Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Dansyl-NA3 conjugates for glycoprotein detection through fluorescent tagging and native gel electrophoresis

(SUPPORTING INFORMATION)

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**CONTENT**

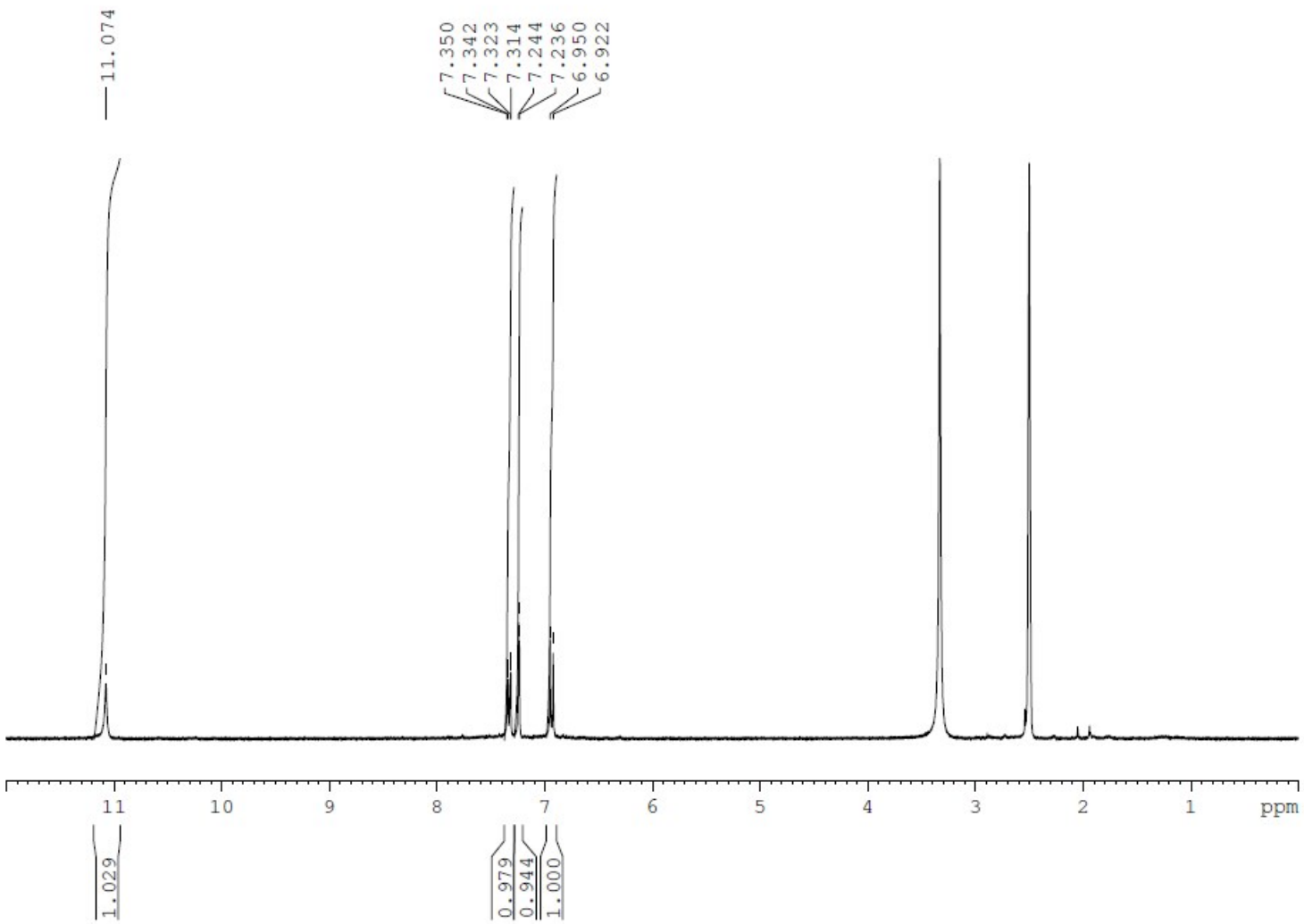


**Figure SI1** $^{1}$H NMR spectrum of 5-azidoisatin (**6**) in DMSO-$D_6$, full view.

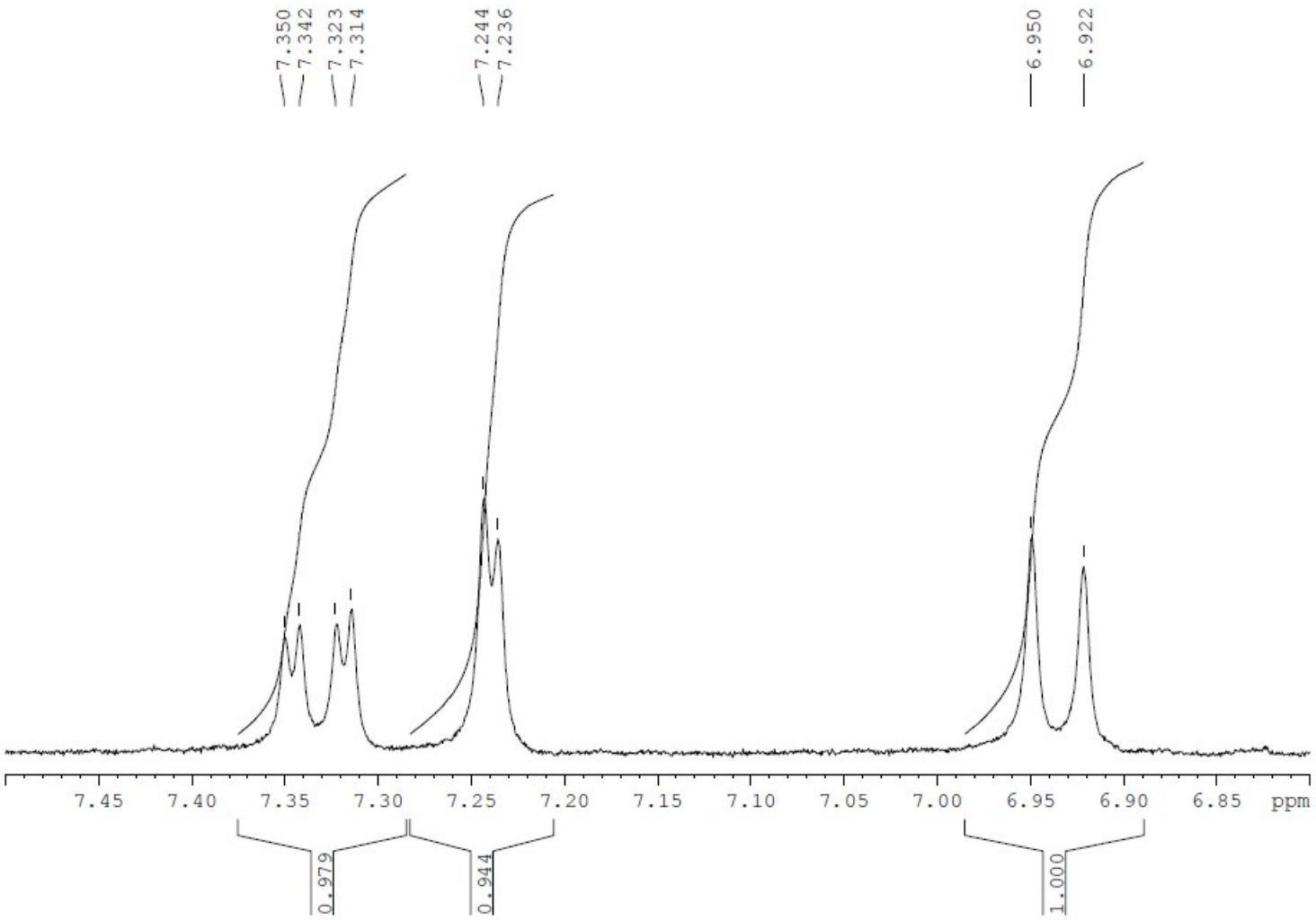


**Figure SI2** $^{1}$H NMR spectrum of 5-azidoisatin (**6**) in DMSO-$D_6$, expanded view.

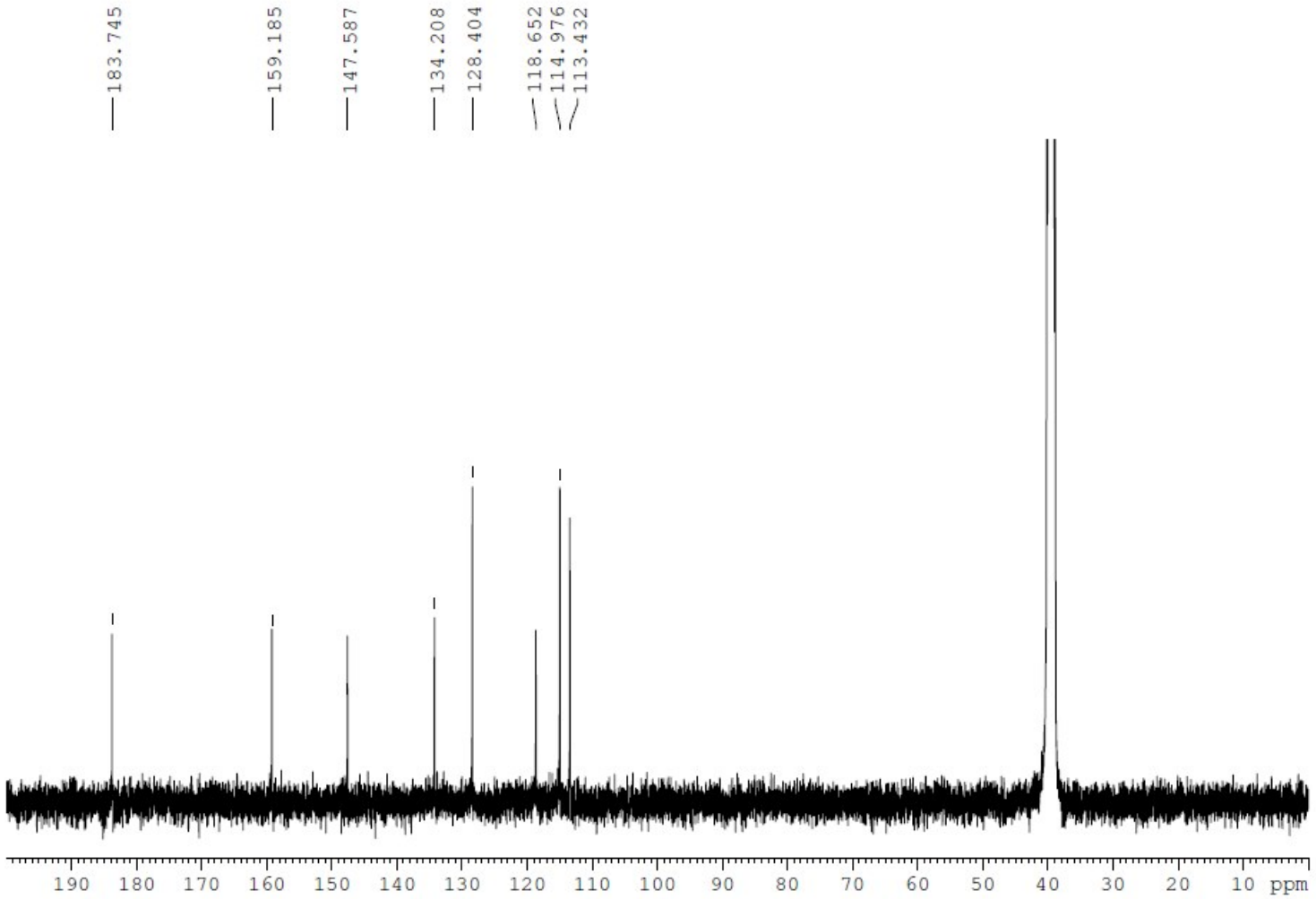


**Figure SI3** $^{13}C$ NMR spectrum of 5-azidoisatin (**6**) in DMSO-$D_6$, full view.

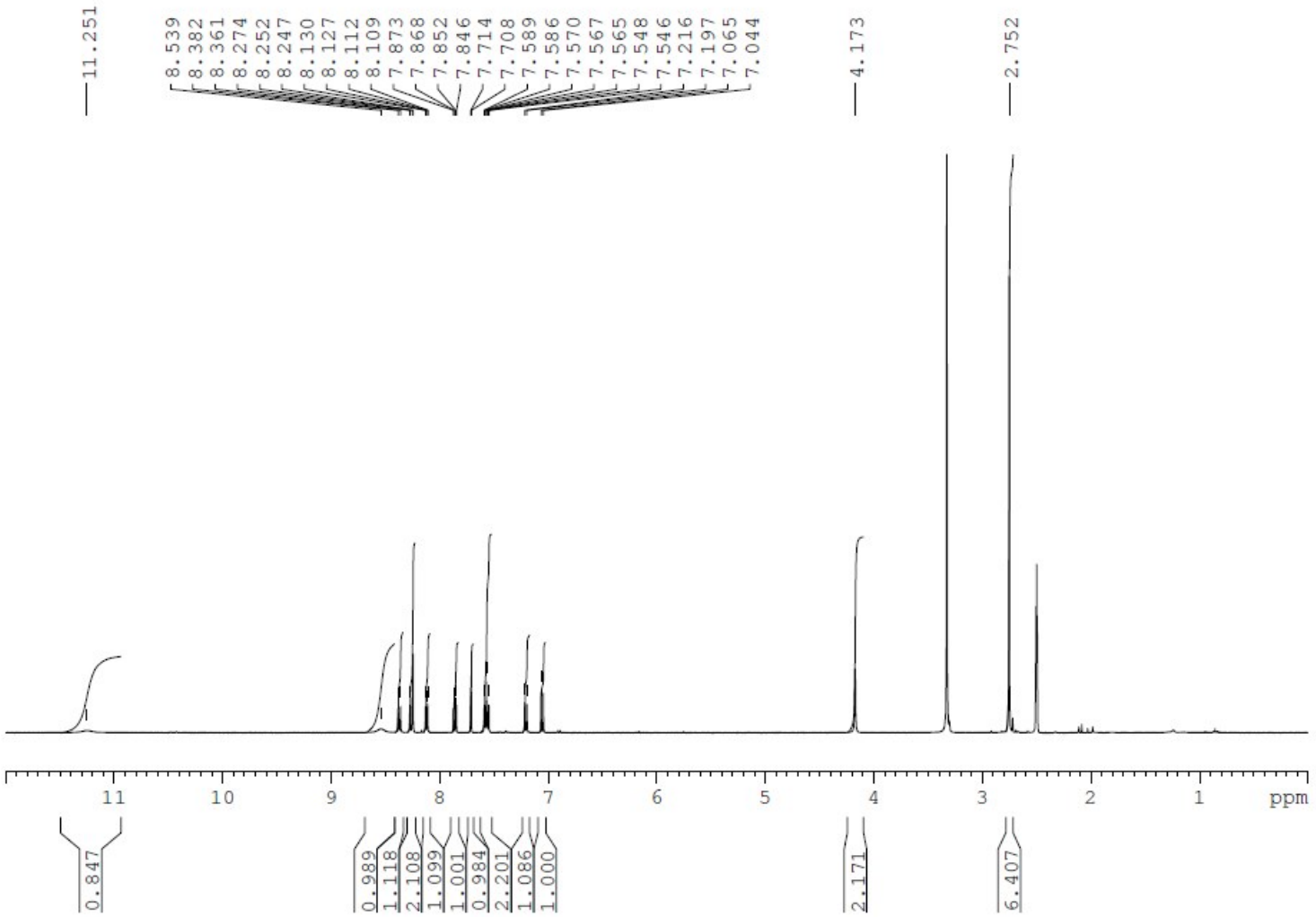


**Figure SI4** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, full view.

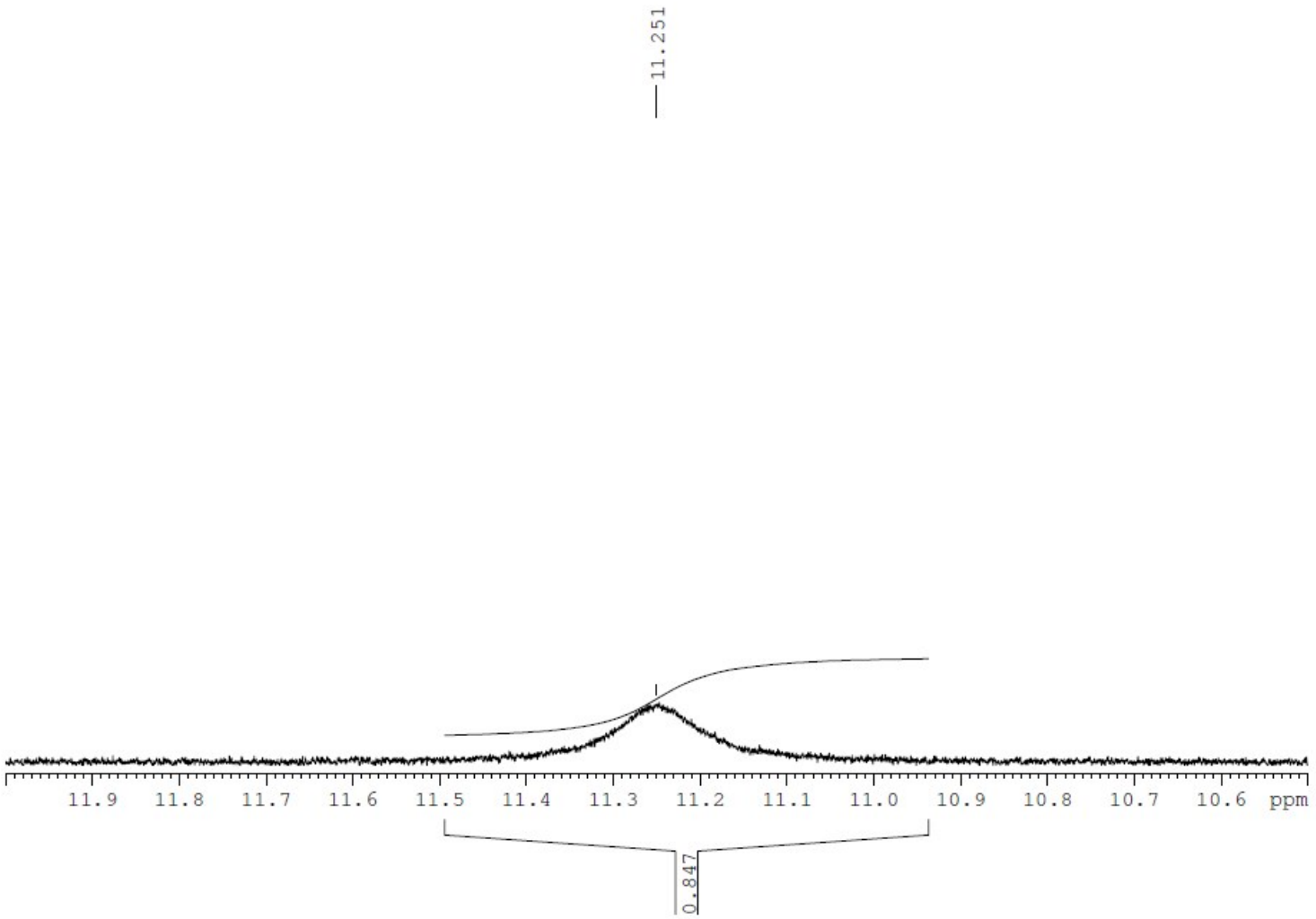


**Figure SI5** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, expanded view 1.

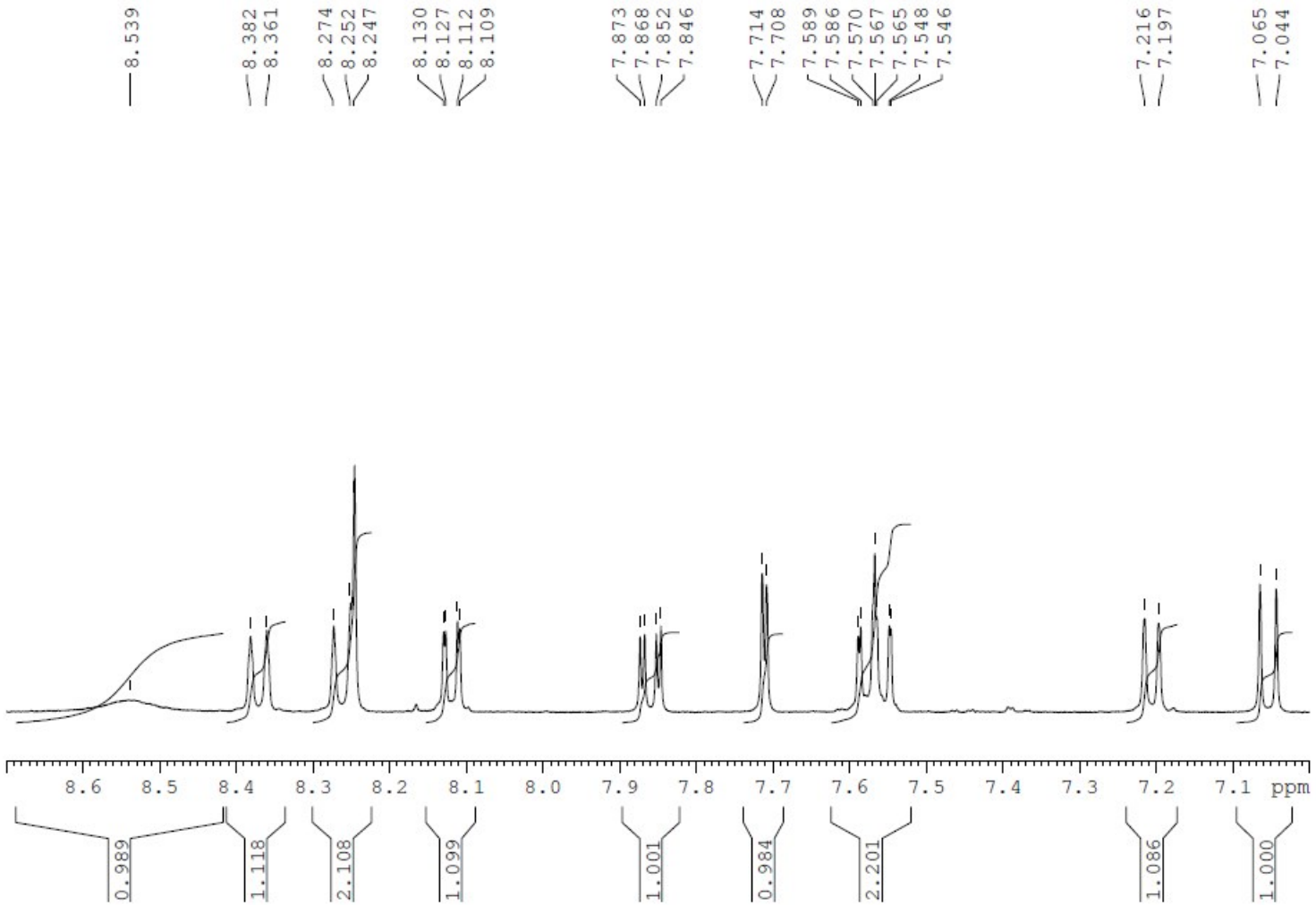


**Figure SI6** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, expanded view 2.

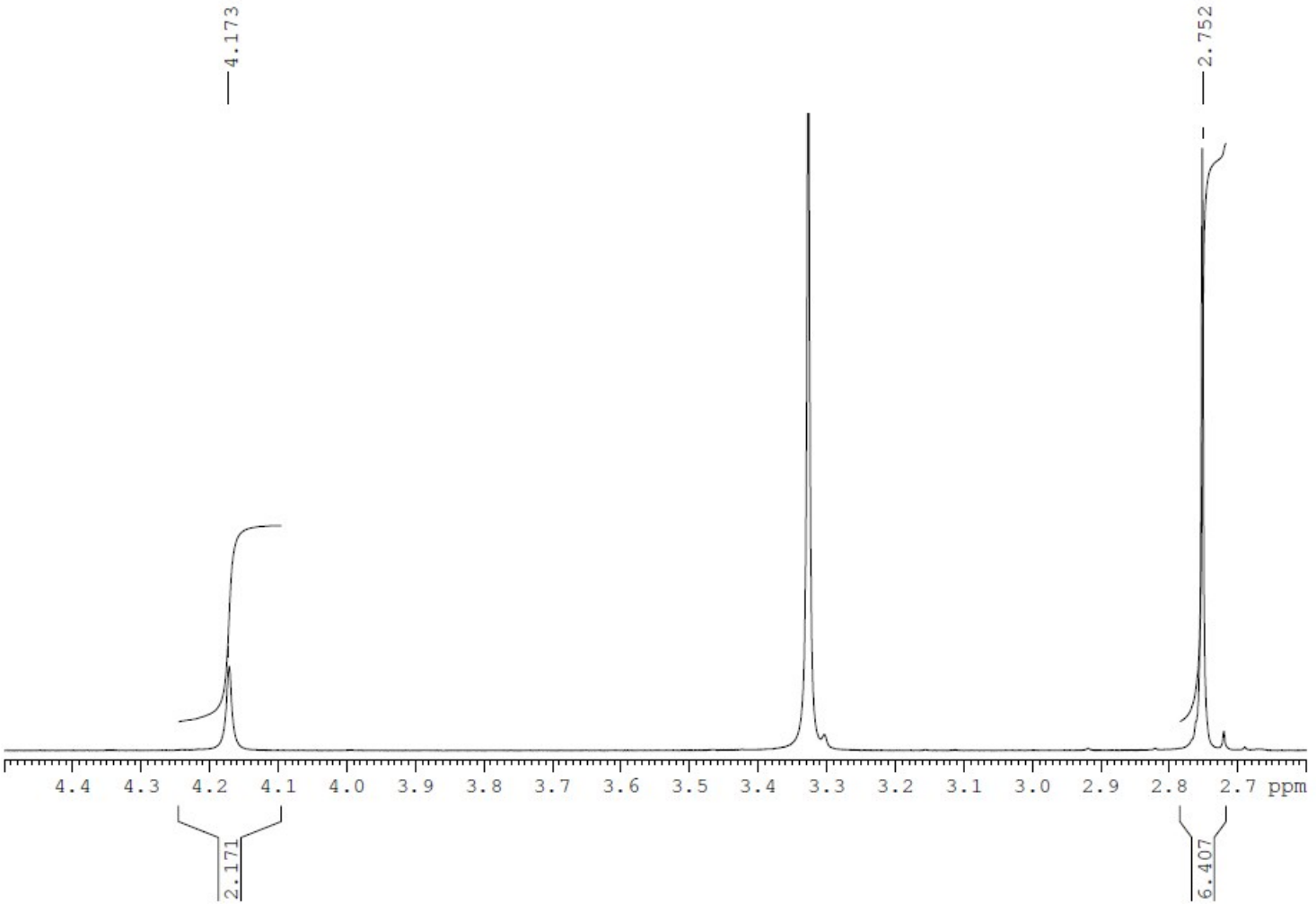


**Figure SI7** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, expanded view 3.

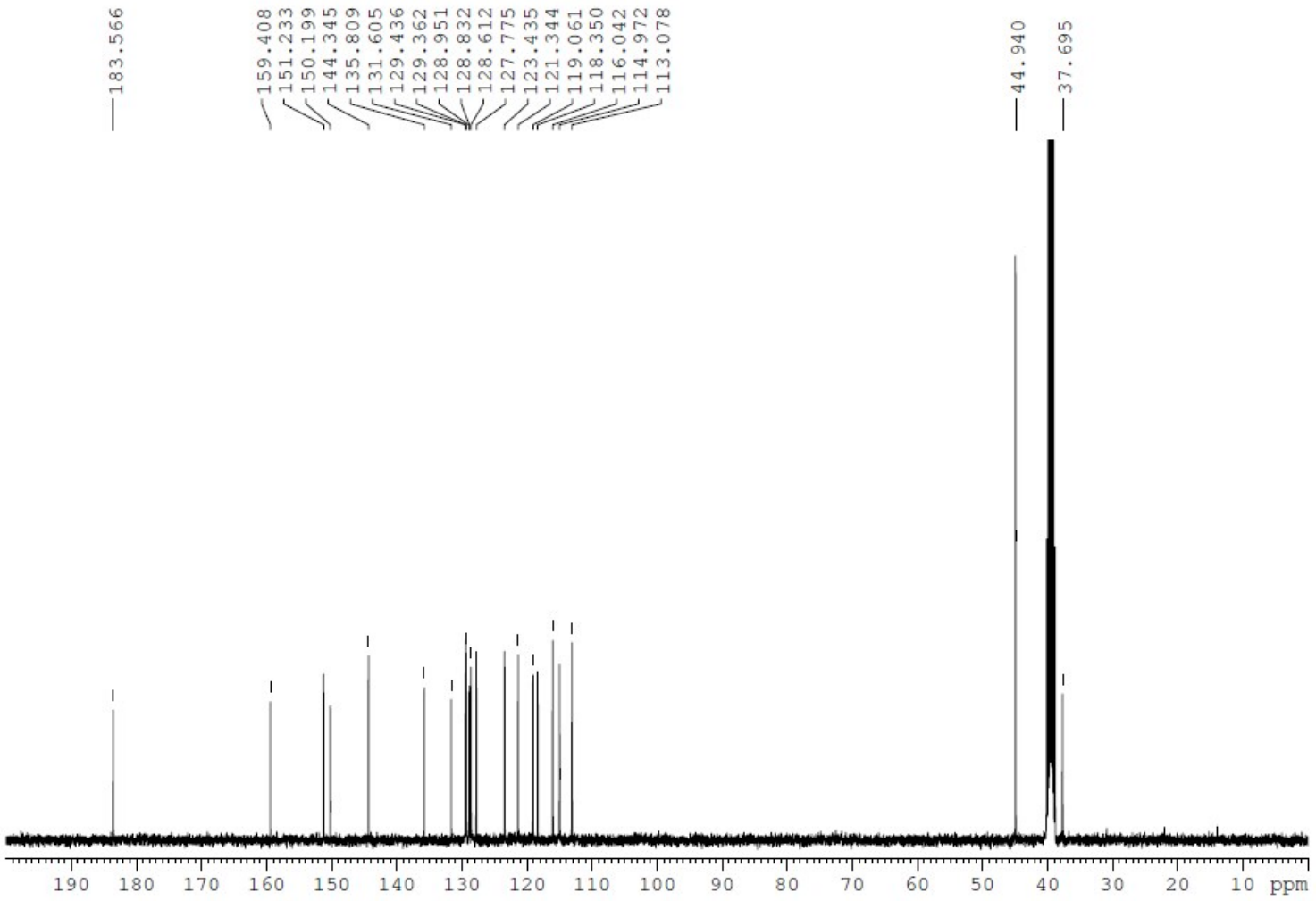


**Figure SI8** $^{13}$C NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, full view.

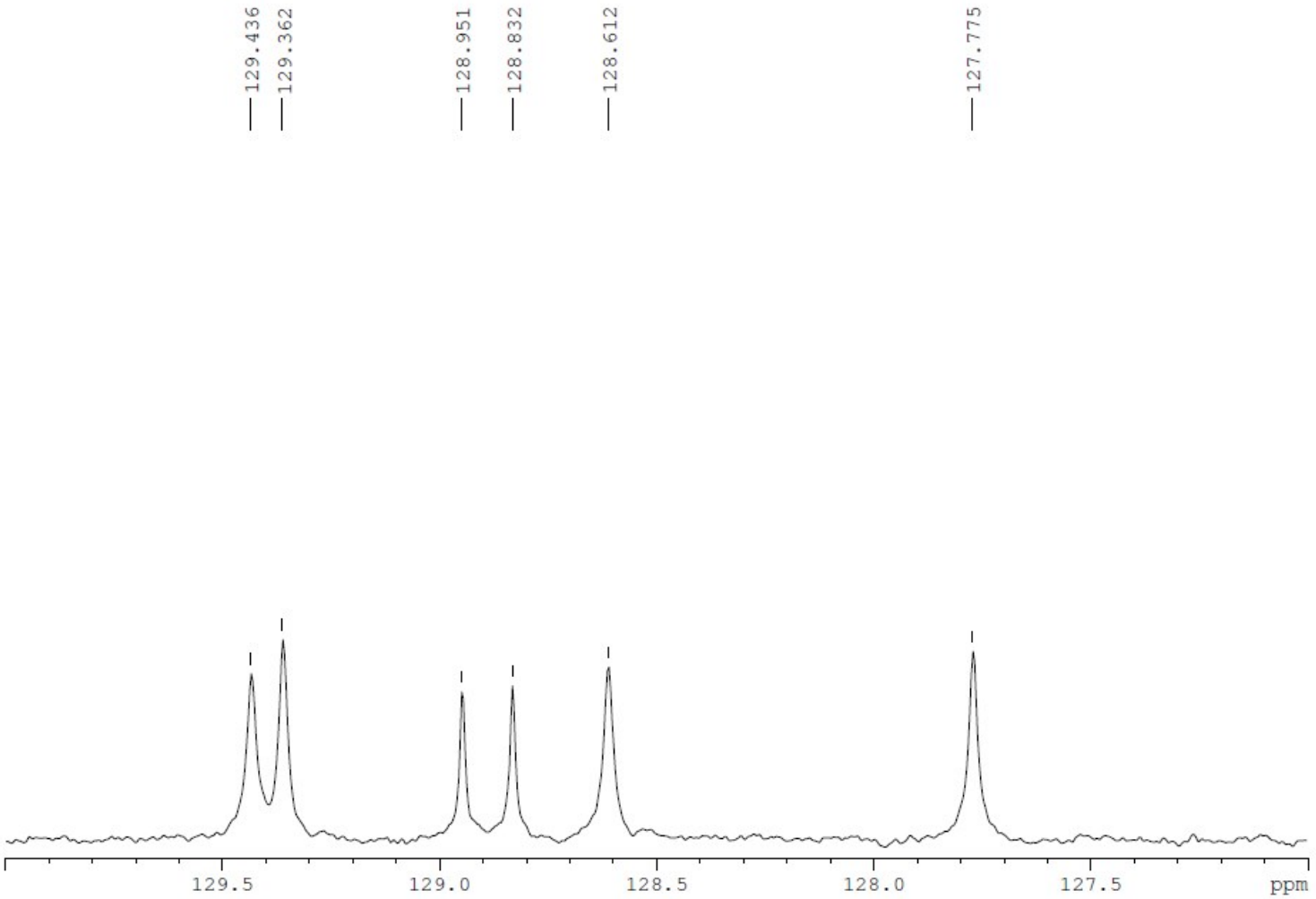


**Figure SI9** $^{13}$C NMR spectrum of 5-(*N*-dansyl-clicked) isatin **4** in DMSO-$D_6$, expanded view.

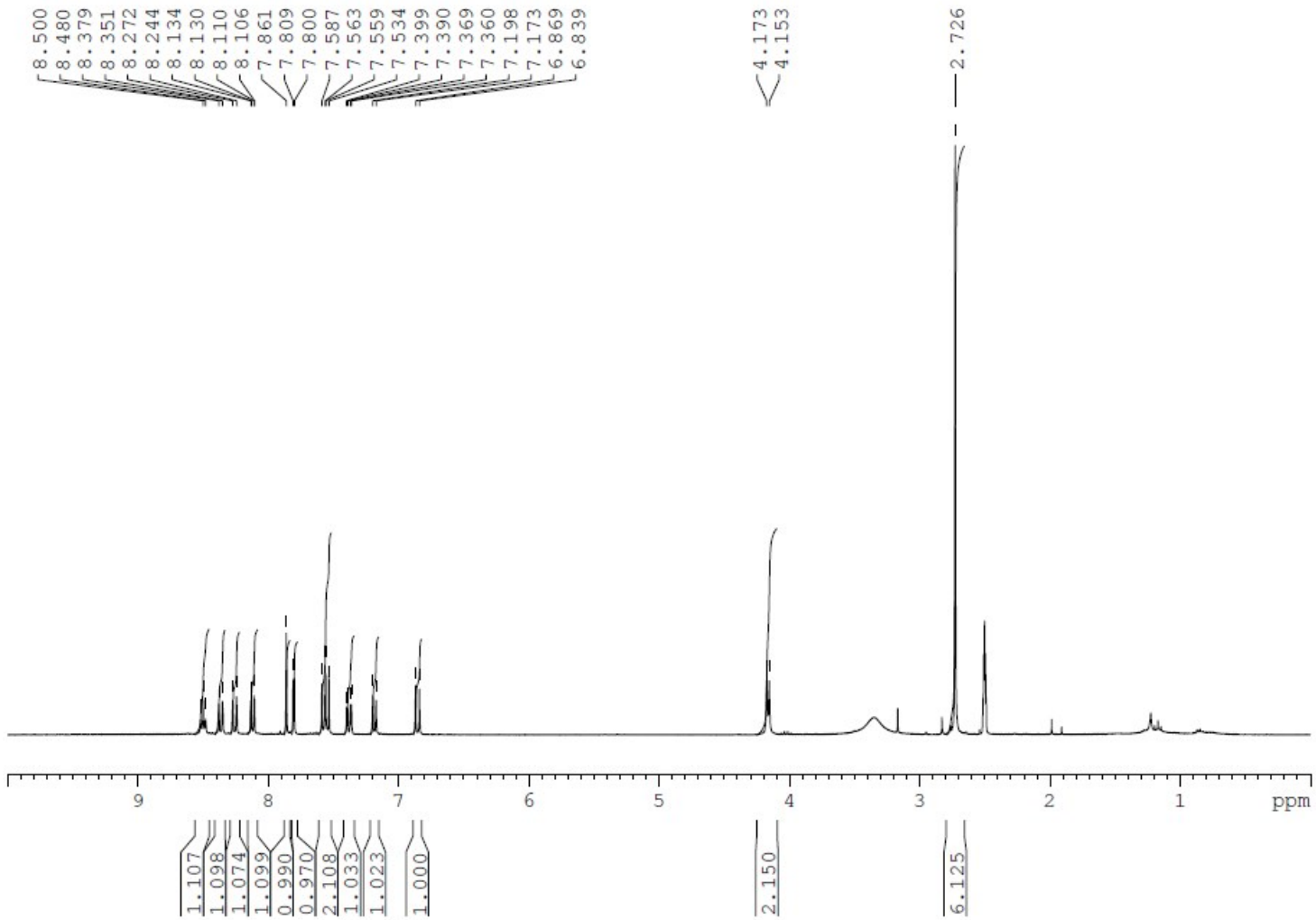


**Figure SI10** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, full view.

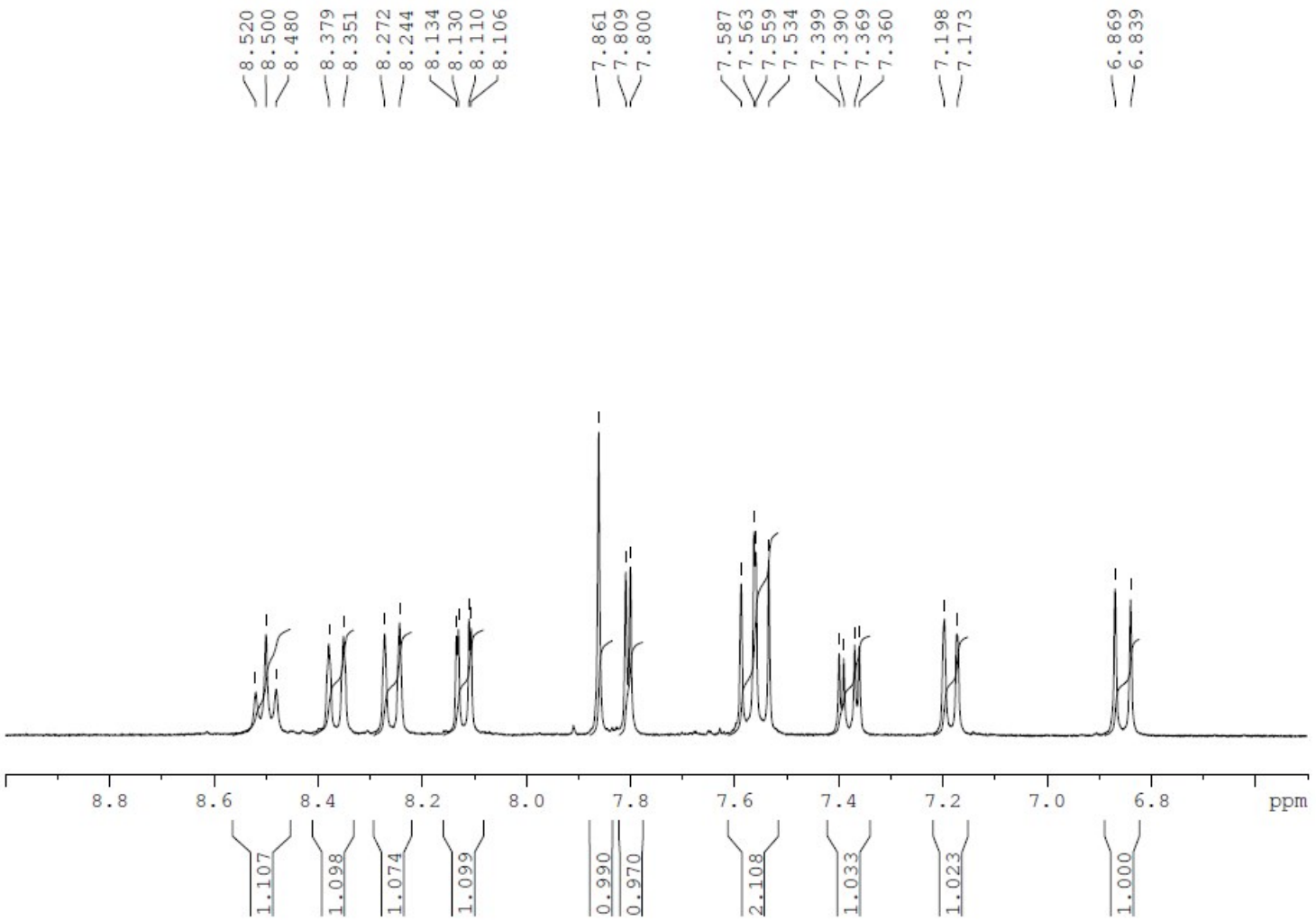


**Figure SI11** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, expanded view 1.

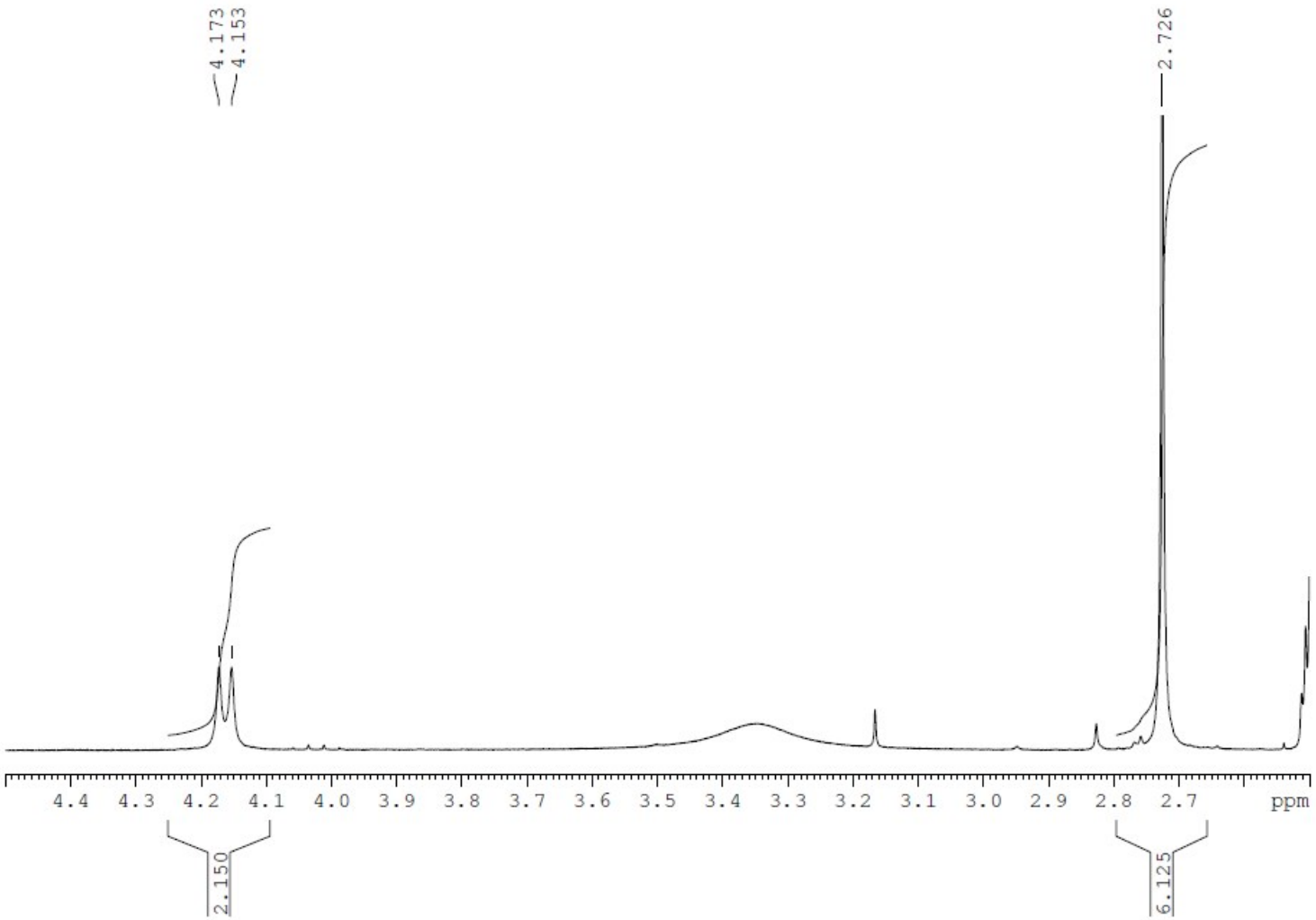


**Figure SI12** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, expanded view 2.

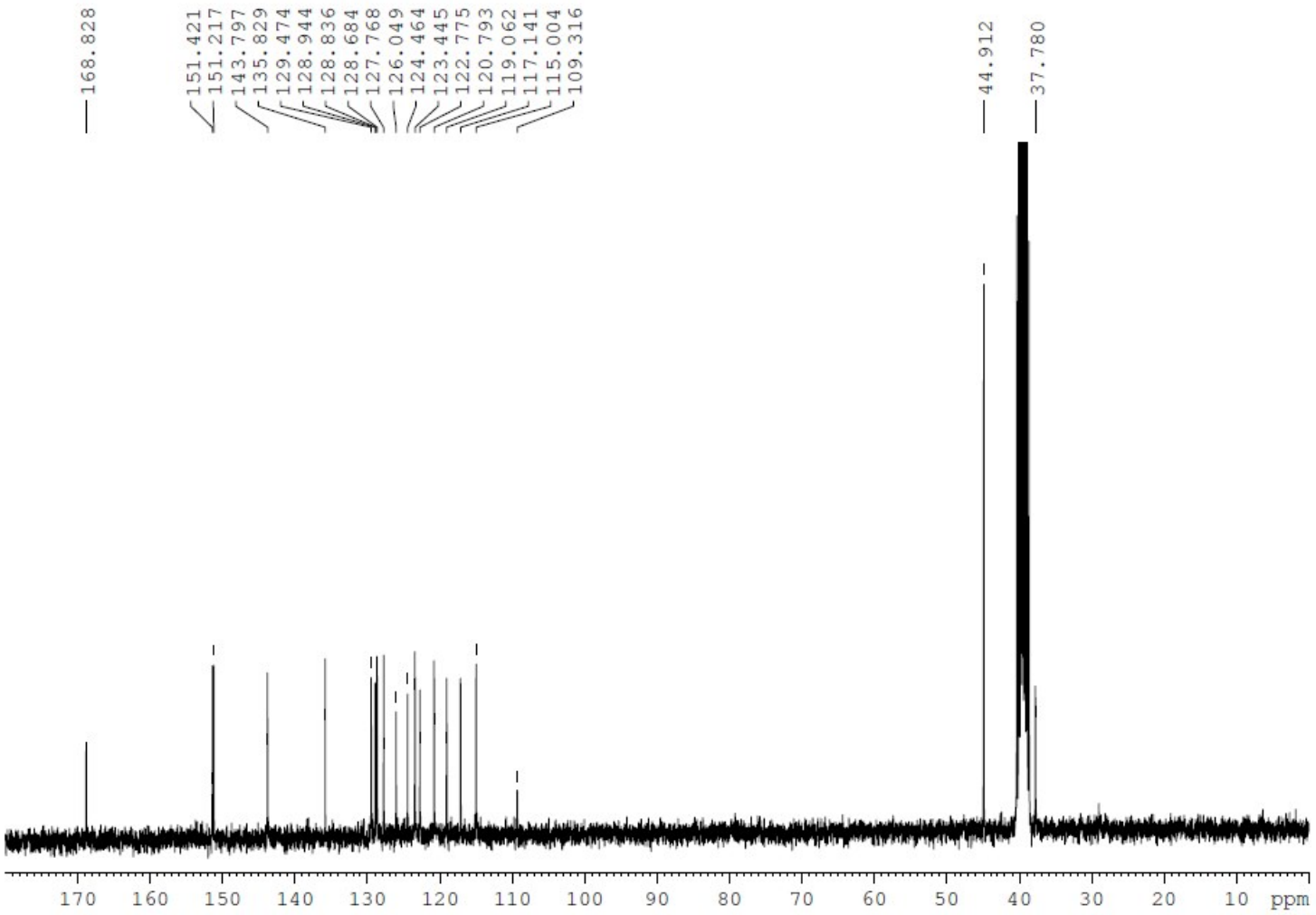


**Figure SI13** $^{13}C$ NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, full view.

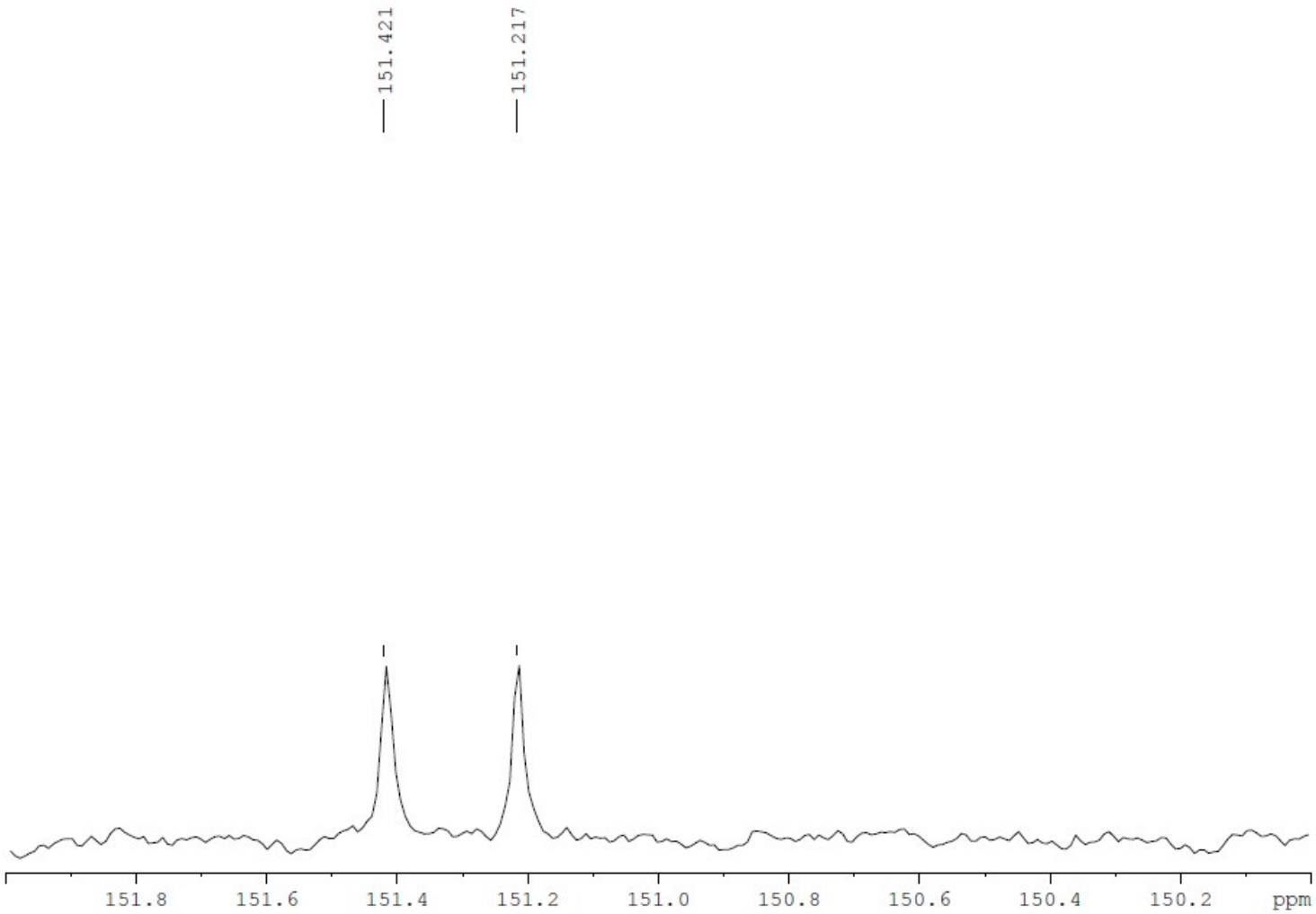


**Figure SI14** $^{13}$C NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, expanded view 1.

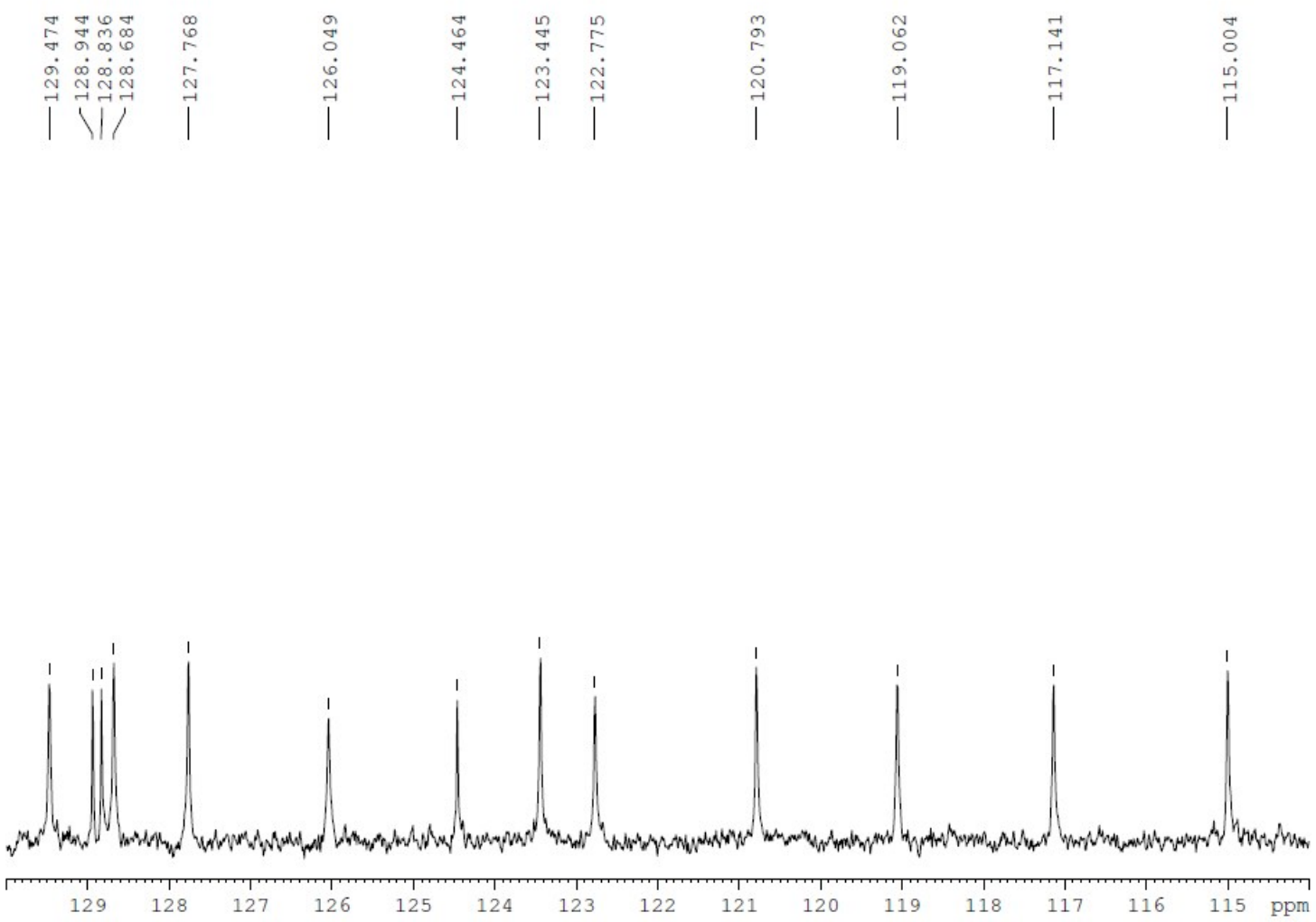


**Figure SI15** $^{13}$C NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, expanded view 2.

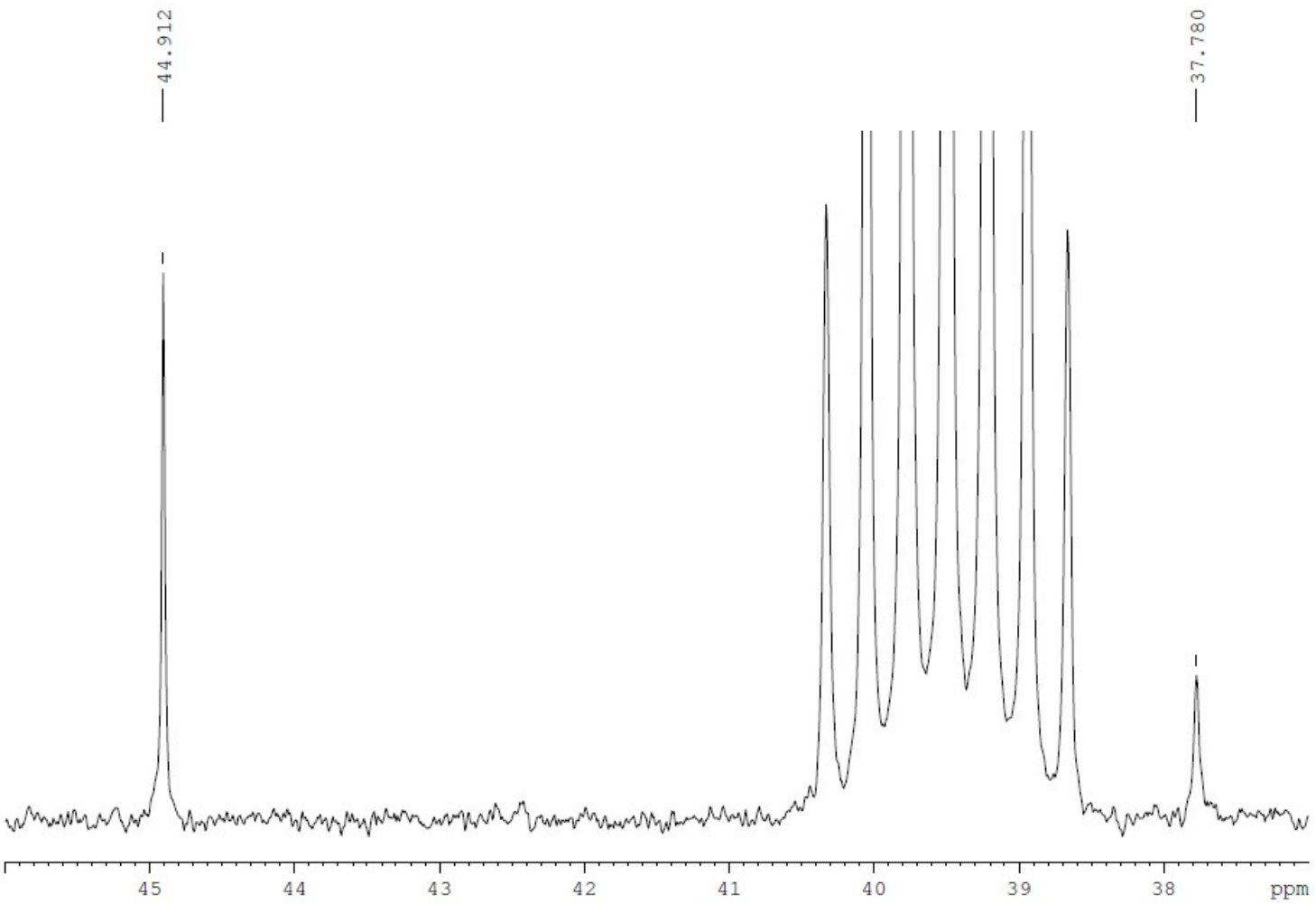


**Figure SI16** $^{13}$C NMR spectrum of 5-(*N*-dansyl-clicked) anthranilic acid **3** in DMSO-$D_6$, expanded view 3.

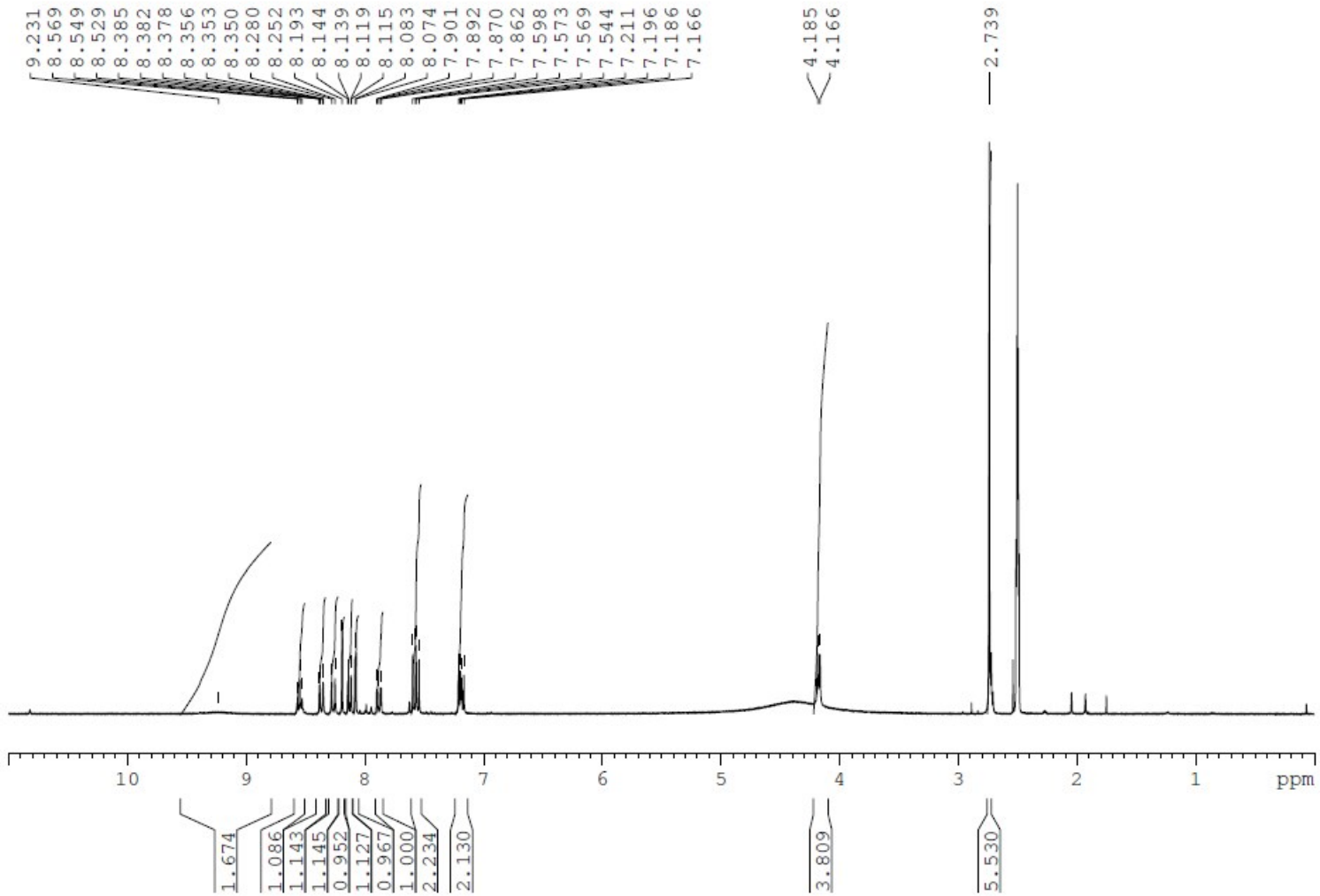


**Figure SI17** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) *N*-aminoanthranilic acid **1** in DMSO-$D_6$, full view.

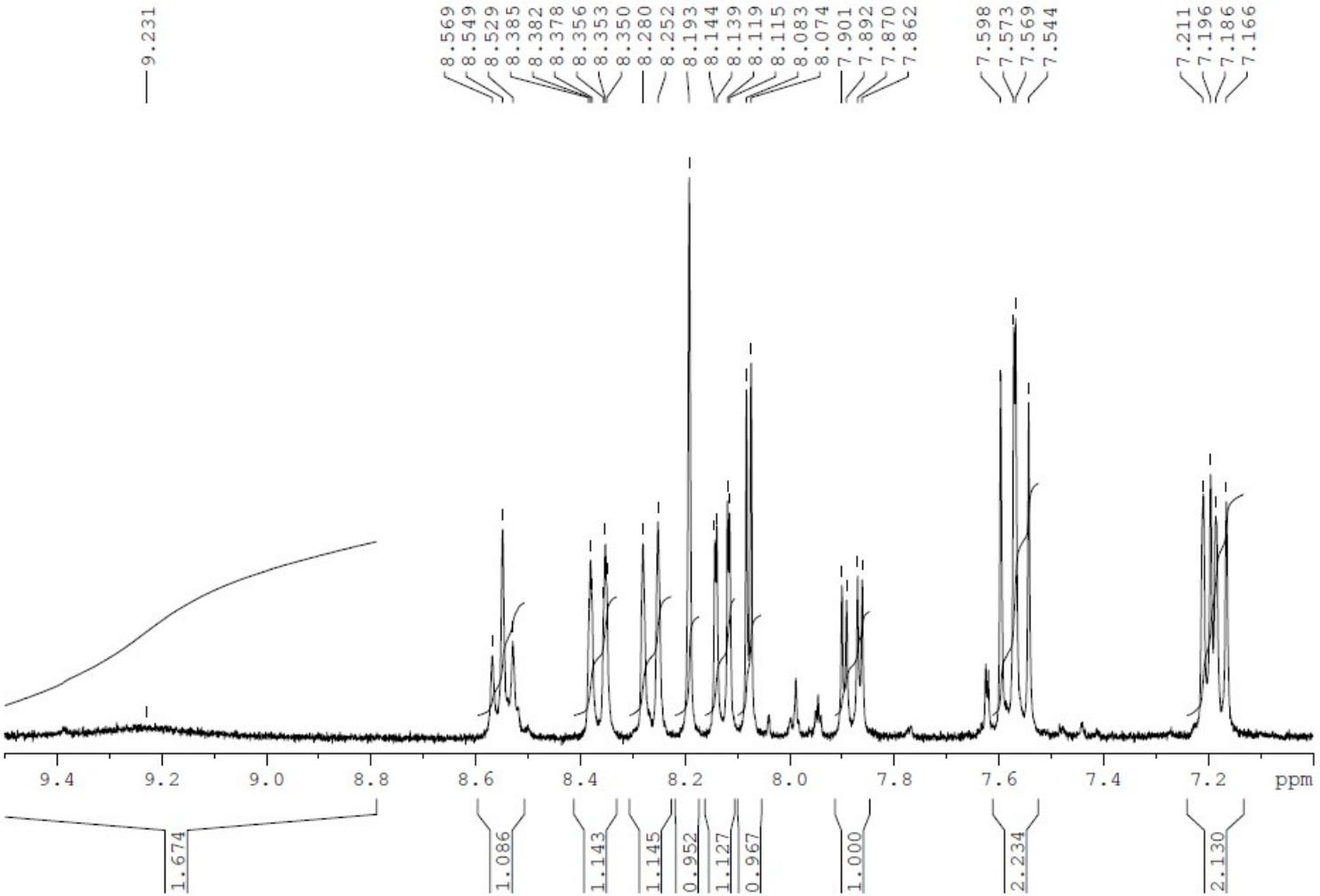


**Figure SI18** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) *N*-aminoanthranilic acid **1** in DMSO-$D_6$, expanded view 1.

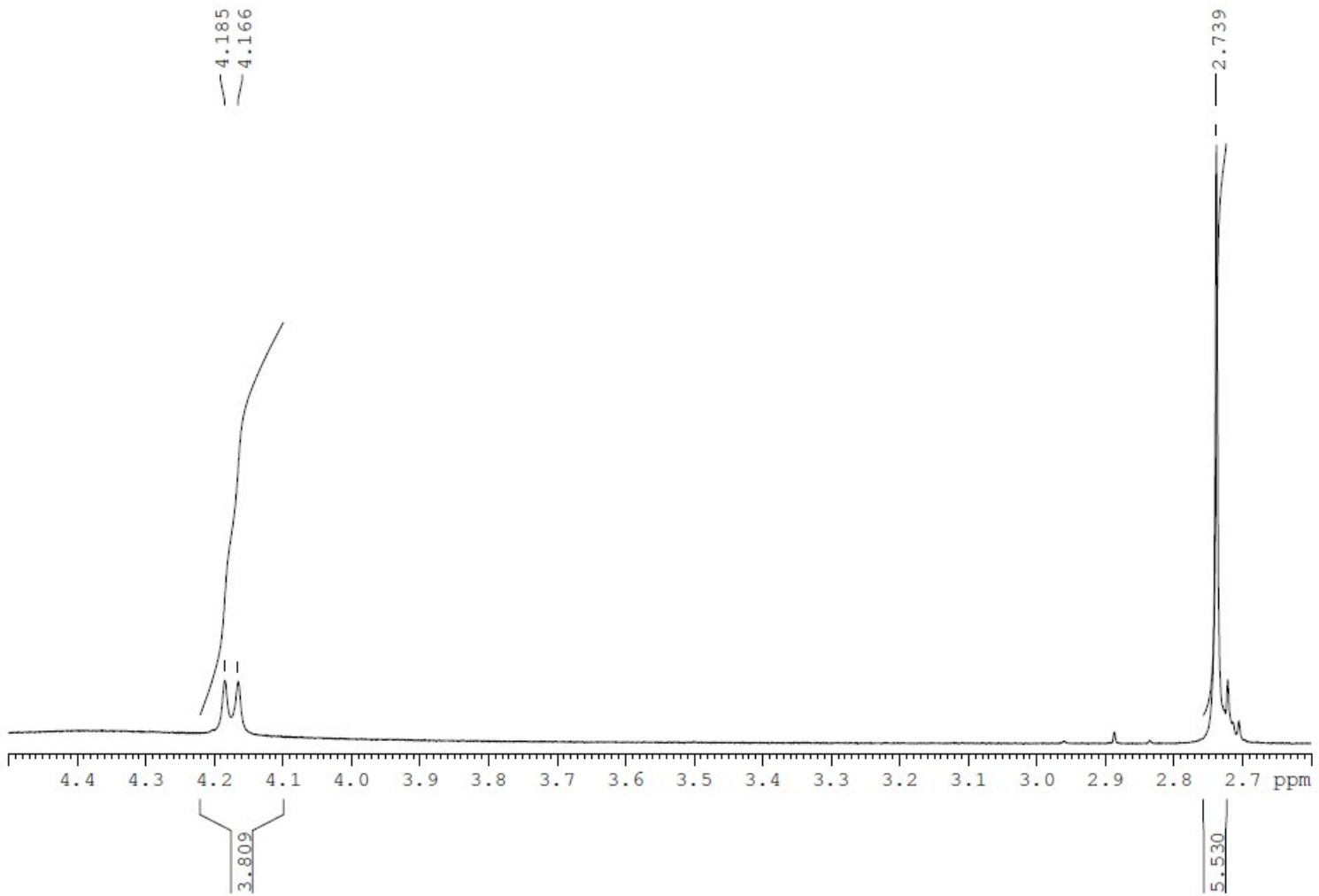


**Figure SI19** $^{1}$H NMR spectrum of 5-(*N*-dansyl-clicked) *N*-aminoanthranilic acid **1** in DMSO-$D_6$, expanded view 2.

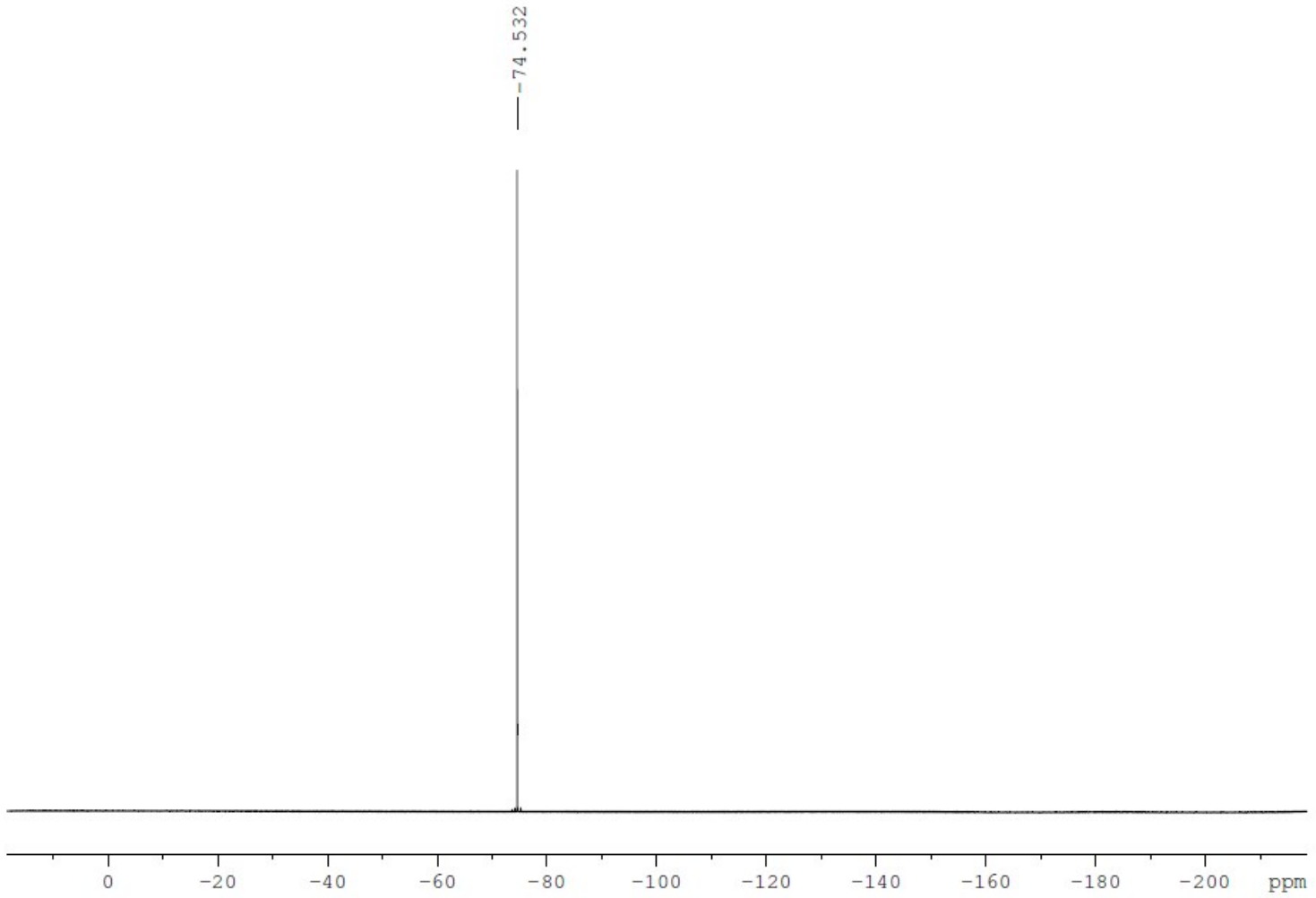


**Figure SI20** $^{19}$F NMR spectrum of 5-(*N*-dansyl-clicked) *N*-aminoanthranilic acid **1** in DMSO-$D_6$, full view

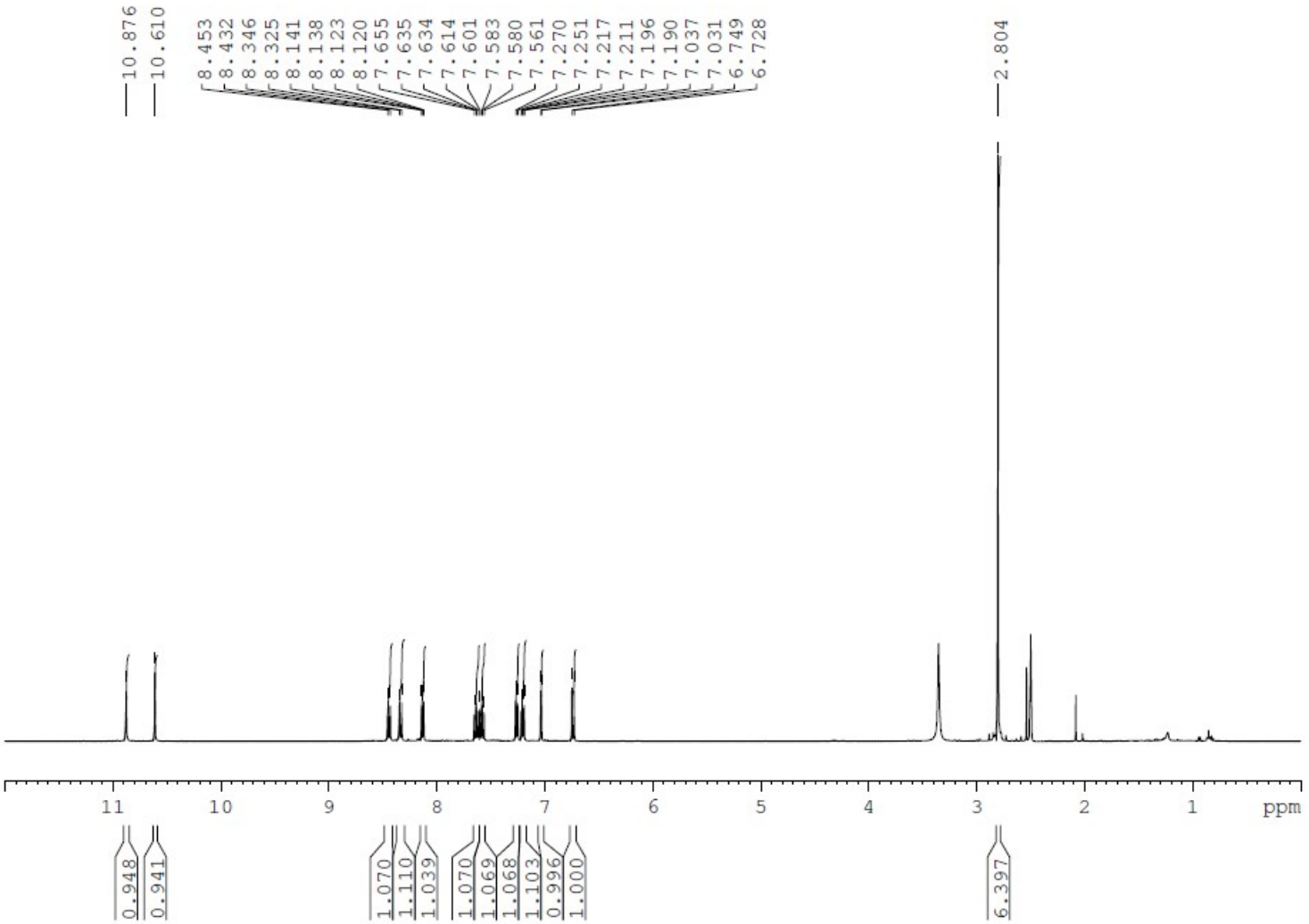


**Figure SI21** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-isatin (**7**) in DMSO-$D_6$, full view.

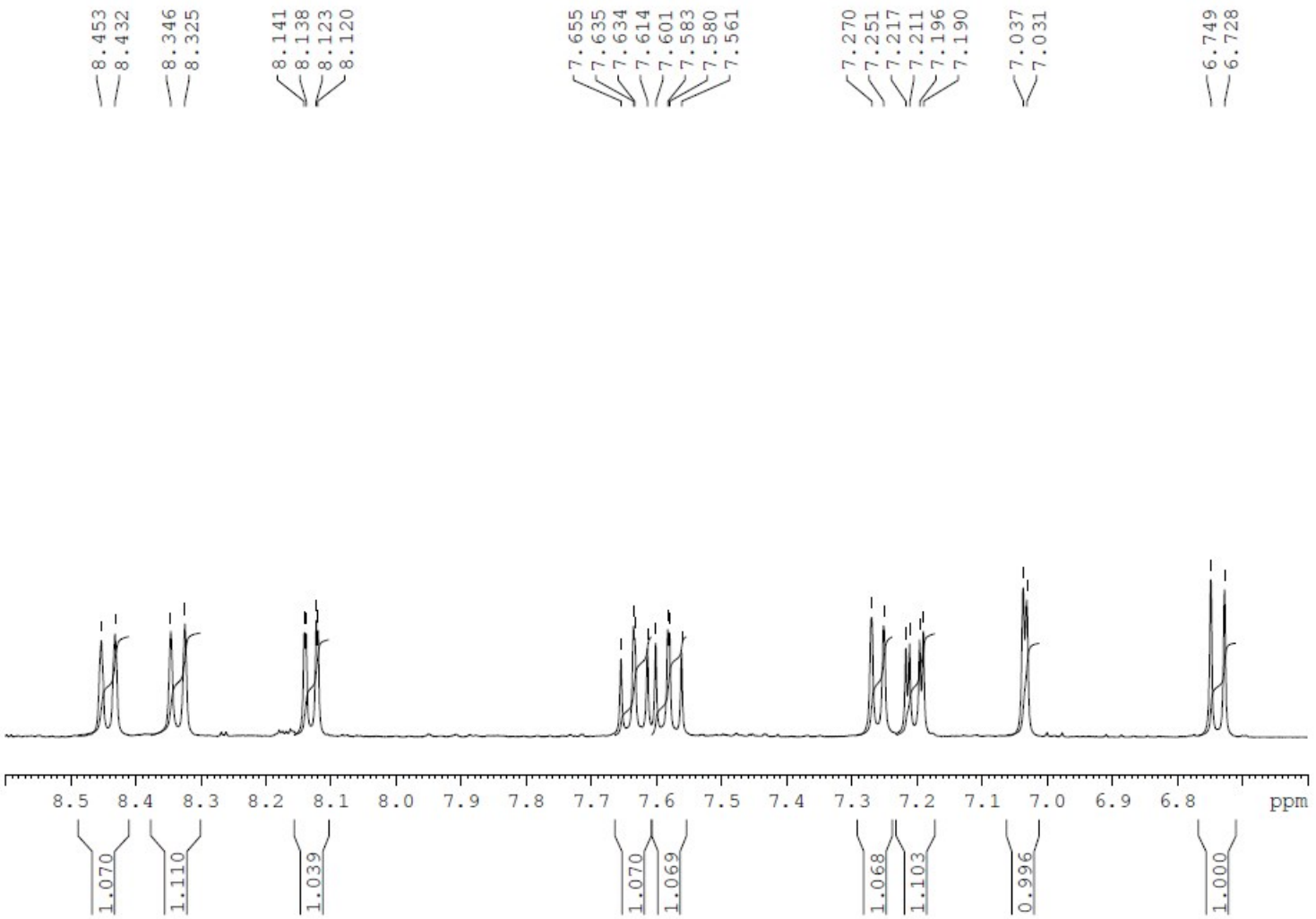


**Figure SI22** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-isatin (**7**) in DMSO-$D_6$, expanded view.

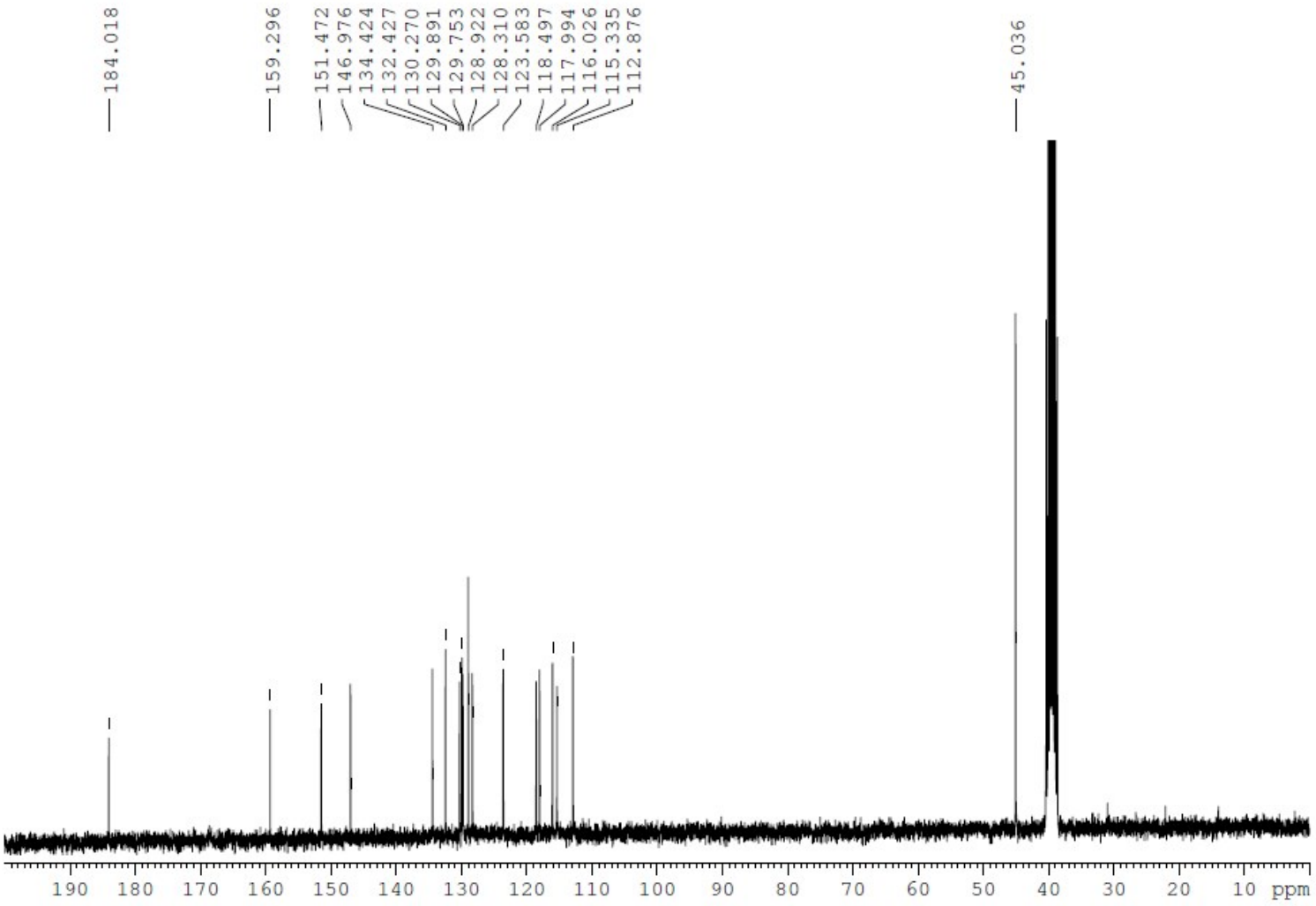


**Figure SI23** $^{13}C$ NMR spectrum of 5-(*N*-dansylamino)-isatin (**7**) in DMSO-$D_6$, full view.

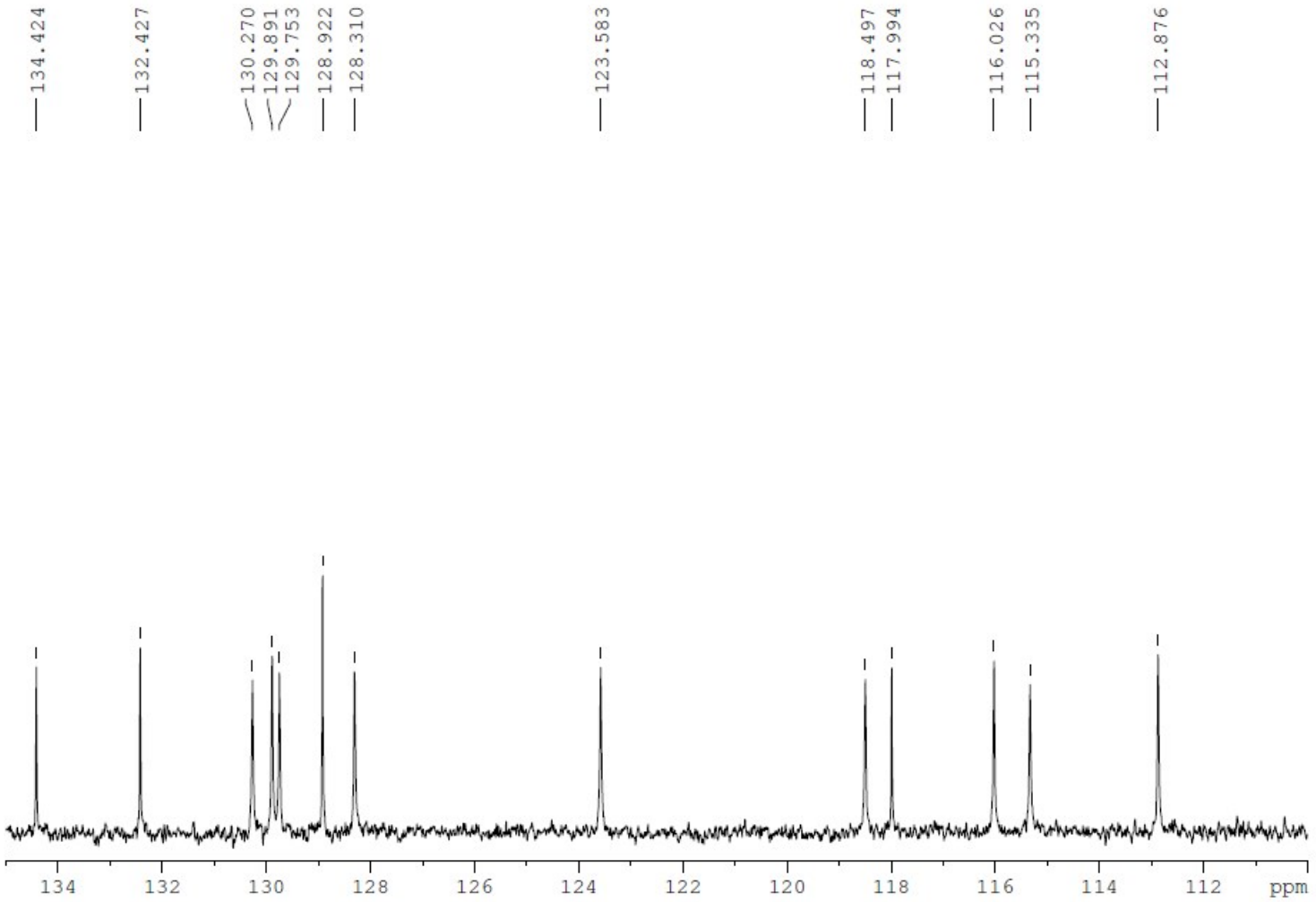


**Figure SI24** $^{13}$C NMR spectrum of 5-(*N*-dansylamino)-isatin (**7**) in DMSO-$D_6$, expanded view.

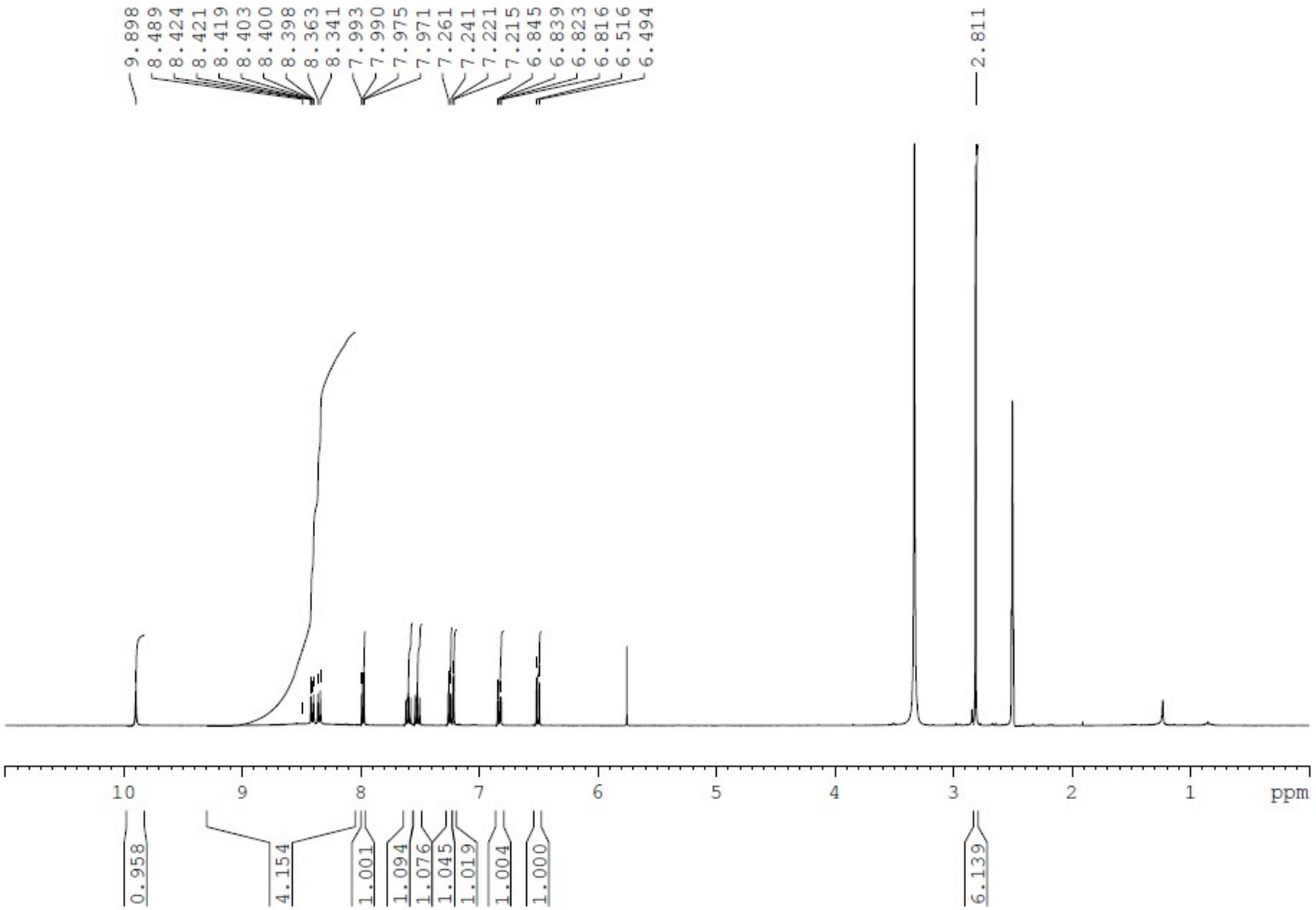


**Figure SI25** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-anthranilic acid (**14**) in DMSO-$D_6$, full view. Minor signal at 5.75 ppm is associated with a small amount of dichloromethane in the sample.

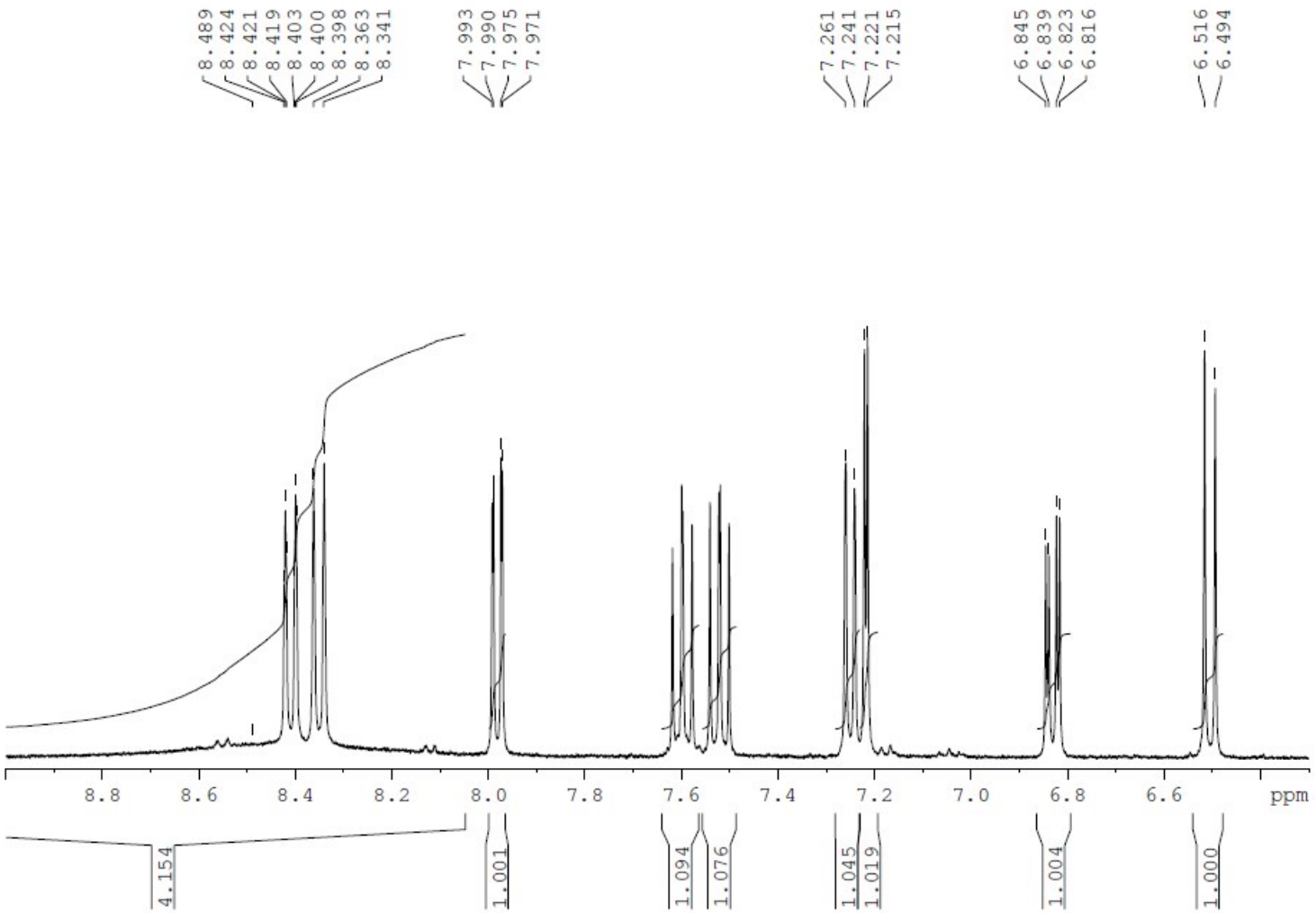


**Figure SI26** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-anthranilic acid (**14**) in DMSO-$D_6$, expanded view.

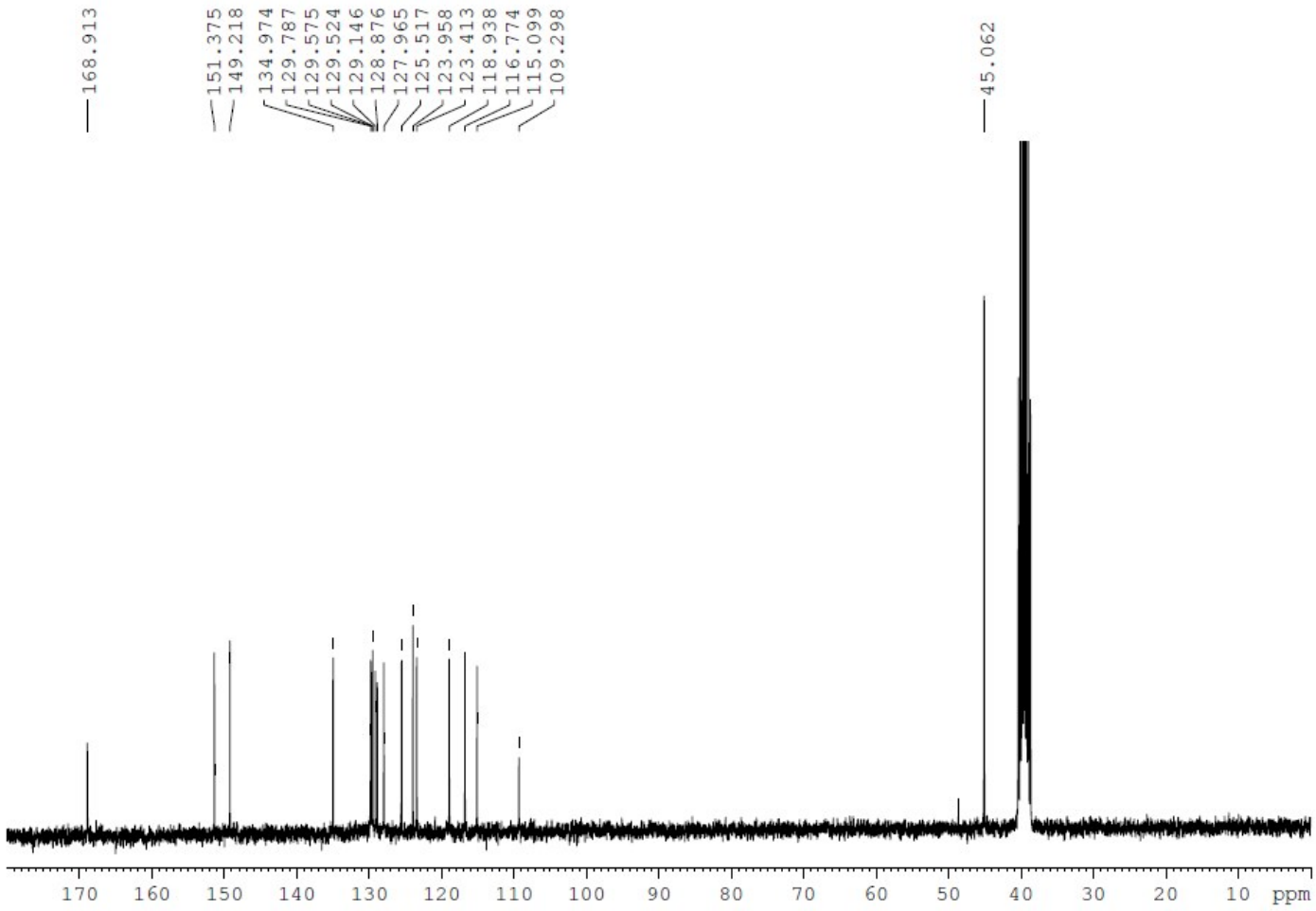


**Figure SI27** $^{13}$C NMR spectrum of 5-(*N*-dansylamino)-anthranilic acid (**14**) in DMSO-$D_6$, full view. Minor signal at 48.5 ppm is associated with a small amount of methanol in the sample.

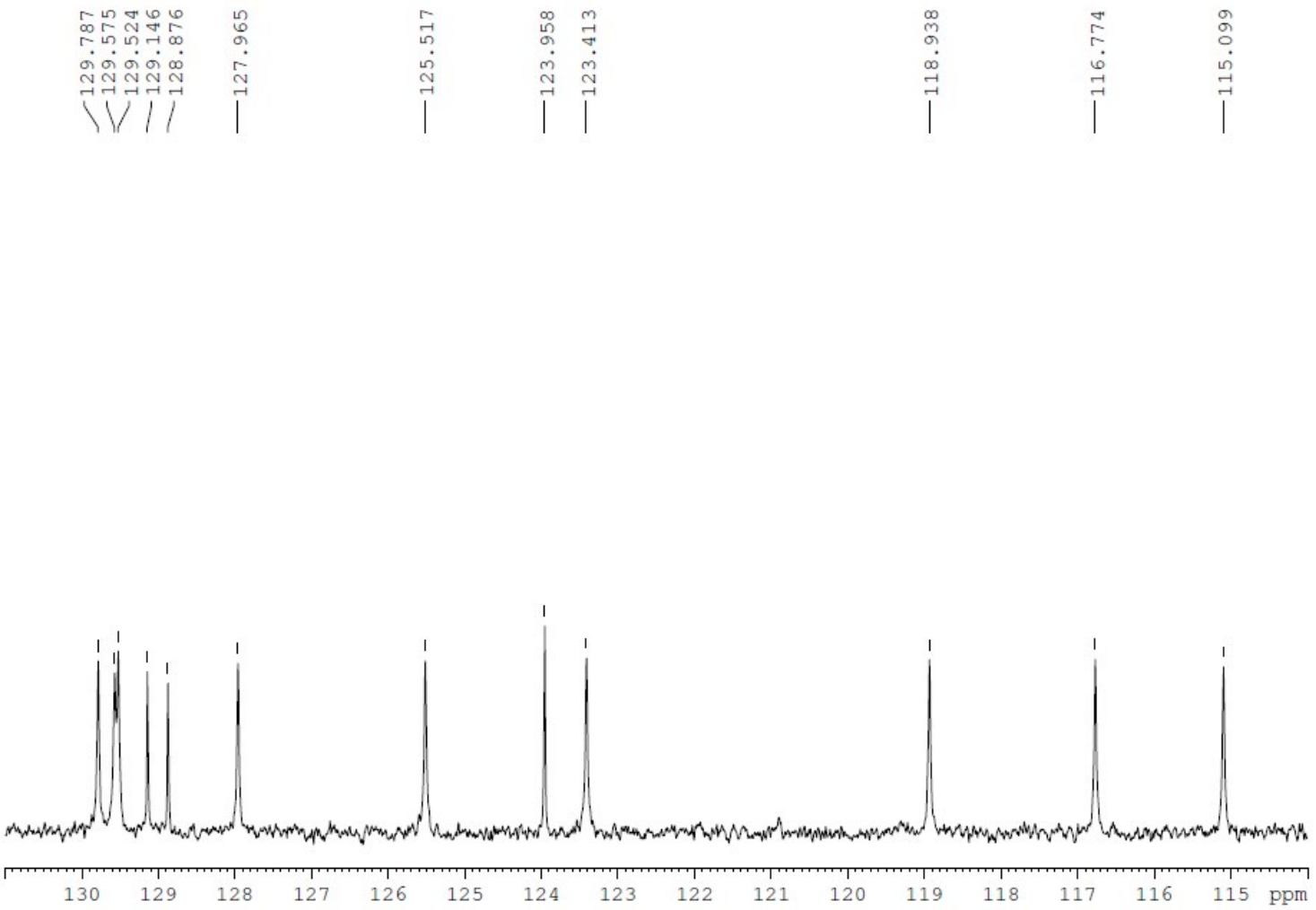


**Figure SI28** $^{13}$C NMR spectrum of 5-(*N*-dansylamino)-anthranilic acid (**14**) in DMSO-$D_6$, expanded view.

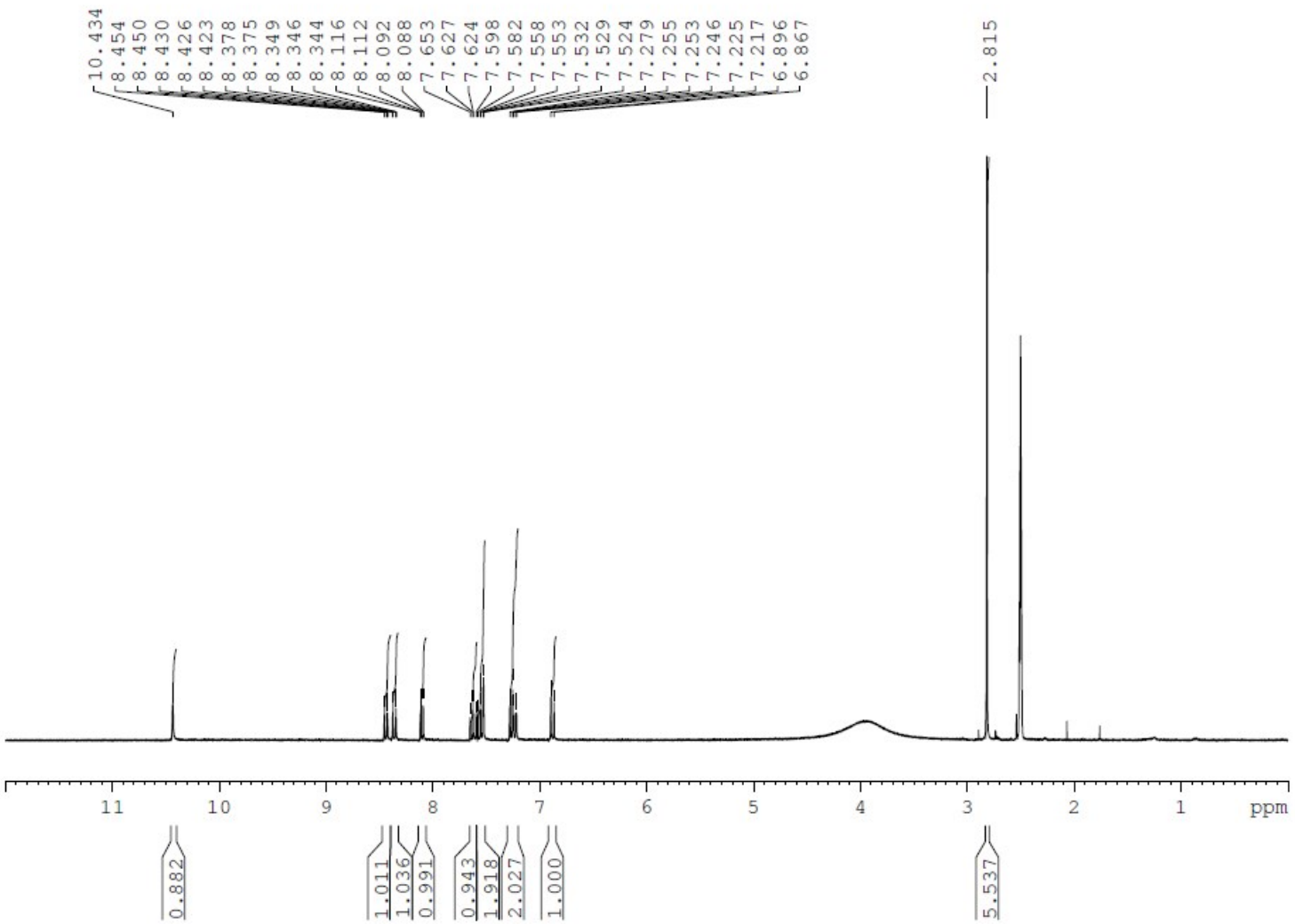


**Figure SI29** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in DMSO-$D_6$, full view.

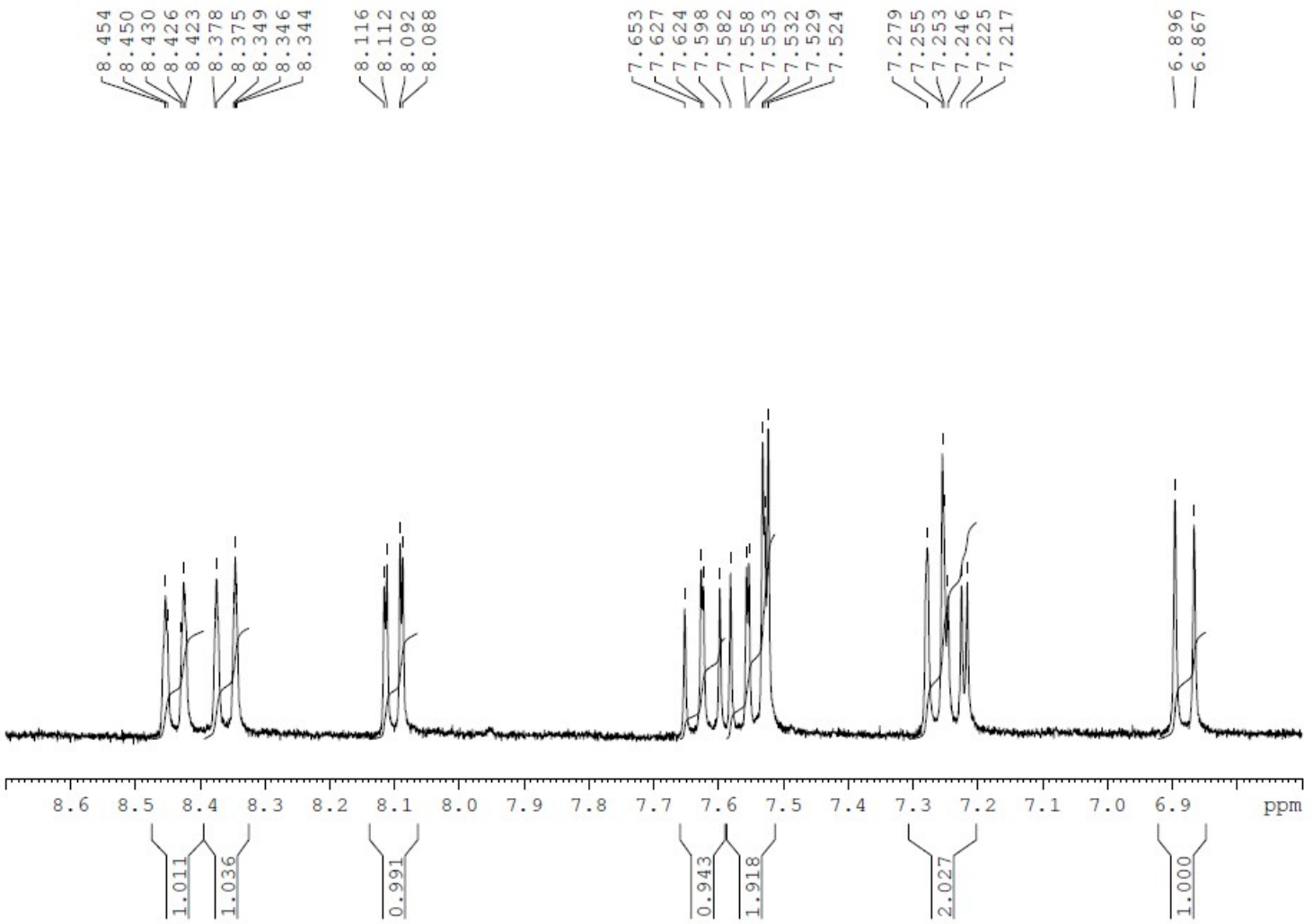


**Figure SI30** $^{1}$H NMR spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in DMSO-$D_6$, expanded view.

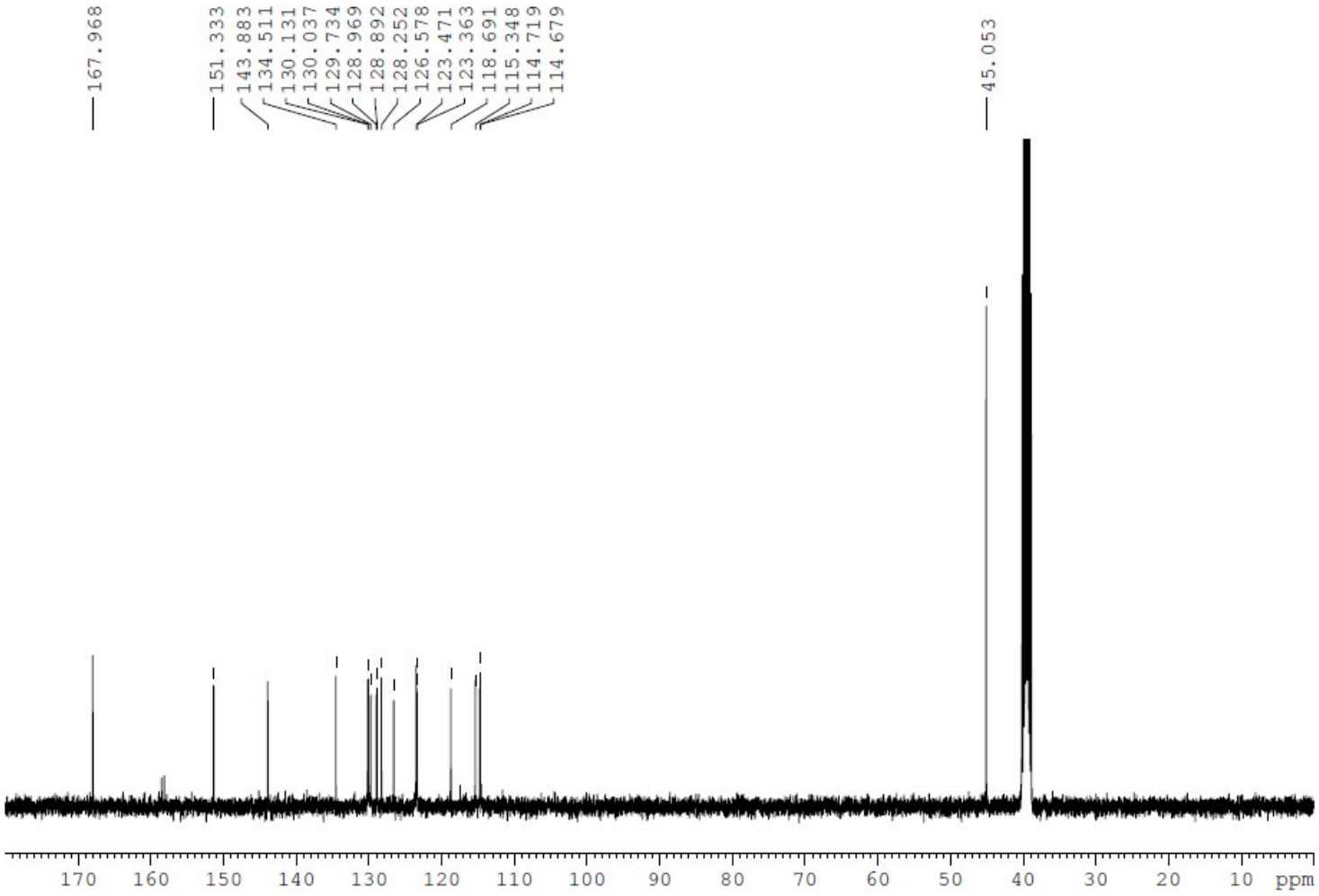


**Figure SI31** $^{13}$C NMR spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in DMSO-$D_6$, full view.

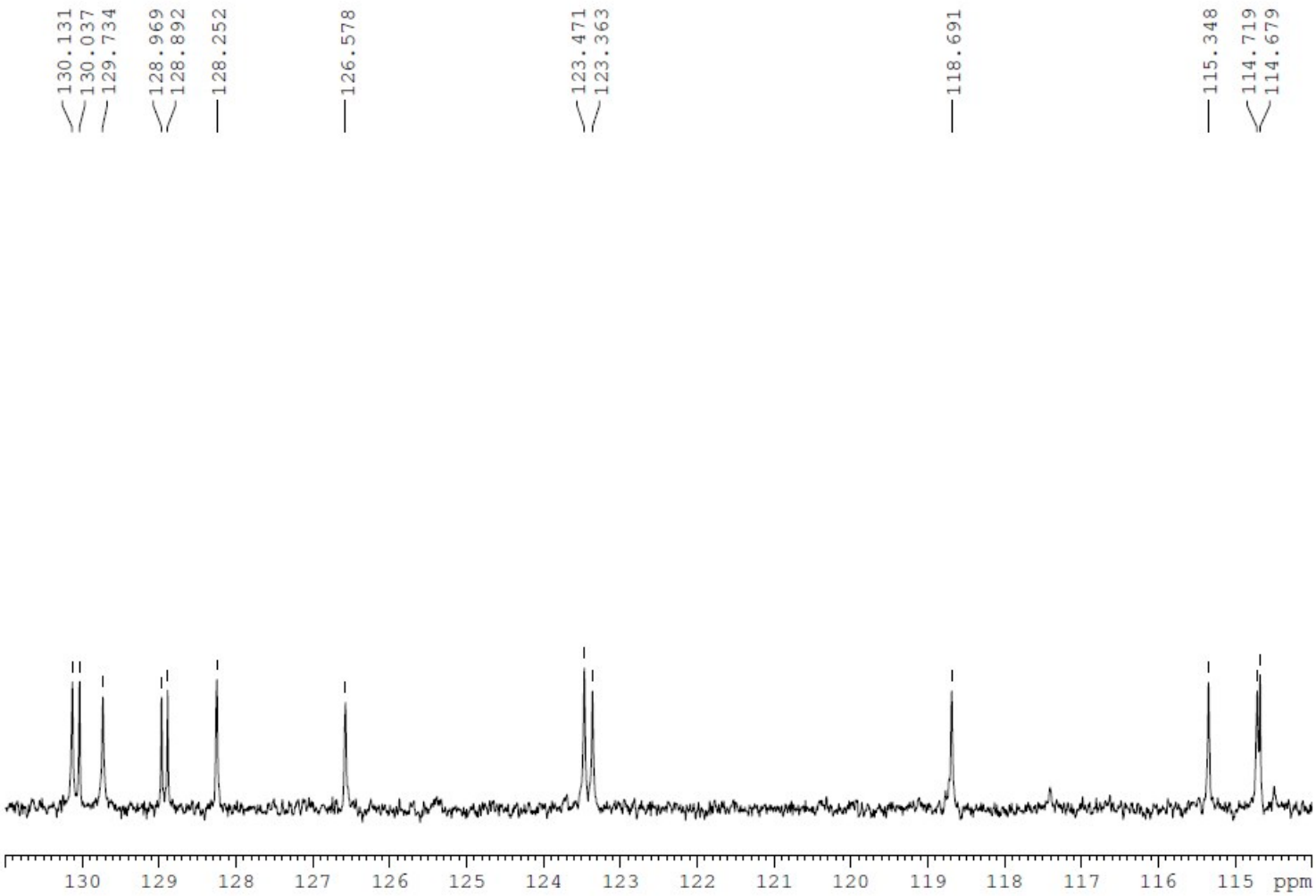


**Figure SI32** $^{13}$C NMR spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in DMSO-$D_6$, expanded view.

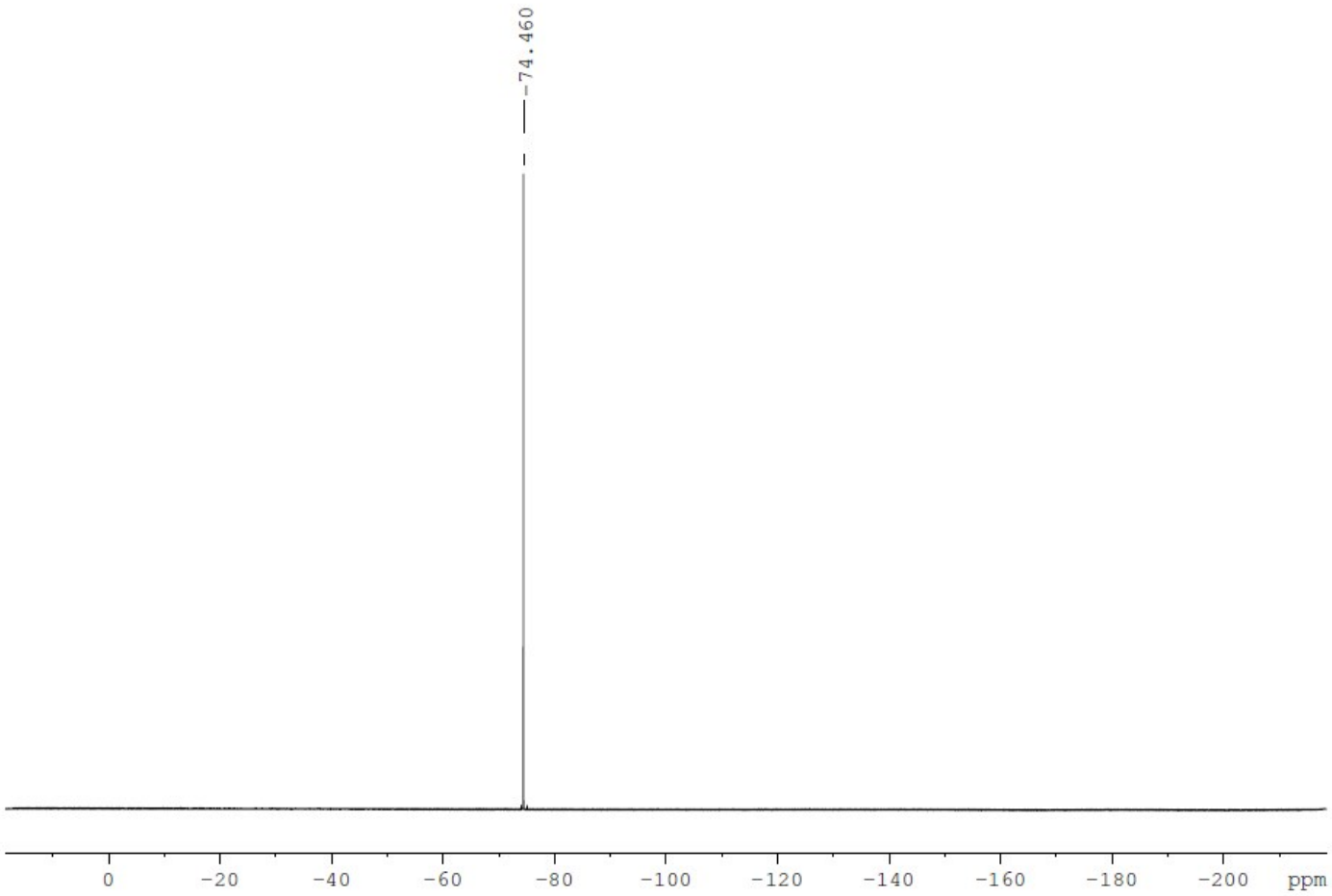


**Figure SI33** $^{19}$F NMR spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in DMSO-$D_6$, full view.

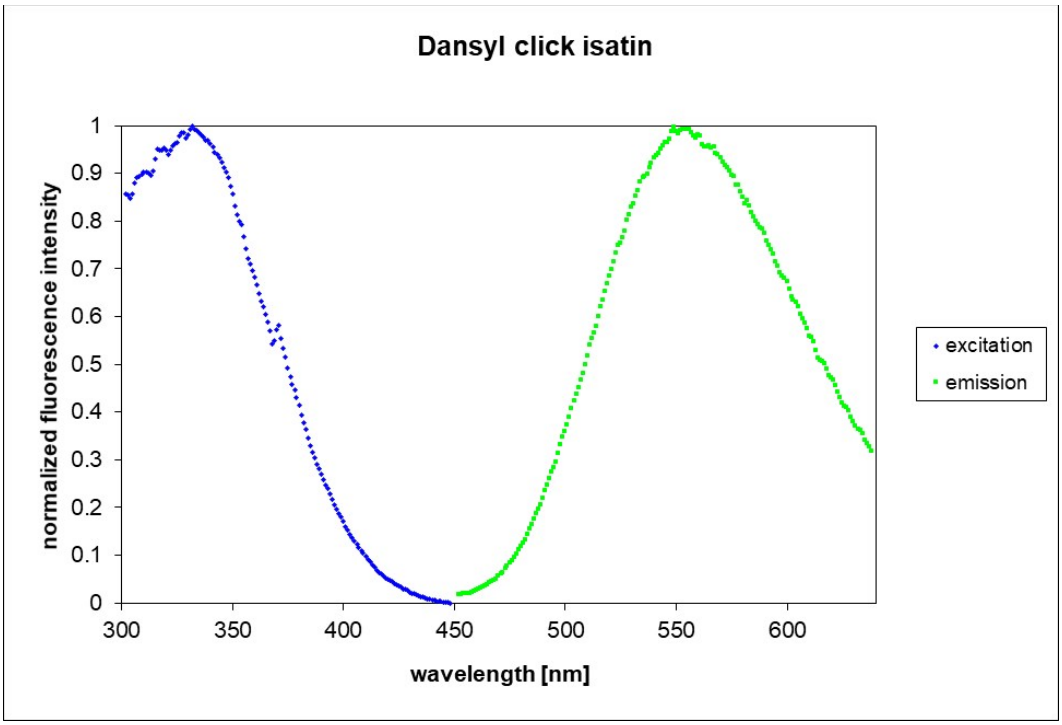


**Figure SI34** Fluorescence spectrum of 5-(*N*-dansyl-clicked) isatin **4** in phosphate buffered saline (PBS) containing 5% DMSO.

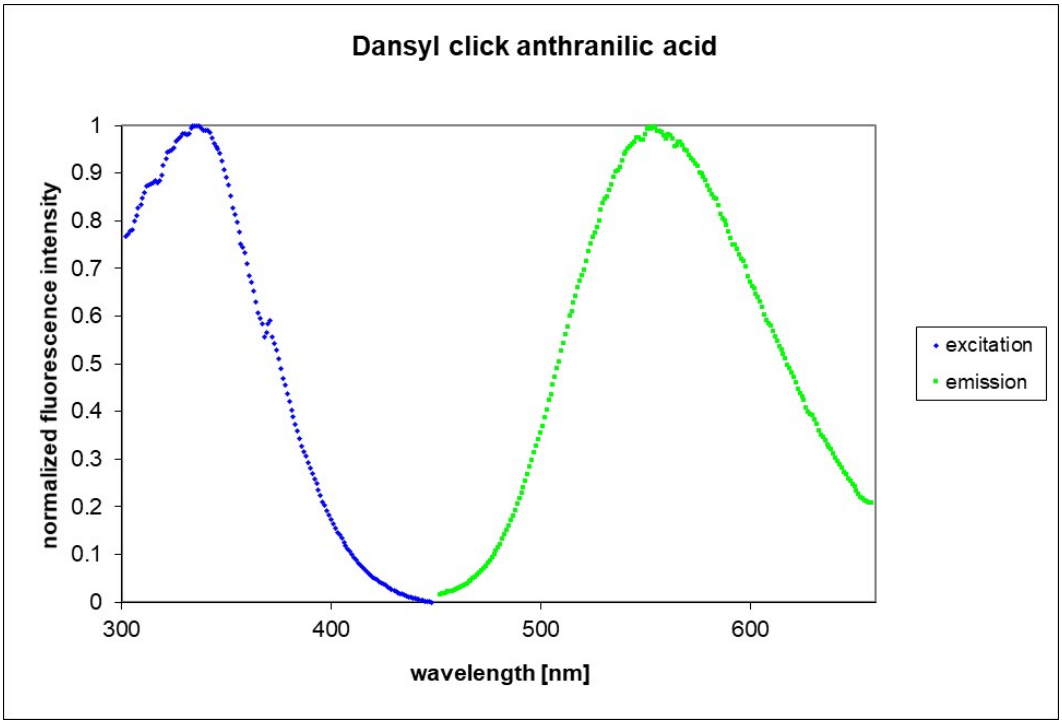


**Figure SI35** Fluorescence spectrum of 5-(*N*-dansyl-clicked) antranilic acid **3** in phosphate buffered saline (PBS) containing 5% DMSO.

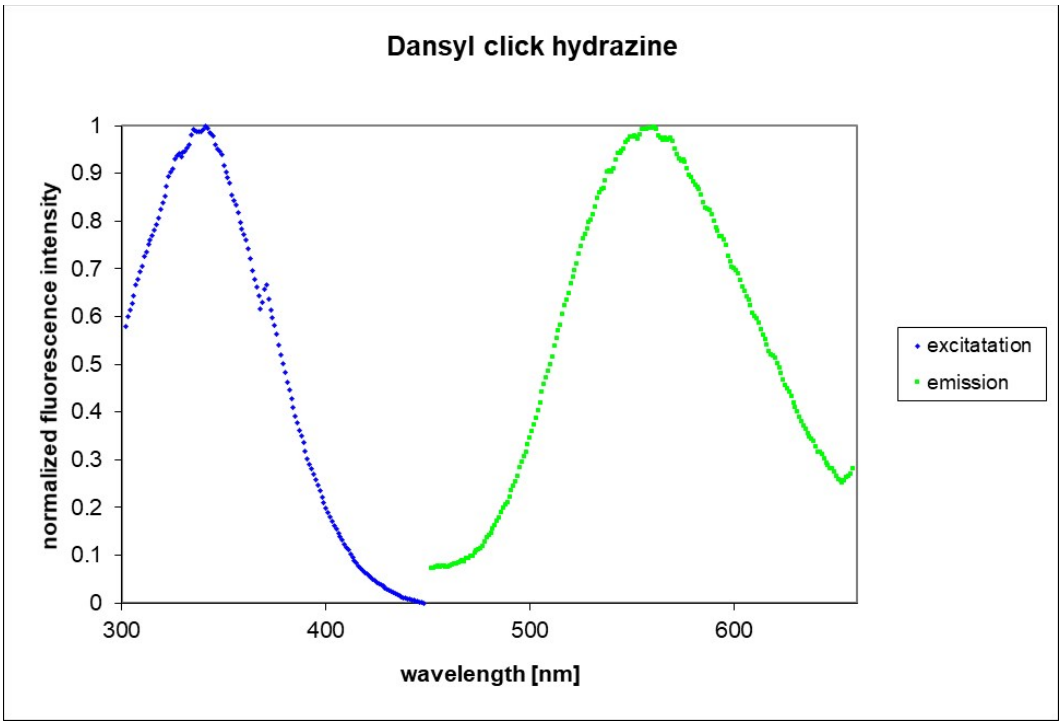


**Figure SI36** Fluorescence spectrum of 5-(*N*-dansyl-clicked) *N*-aminoantranilic acid **1** in phosphate buffered saline (PBS) containing 5% DMSO.

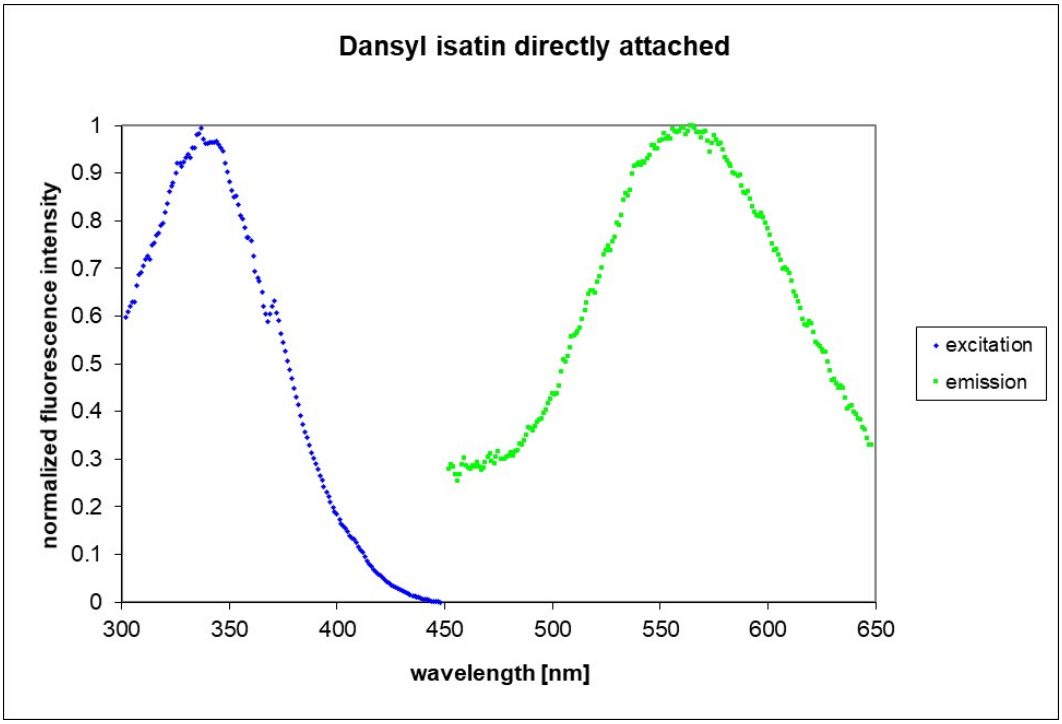


**Figure SI37** Fluorescence spectrum of 5-(*N*-dansylamino)-isatin (**7**) in phosphate buffered saline (PBS) containing 5% DMSO.

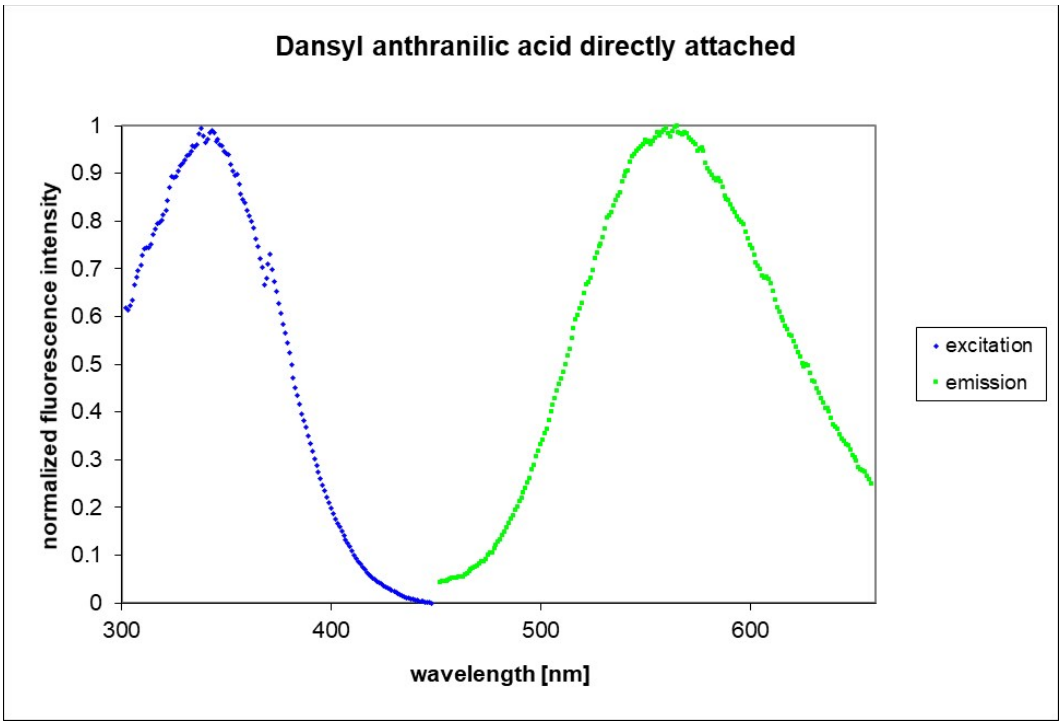


**Figure SI38** Fluorescence spectrum of 5-(*N*-dansylamino)-anthranilic acid (**14**) in phosphate buffered saline (PBS) containing 5% DMSO.

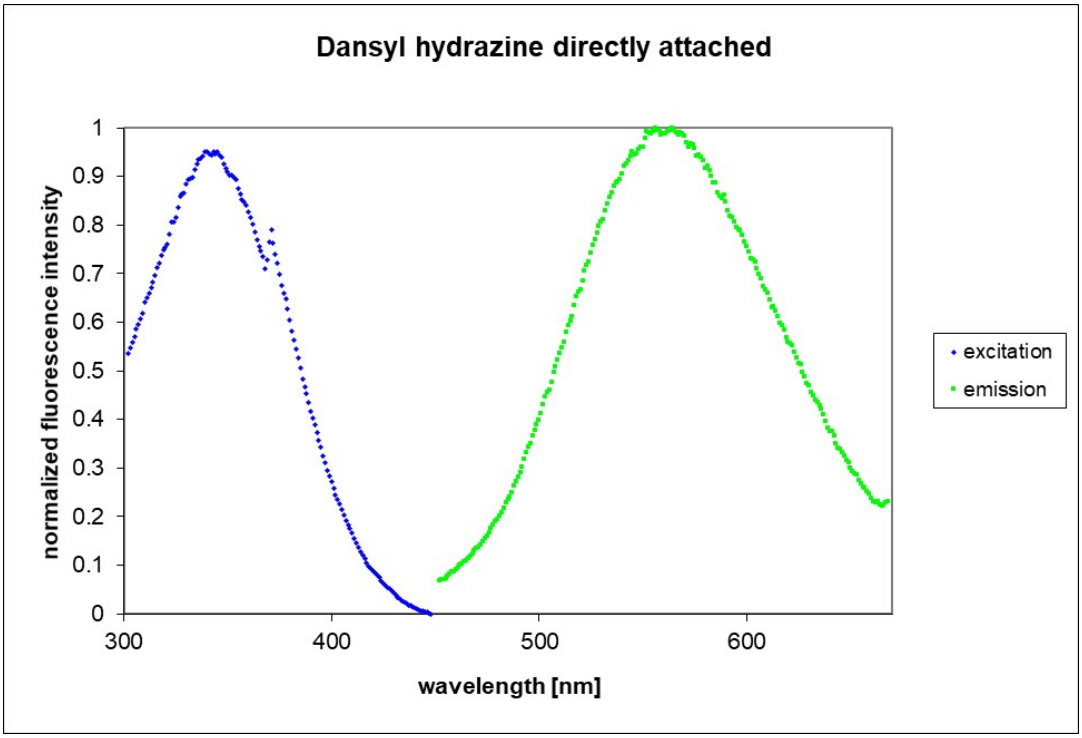


**Figure SI39** Fluorescence spectrum of 5-(*N*-dansylamino)-*N*-aminoanthranilic acid (**2**) in phosphate buffered saline (PBS) containing 5% DMSO.

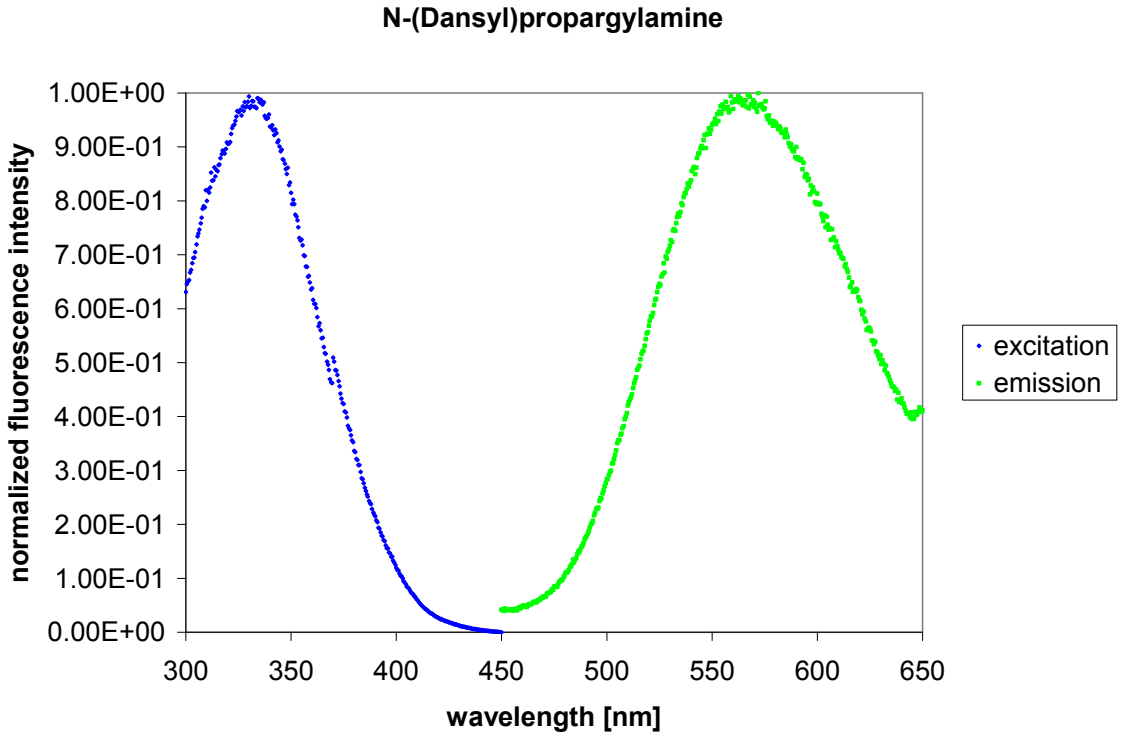


**Figure SI40** Fluorescence spectrum of *N*-(Dansyl)-propargylamine (**6**) in phosphate buffered saline (PBS) containing 5% DMSO.

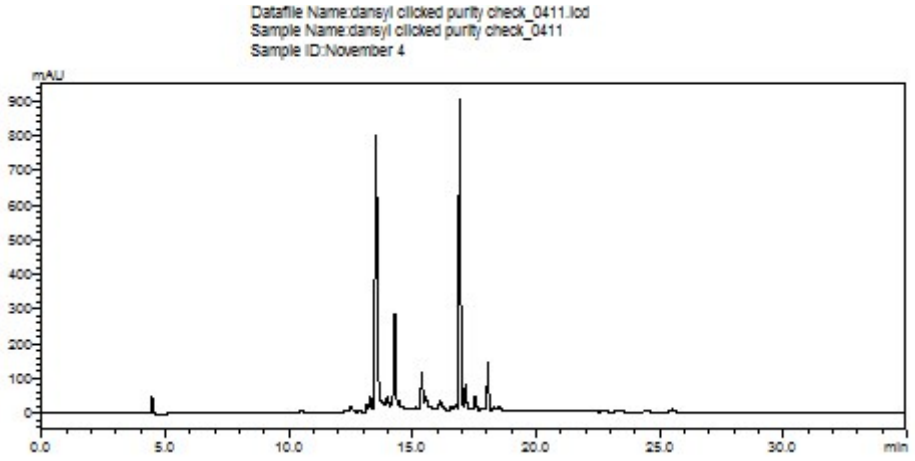


**Figure SI41** HPLC trace (Method B) of 5-(*N*-dansyl-clicked) *N*-aminoantranilic acid **1** ($t_R$ ~ 13 min) upon storing for 12 months at -20 °C.

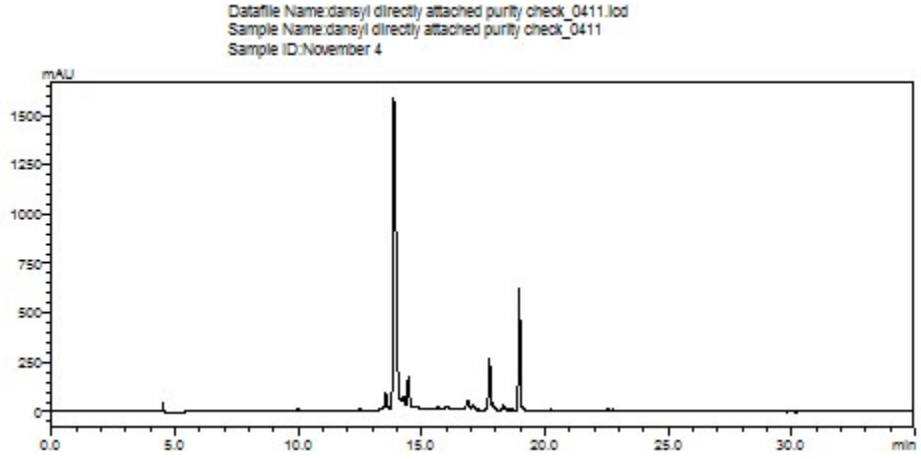


**Figure SI42** HPLC trace (Method B) of 5-(*N*-dansylamino)-*N*-aminoantranilic acid (**2**, $t_R$ ~ 14 min) upon storing for 12 months at -20 °C. Note significantly increased stability compared to compound **1**.

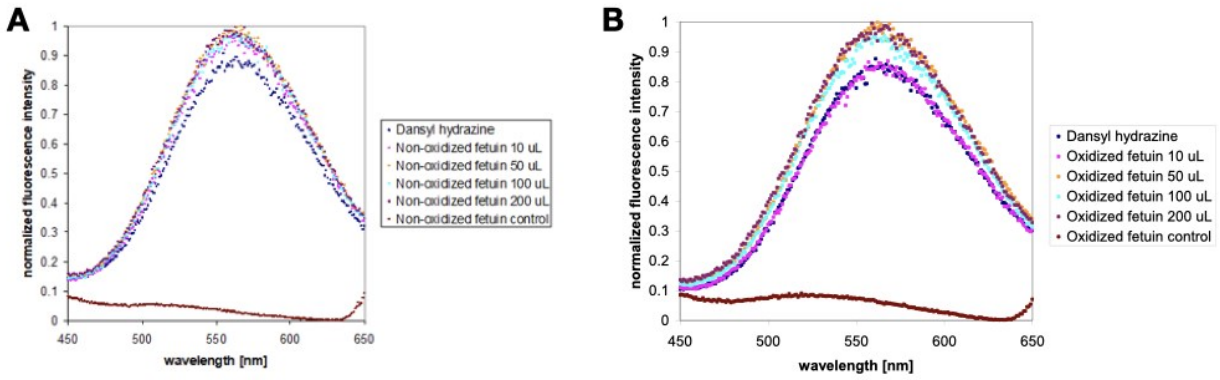


**Figure SI43** Emission spectra of dansyl-NA$^3$ (**2**) with native (A) or oxidized (B) fetuin. Total solution volume was 1 mL after addition of dansyl-NA$^3$ and indicated volume of protein solution, and excitation was set to 339 nm.

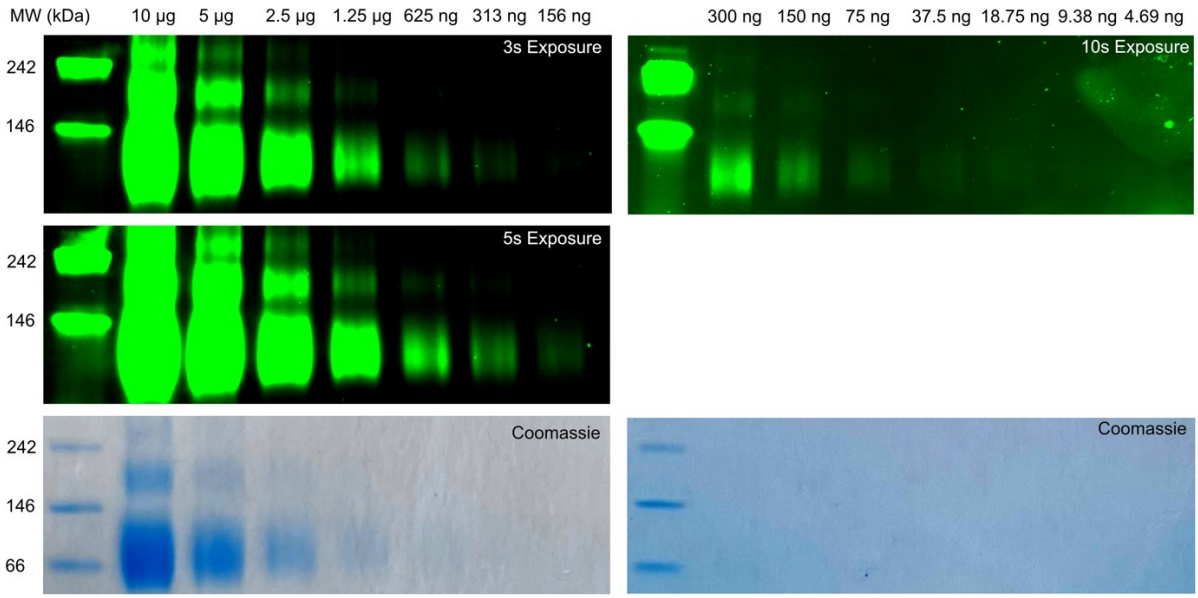


**Figure SI44** The limit of detection of glycoprotein identification following oxidation and tagging with compound **2**. The visualization of a native protein gel was performed by Coomassie staining (*top*) and fluorescence imaging (*bottom*). A serially diluted fetuin sample was evaluated, resulting in the final protein amounts indicated above the respective lanes; the limit of detection is ~ 18 ng of protein.