

Supplementary Material

Synthesis, Stability and Relaxivity of TEEPO-Met: An Organic Radical as a Potential Tumour Targeting Contrast Agent for Magnetic Resonance Imaging

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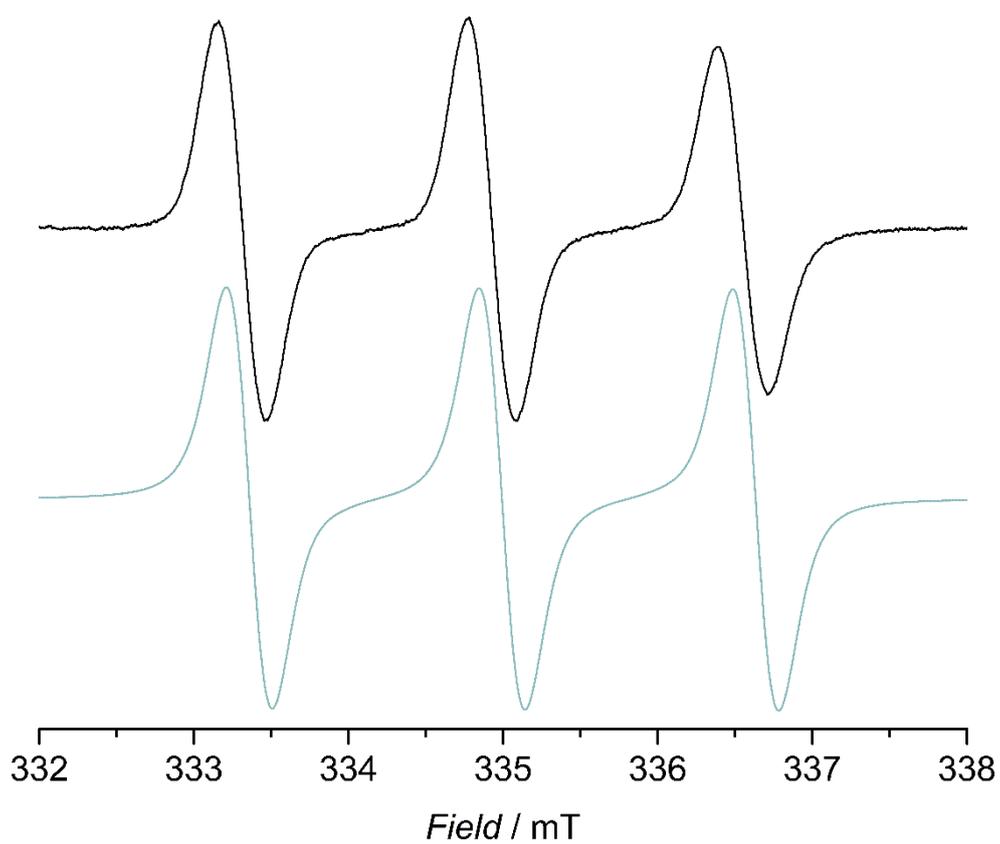


Figure S1. Solution-state X-band EPR spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetraethylpiperidin-1-oxyl (TEEPO-Met, **5**) in PBS (black) and simulated EPR spectrum (green).

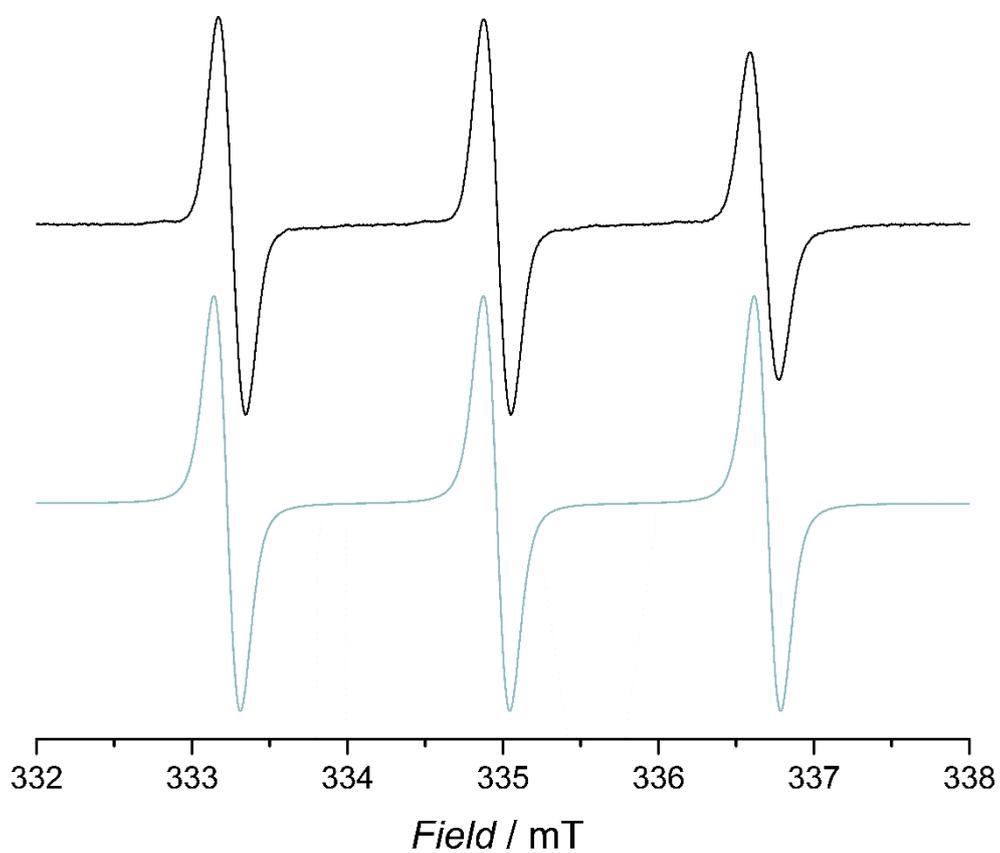


Figure S2. Solution-state X-band EPR spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO-Met, **7**) in PBS (black) and simulated EPR spectrum (green).

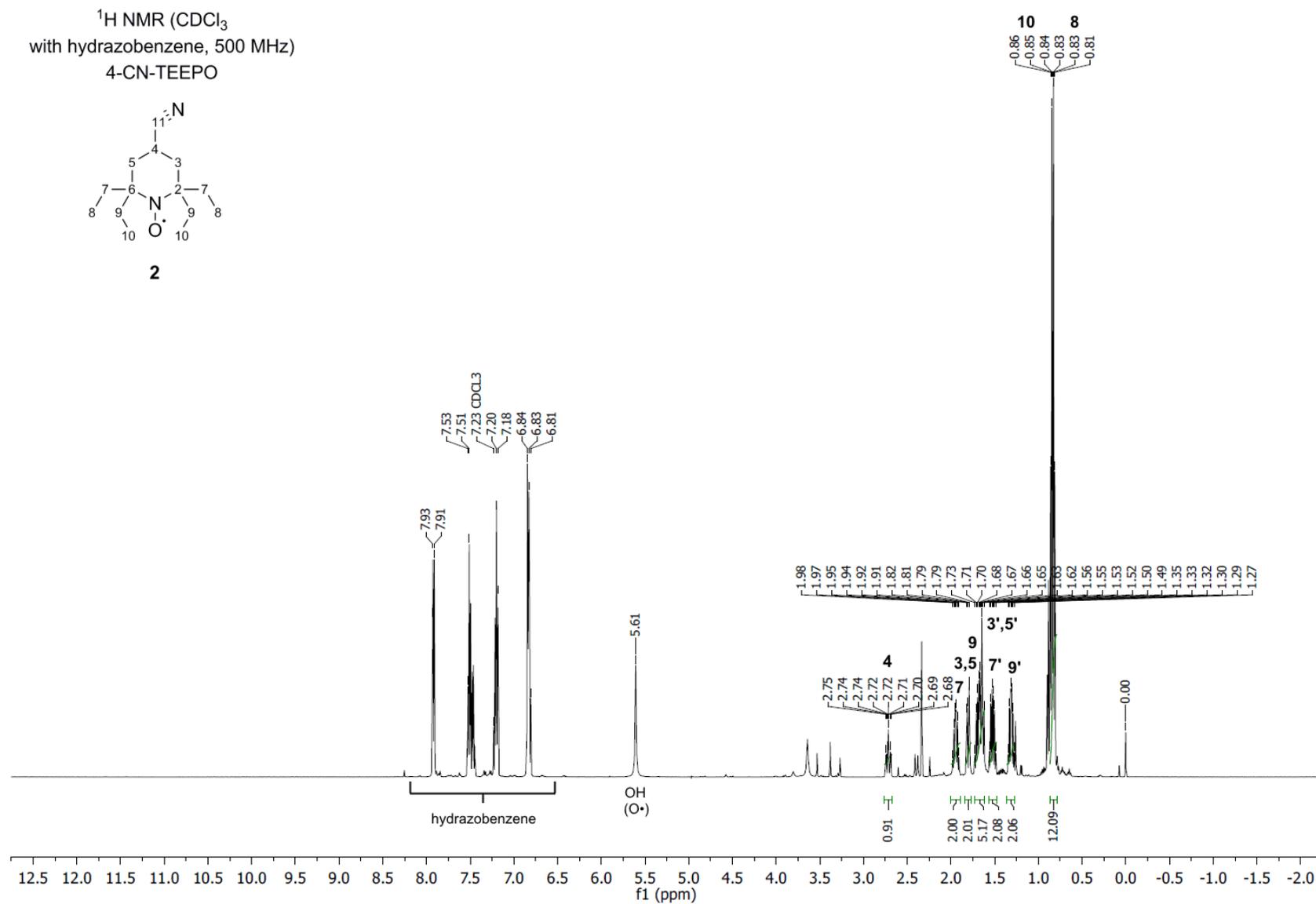


Figure S3. ¹H spectrum of 4-Carbonitrile-2,2,6,6-tetraethylpiperidin-1-oxyl (4-CN-TEEPO, **2**) in CDCl₃.

^{13}C NMR (CDCl_3)
with hydrazobenzene, 126 MHz
4-CN-TEEPO

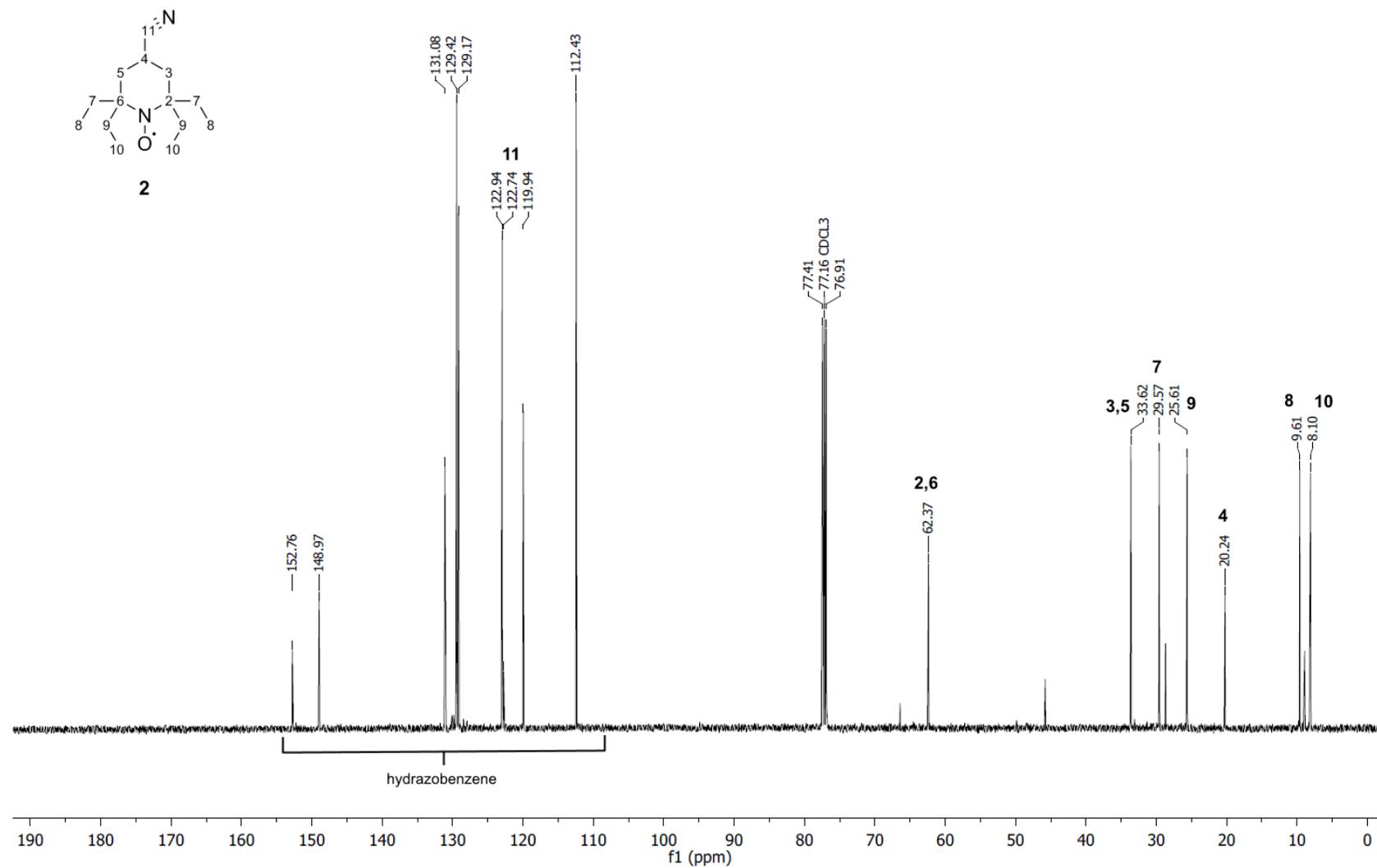


Figure S4. ^{13}C spectrum of 4-Carbonitrile-2,2,6,6-tetraethylpiperidin-1-oxyl ((4-CN-TEEPO, 2) in CDCl_3 .

^1H NMR (CD_3OD
with hydrazobenzene, 500 MHz)
4-COOH-TEEPO

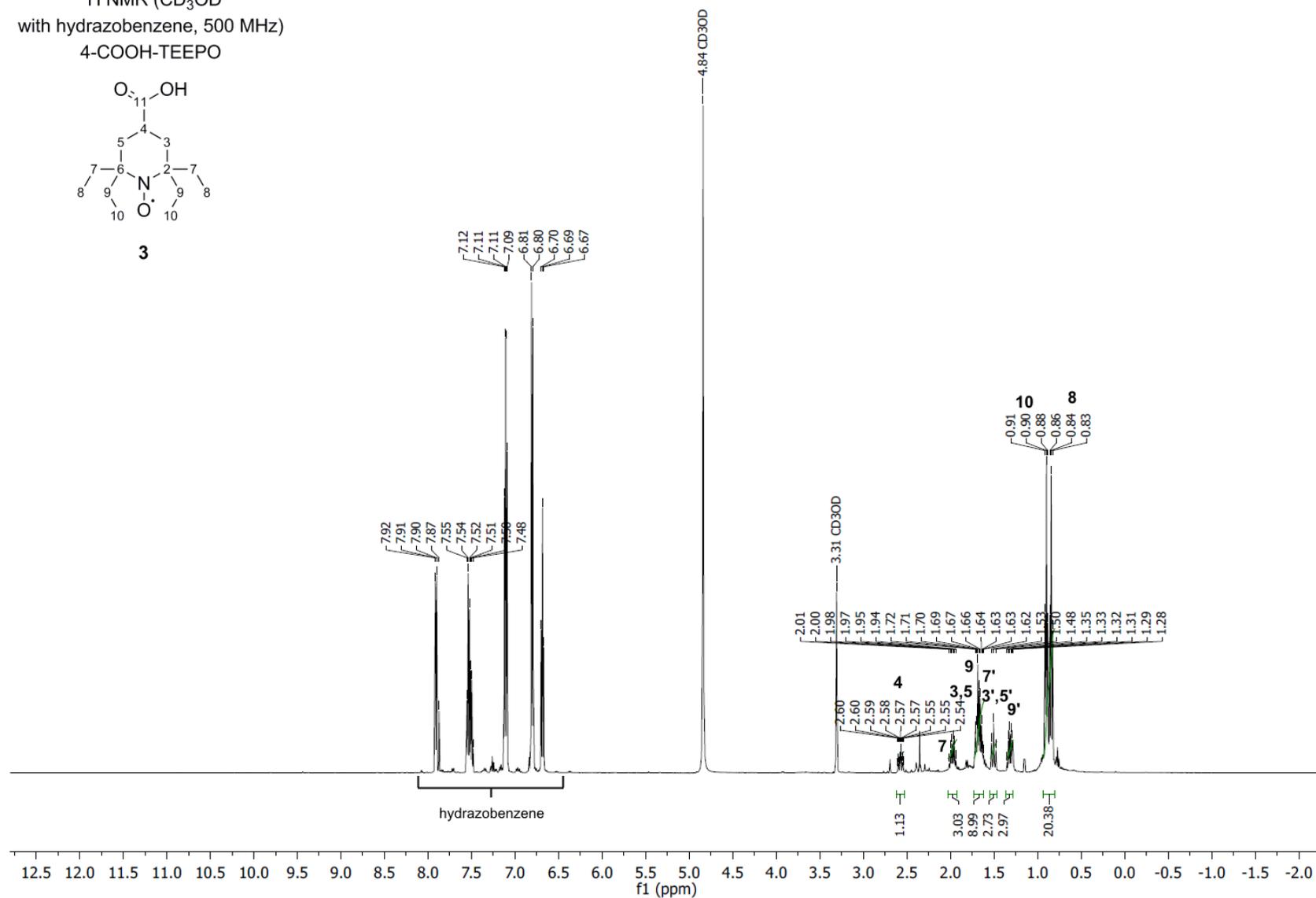
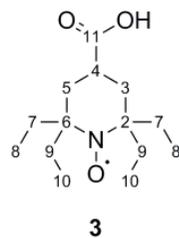


Figure S5. ^1H spectrum of 4-Carboxy-2,2,6,6-tetraethylpiperidin-1-oxyl (4-COOH-TEEPO, **3**) in CD_3OD .

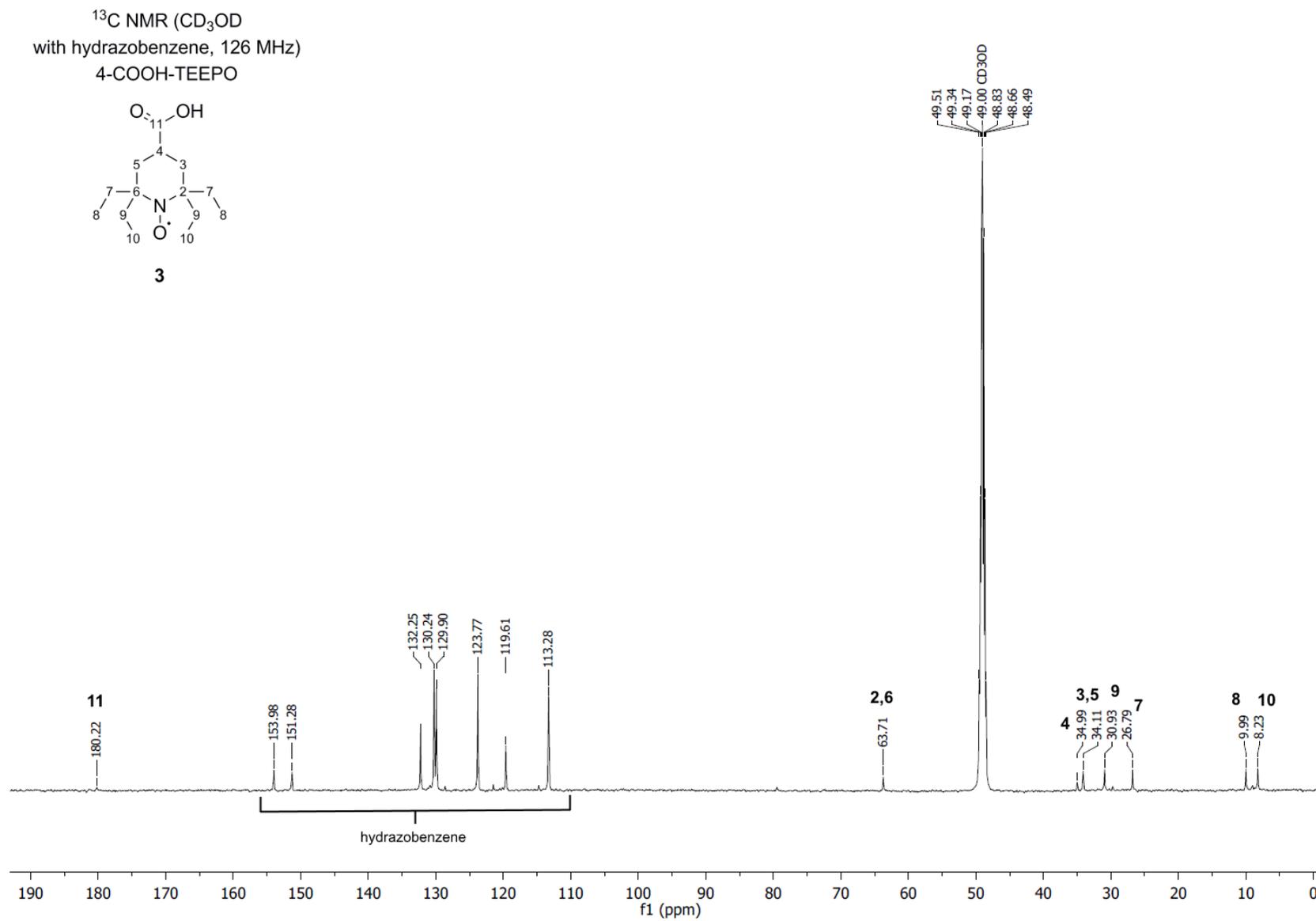


Figure S6. ¹³C spectrum of 4-Carboxy-2,2,6,6-tetraethylpiperidin-1-oxyl (4-COOH-TEEPO, **3**) in CD₃OD.

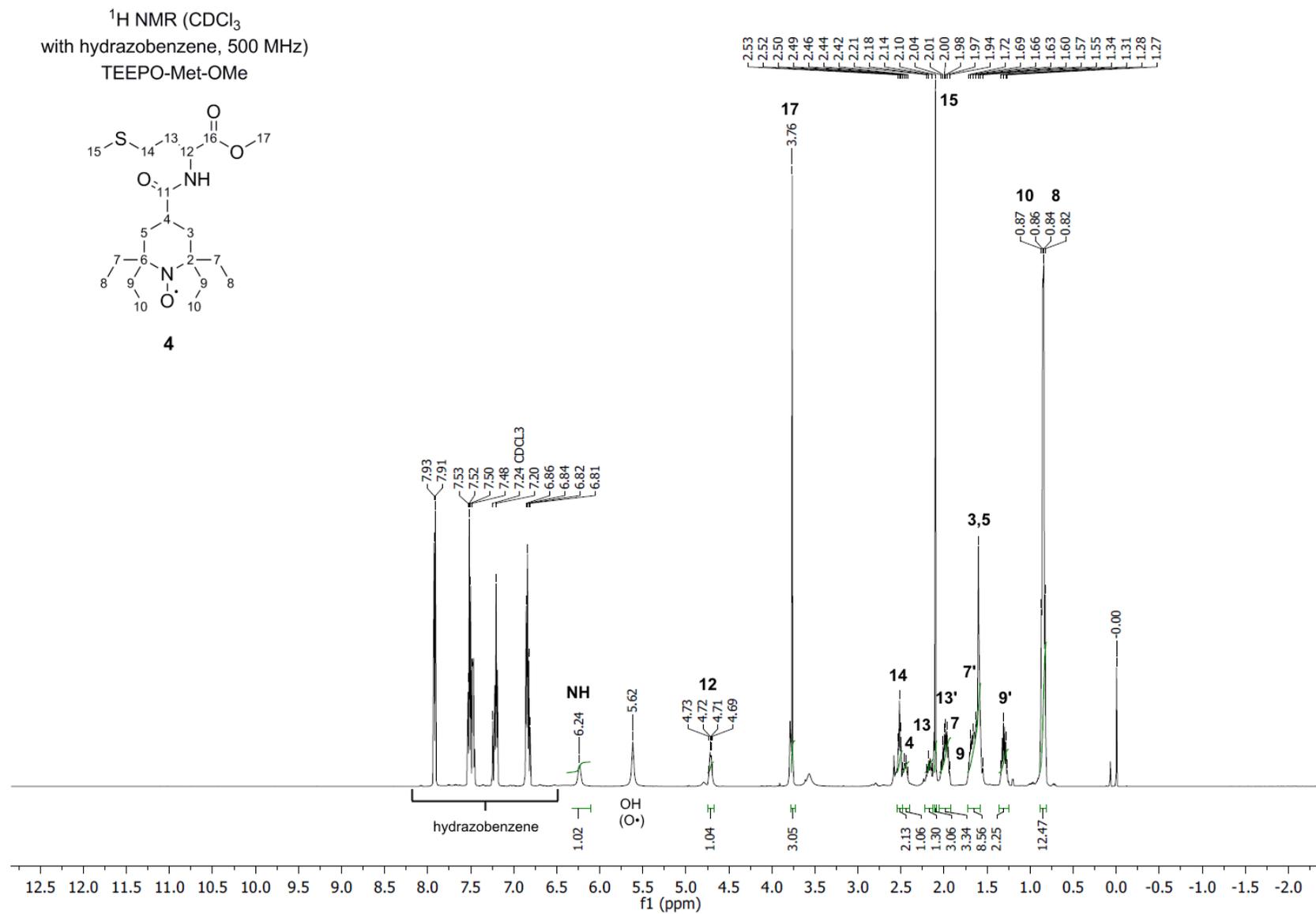


Figure S7. ¹H spectrum of 4-[(L-Methionine methyl ester)carbonyl]-2,2,6,6-tetraethylpiperidin-1-oxyl (TEEPO-Met-OMe, **4**) in CDCl₃.

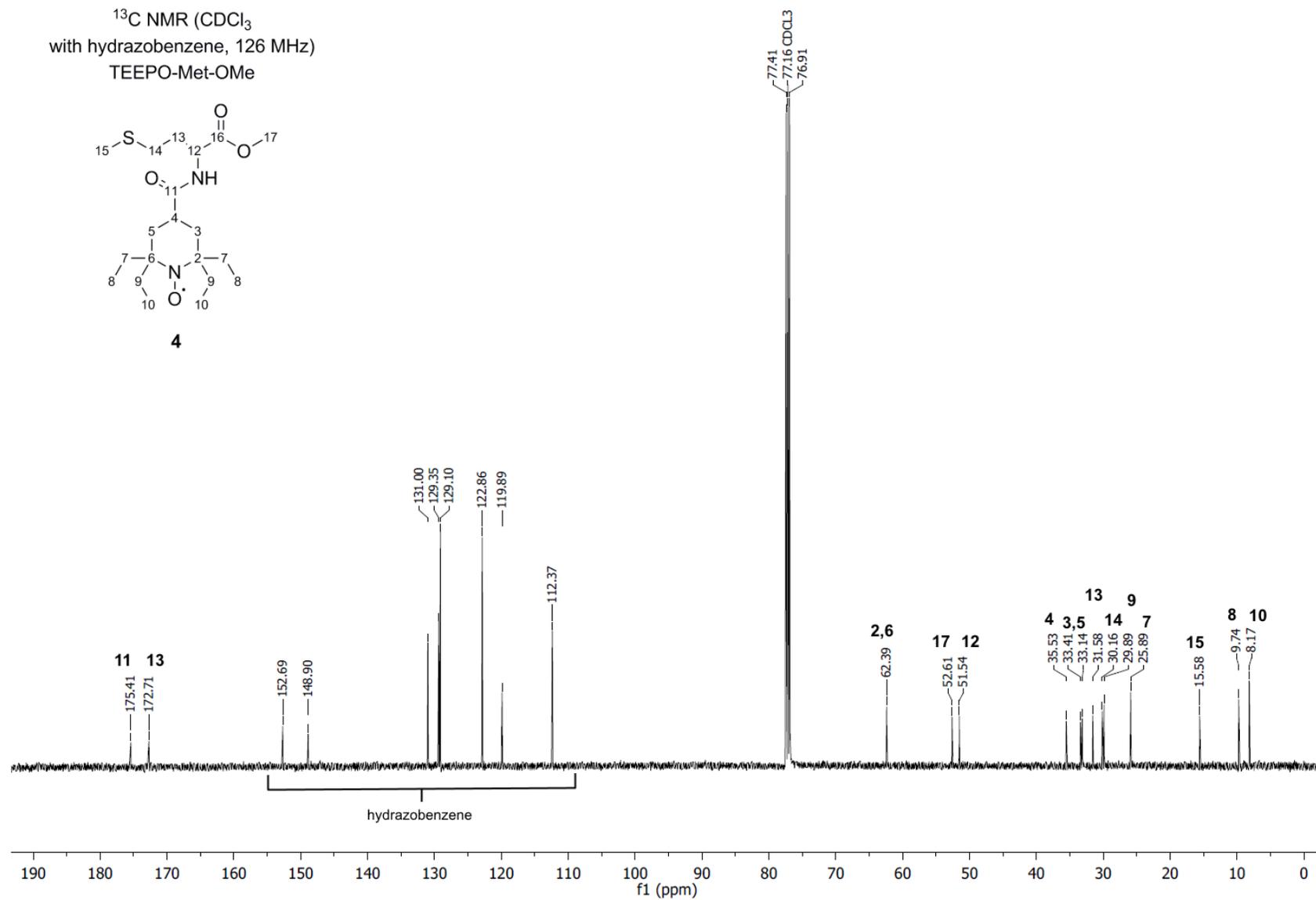


Figure S8. ¹³C spectrum of 4-[(L-Methionine methyl ester)carbonyl]-2,2,6,6-tetraethylpiperidin-1-oxyl (TEEPO-Met-OMe, **4**) in CDCl₃.

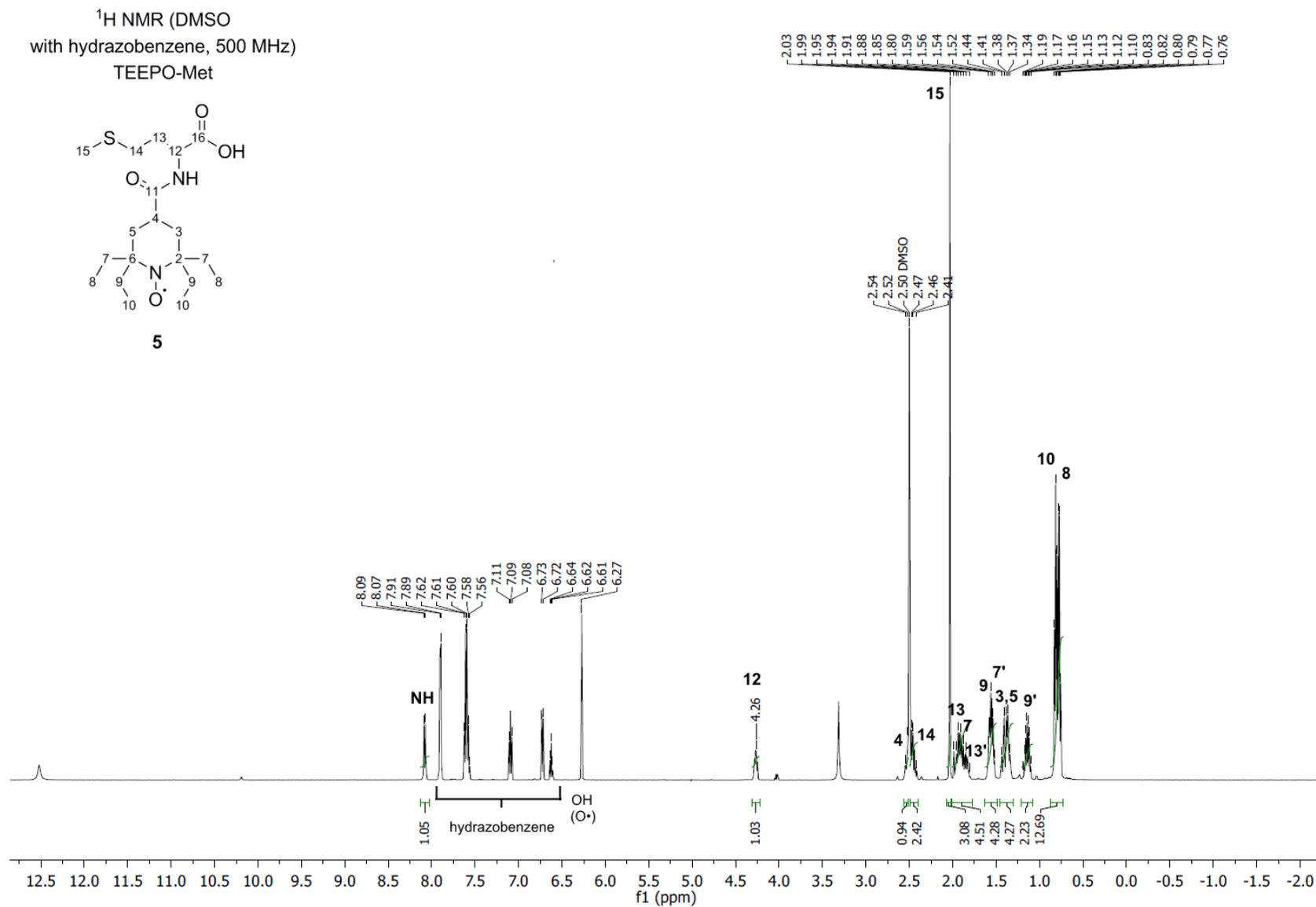


Figure S9. ¹H spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetraethylpiperidin-1-oxyl (TEEPO-Met, **5**) in DMSO.

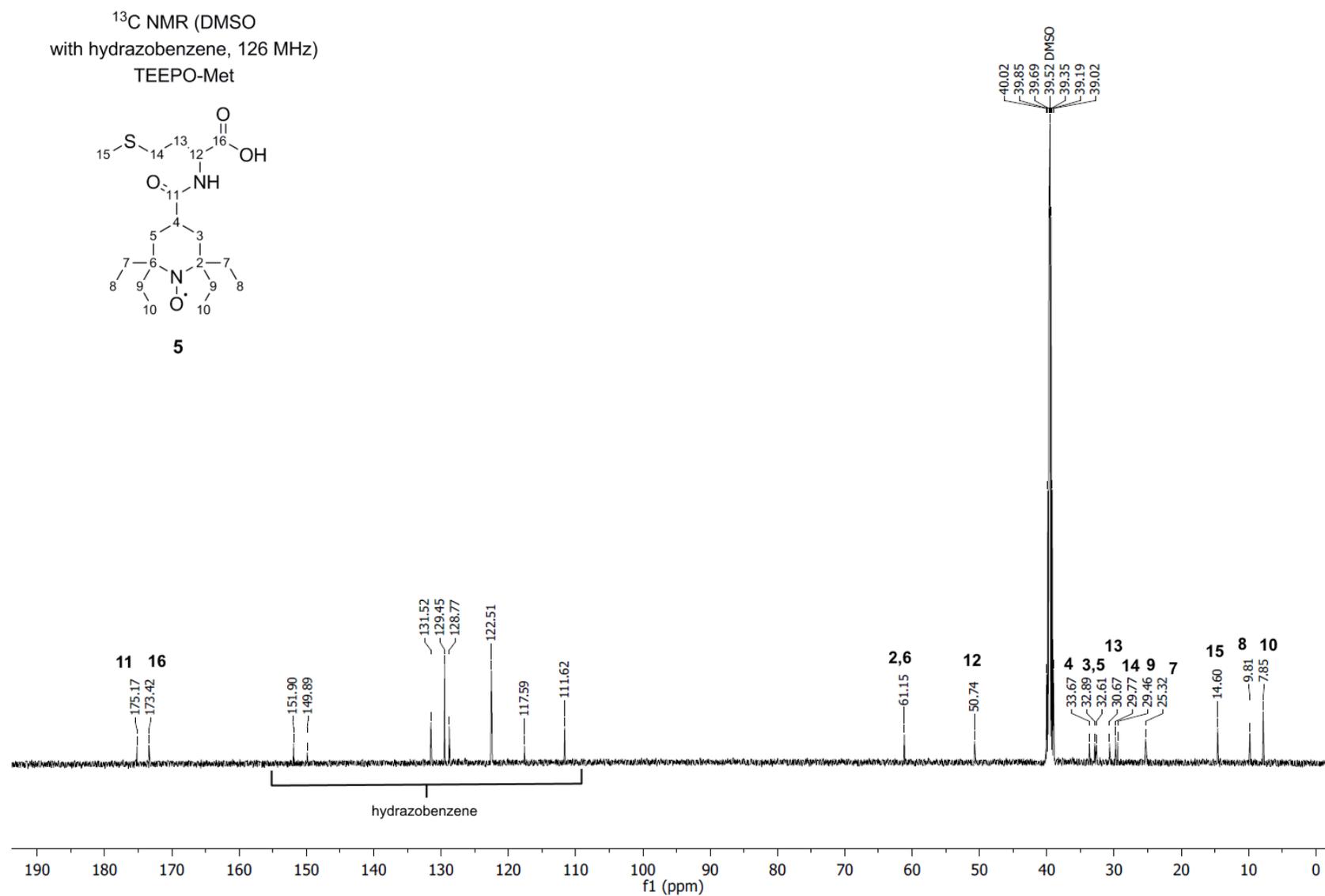


Figure S10. ¹³C spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetraethylpiperidin-1-oxyl (TEEPO-Met, **5**) in DMSO.

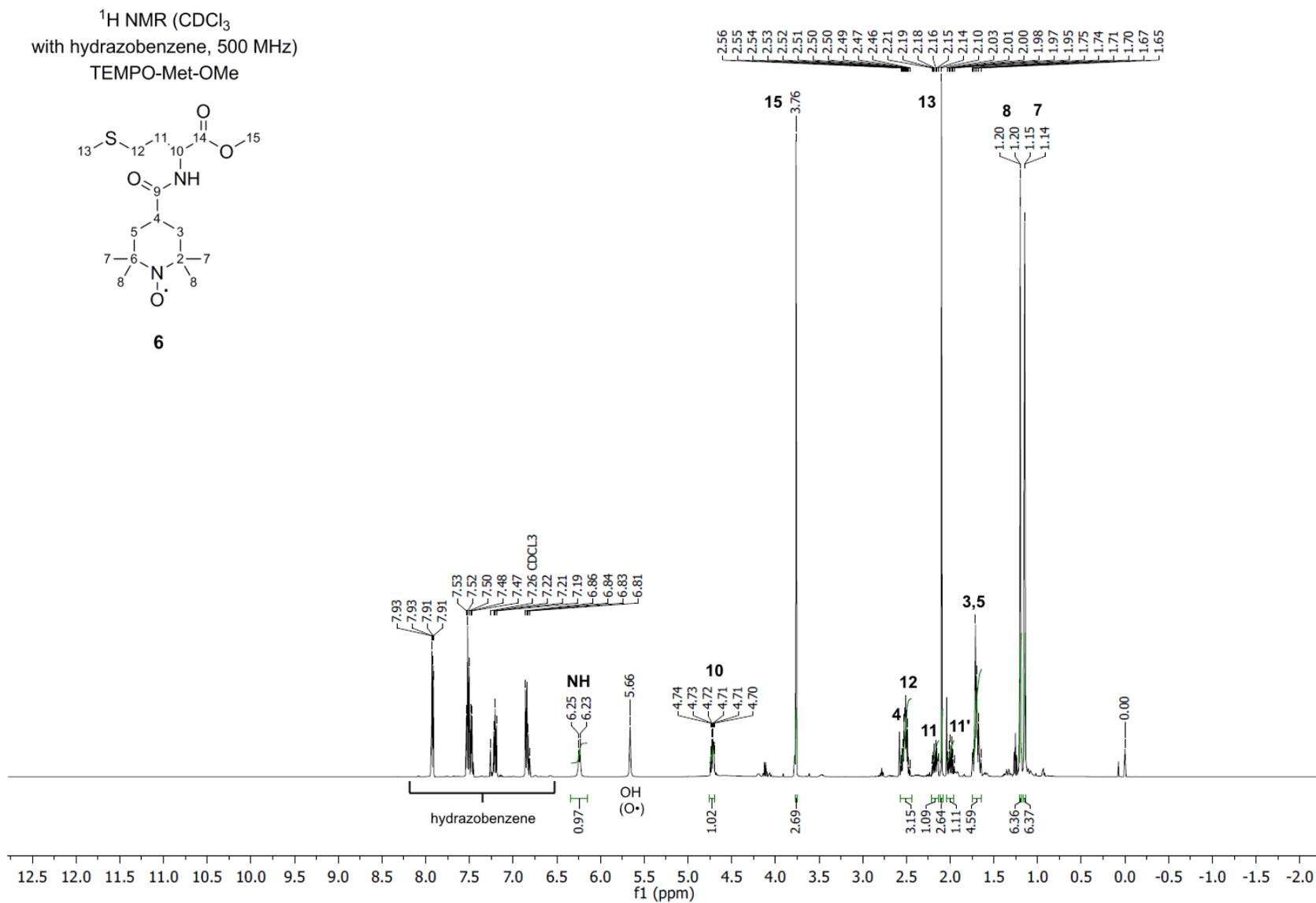


Figure S11. ¹H spectrum of 4-[(L-Methionine methyl ester)carbonyl]-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO-Met-OMe, **6**) in CDCl₃.

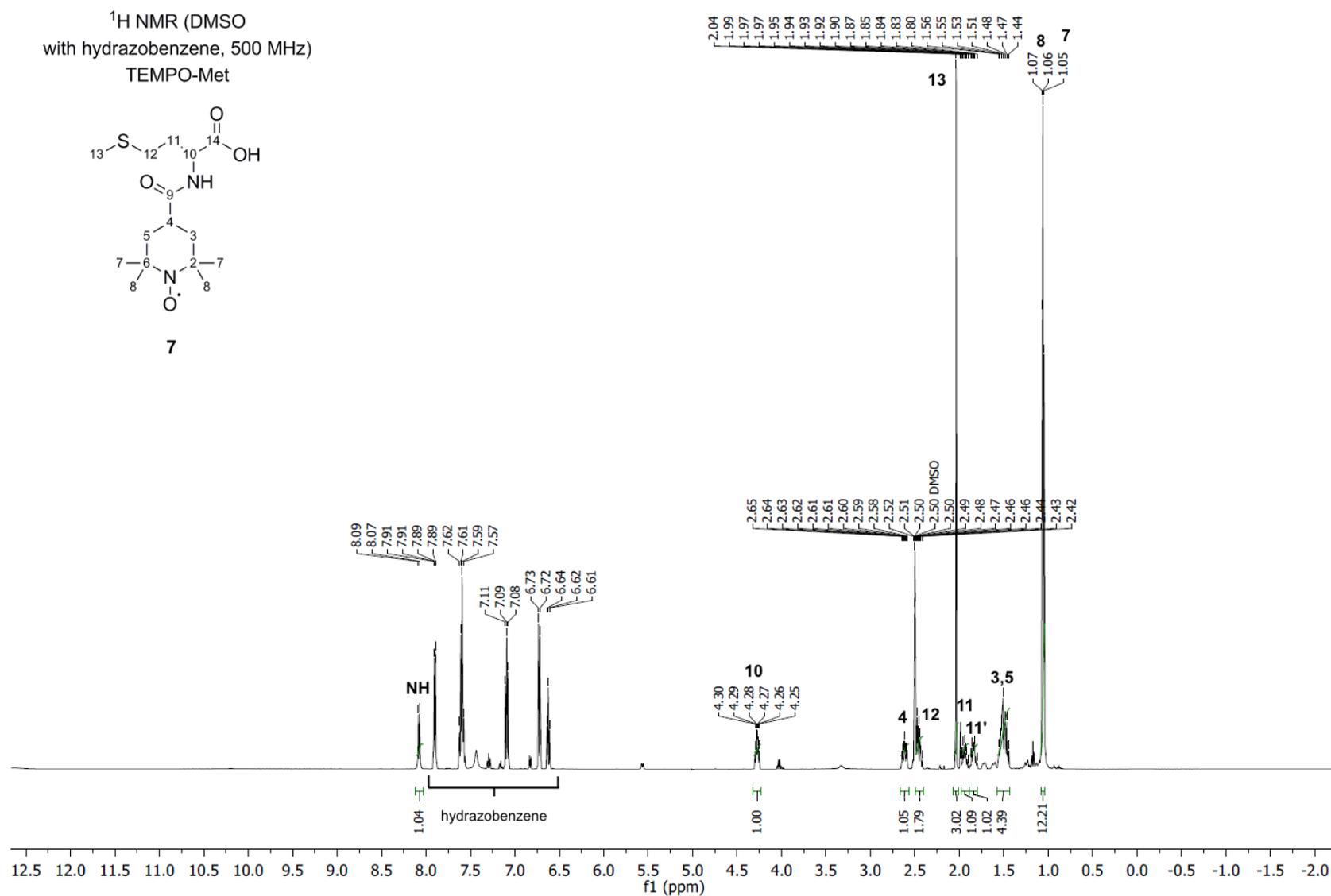


Figure S13. ¹H spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO-Met, 7) in DMSO.

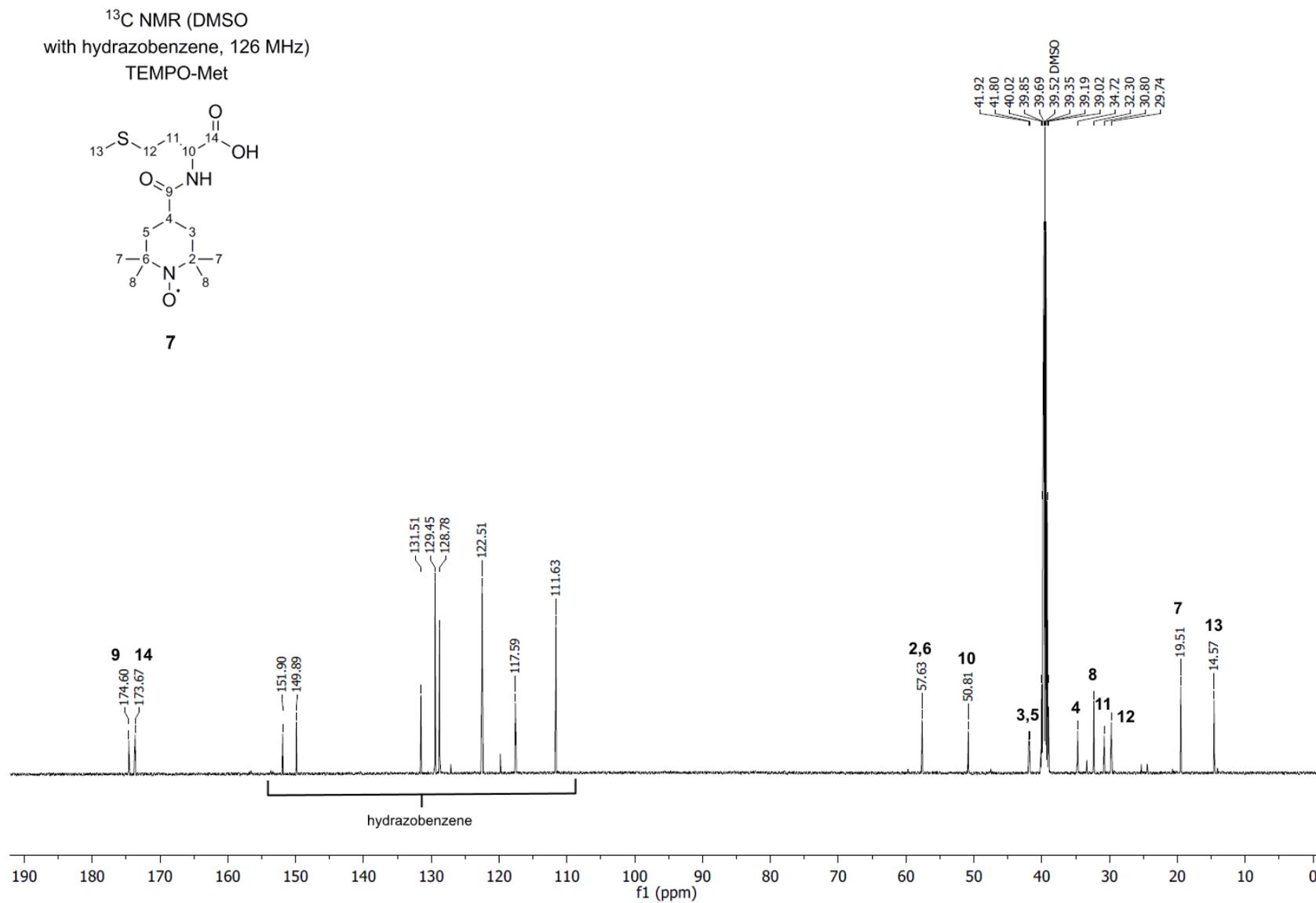


Figure S14. ¹³C spectrum of 4-[(L-Methionine)carbonyl]-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO-Met, 7) in DMSO.