

Supplementary data

Unveiling the structural aspects of novel azo-dyes with promising anti-virulence activity against MRSA: A deep dive into the spectroscopy via integrated experimental and computational approaches

Ahmed M. Hegazy,^{*} ^{a,b} Michael G. Shehat,^c Alaa. Abouelfetouh,^{c,d} Mohamed Teleb,^{e,f,g} Sherine N. Khattab,^{*, a} Nesreen S. Haiba ^h

^a Chemistry Department, Faculty of Science, Alexandria University, Alexandria 21321, Egypt.

^b Department of Materials Science, Institute of Graduate Studies and Research, Alexandria University, Alexandria, Egypt.

^c Department of Microbiology and Immunology, Faculty of Pharmacy, Alexandria University, 21521 Alexandria, Egypt.

^d Department of Microbiology and Immunology, Faculty of Pharmacy, Alamein International University, 51718 Alamein, Egypt.

^e Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Alexandria University, 21521 Alexandria, Egypt.

^f Cancer Nanotechnology Research Laboratory (CNRL), Faculty of Pharmacy, Alexandria University, 21521 Alexandria, Egypt.

^g Department of Medicinal Chemistry, Faculty of Pharmacy, Alamein International University (AIU), Alamein City 5060310, Egypt.

^h Department of Physics and Chemistry, Faculty of Education, Alexandria University, Egypt.

***Corresponding authors** sherinekhattab@alexu.edu.eg; ahmed.hegazy@alexu.edu.eg

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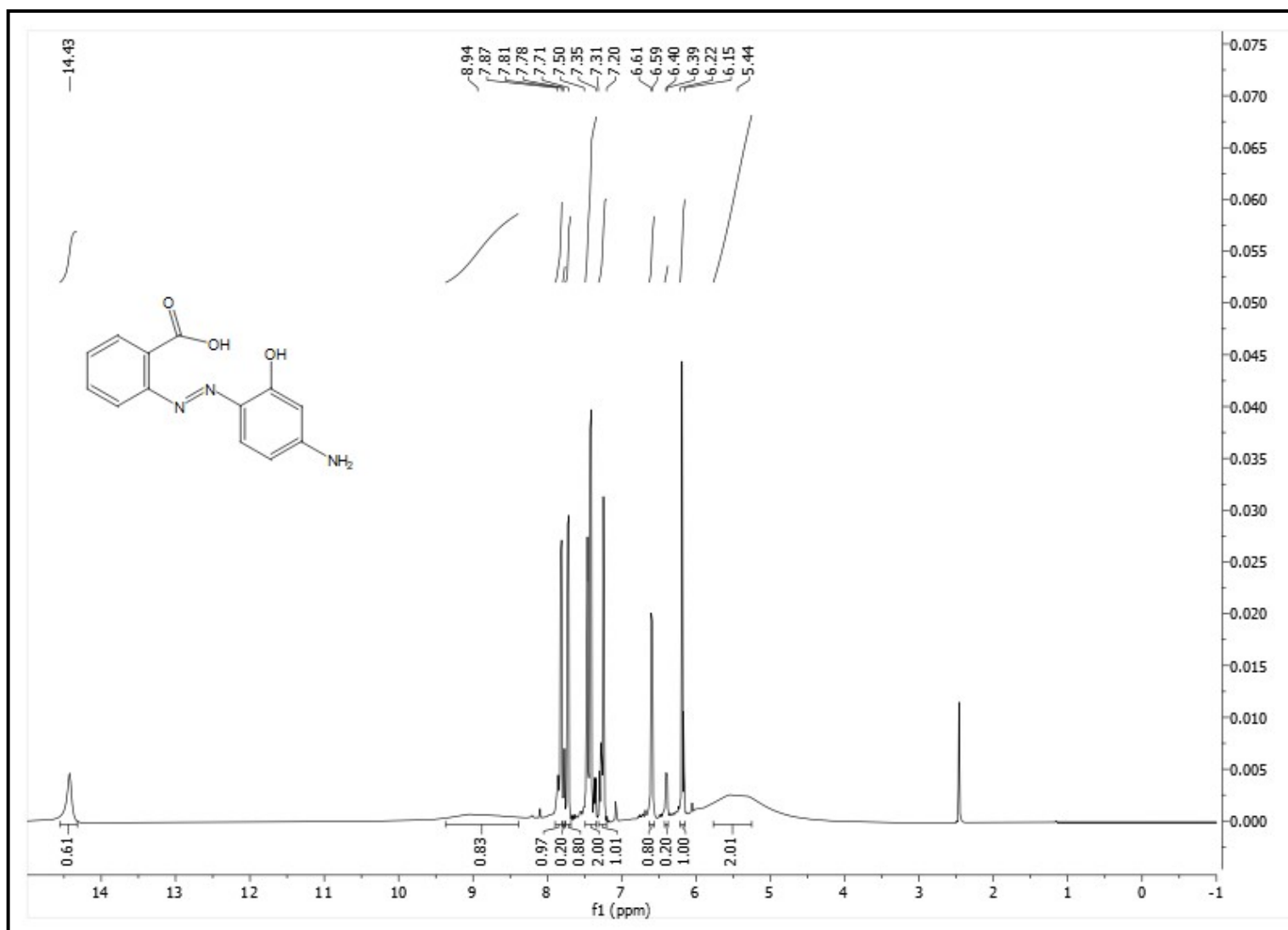


Figure S1a: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 2-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D1**)

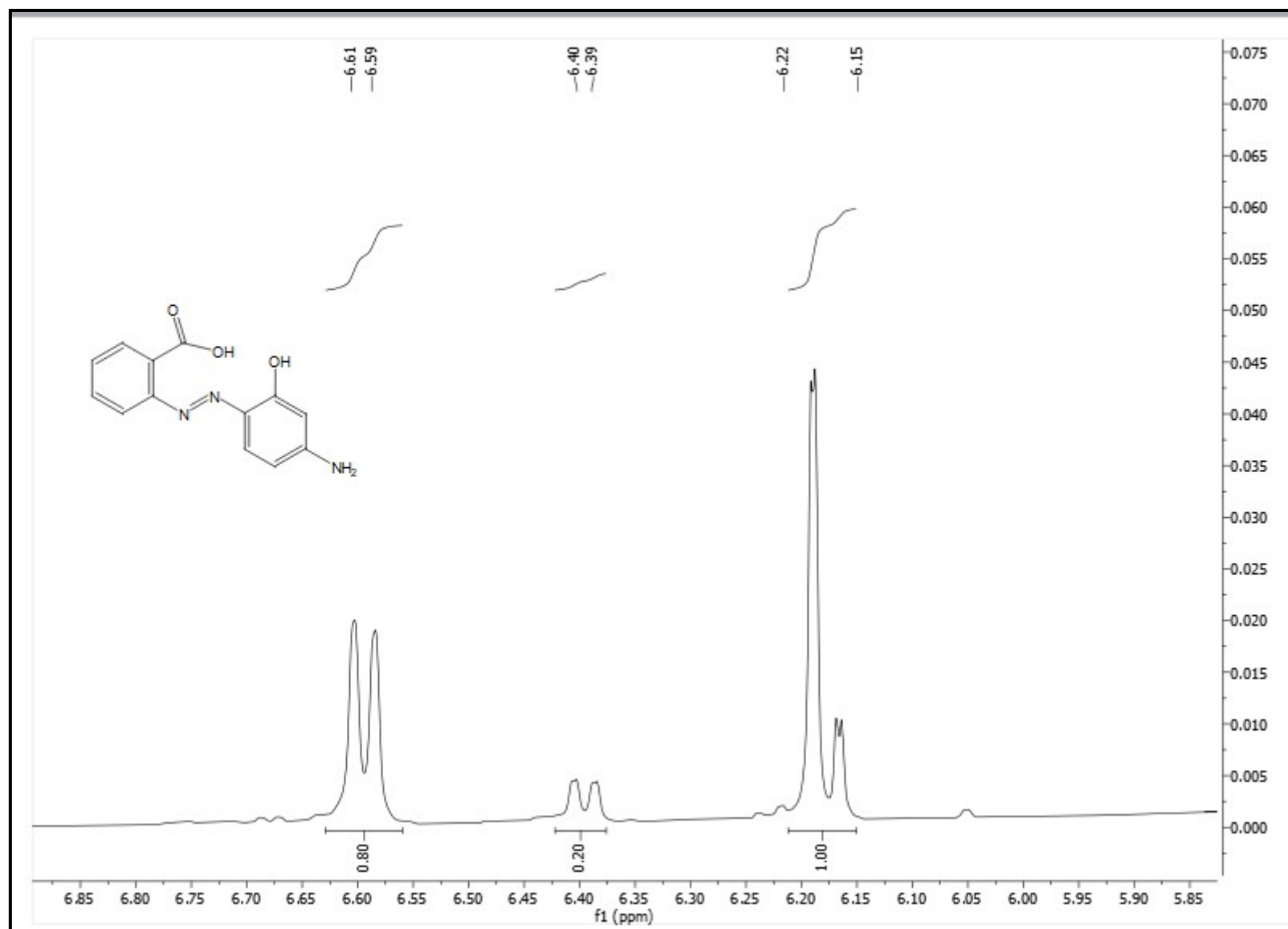


Figure S1b: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 2-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D1**)

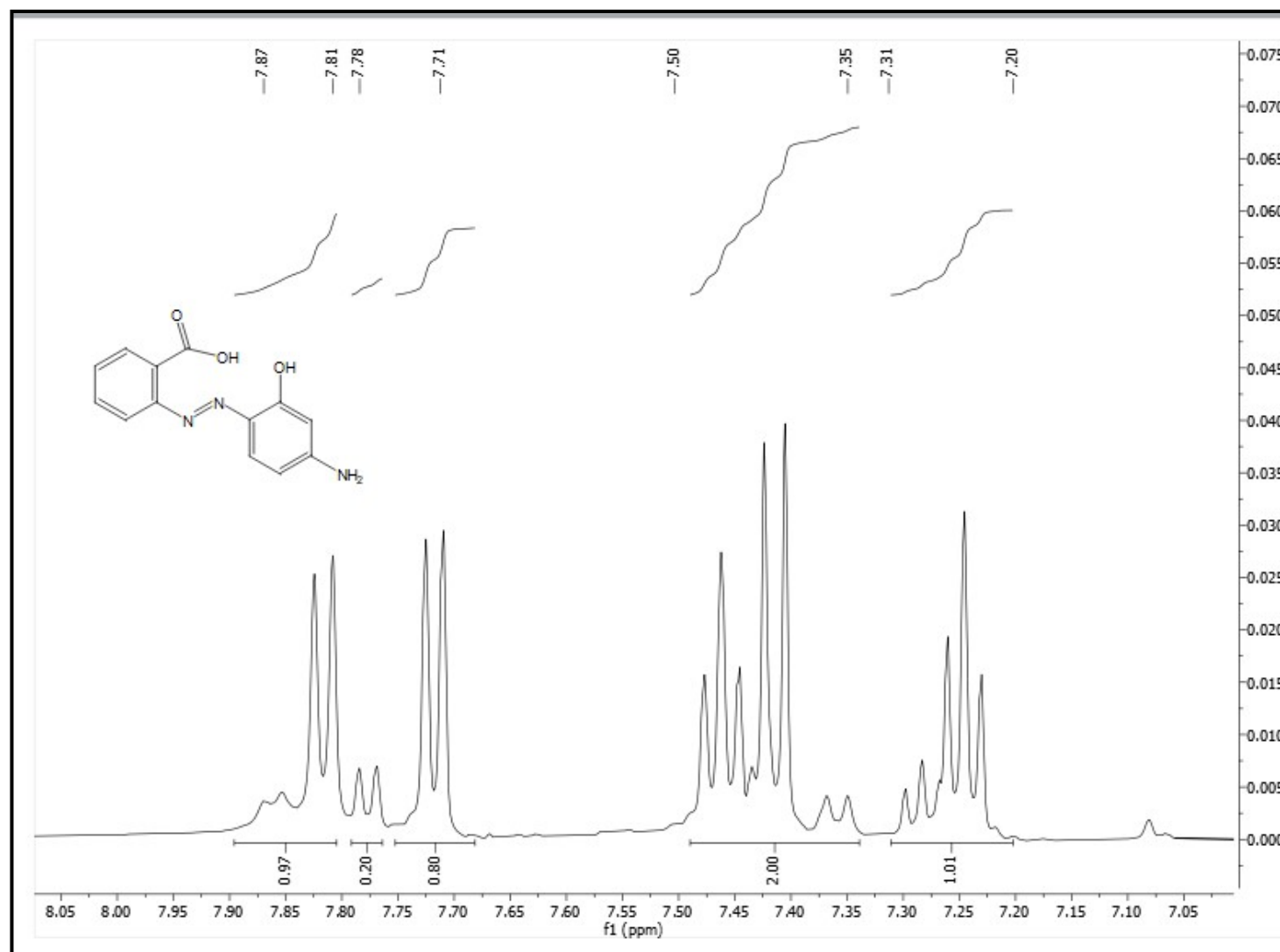


Figure S1c: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 2-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D1**)

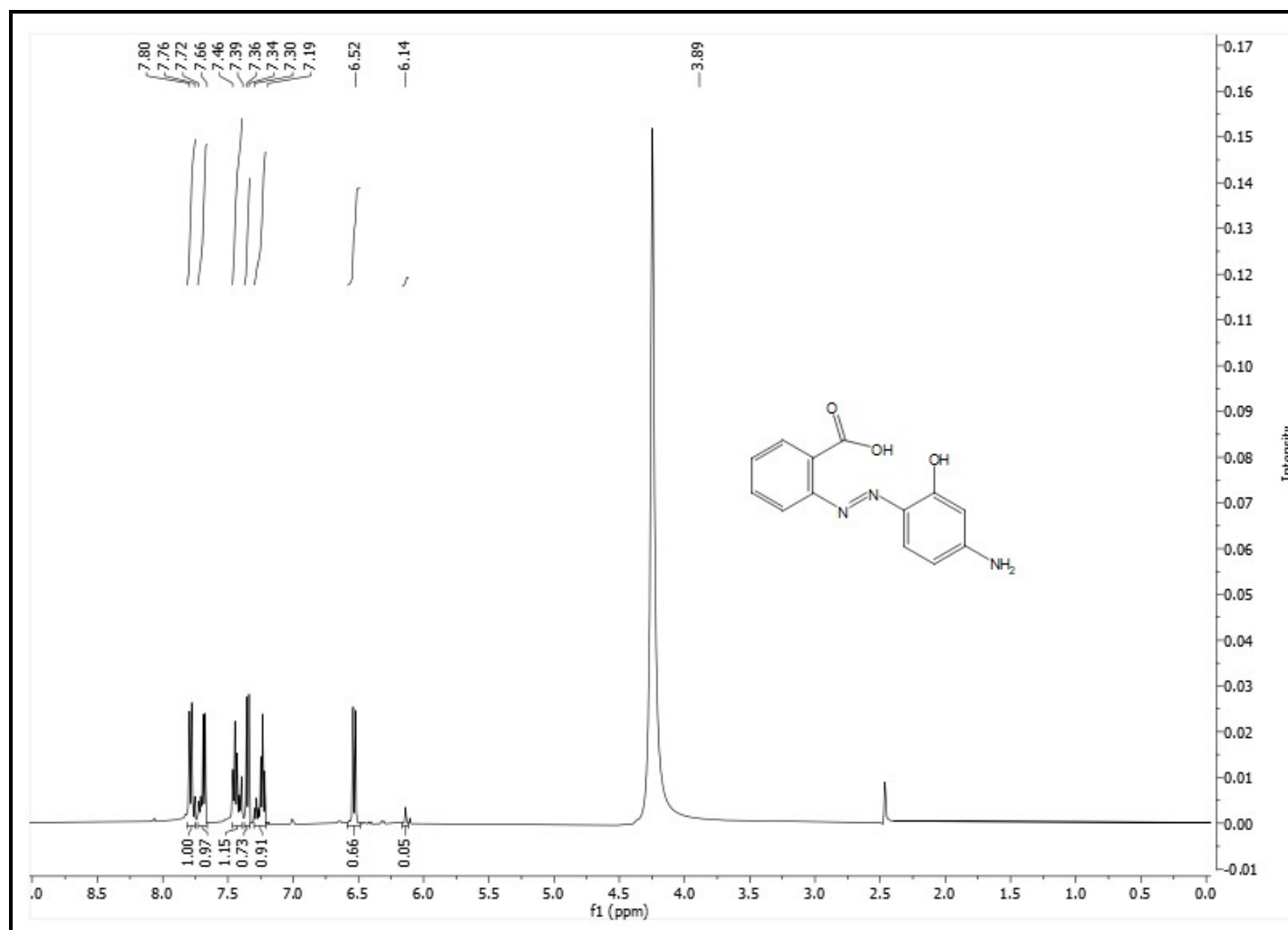


Figure S2: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$ - D_2O) spectrum of 2-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D1**)

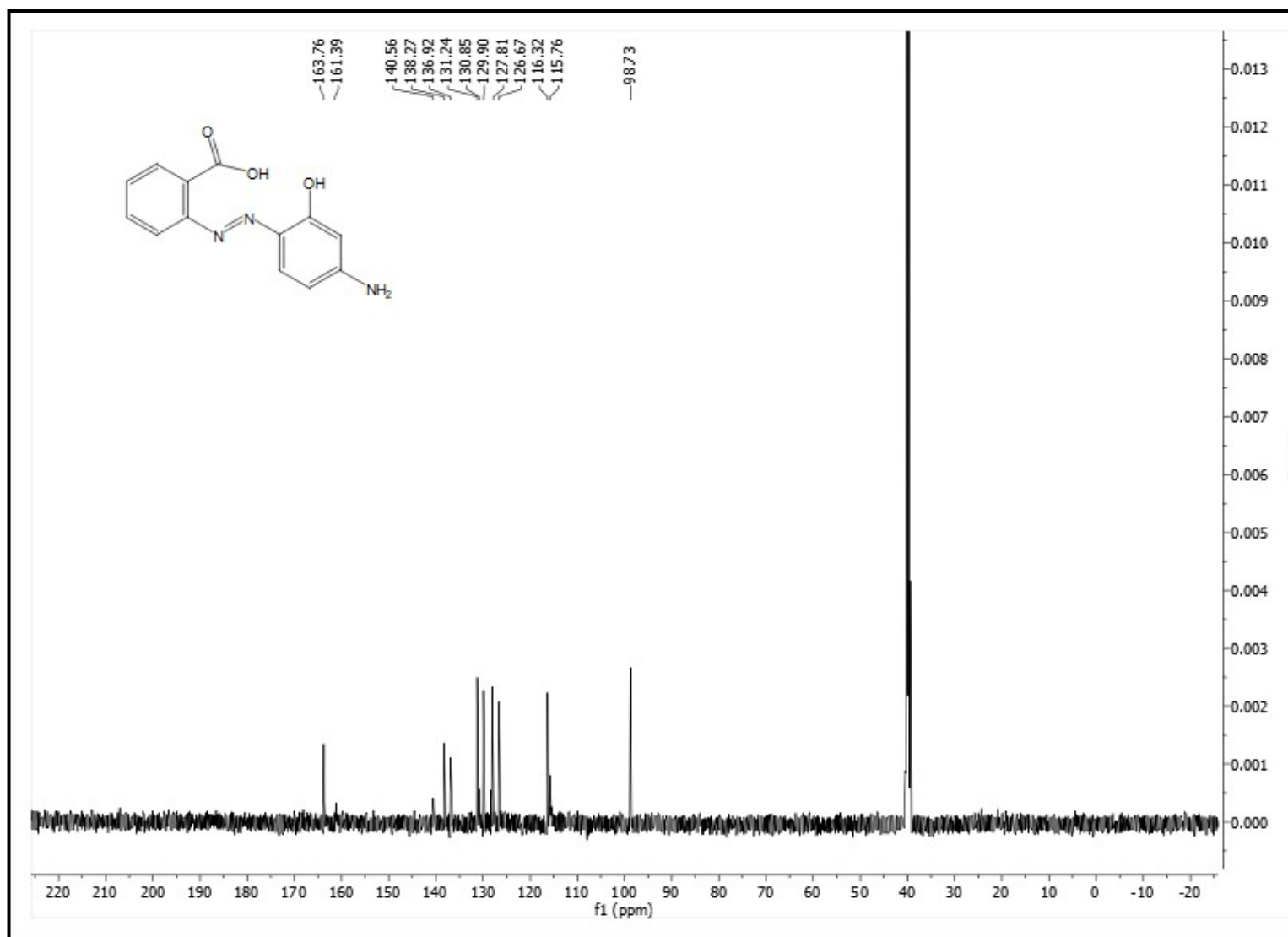


Figure S3: ¹³C-NMR (125 MHz, DMSO-*d*₆) spectrum of 2-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D1**)

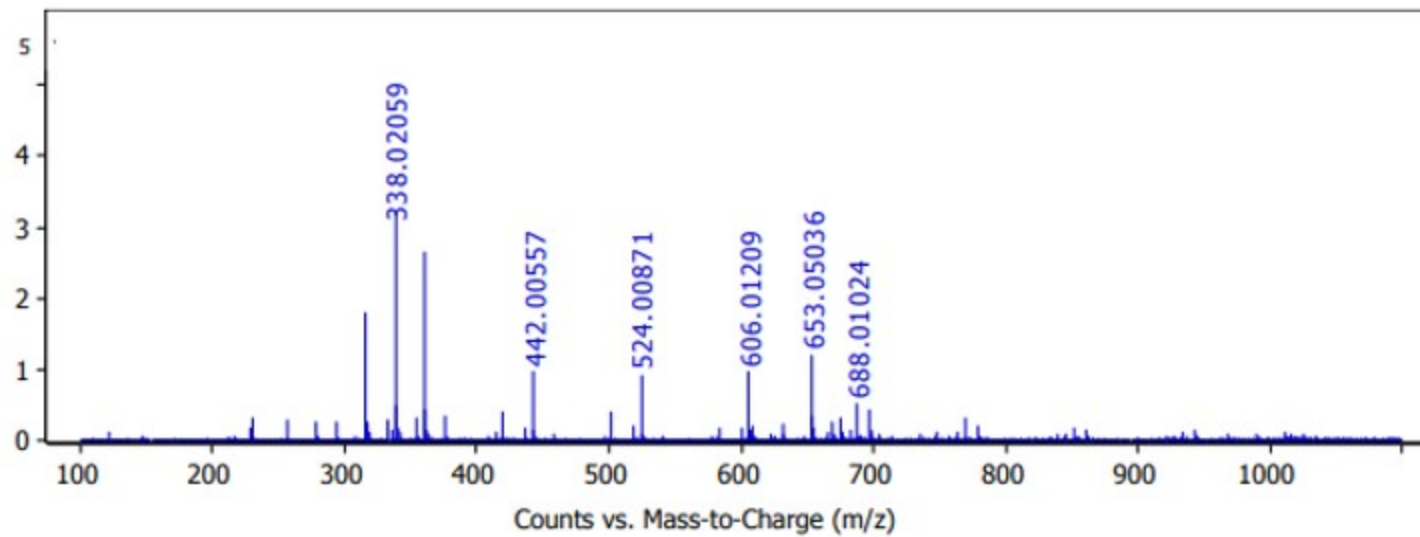


Figure S4: The High- resolution mass (HRMS) spectrum of **D1**

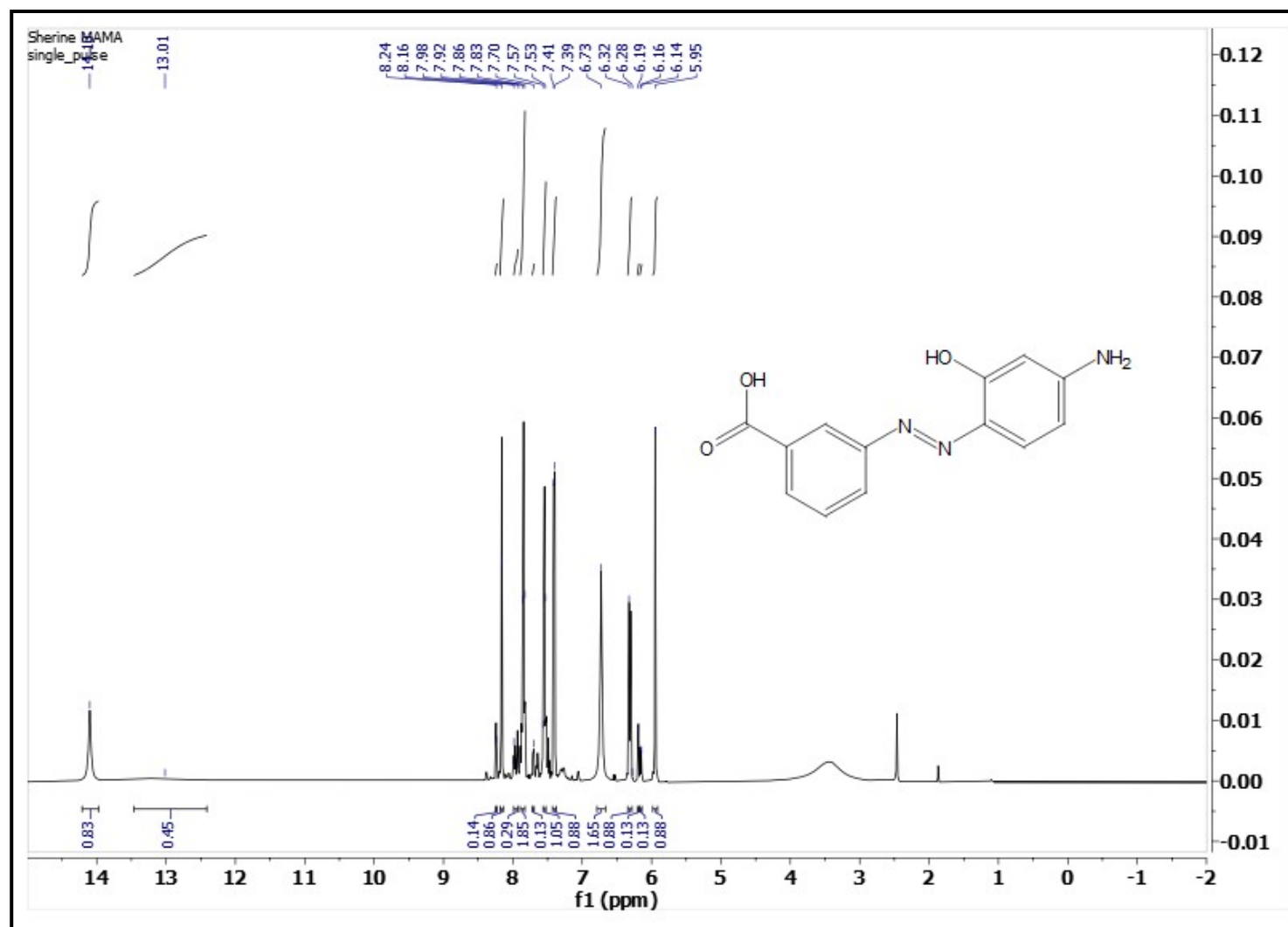


Figure S4a: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 3-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid **D2**

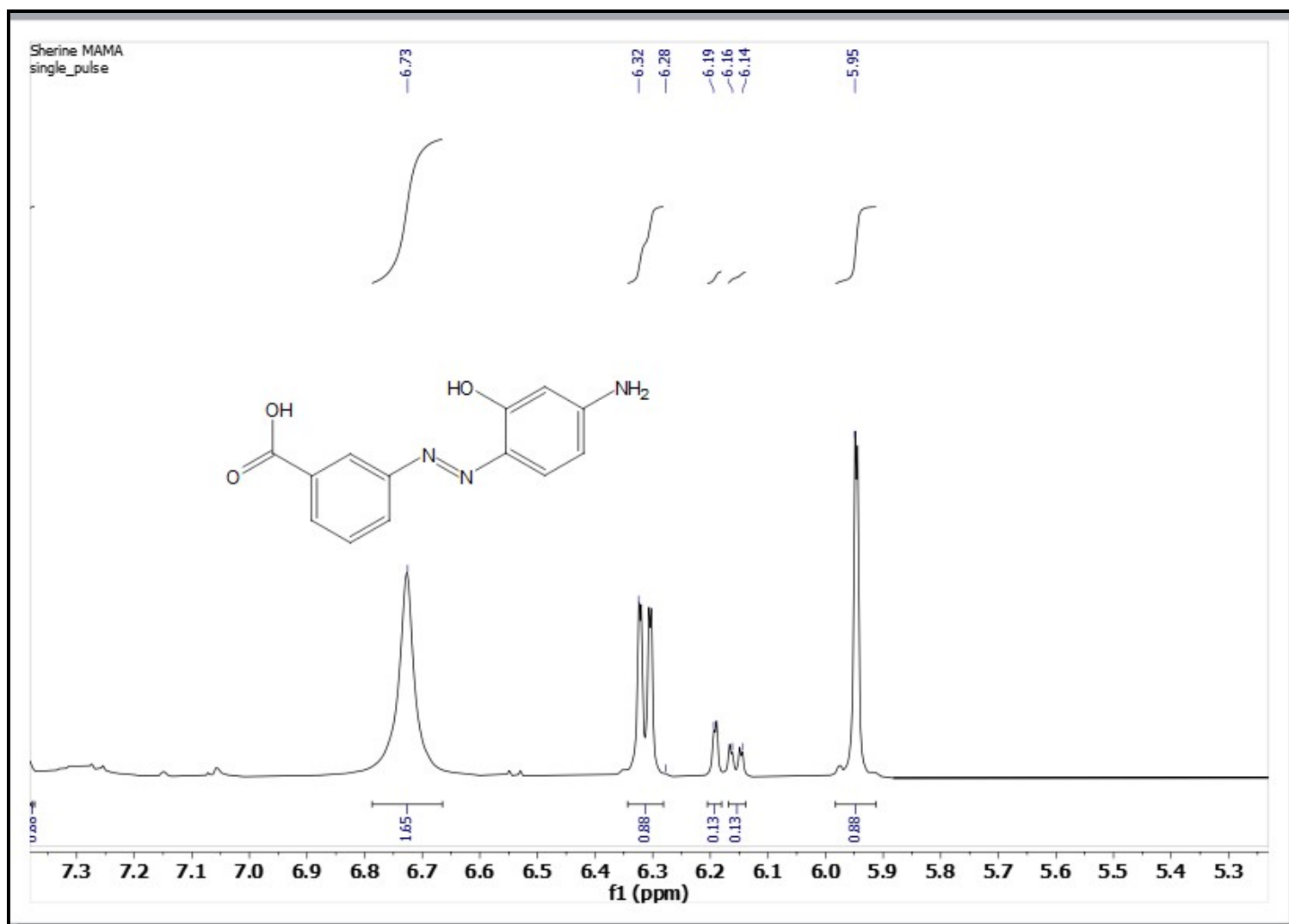


Figure S4b: ^1H -NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of 3-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid **D2**

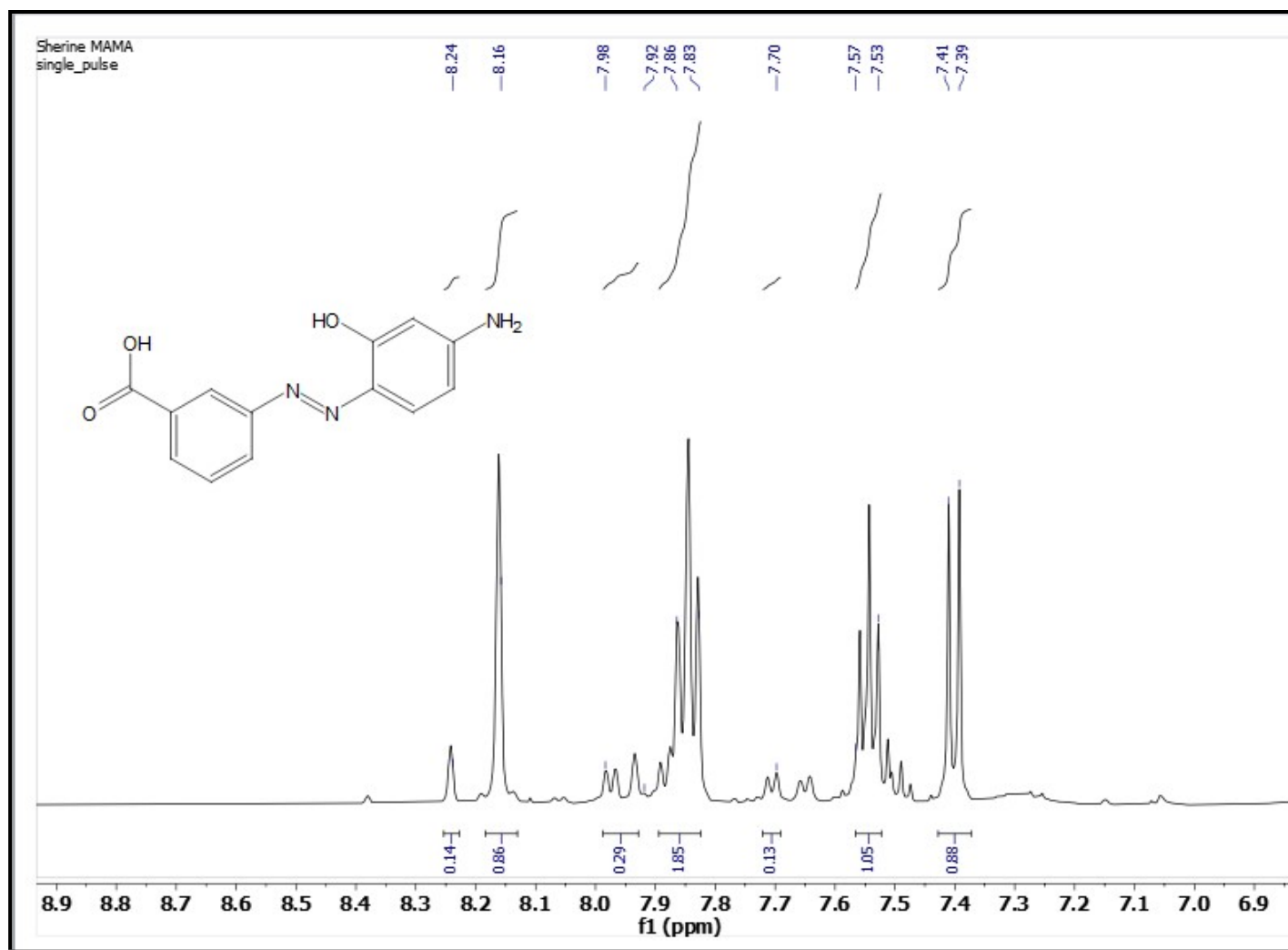


Figure S4c: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 3-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid **D2**

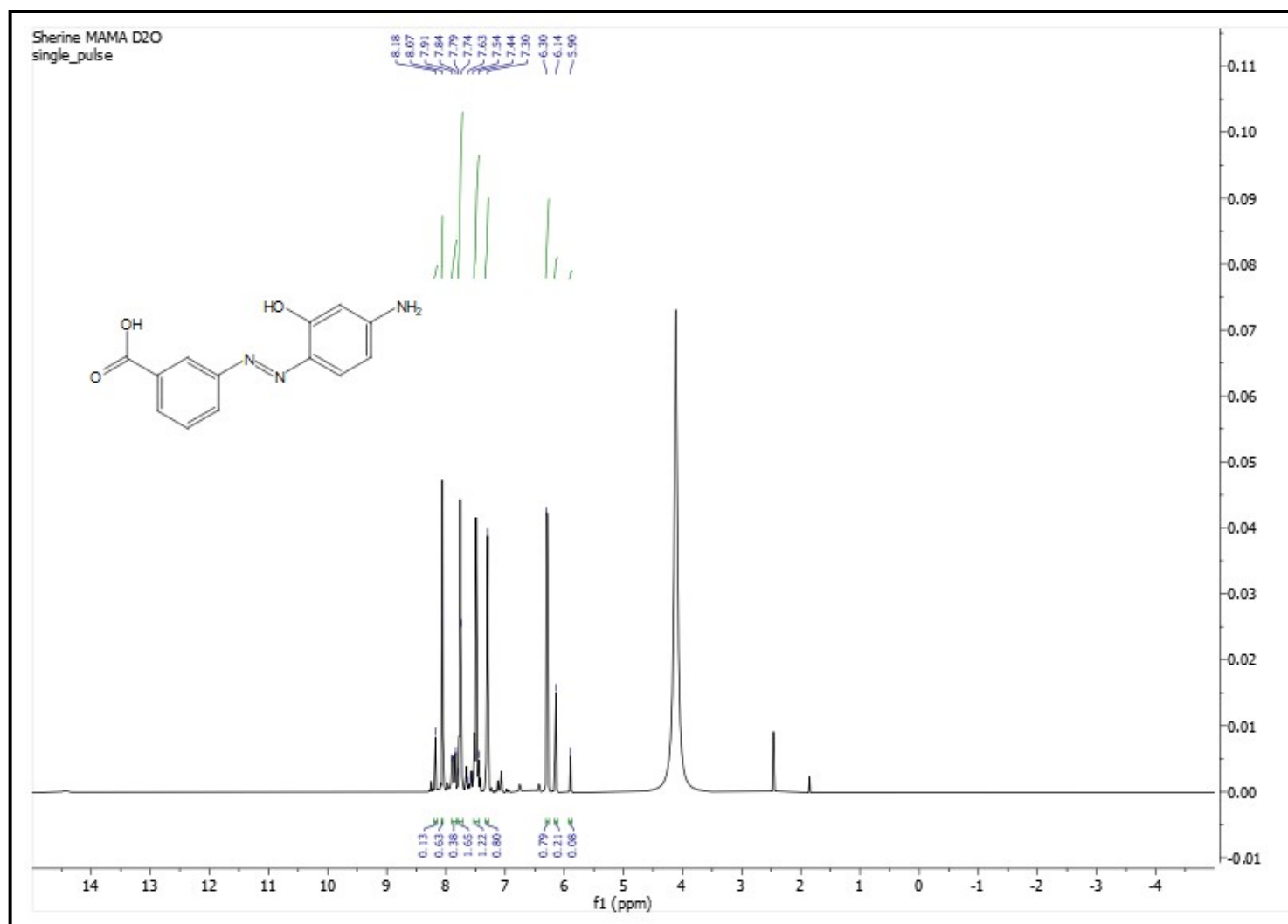


Figure S5: ^1H -NMR (500 MHz, $\text{DMSO-}d_6$ - D_2O) spectrum of 3-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid **D2**

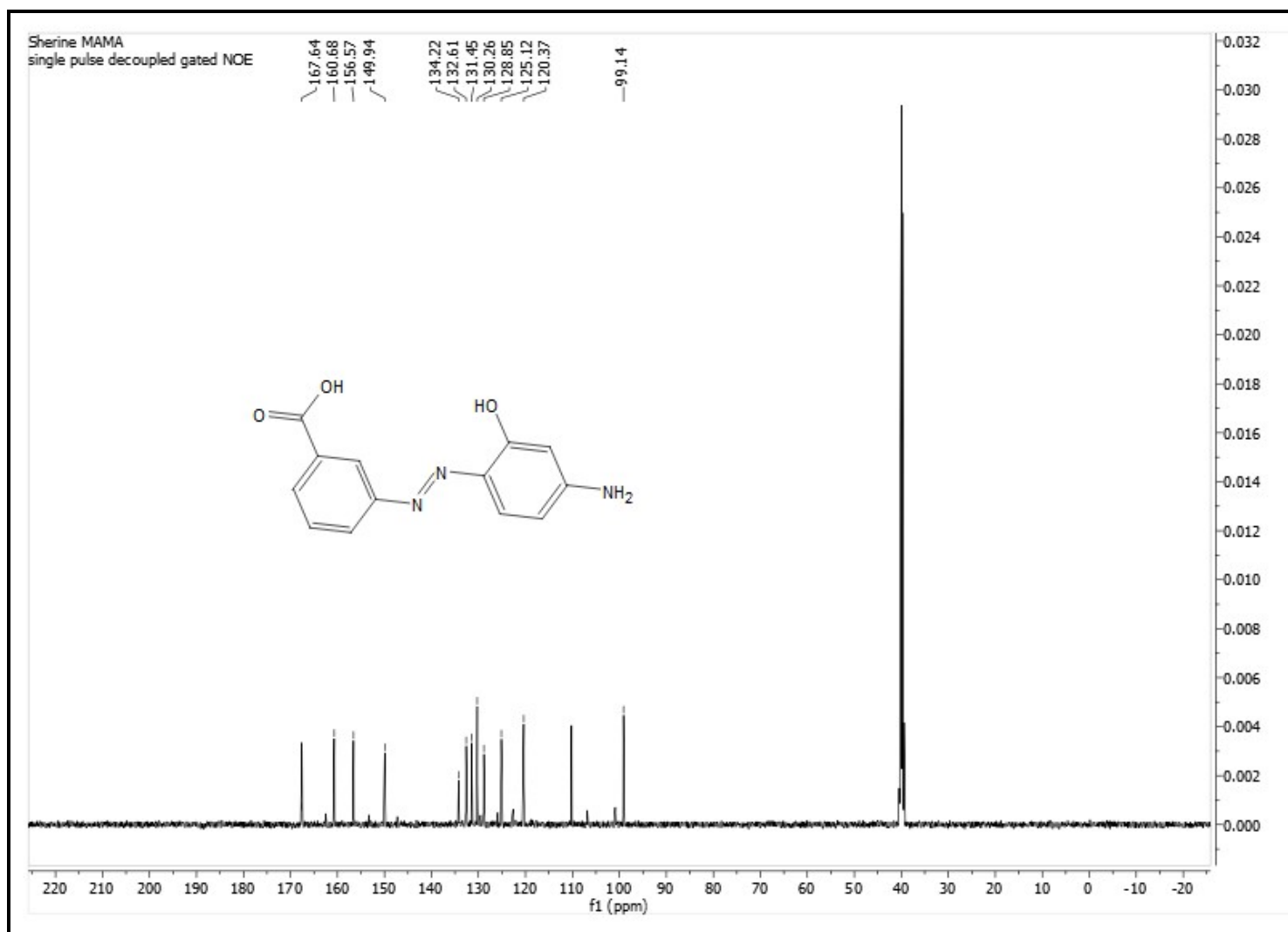


Figure S6: ¹³C-NMR (125 MHz, DMSO-*d*₆) spectrum of 3-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid **D2**

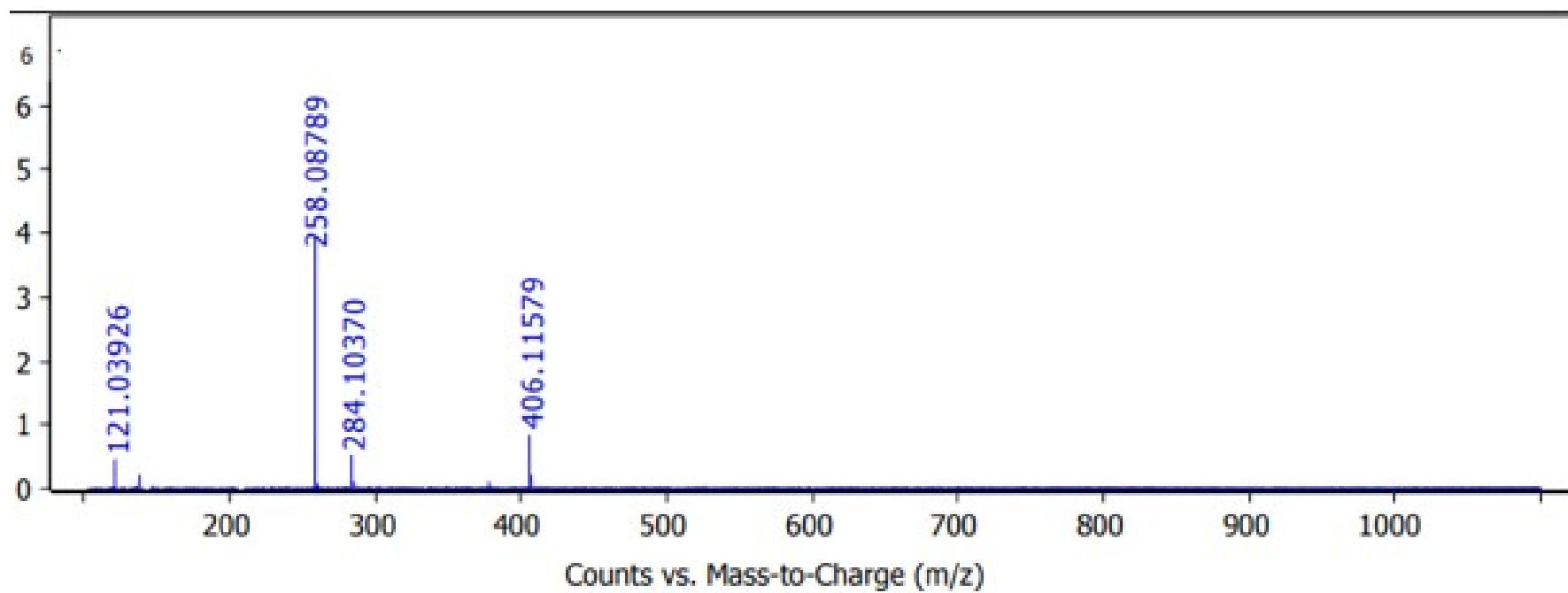


Figure S8: The High- resolution mass (HRMS) spectrum of **D2**

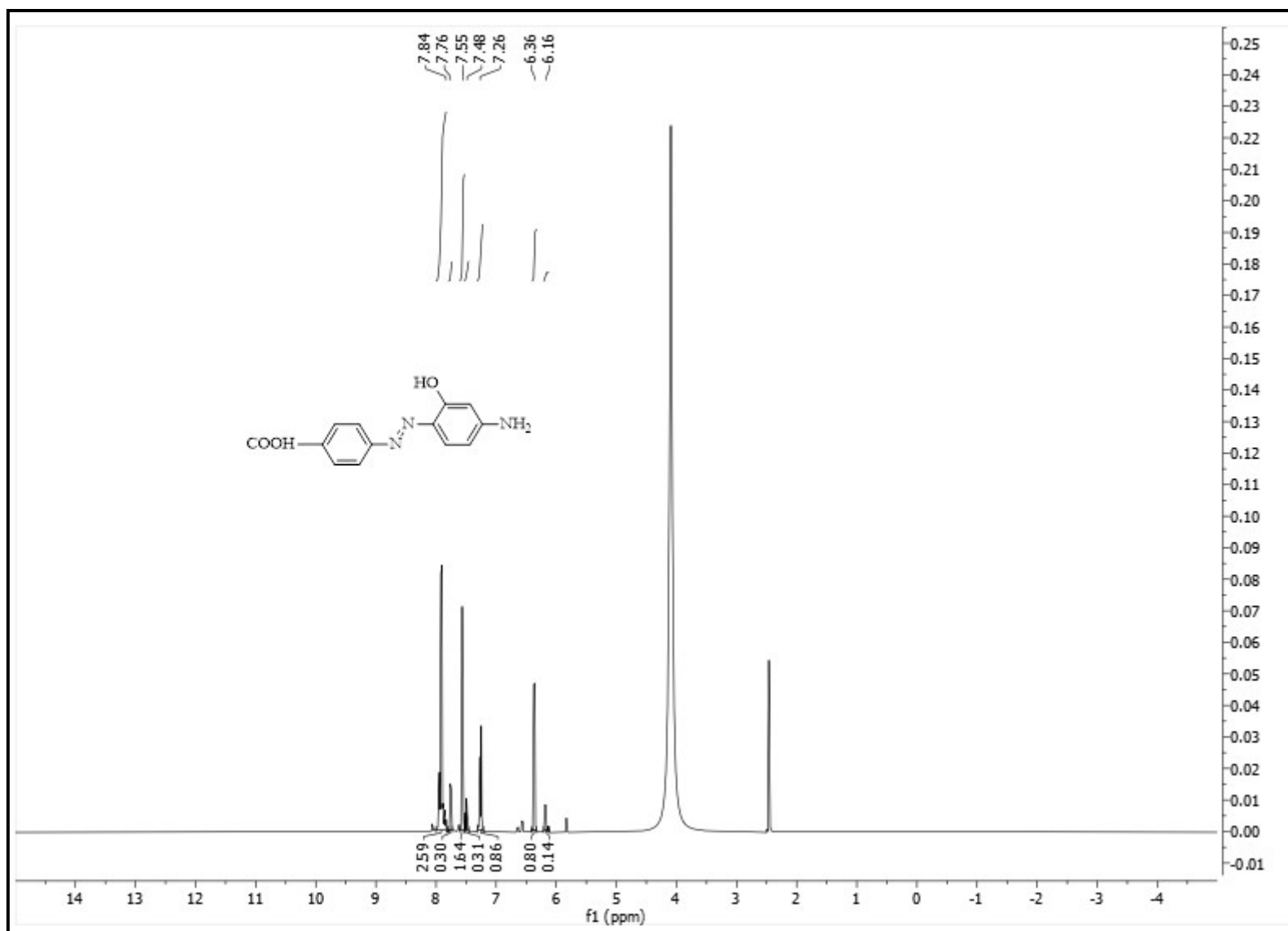


Figure S9a: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 4-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D3**)

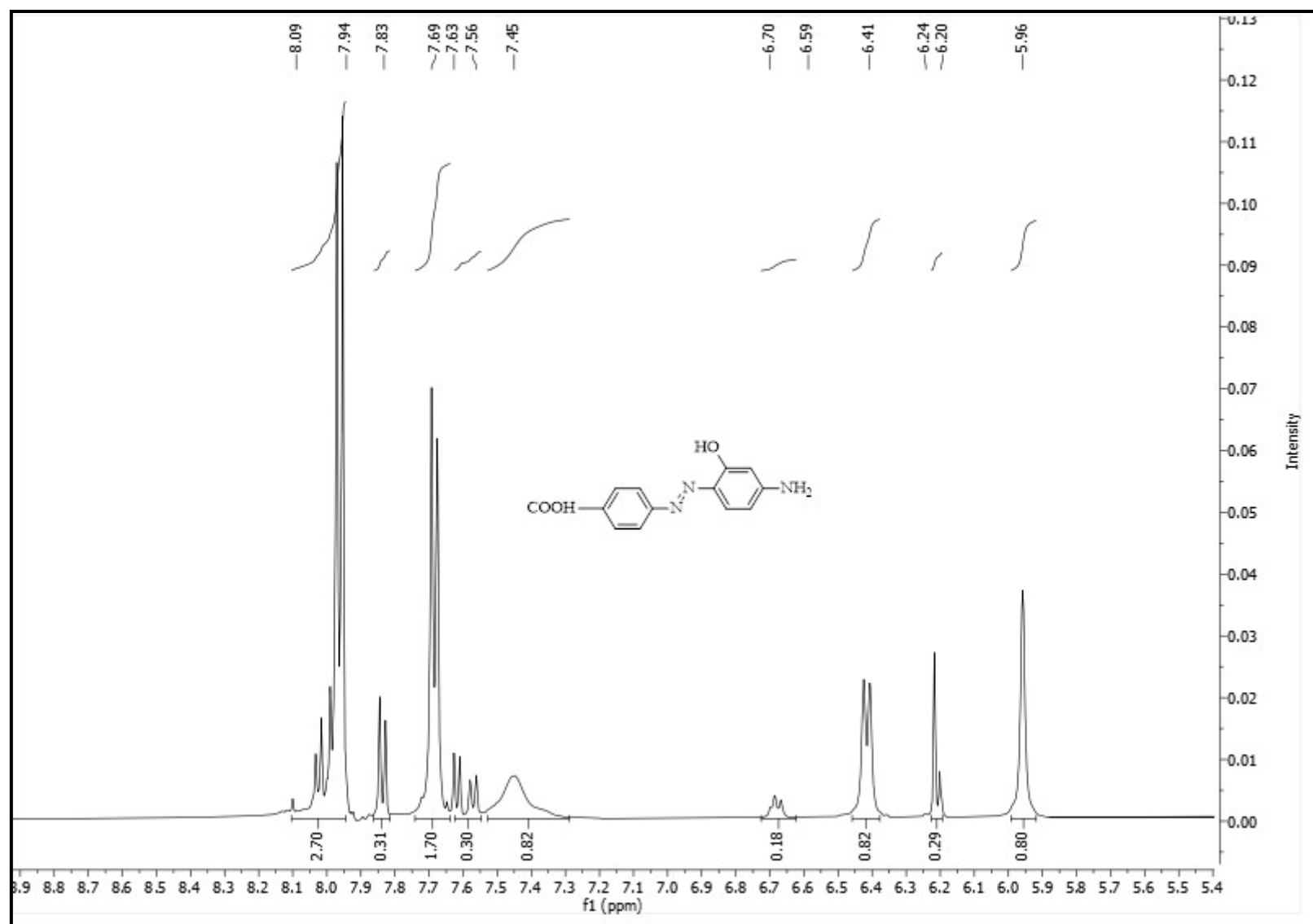


Figure S9b: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 4-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D3**)

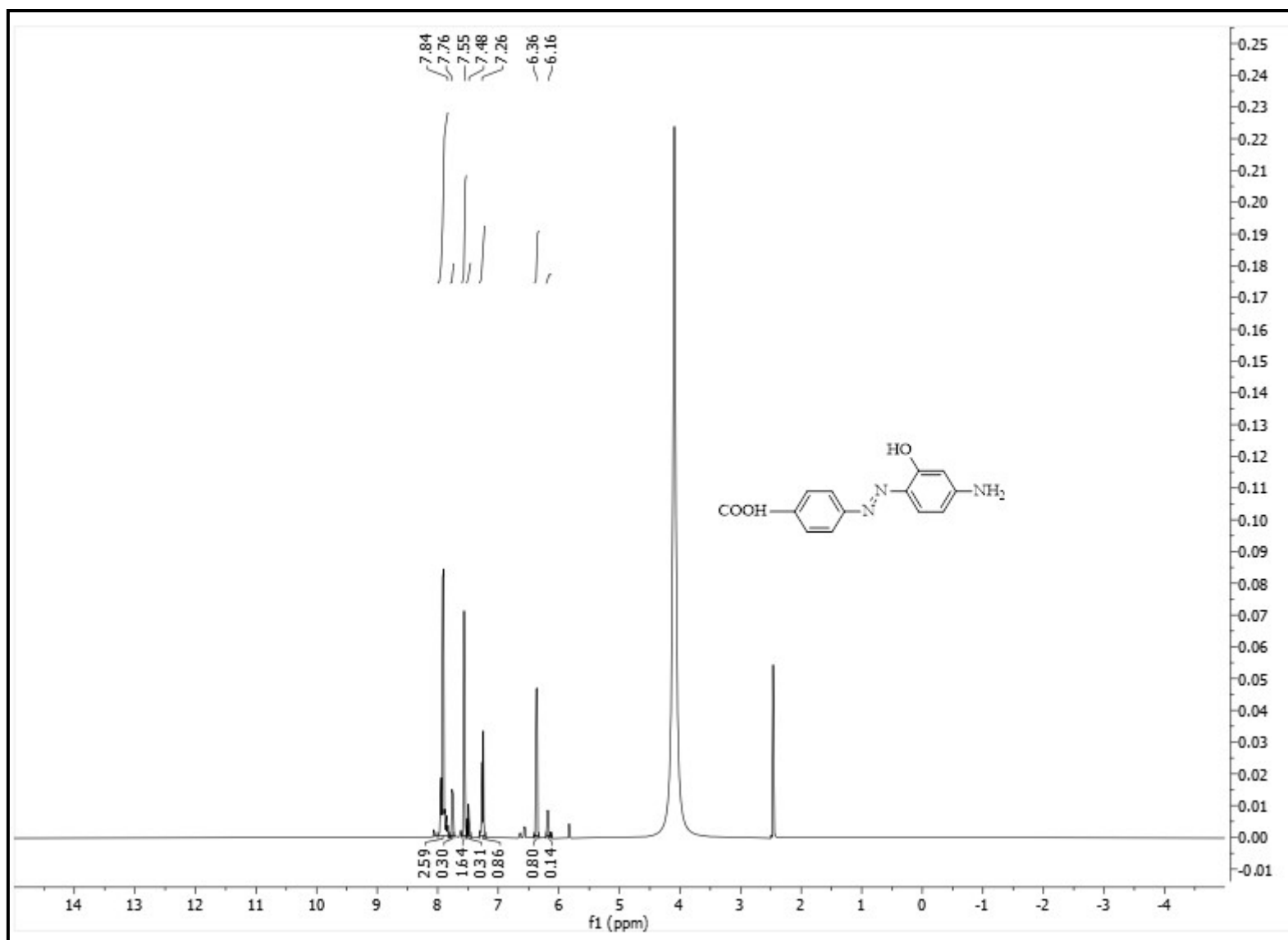


Figure S10: ^1H -NMR (500 MHz, $\text{DMSO}-d_6/\text{D}_2\text{O}$) spectrum of 4-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D3**)

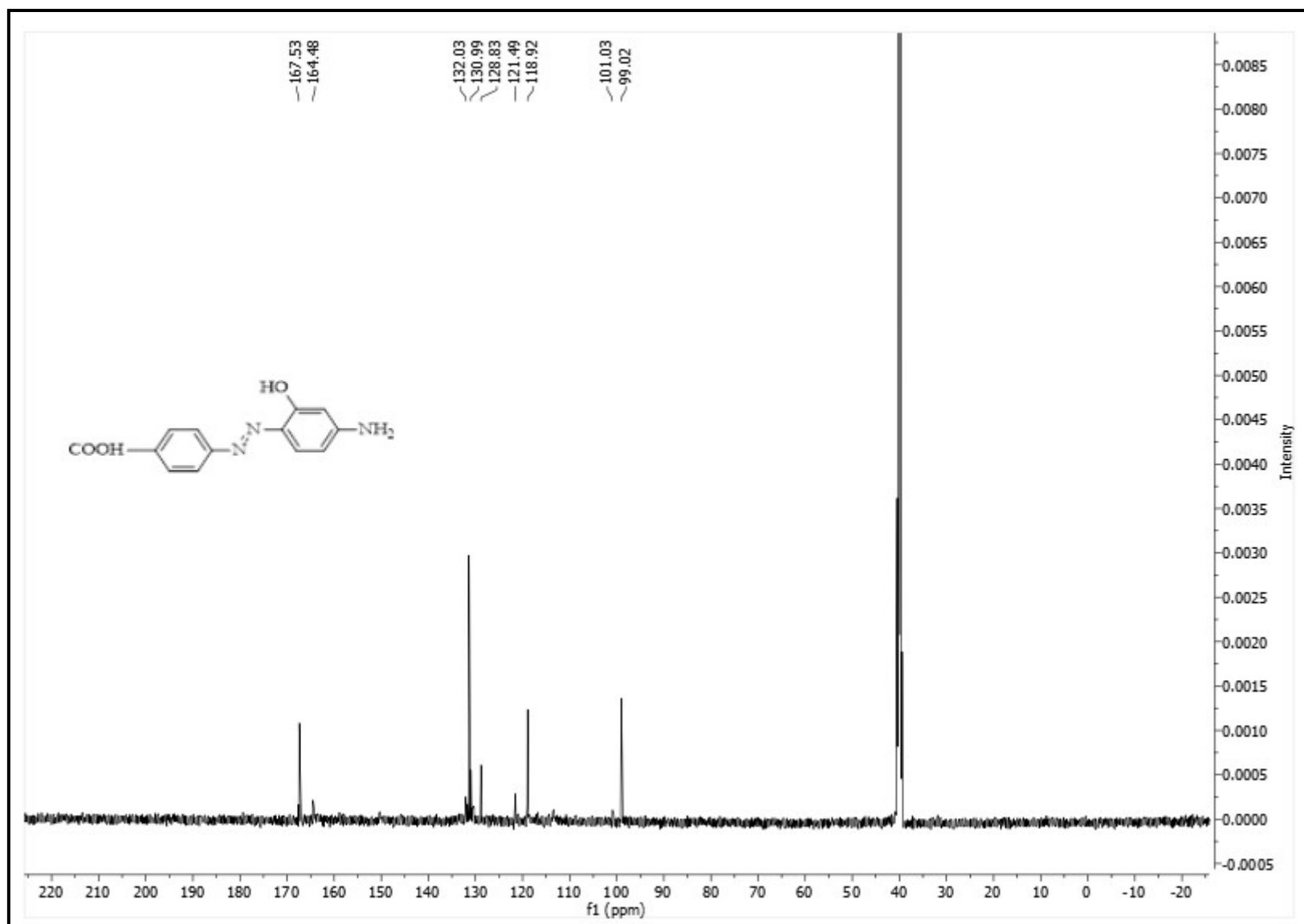


Figure S11: ^{13}C -NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of 4-((4-amino-2-hydroxyphenyl)diazenyl)benzoic acid (**D3**)

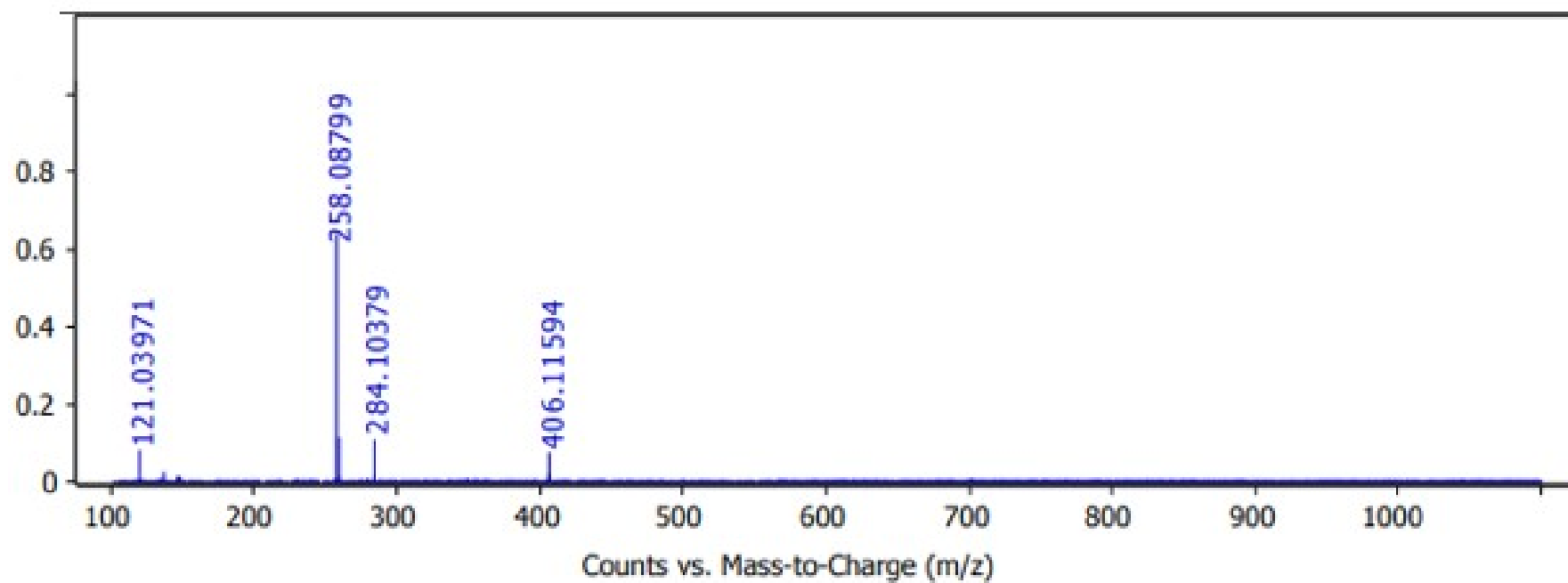


Figure S12: The High- resolution mass (HRMS) spectrum of **D3**

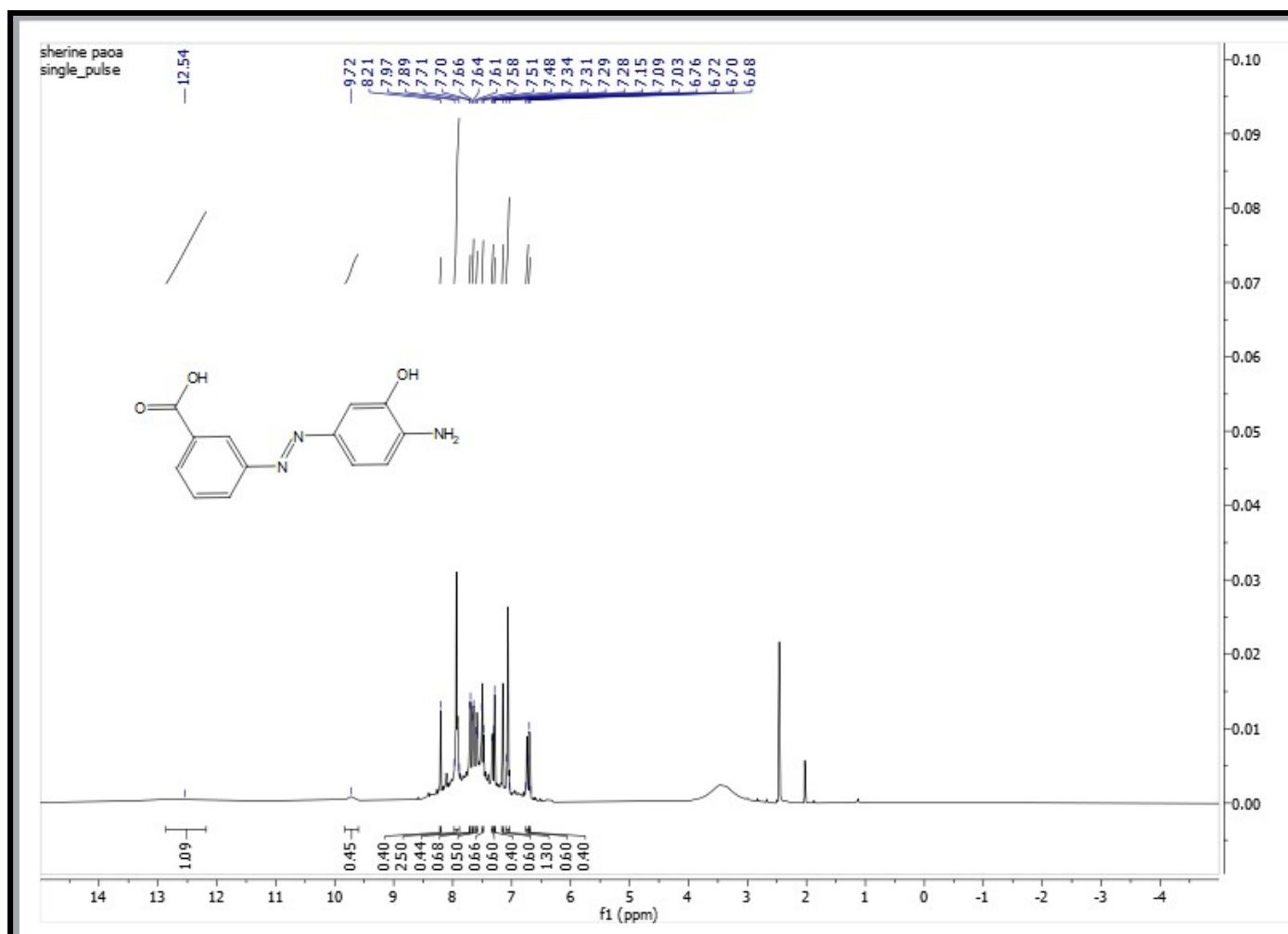


Figure S13a: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

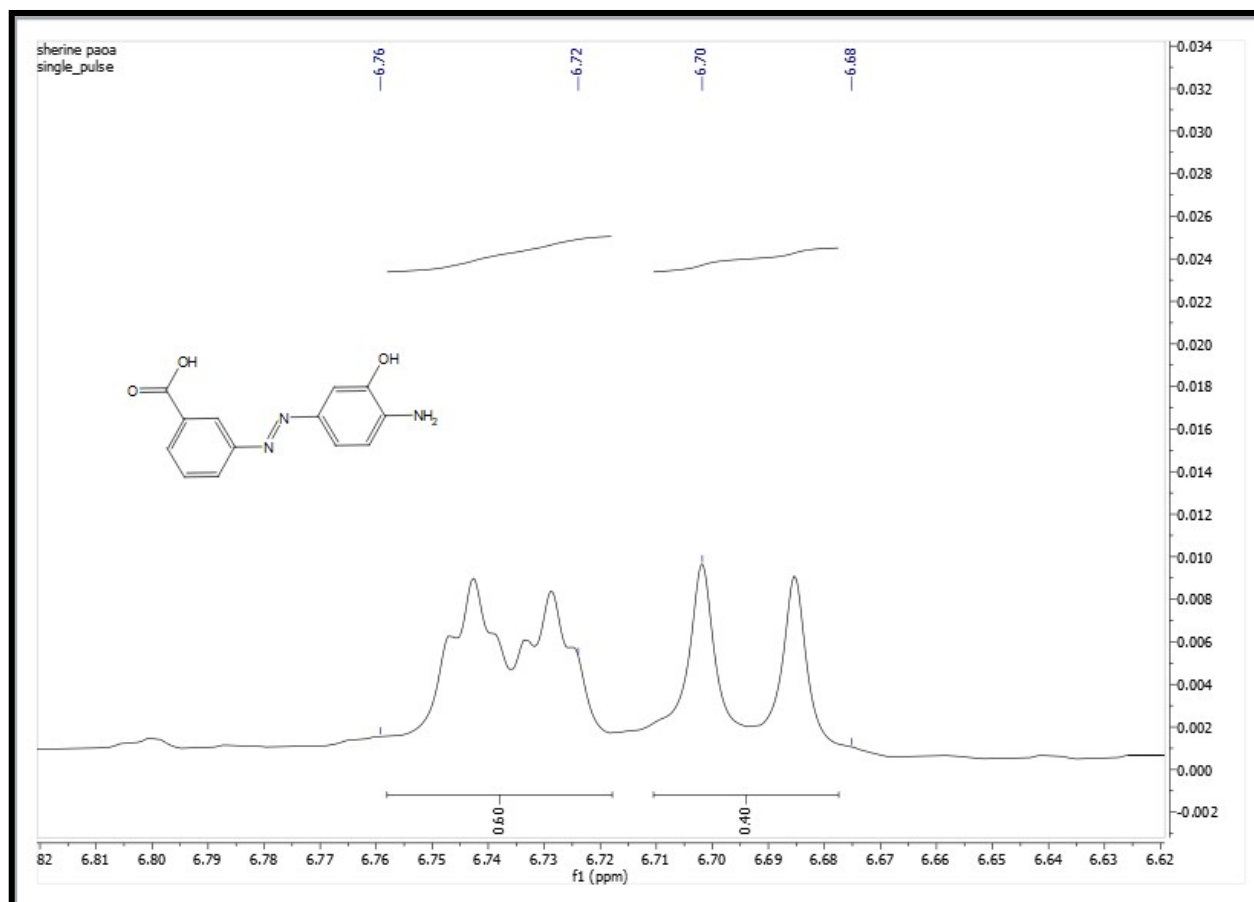


Figure S13b: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

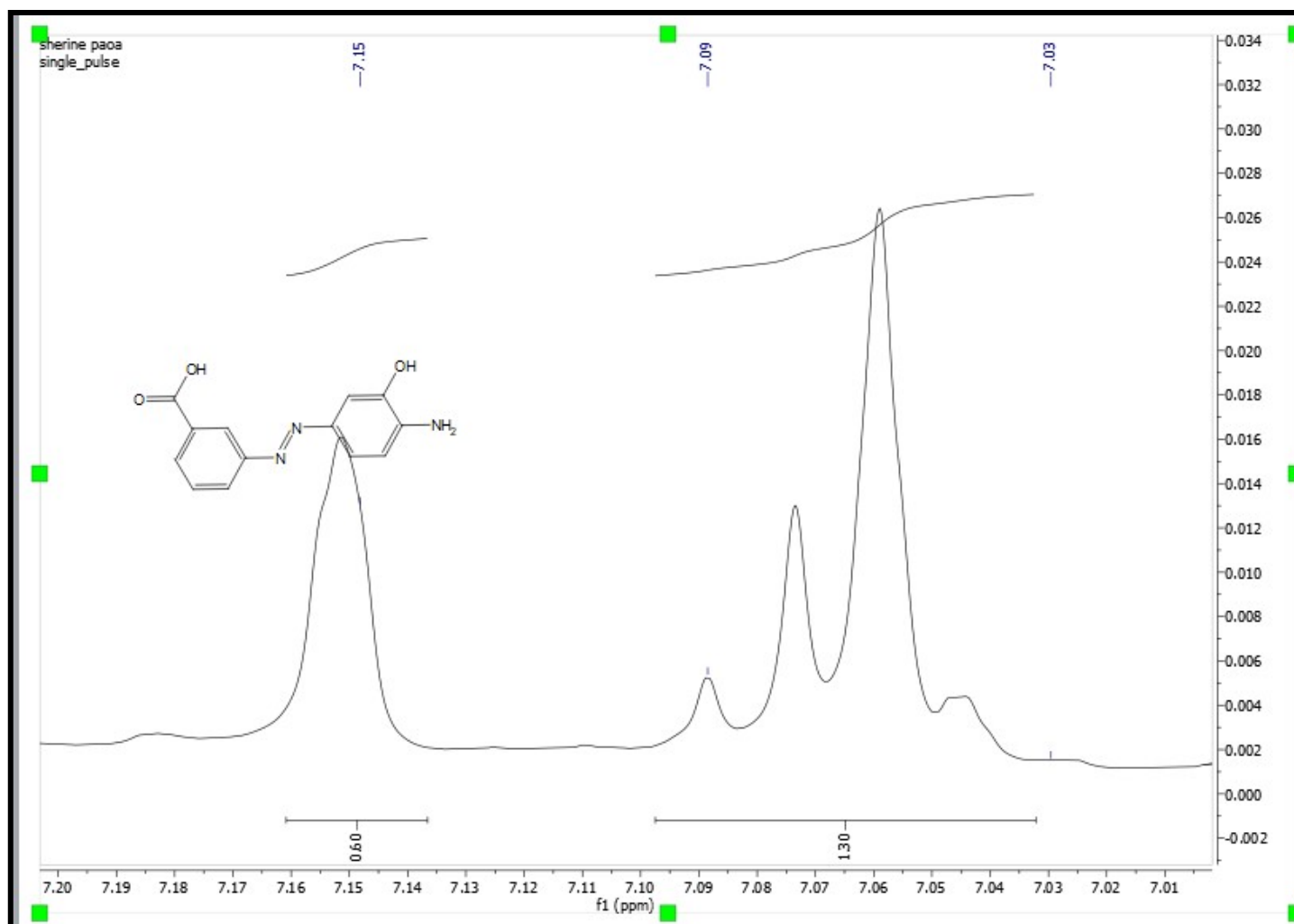


Figure S13c: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (D4)

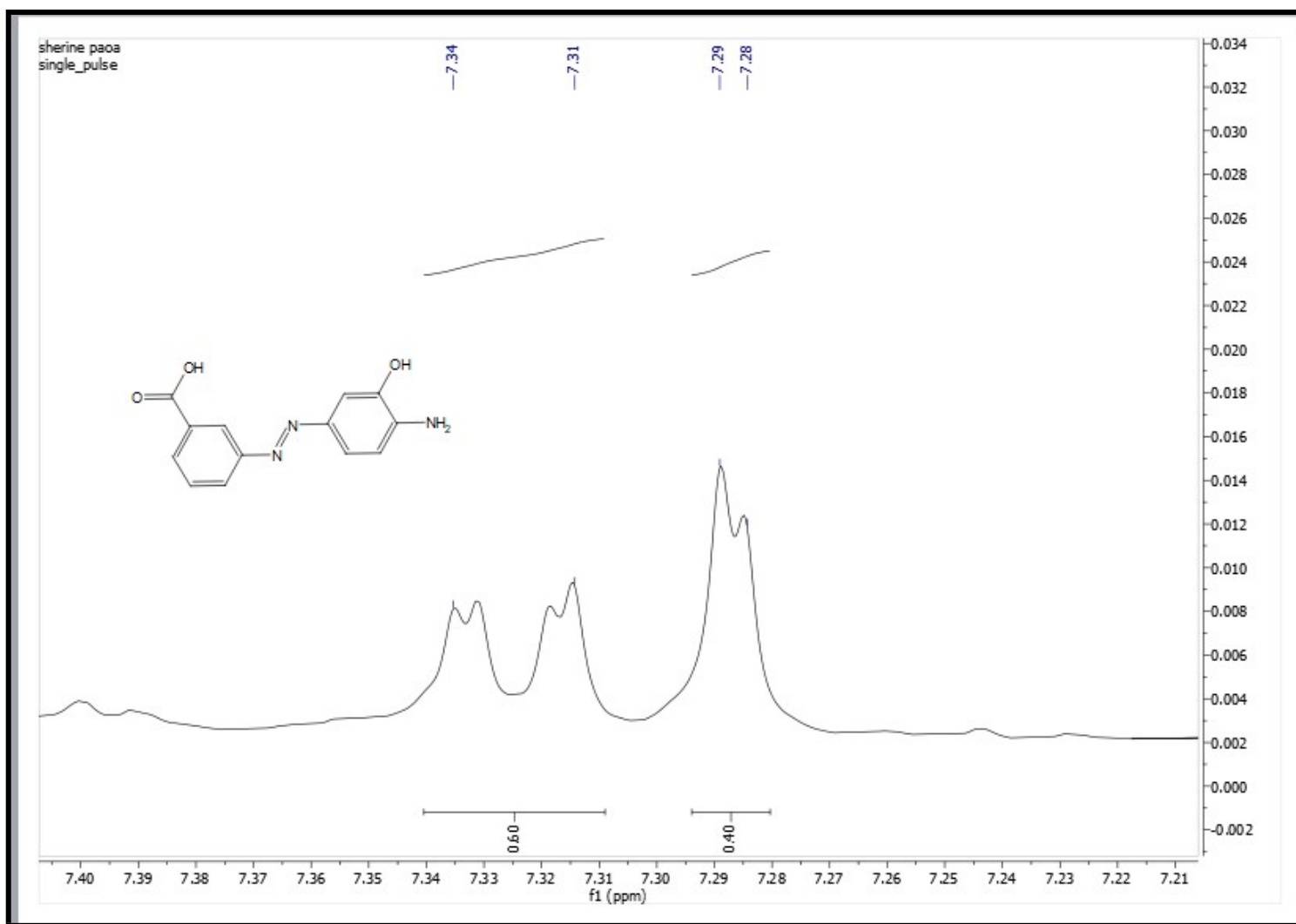


Figure S13d: ^1H -NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

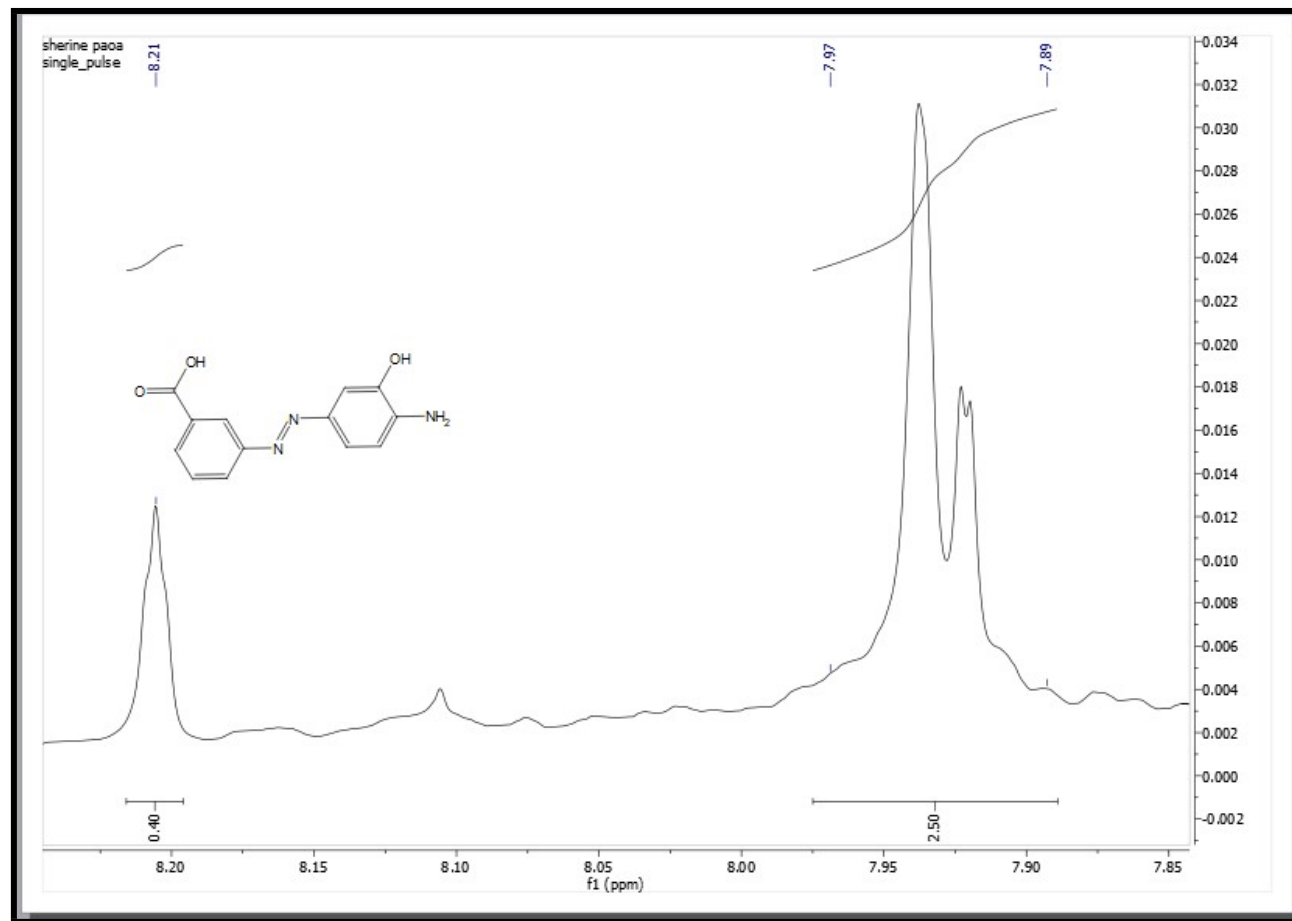


Figure S13e: ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

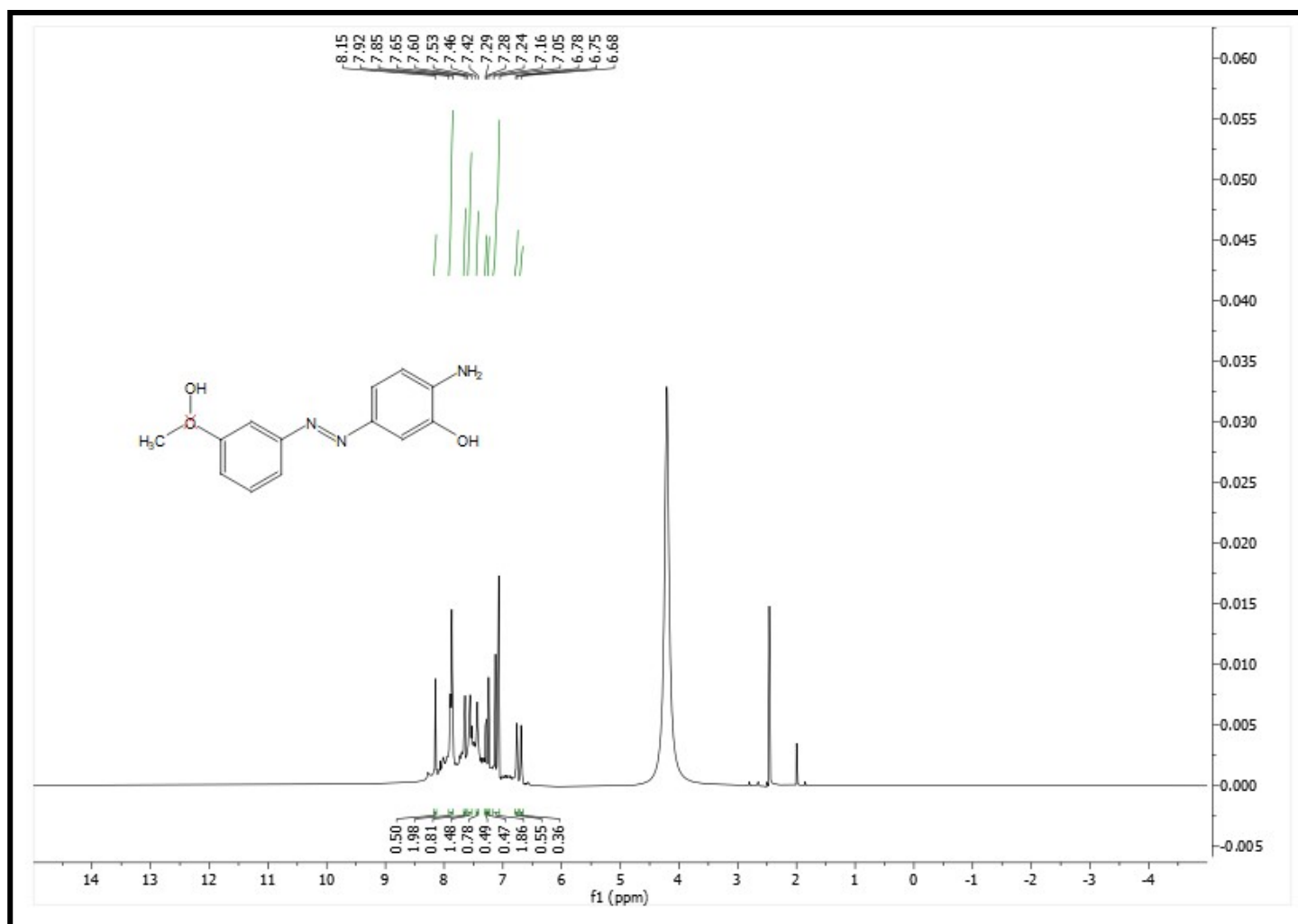


Figure S14: ¹H-NMR (500 MHz, DMSO-*d*₆/D₂O) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

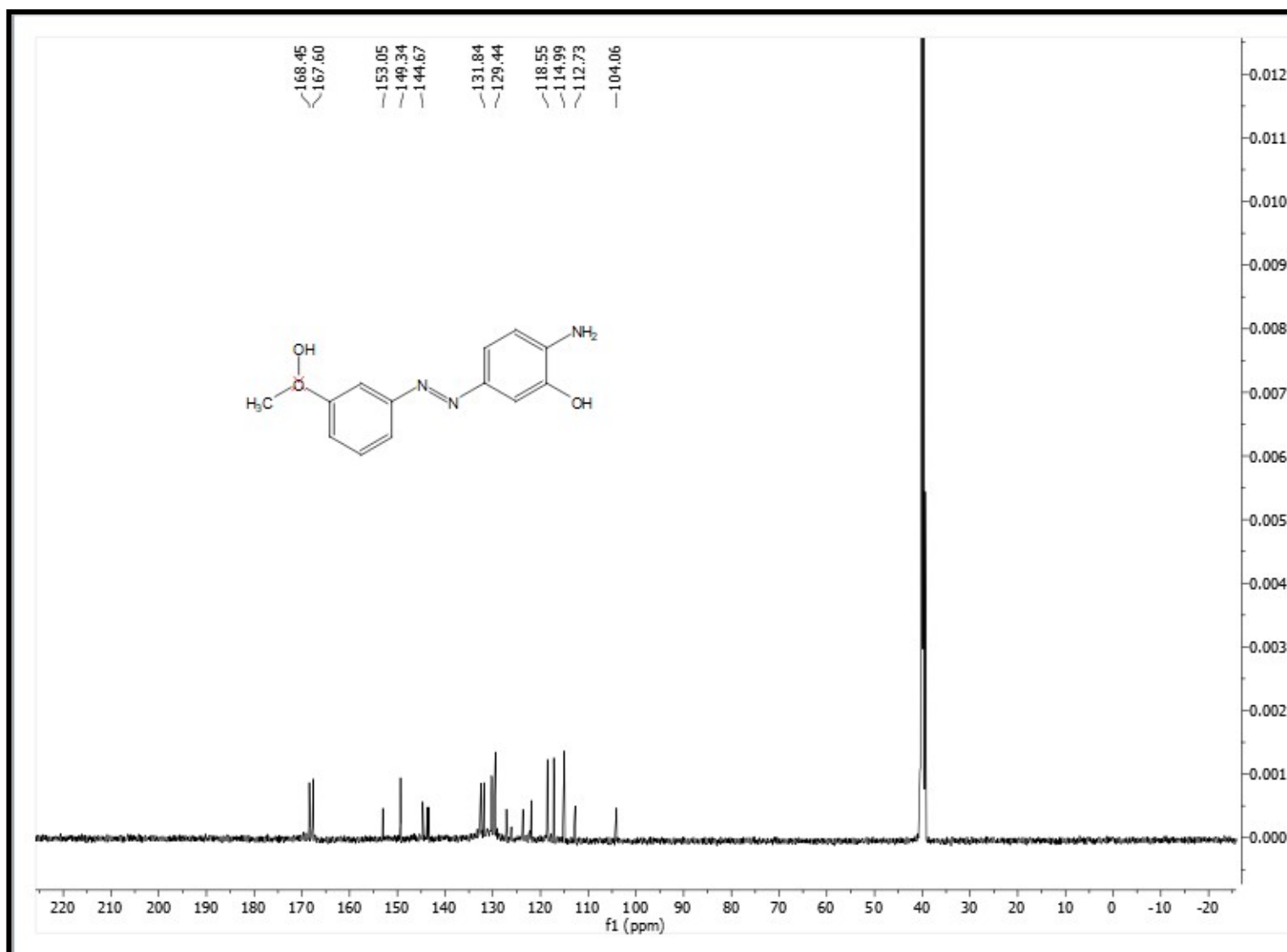


Figure S15: ¹³C-NMR (125 MHz, DMSO-*d*₆) spectrum of 3-((4-amino-3-hydroxyphenyl)diazenyl)benzoic acid (**D4**)

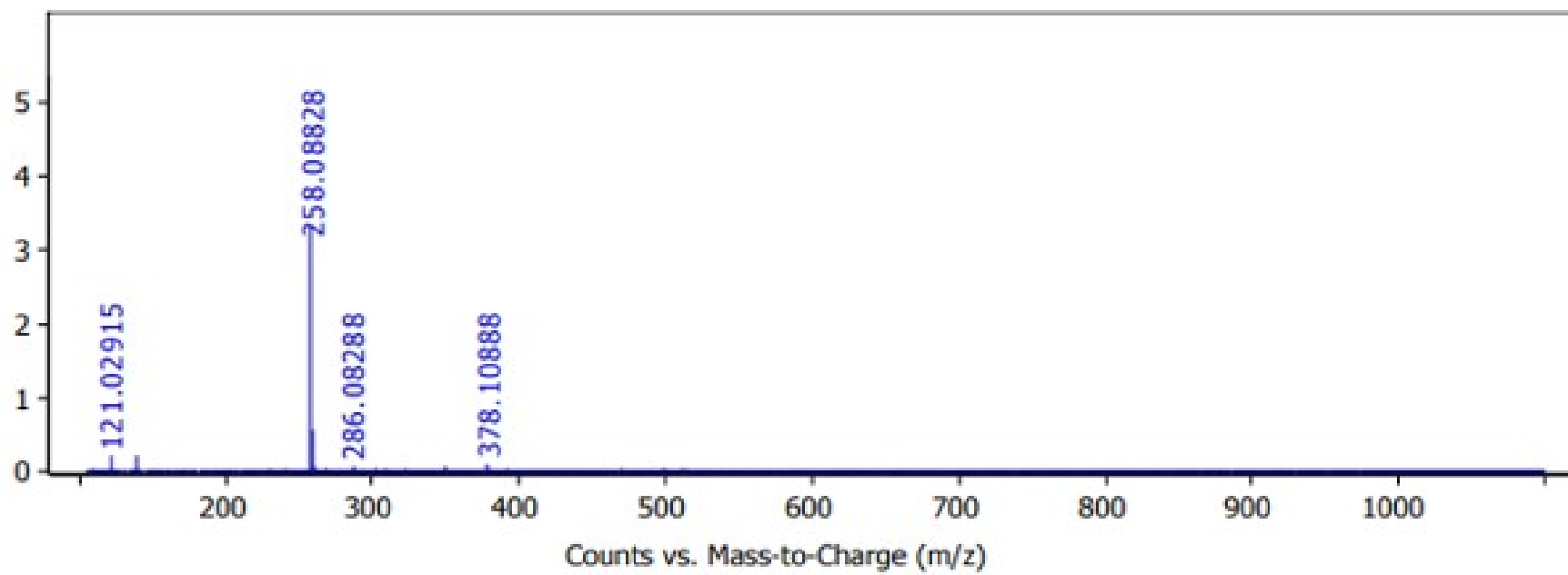


Figure S16: The High- resolution mass (HRMS) spectrum of **D4**.

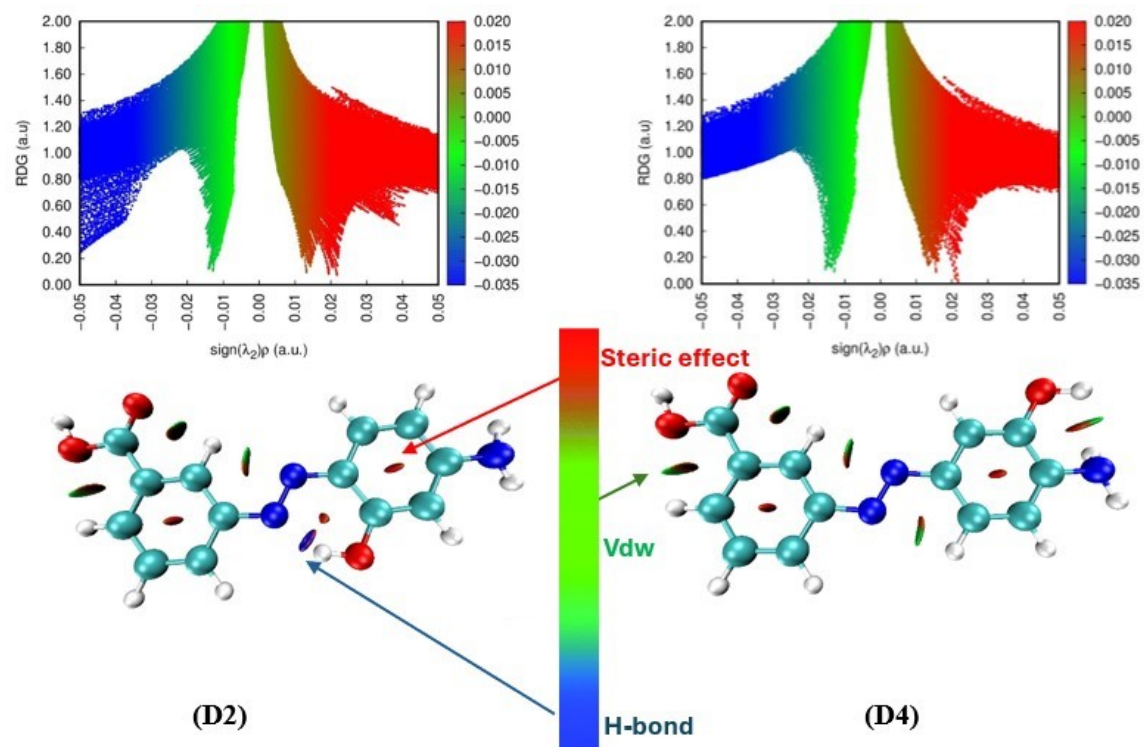


Figure S17. The reduced density gradient (RDG) scatter plot of dyes **D2** and **D4**.

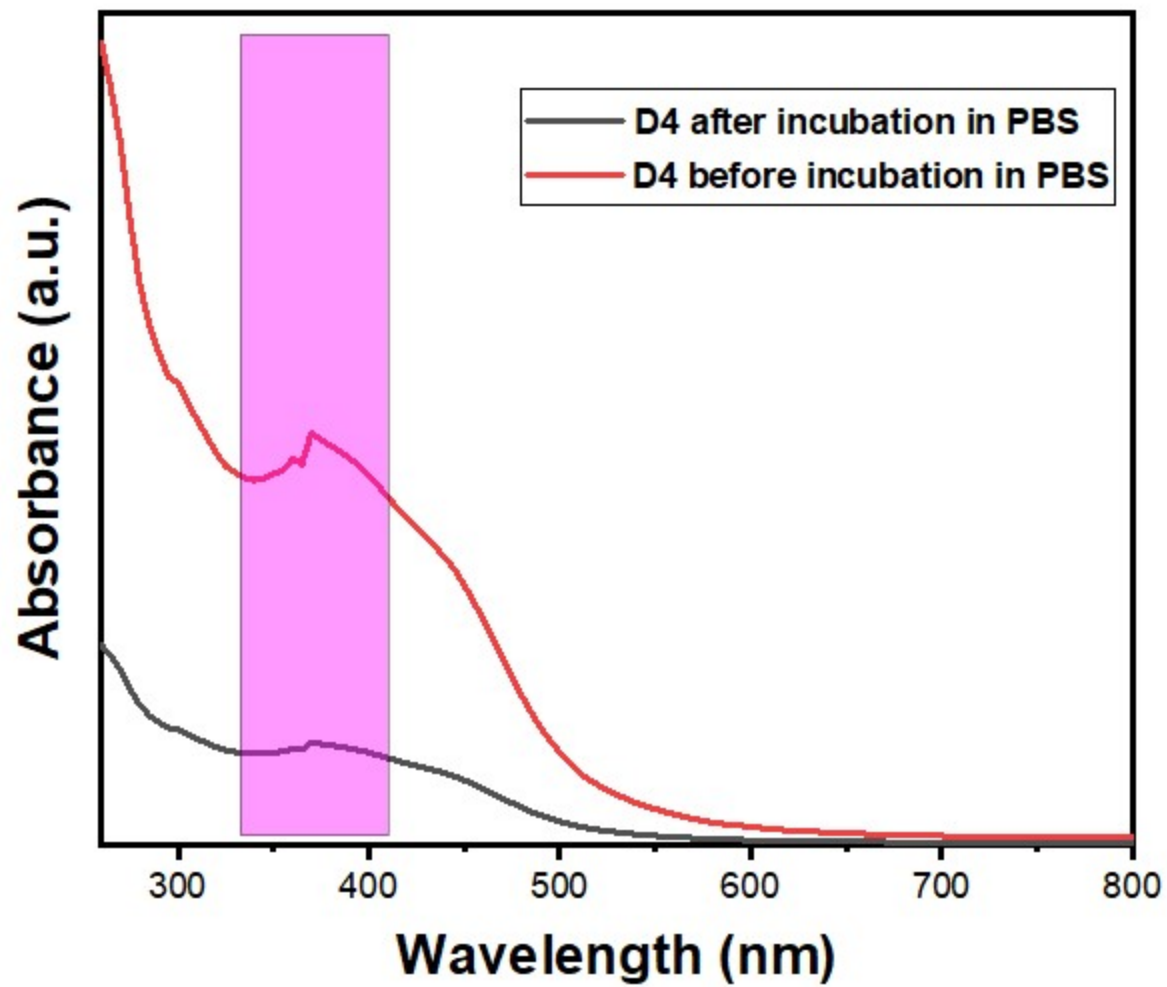


Figure S18. UV-Vis spectra of dye **D4** after and before incubation in PBS solution for 24 hours.