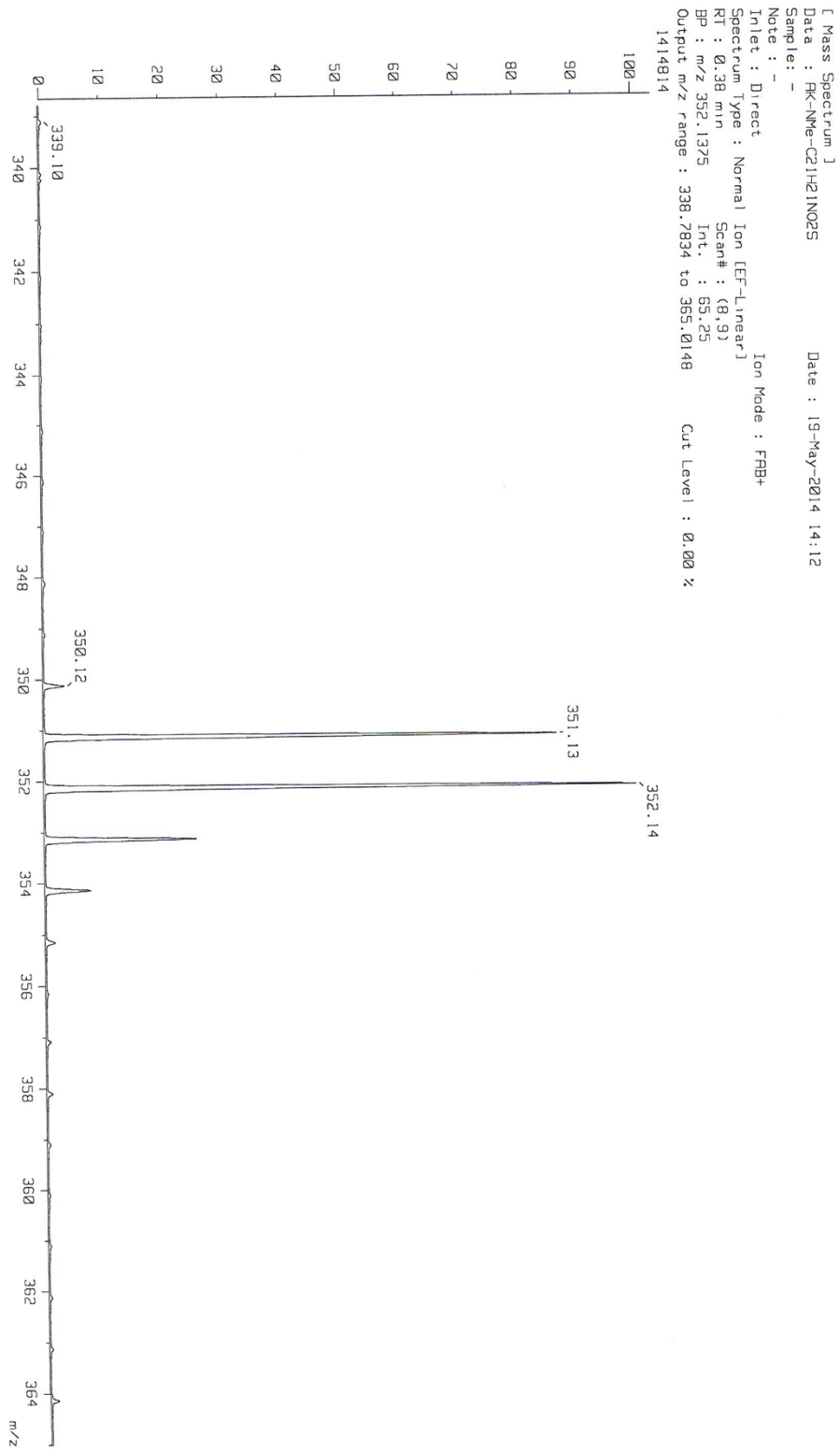
¹H NMR of probe **5** aromatic region in CDCl₃.



^{13}C NMR of probe 5 in CDCl_3 .



HRMS of probe 5



HRMS of probe 5

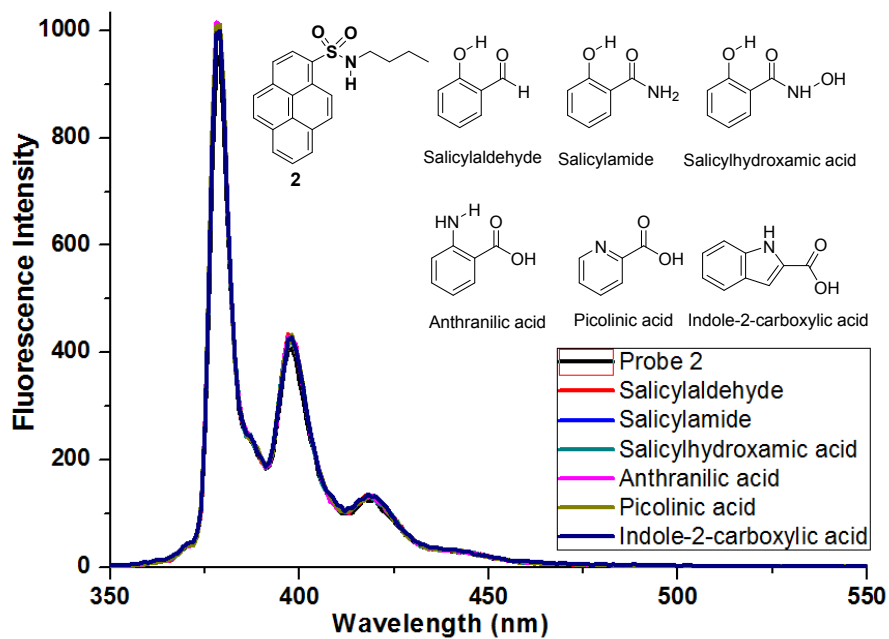


Fig. SI 1: Fluorescence study of probe 2 (1 μM , EtOH) with different salicylic derivatives/similar moieties, $\lambda_{ex} = 336$ nm, slit width 3,3.

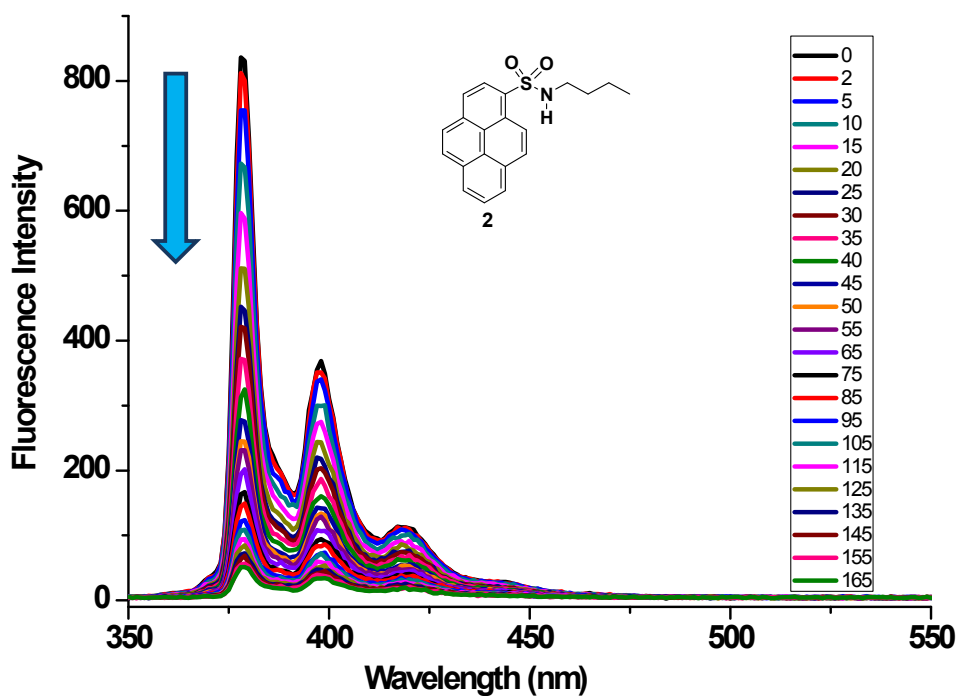


Fig. SI 2: Fluorescence titration of probe 2 (1 μM , EtOH) with 3,5-Dinitrosalicylic acid, $\lambda_{ex} = 336$ nm.

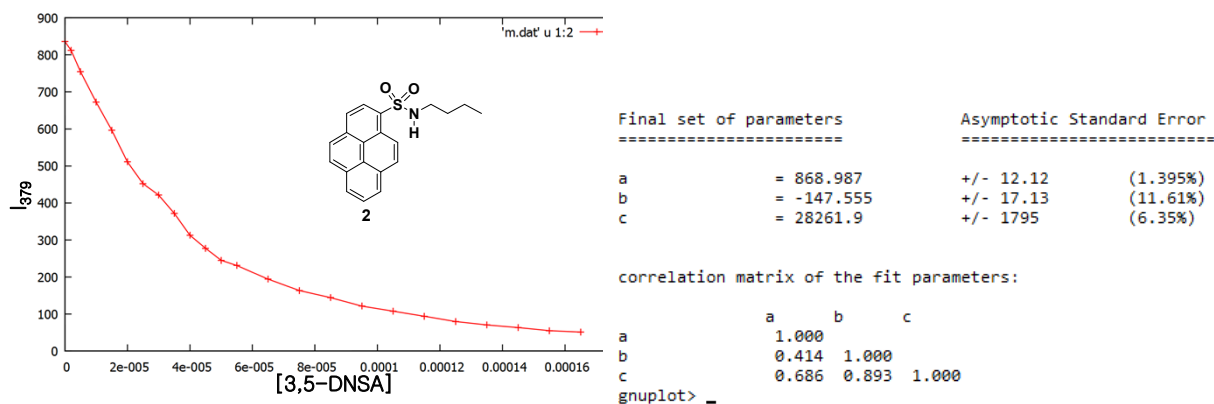


Fig. SI 3: Fluorescence spectral fitting of probe **2** (1 μ M, EtOH) with [3,5-Dinitrosalicylic Acid] and association constant.

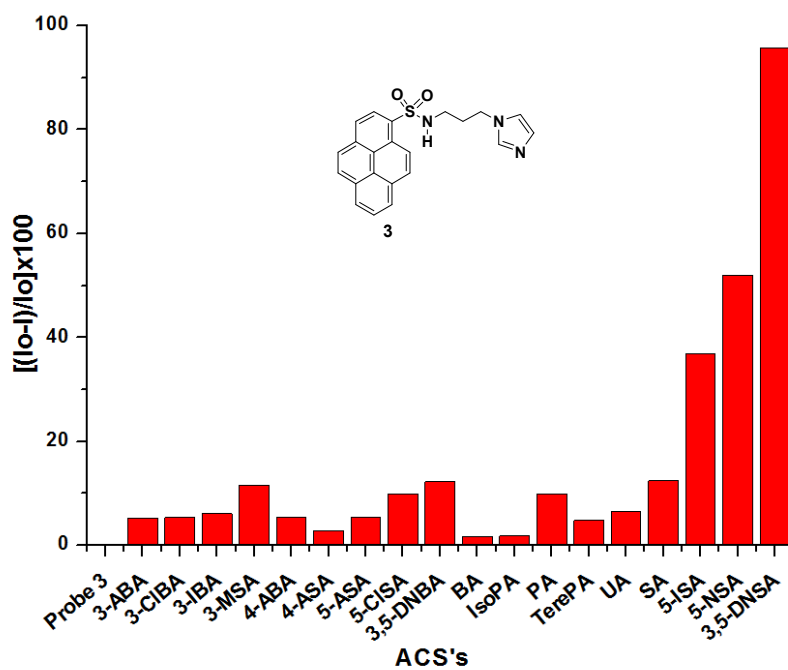


Fig. SI 4: Relative fluorescence intensity bar diagram of probe **3** (1 μ M, EtOH) with different aromatic carboxylic acids, $\lambda_{ex} = 336$ nm.

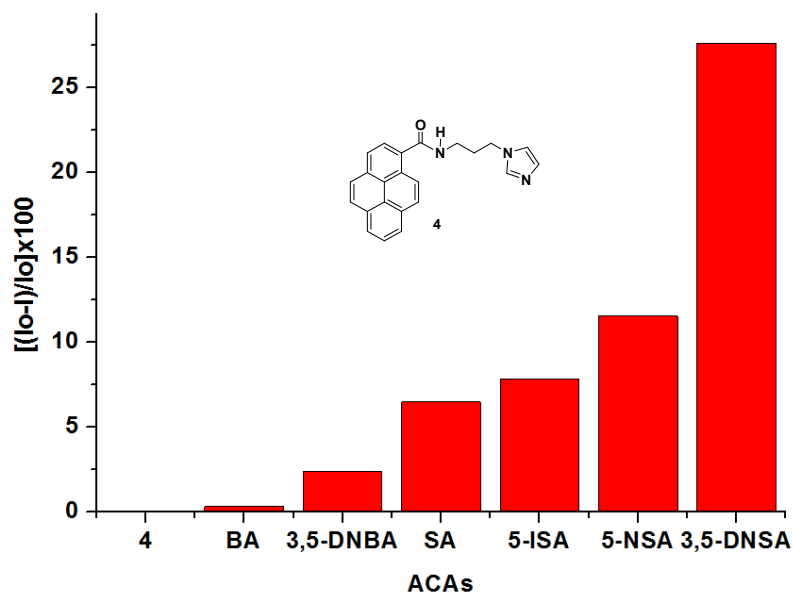


Fig. SI 5: Relative fluorescence intensity bar diagram of probe **4** (1 μ M, EtOH) with different carboxylic acids, λ_{ex} = 336 nm, slit width 3,3.

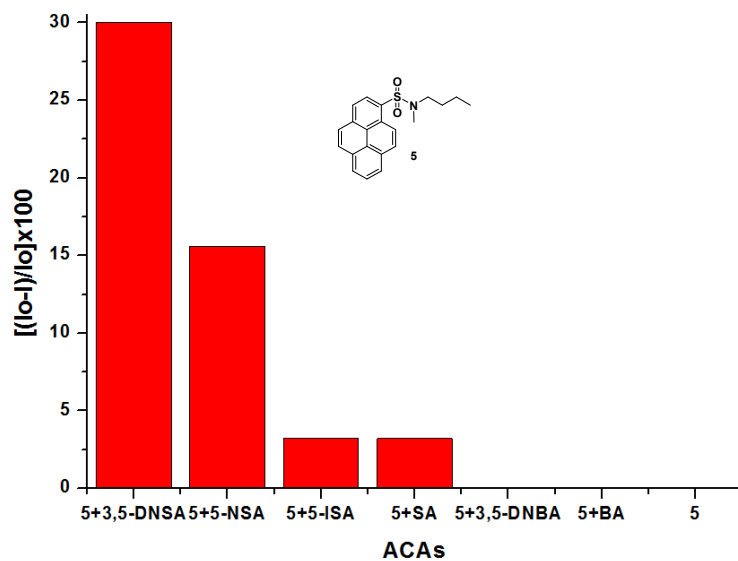


Fig. SI 6: Relative fluorescence intensity bar diagram of probe **5** (1 μ M, EtOH) with different carboxylic acids, λ_{ex} = 336 nm, slit width 3,3.

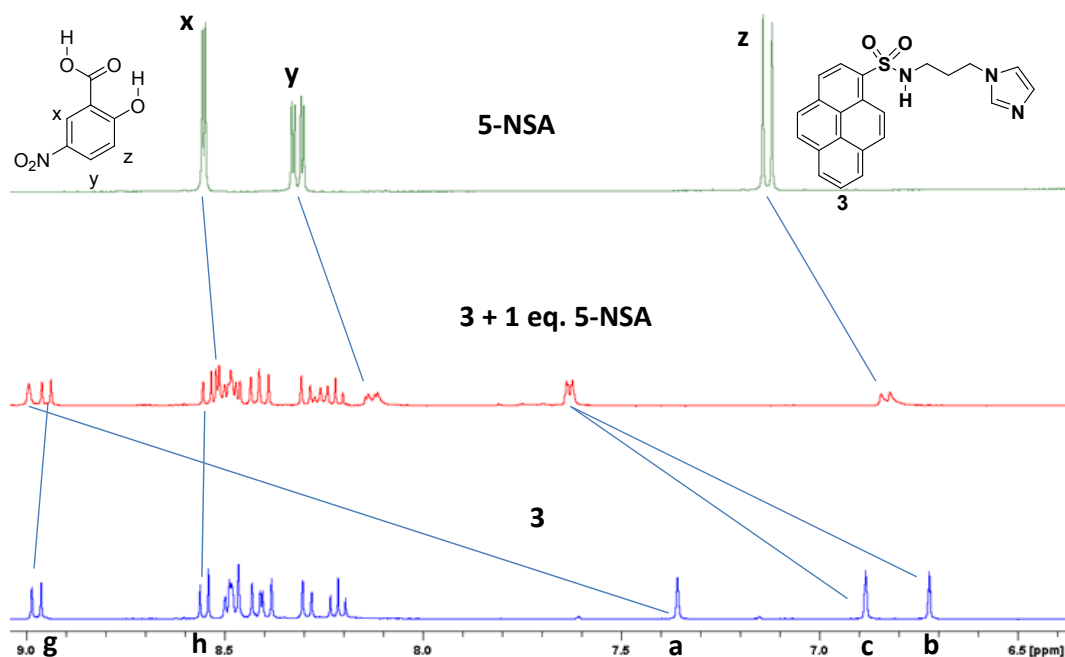


Fig. SI 7: Partial ^1H NMR spectra of aromatic region of 5-NSA and probe **3** on addition of 1 eq. of 5-NSA in DMSO-d_6 .

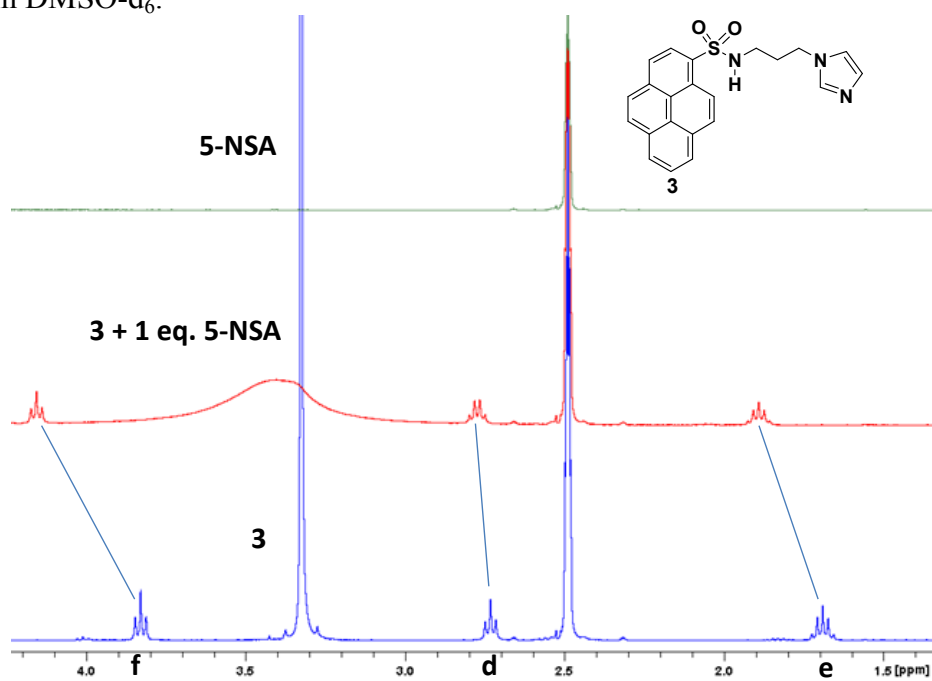


Fig. SI 8: Partial ^1H NMR spectra of aliphatic region of 5-NSA and probe **3** on addition of 1 eq. of 5-NSA in DMSO-d_6 .

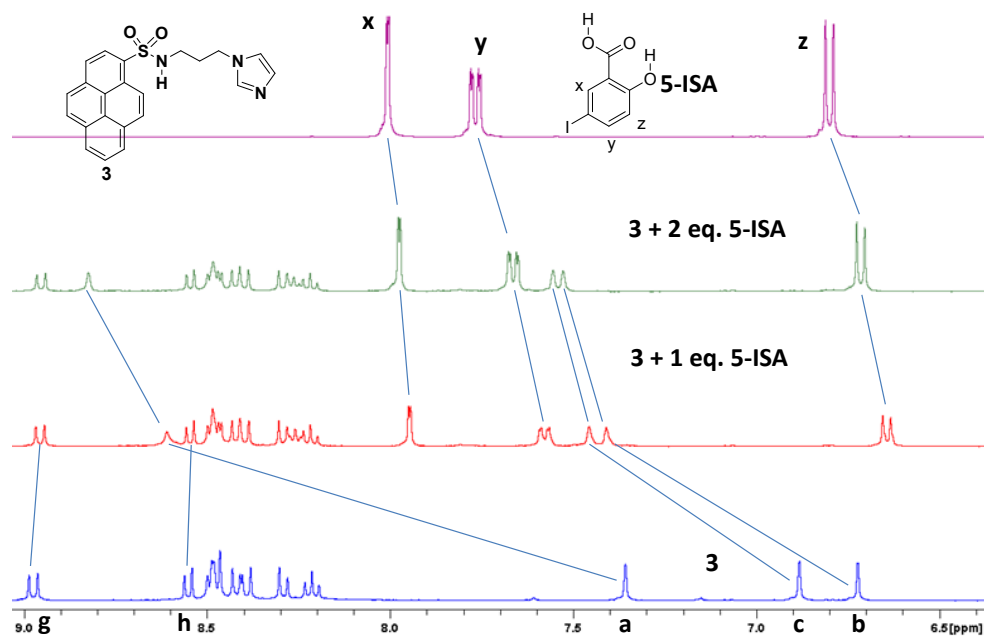


Fig. SI 9: Partial ¹H NMR spectra of aromatic region of 5-ISA and probe **3** on addition of 1 eq. of 5-ISA, 2 eq. of 5-ISA in DMSO-d₆.

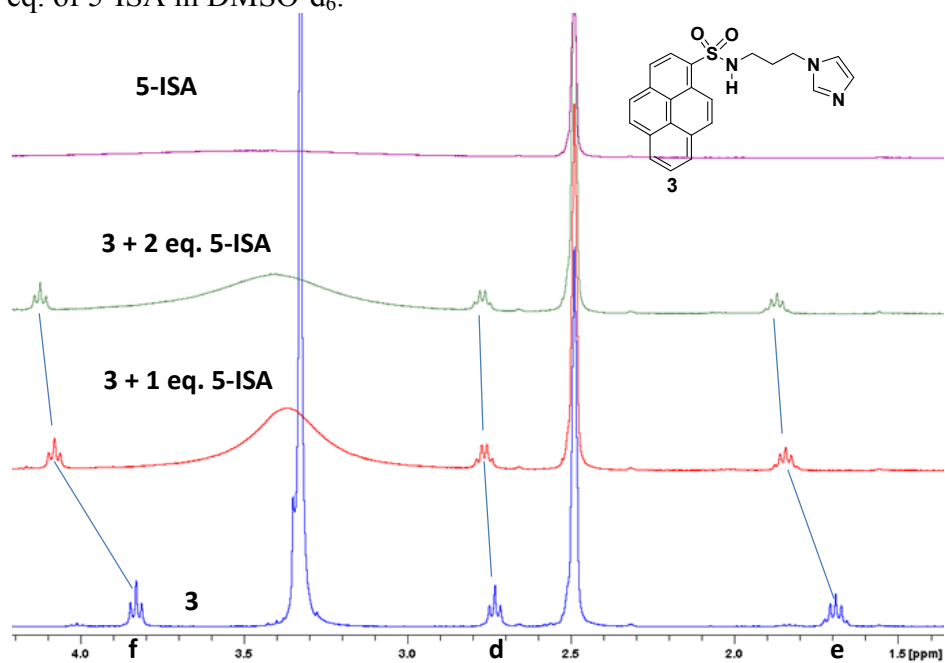


Fig. SI 10: Partial ¹H NMR spectra of aliphatic region 5-ISA and probe **3** on addition of 1 eq. of 5-ISA, 2 eq. of 5-ISA in DMSO-d₆.

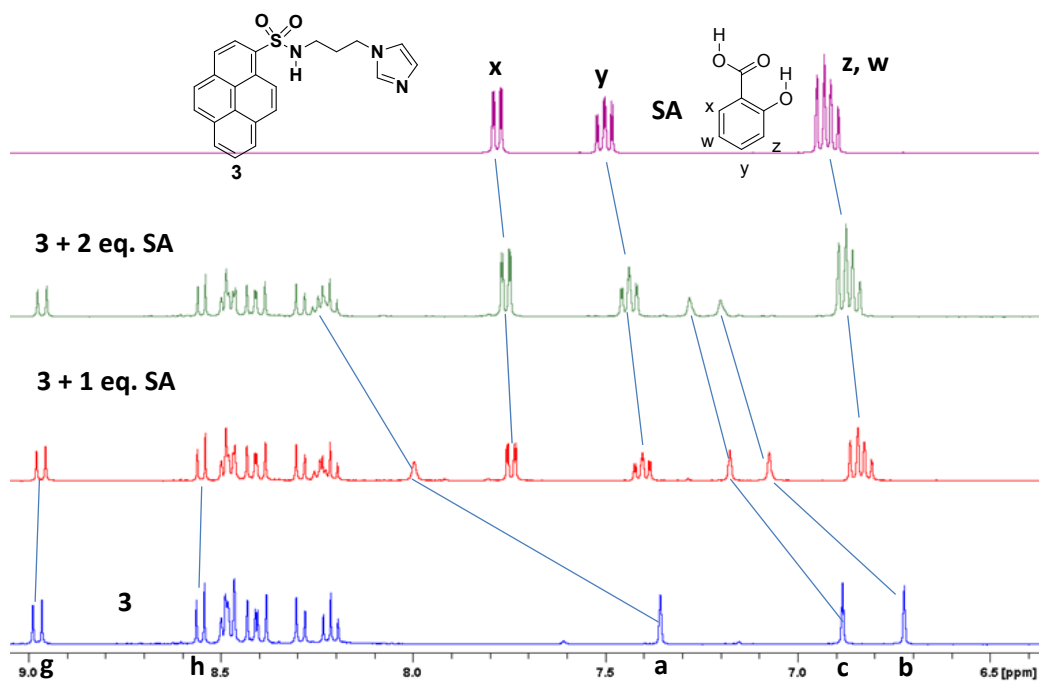


Fig. SI 11: Partial ^1H NMR spectra of aromatic region of SA and probe **3** on addition of 1 eq. of SA, 2 eq. of SA in DMSO-d_6 .

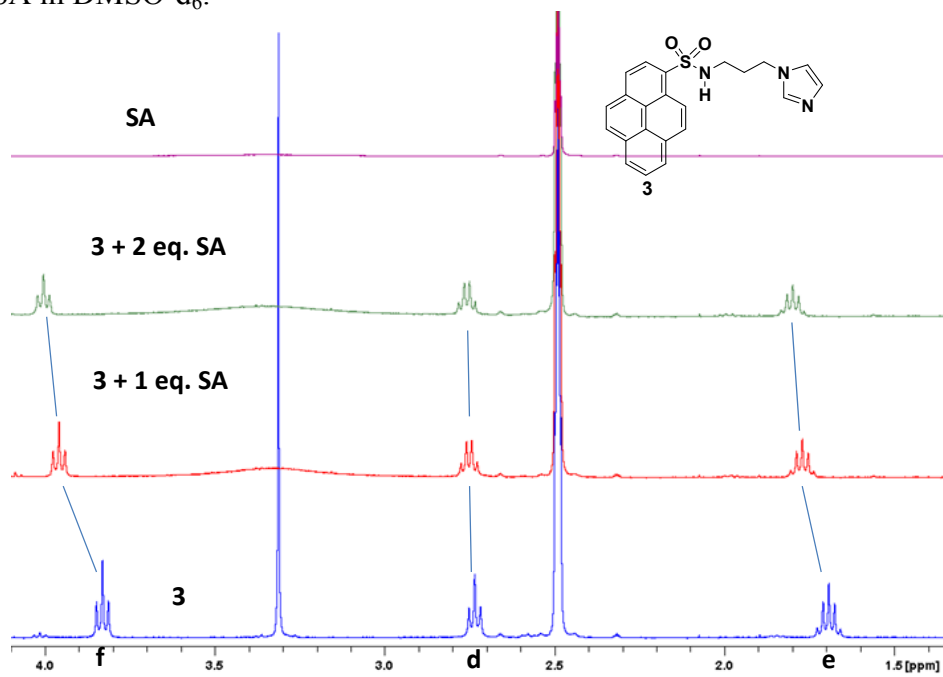


Fig. SI 12: Partial ^1H NMR spectra of aliphatic aromatic region of SA and probe **3** on addition of 1 eq. of SA, 2 eq. of SA in DMSO-d_6 .

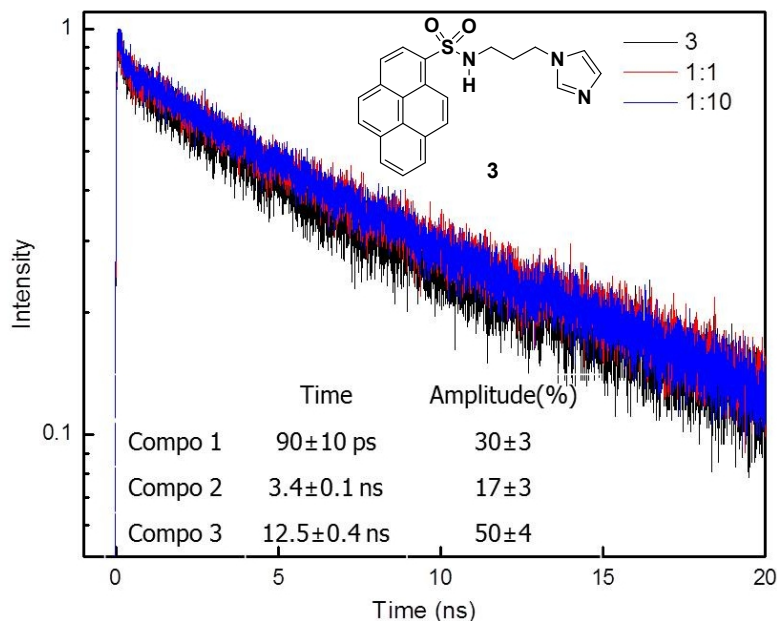


Fig. SI 13: The lifetimes of samples (Compo 1 = probe 3 (black), Compo 2 = 1:1 complex with 3,5-dinitrobenzoic acid (red) and Compo 3 = 1:10 complex with 3,5-dinitrobenzoic acid (blue)) are almost similar.

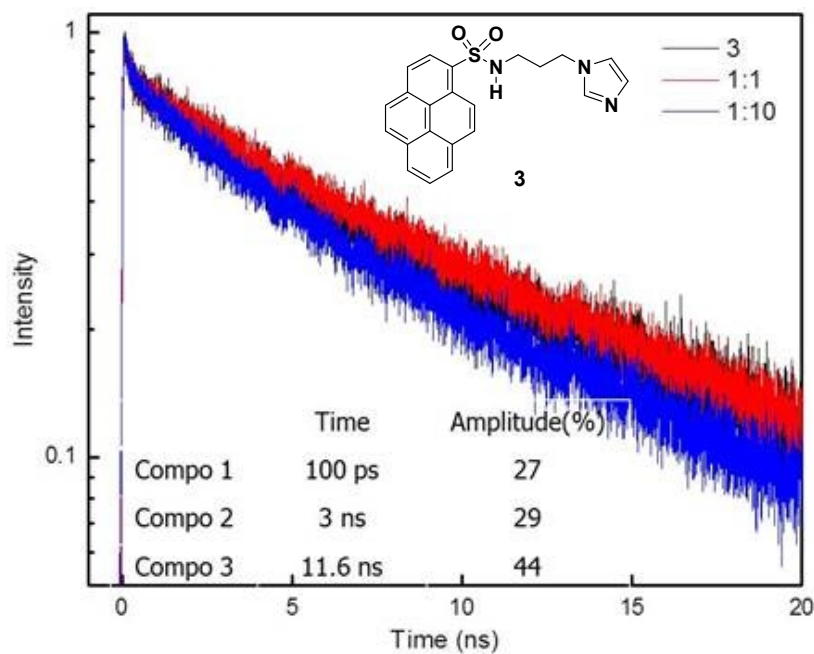


Fig. SI 14: The lifetimes of samples (Compo 1 = probe 3 (black), Compo 2 = 1:1 complex with 3,5-dinitrosalicylic acid (red) and Compo 3 = 1:10 complex with 3,5-dinitrosalicylic acid (blue)) are slightly different.

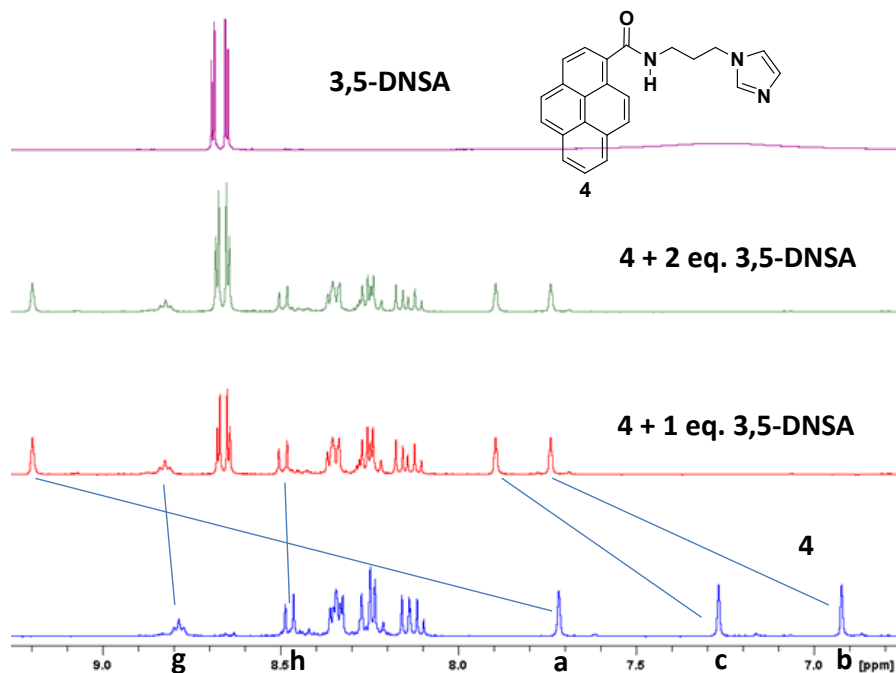


Fig. SI 15: Partial ^1H NMR spectra of aromatic region of 3,5-DNSA and probe **4** on addition of 1 eq. of 3,5-DNSA, 2 eq. of 3,5-DNSA in DMSO-d_6 .

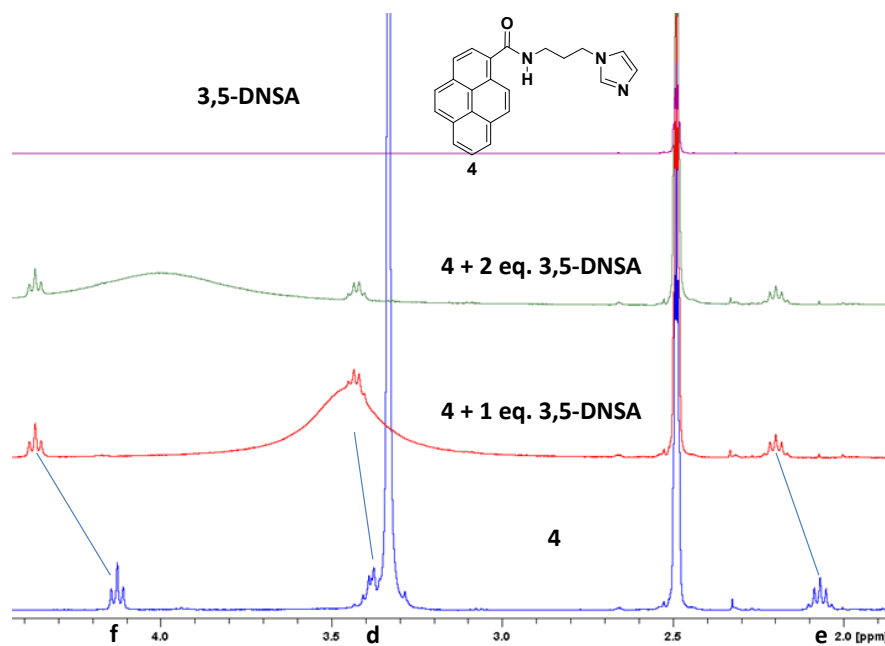


Fig. SI 16: Partial ^1H NMR spectra of aliphatic region of 3,5-DNSA and probe **4** on addition of 1 eq. of 3,5-DNSA, 2 eq. of 3,5-DNSA in DMSO-d_6 .

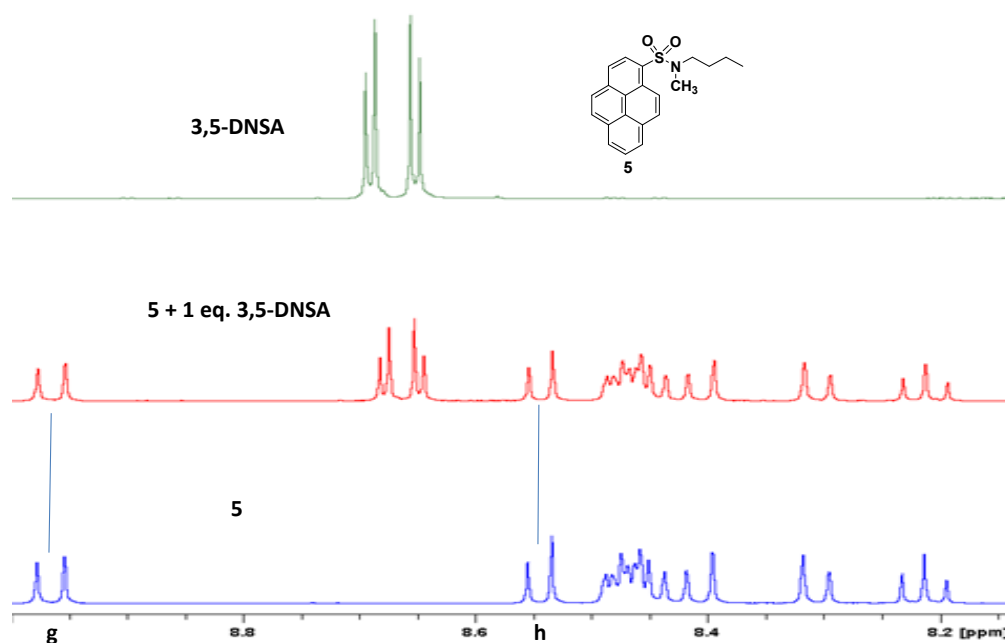


Fig. SI 17: Partial ^1H NMR spectra of aromatic region of 3,5-DNSA and probe **5** on addition of 1 eq. of 3,5-DNSA in DMSO-d_6 .

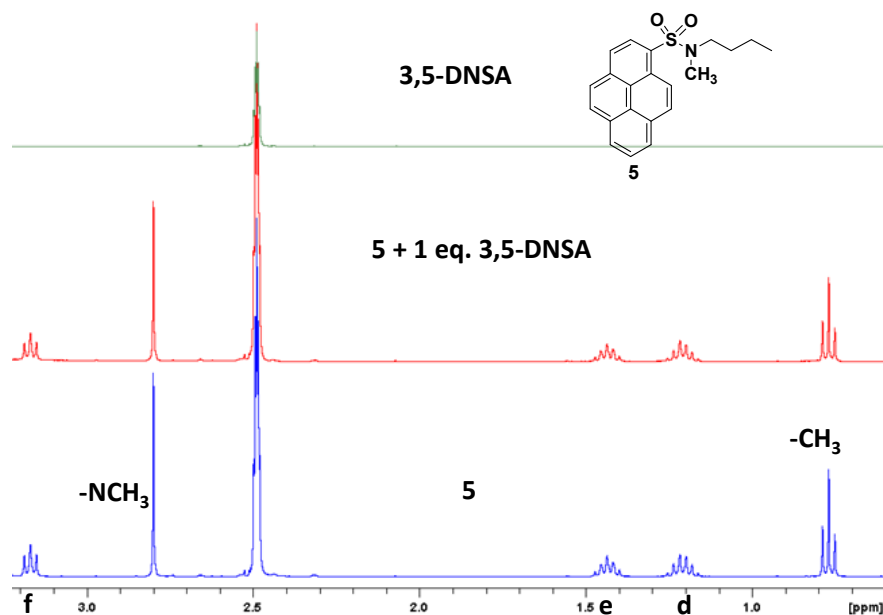


Fig. SI 18: Partial ^1H NMR spectra of aliphatic region of 3,5-DNSA and probe **5** on addition of 1 eq. of 3,5-DNSA in DMSO-d_6 .

SI Table 1: The contributions of each electronic oscillator (orbital transitions) to the lowest energy transition.

Molecule/Complex	State	Absorption	Coefficient	$-\Delta E_{\text{HOMO/LUMO}}$
5-NSA	S ₄	H → L	0.95	4.391
3,5-DNSA	S ₆	H → L + 1	0.89	4.480
Probe 3	S ₁	H → L	0.95	3.537
Probe 3 + 5-NSA	S ₂	H → L	0.91	3.530
Probe 3 + 3,5-DNSA	S ₇	H → L + 2	0.95	3.518

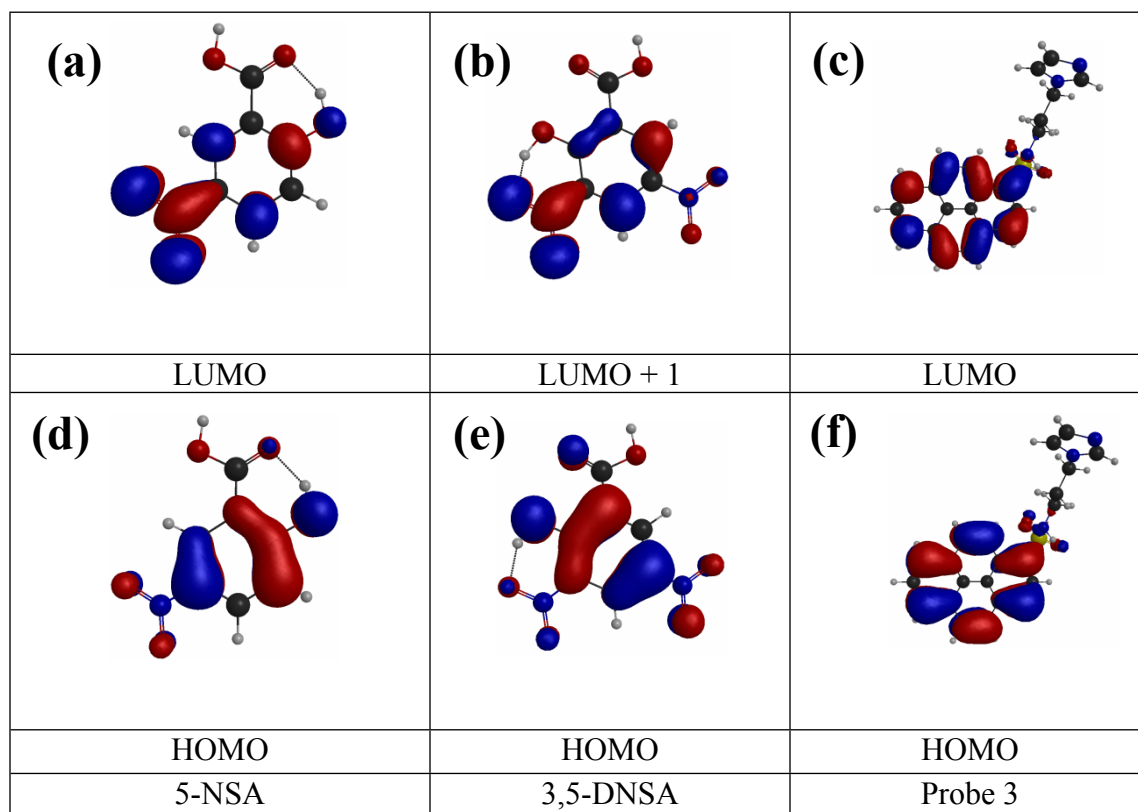


Fig. SI 19: B3LYP/6-31G* calculated molecular orbitals of 5-NSA, 3,5-DNSA and probe 3.

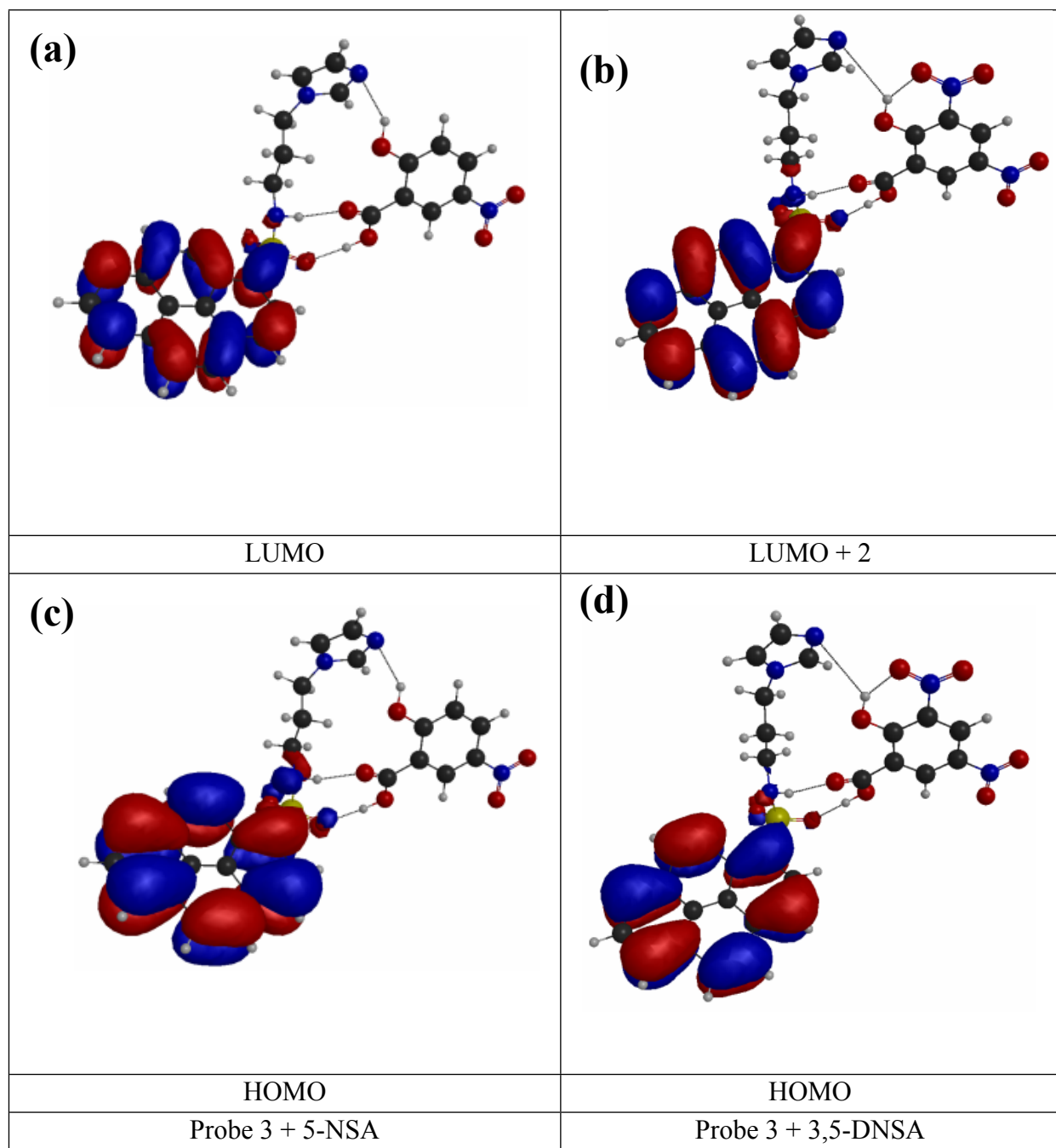


Fig. SI 20: B3LYP/6-31G* calculated molecular orbitals of probe **3** + 5-NSA and probe **3** + 3,5-DNSA.

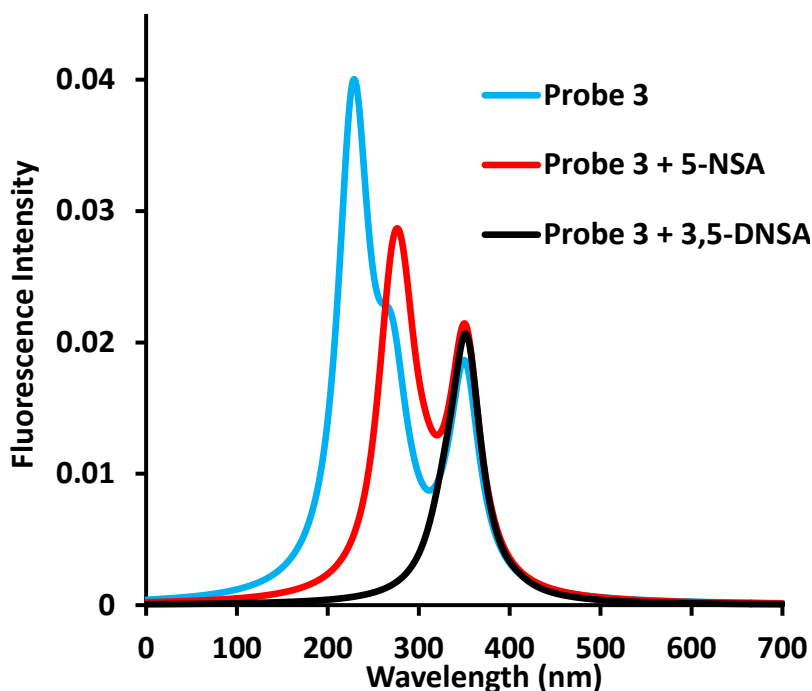


Fig. SI 21: Fluorescence emission spectra of probe **3** and its complexes with 3,5-DNSA and 5-NSA, obtained by using B3LYP/6-31G*.

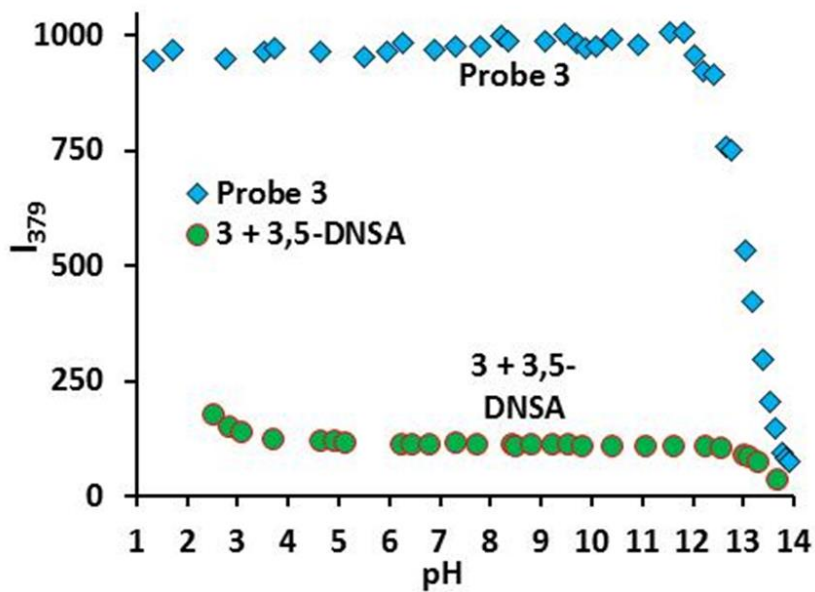


Fig. SI 22: Fluorescence intensity at $\lambda_{max} = 379$ nm of probe **3** and [**3**•3,5-DNSA] (1 μ M, EtOH-H₂O 10%) vs pH, $\lambda_{ex} = 336$ nm, slit width 3,3.