Supplementary Information

Two Novel Donepezil-Lipoic Acid Hybrids: Synthesis, Anticholinesterase and Antioxidant Activities and Theoretical Studies

Bruna S. Terra,[a] Pedro H. C. da Silva,[a] Anna Tramarin,[b] Lucas L. Franco,[a] Elaine F. F. da Cunha,[c] Fernando Macedo Junior,[d] Teodorico C. Ramalho,[c] Manuela Bartolini,[b] Maria L. Bolognesi[b] and Ângelo de Fátima*[a]

[a]Departamento de Química, Universidade Federal de Minas Gerais (UFMG), Av. Pres. Antônio Carlos, 6627, 31270-901 Belo Horizonte-MG, Brazil

[b]Department of Pharmacy and Biotechnology, Alma Mater Studiorum University of Bologna, via Belmeloro, 6, 40126 Bologna, Italy

[c]Departamento de Química, Universidade Federal de Lavras (UFLA), Av. Doutor Sylvio Menicucci, 1001, Kennedy, 37200-000 Lavras-MG, Brazil

[d]Departamento de Química, Universidade Estadual de Londrina (UEL), Rodovia Celso Garcia Cid, Pr 445, km 380, 86057-970 Londrina-PR, Brazil

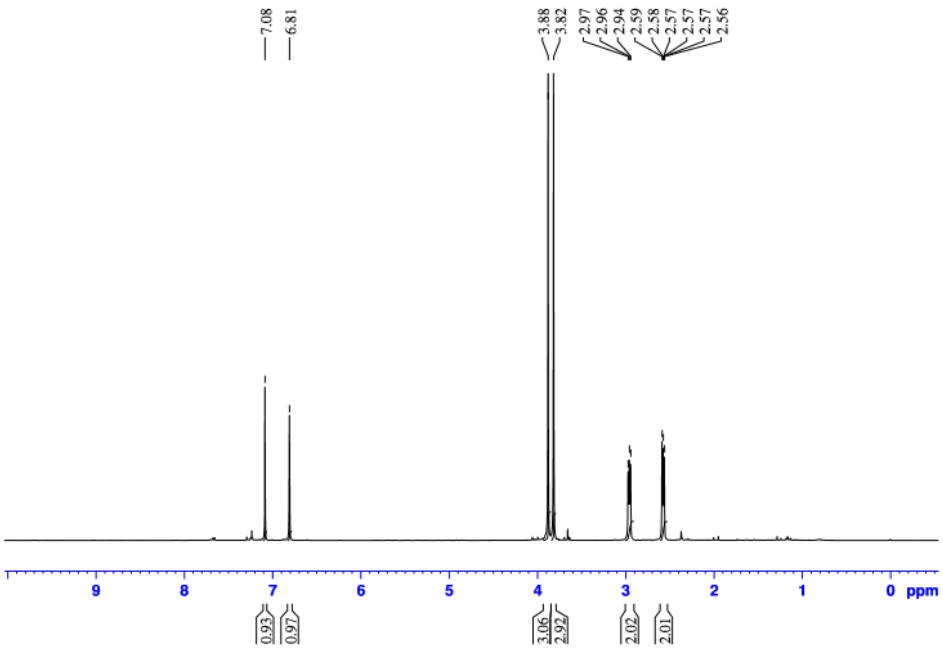

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound (**6**).

*e-mail: adefatima@qui.ufmg.br

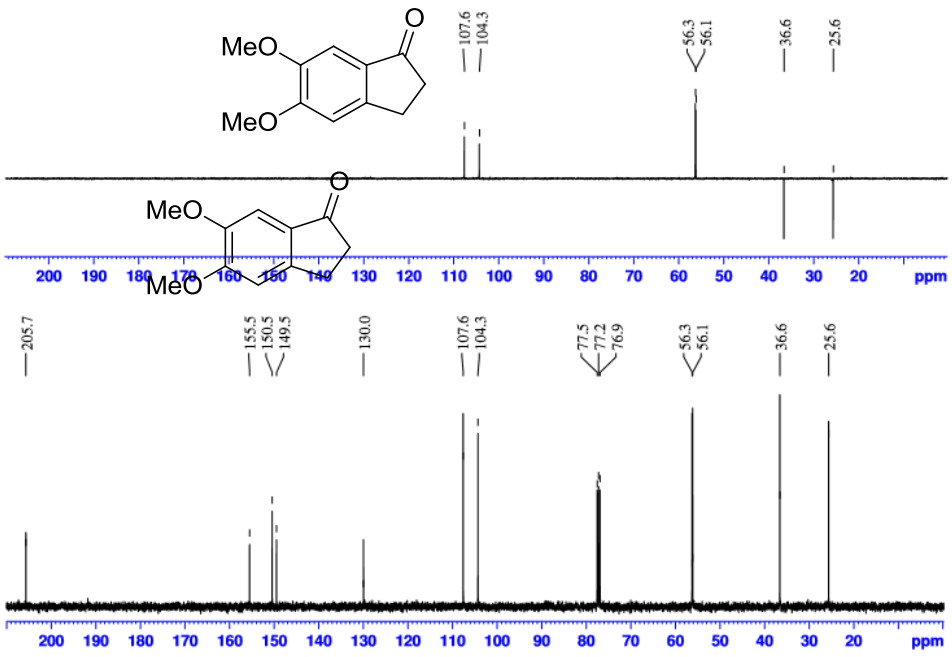

Figure S2. ^{13}C NMR spectrum (down) and DEPT 135 (up) (100 MHz, $CDCl_3$) of compound (**6**).

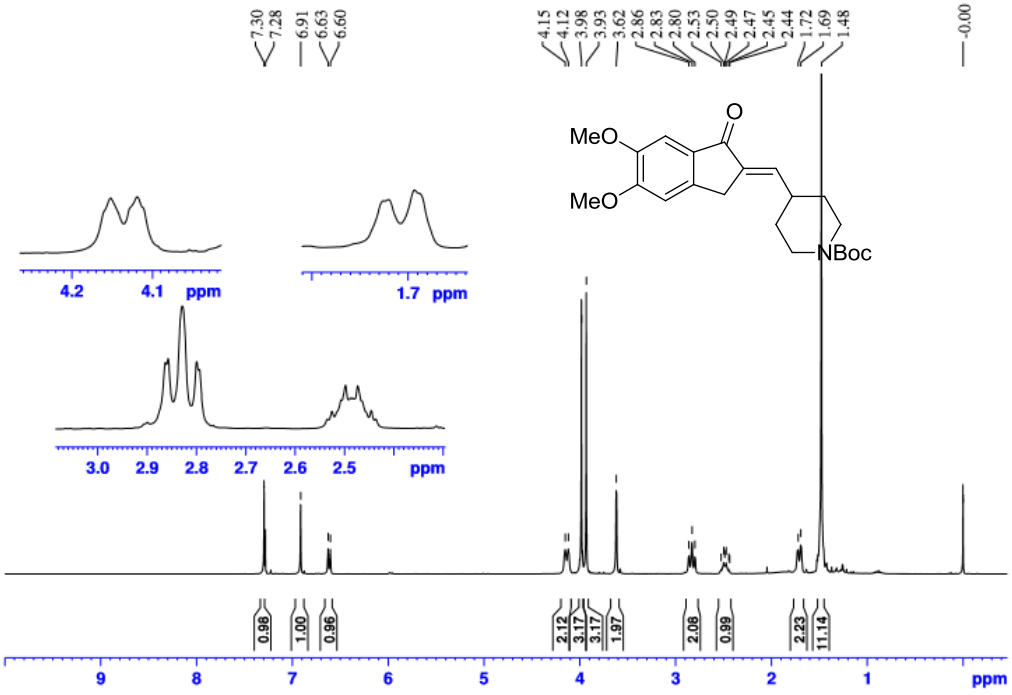

Figure S3. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound (**7**).

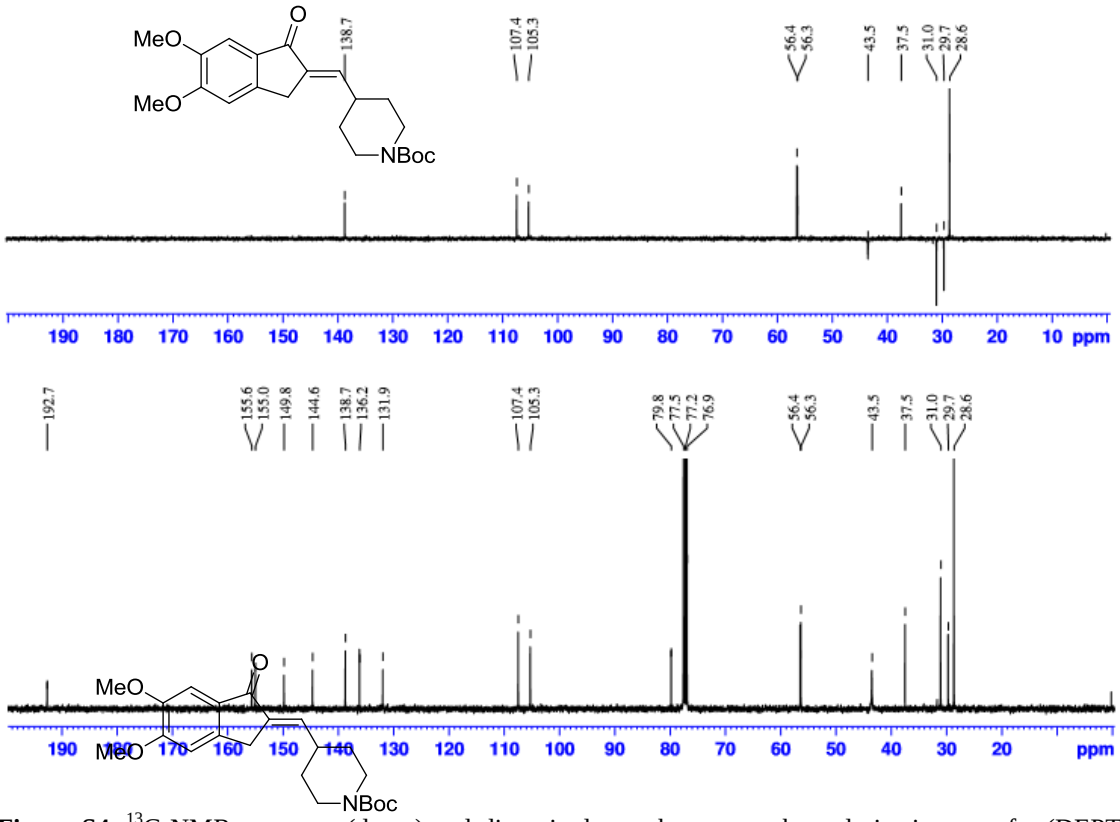

Figure S4. ^{13}C NMR spectrum (down) and distortionless enhancement by polarization transfer (DEPT) 135 (up) (50 MHz, $CDCl_3$) of compound (**7**).

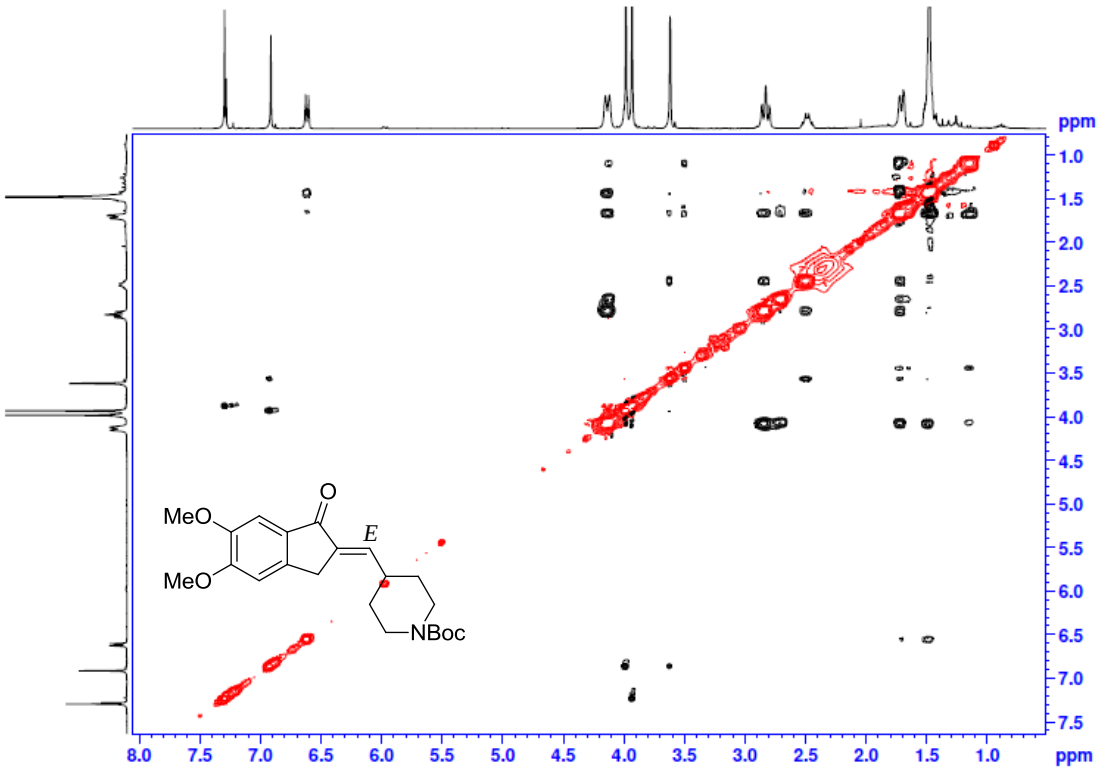

Figure S5. Nuclear Overhauser effect (NOESY) spectrum (400 MHz, $CDCl_3$) of compound (**7**).

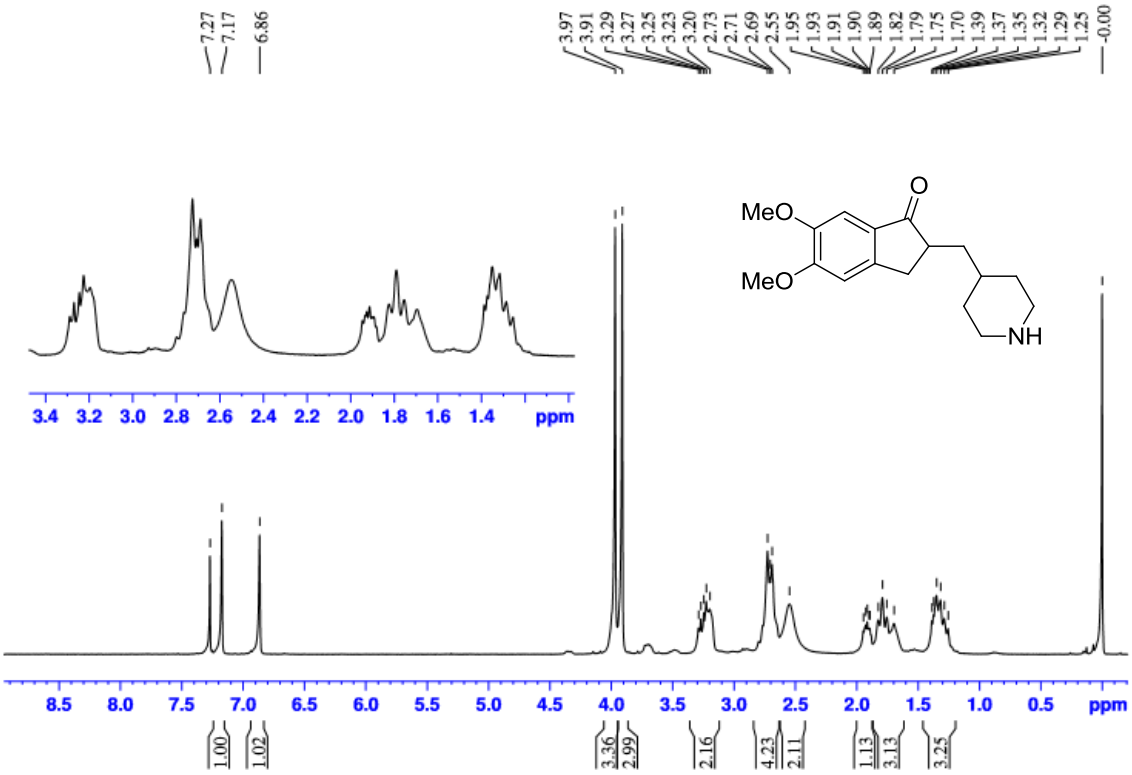

Figure S6. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound (**4**).

Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound (**1**).

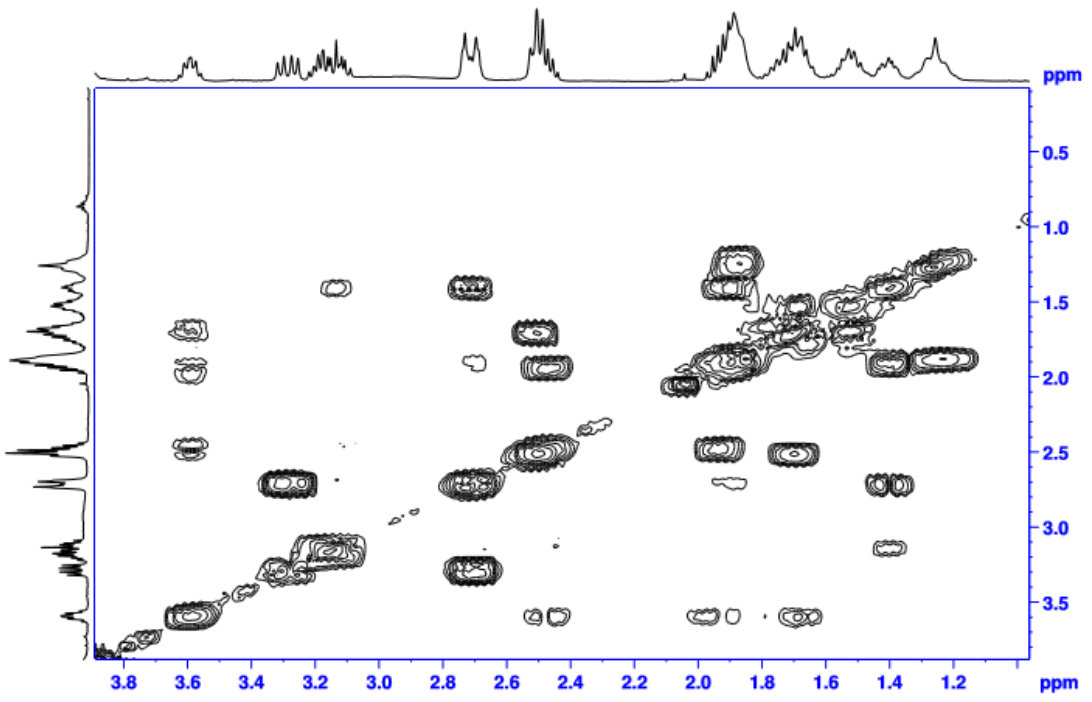

Figure S8. Correlated spectroscopy (COSY) correlations spectrum (400 MHz, $CDCl_3$) of compound (**1**).

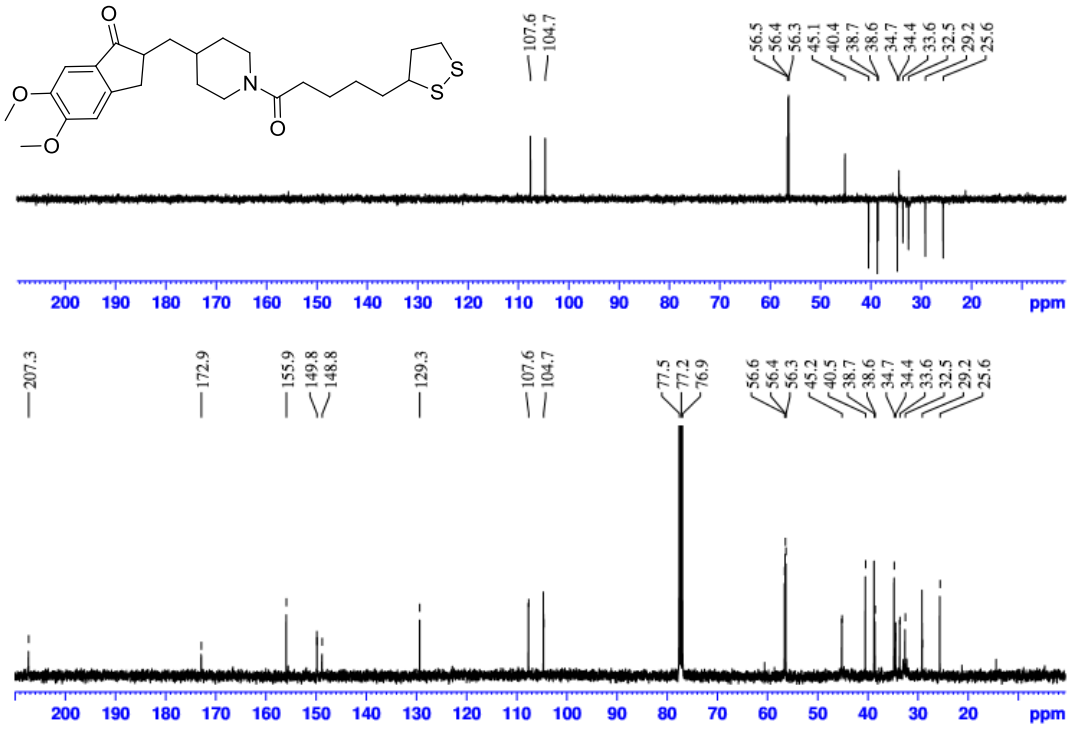

Figure S9. ^{13}C NMR spectrum (down) and DEPT 135 (up) (100 MHz, $CDCl_3$) of compound (**1**).

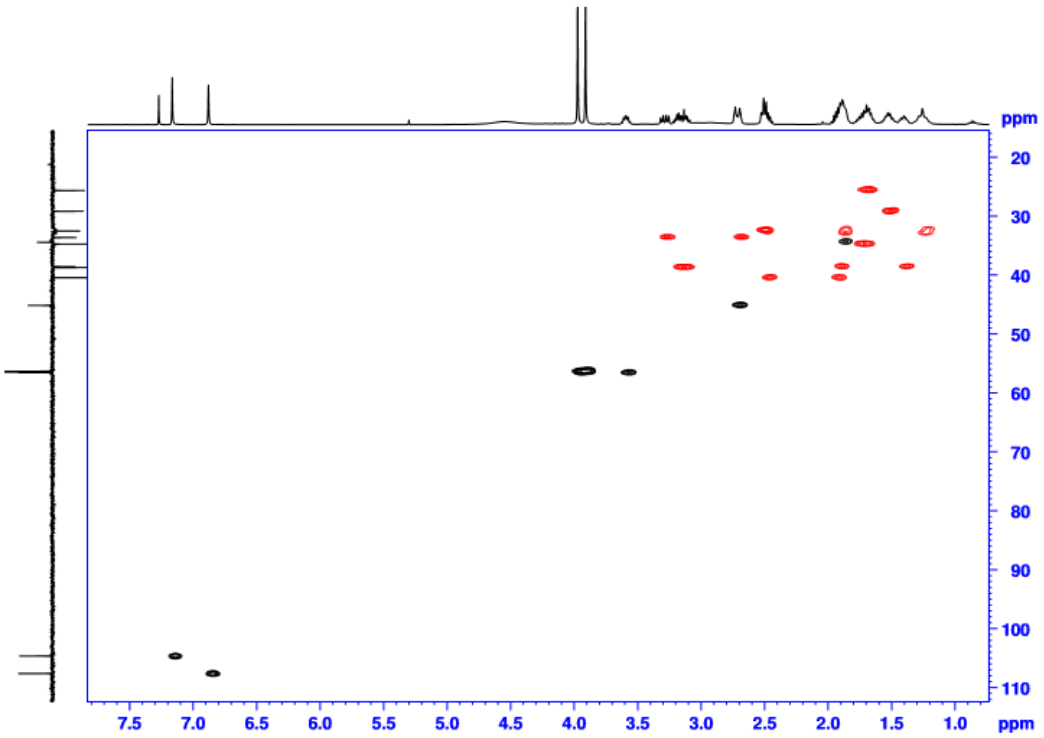

Figure S10. Heteronuclear single quantum correlation (HSQC) spectrum (400 MHz, $CDCl_3$) of compound (**1**).

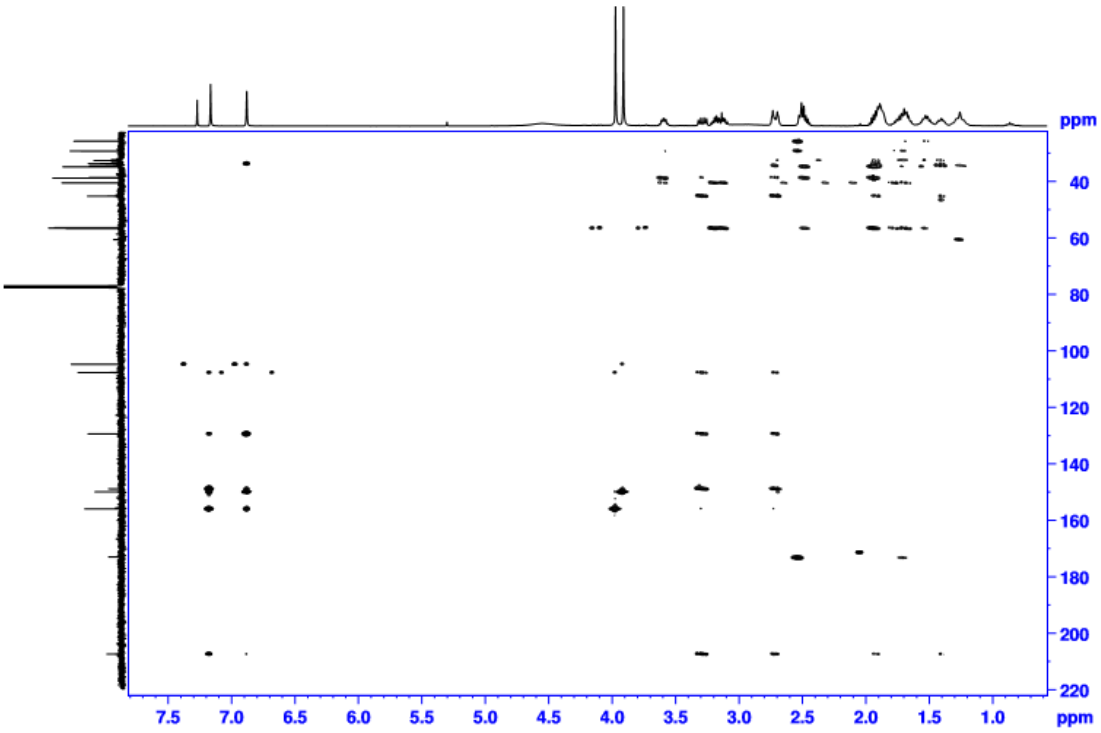

Figure S11. Heteronuclear multiple bond correlation (HMBC) spectrum (400 MHz, $CDCl_3$) of compound (**1**).

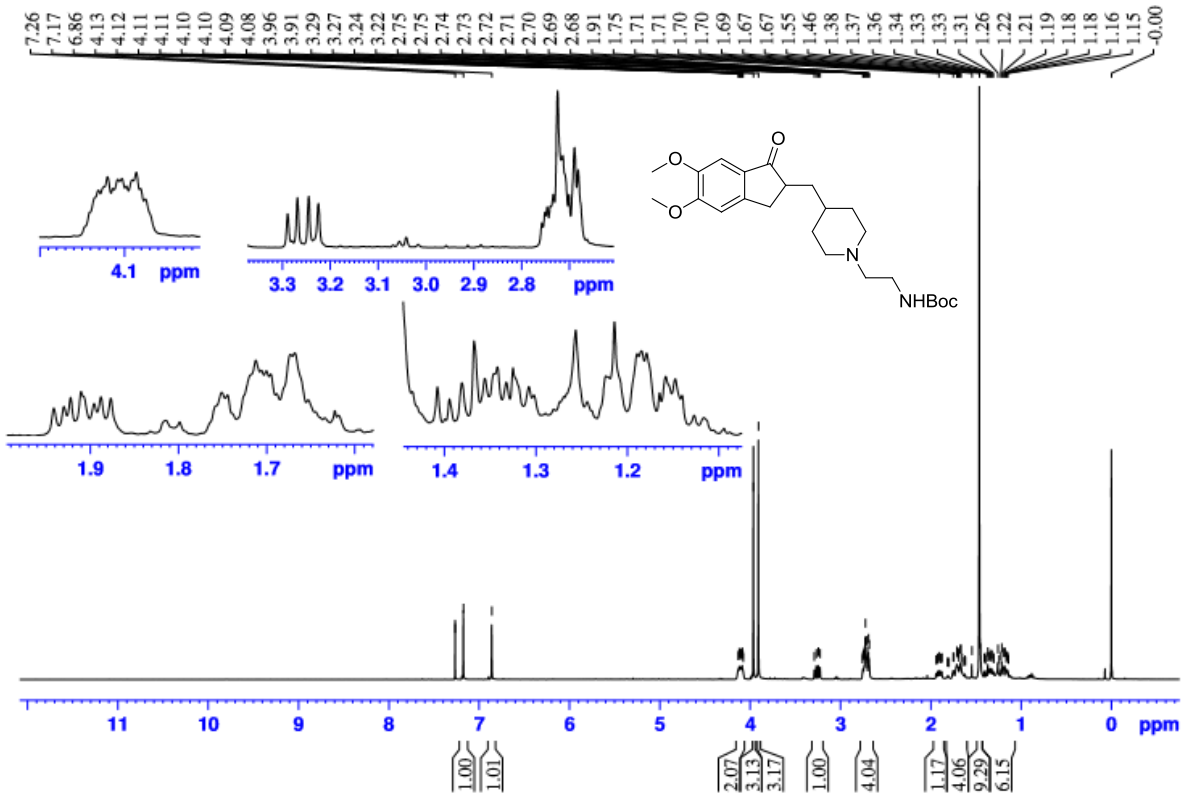

Figure S12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound (**8**).

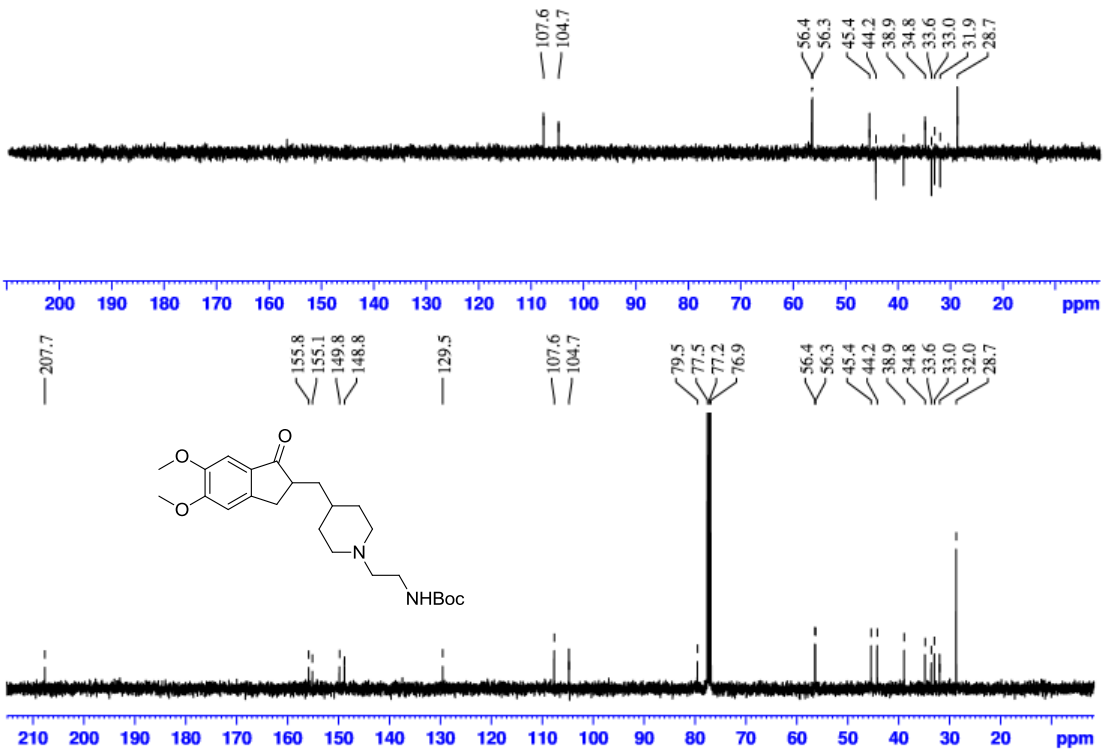

Figure S13. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound (**8**).

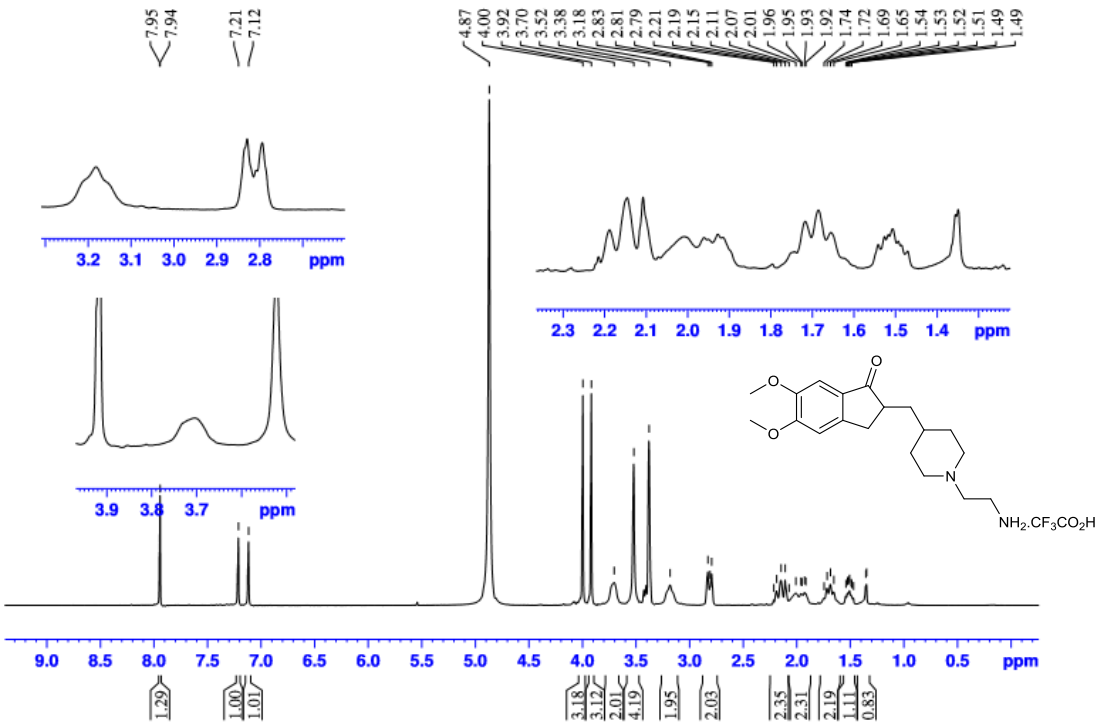

Figure S14. ^{1}H NMR spectrum (400 MHz, CD_3OD) of compound (**9**).

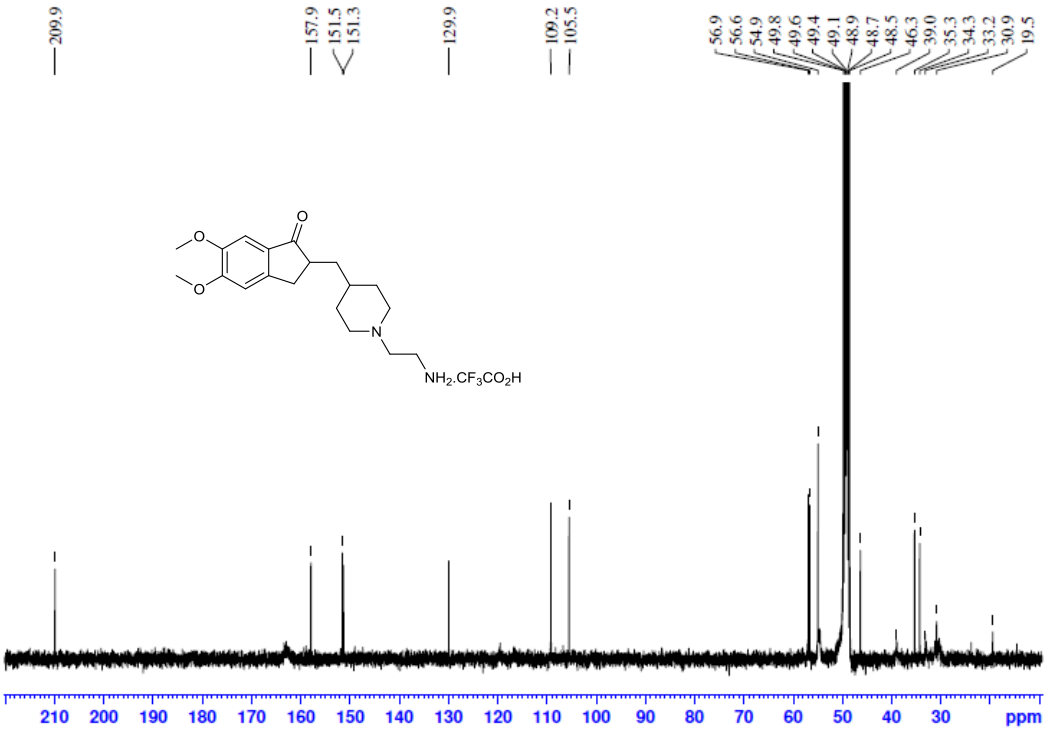

Figure S15. ^{13}C NMR spectrum (100 MHz, CD_3OD) of compound (**9**).

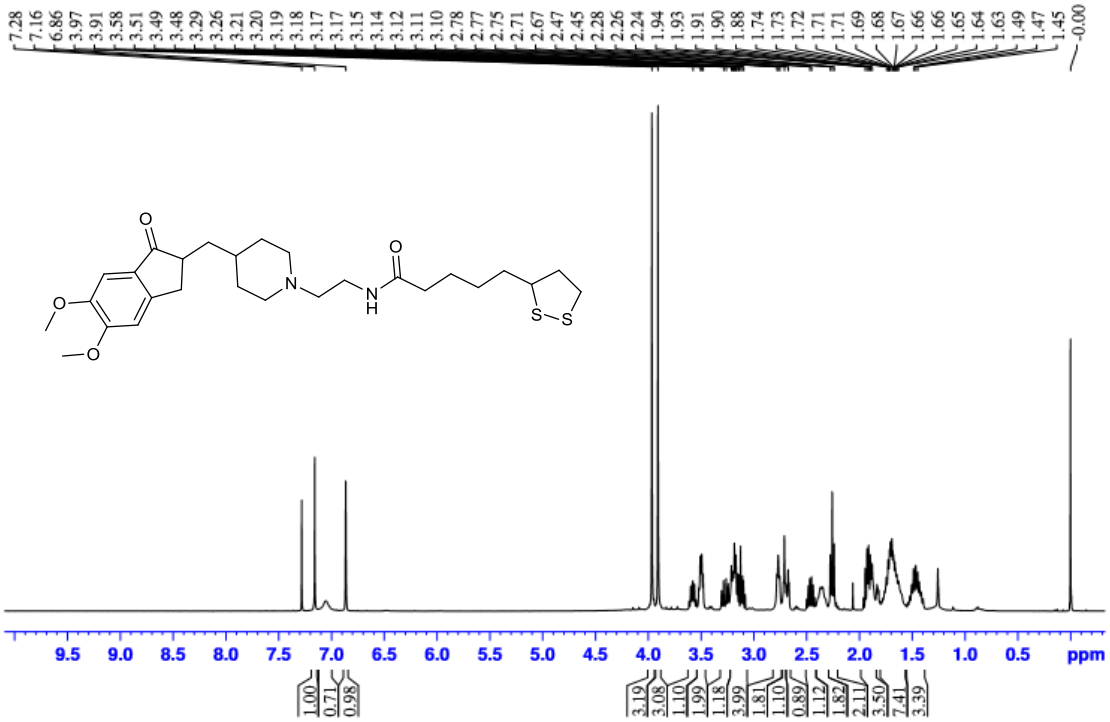

Figure S16. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound (**2**).

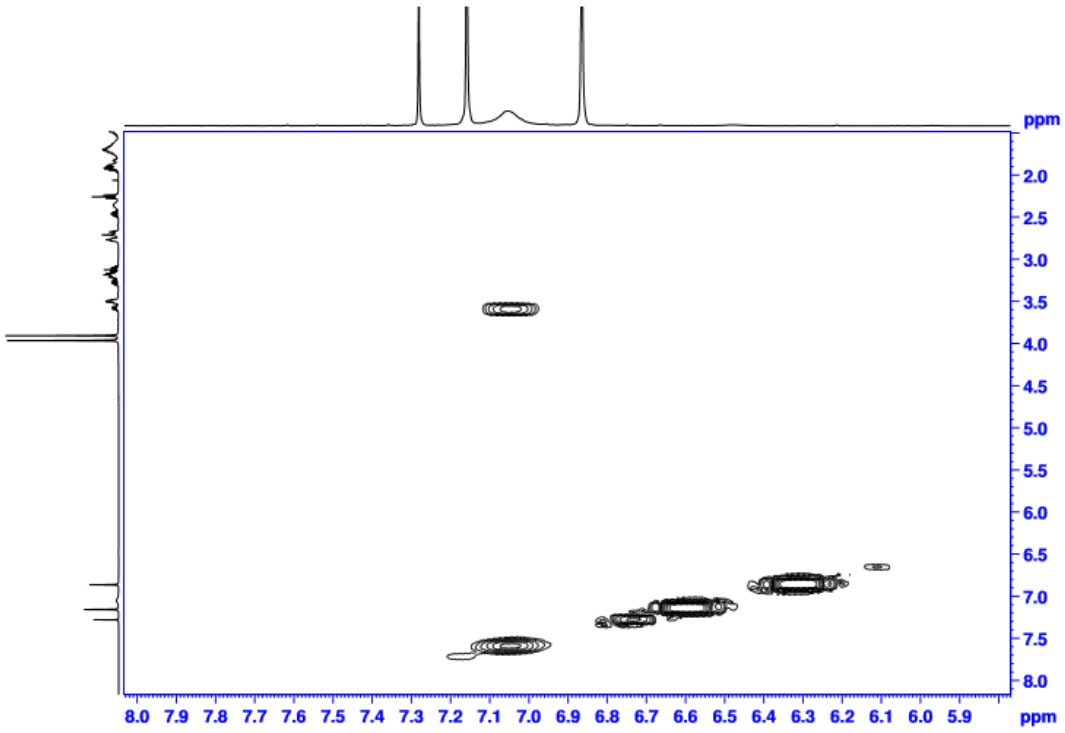

Figure S17. COSY spectrum (400 MHz, $CDCl_3$) of compound (**2**).

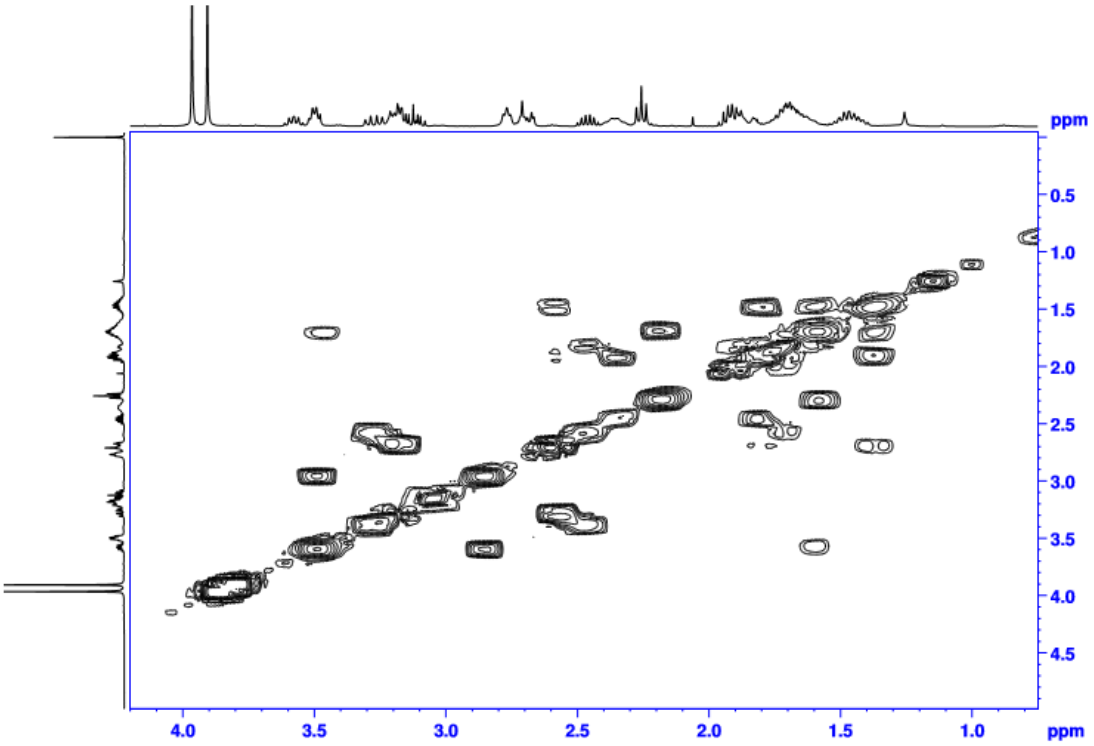

Figure S18. COSY spectrum (400 MHz, $CDCl_3$) of compound (**2**).

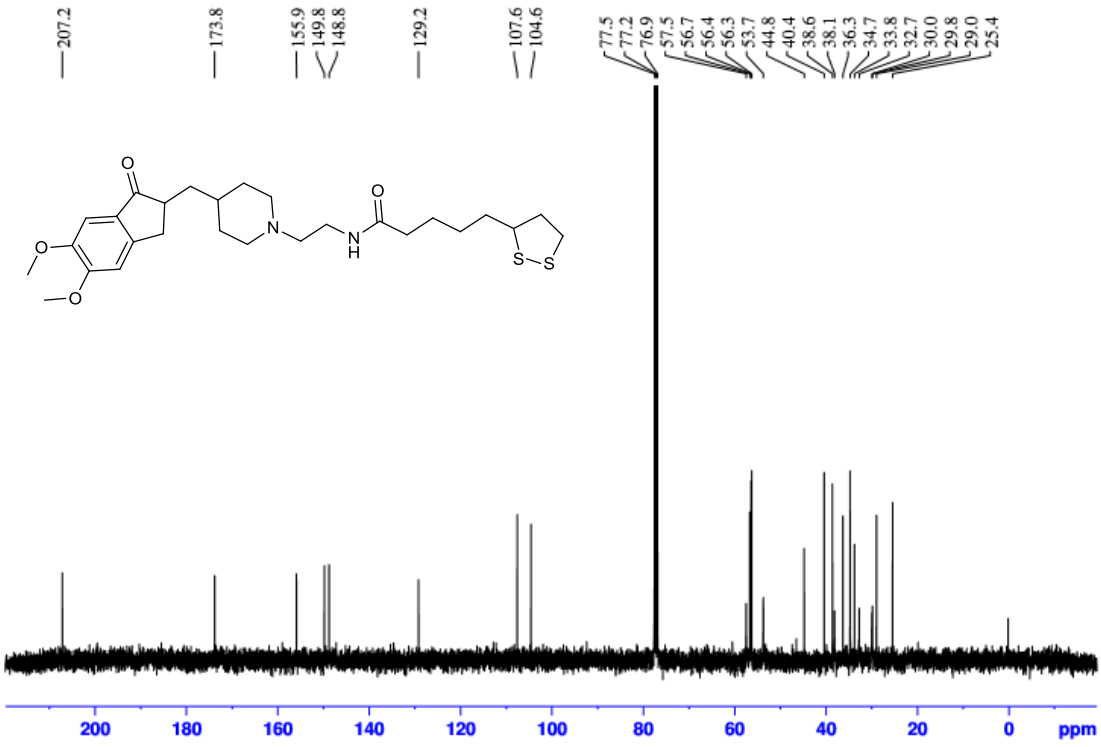

Figure S19. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound (**2**).

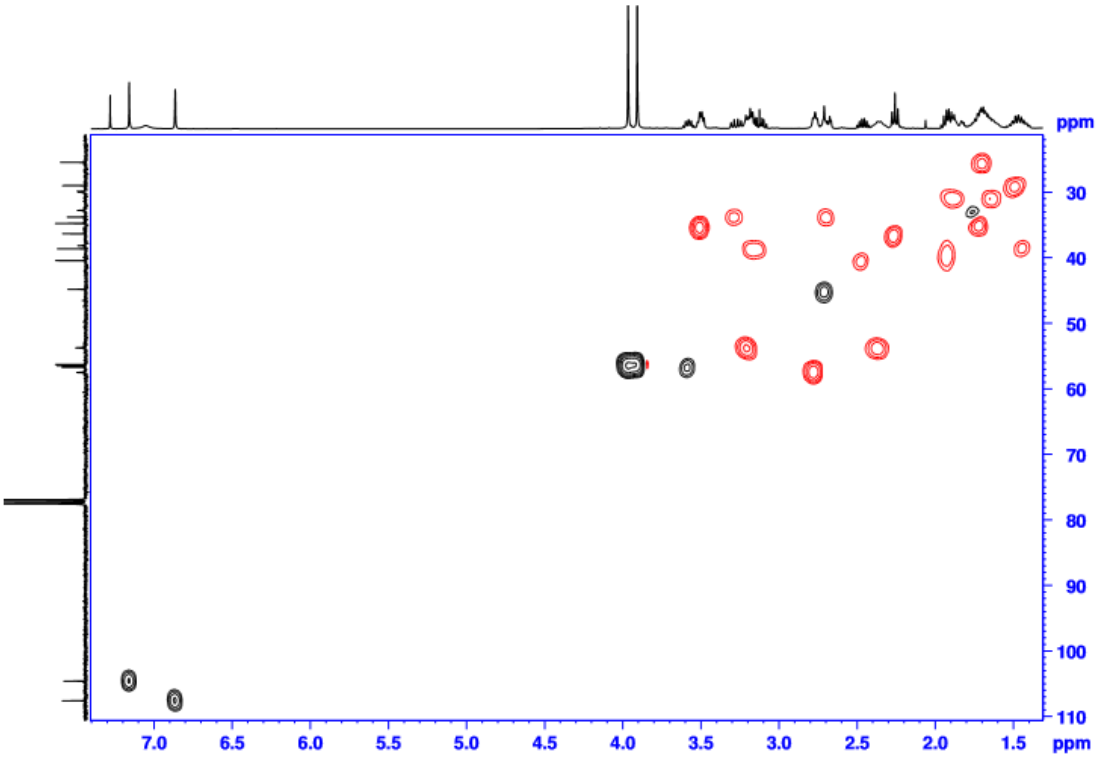

Figure S20. HSQC spectrum (400 MHz, $CDCl_3$) of compound (**2**).