Supplementary material for the article:

Elshaflu, H.; Todorović, T. R.; Nikolić, M.; Lolić, A.; Višnjevac, A.; Hagenow, S.; Padrón, J. M.; García-Sosa, A. T.; Djordjevic, I. S.; Grubišic, S.; et al. Selenazolyl-Hydrazones as Novel Selective MAO Inhibitors with Antiproliferative and Antioxidant Activities: Experimental and In-Silico Studies. *Frontiers in Chemistry* **2018**, *6* (JUL). https://doi.org/10.3389/fchem.2018.00247

frontiers

Supplementary Material

Selenazolyl-hydrazones as Novel Selective MAO Inhibitors with Antiproliferative and Antioxidant Activities: Experimental and *In-silico* Studies

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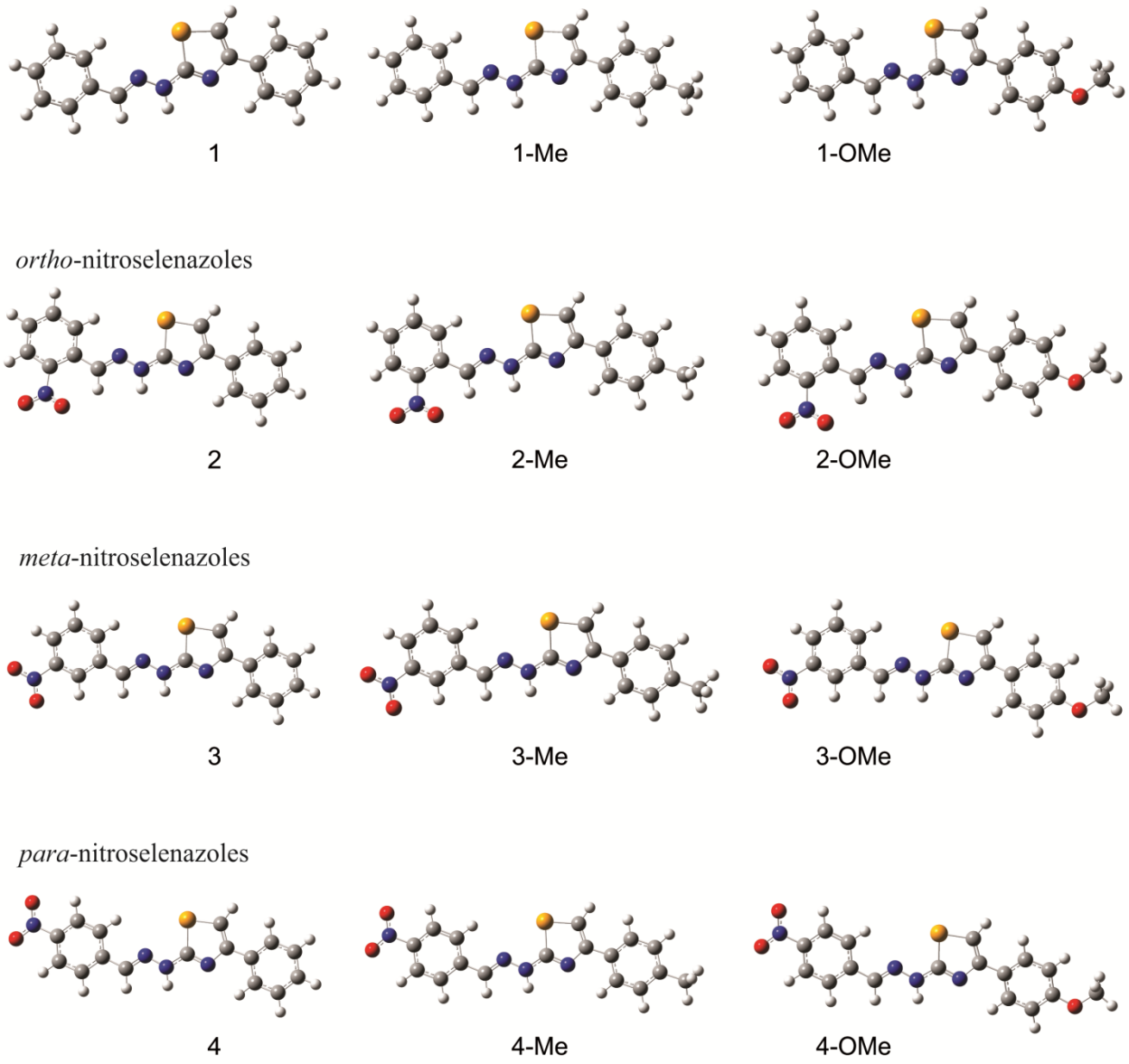
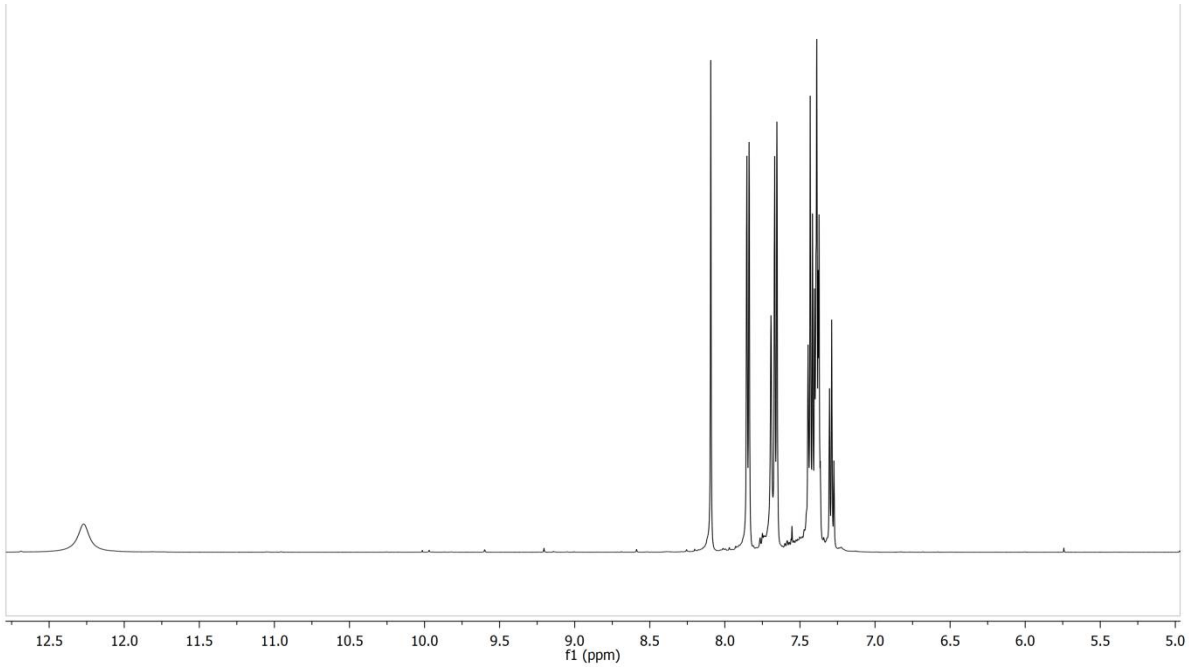
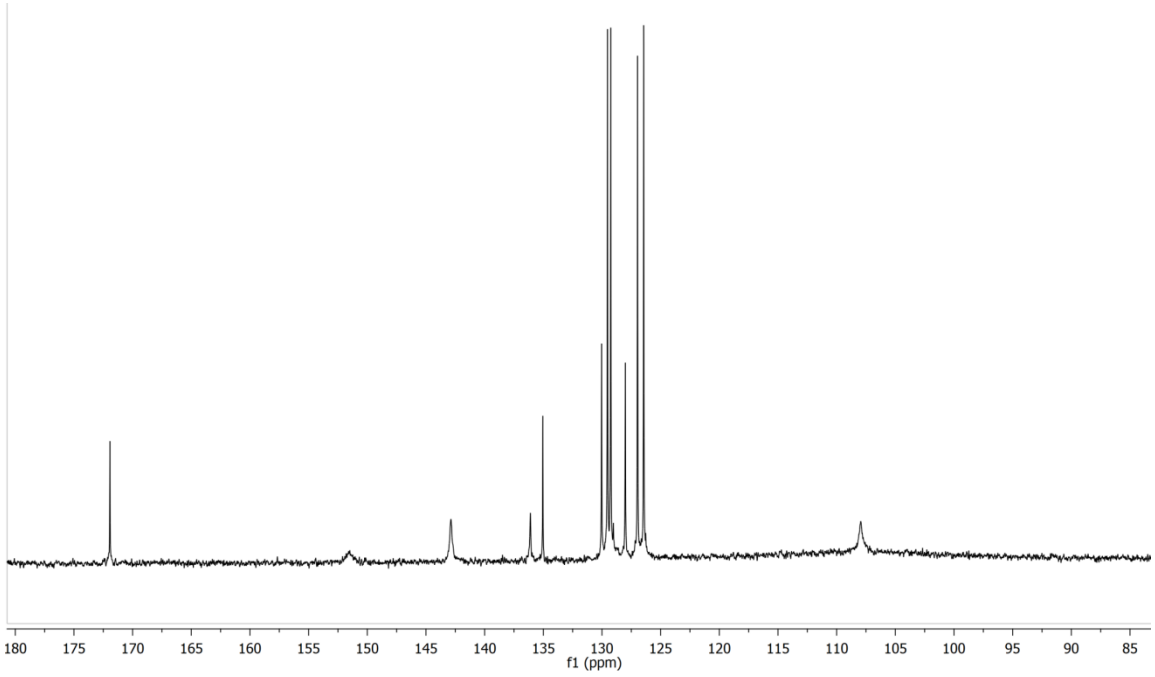
1 Supplementary Figures and Tables



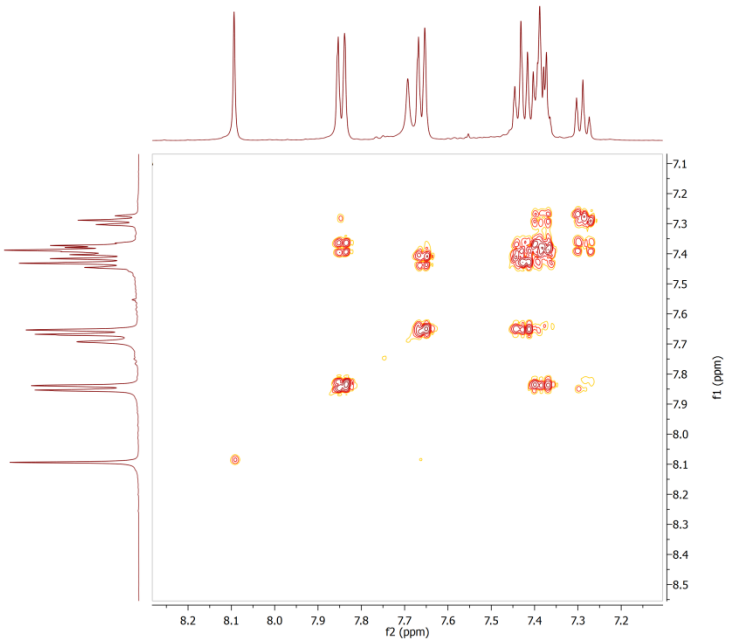
Supplementary Figure S2. Optimized geometries of benzylidene-based (1,3-selenazol-2-yl)hydrazones in the gas phase obtained with DFT/B3LYP/6-31G(d,p) method.



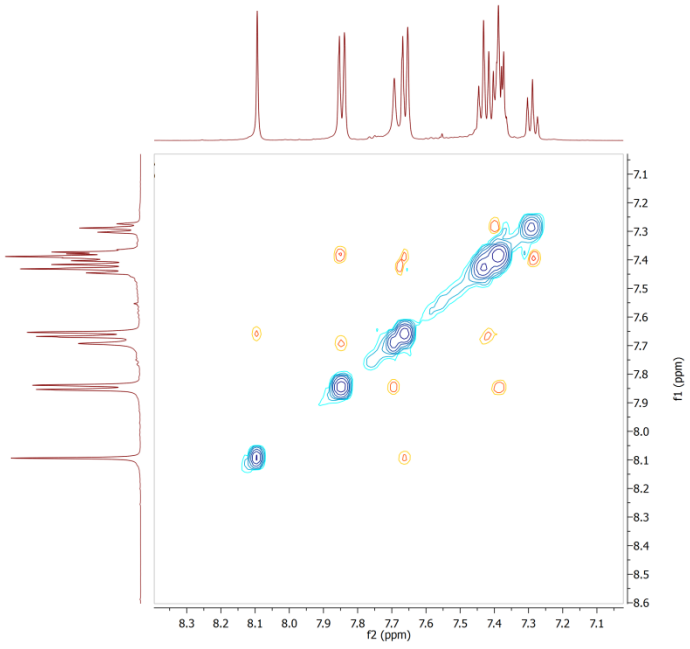
Supplementary Figure S2. ^{1}H NMR spectrum of **1** in DMSO-d_6.



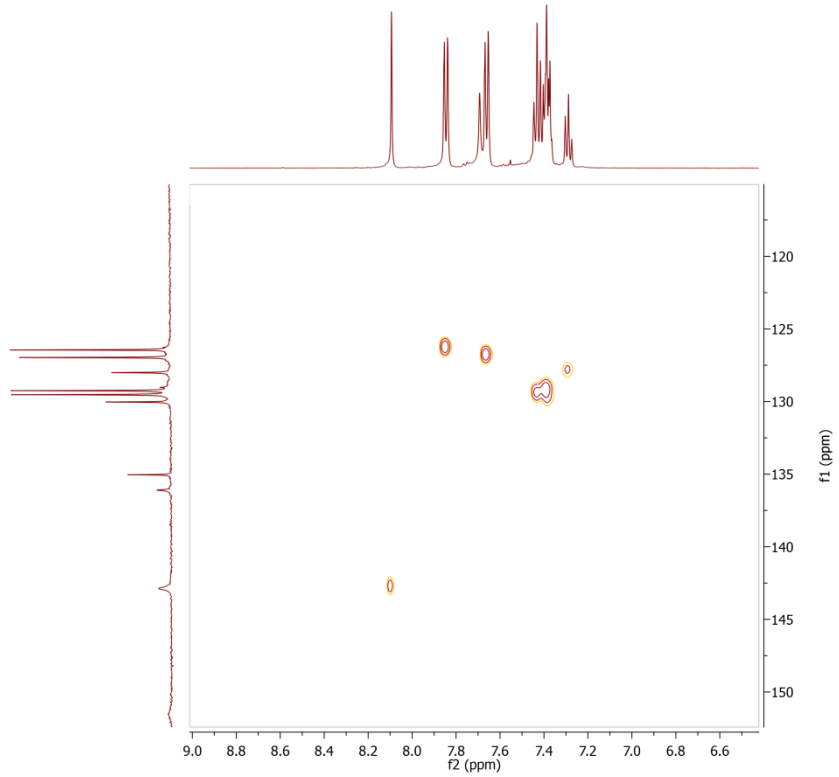
Supplementary Figure S3. ^{13}C NMR spectrum of **1** in DMSO-d_6.



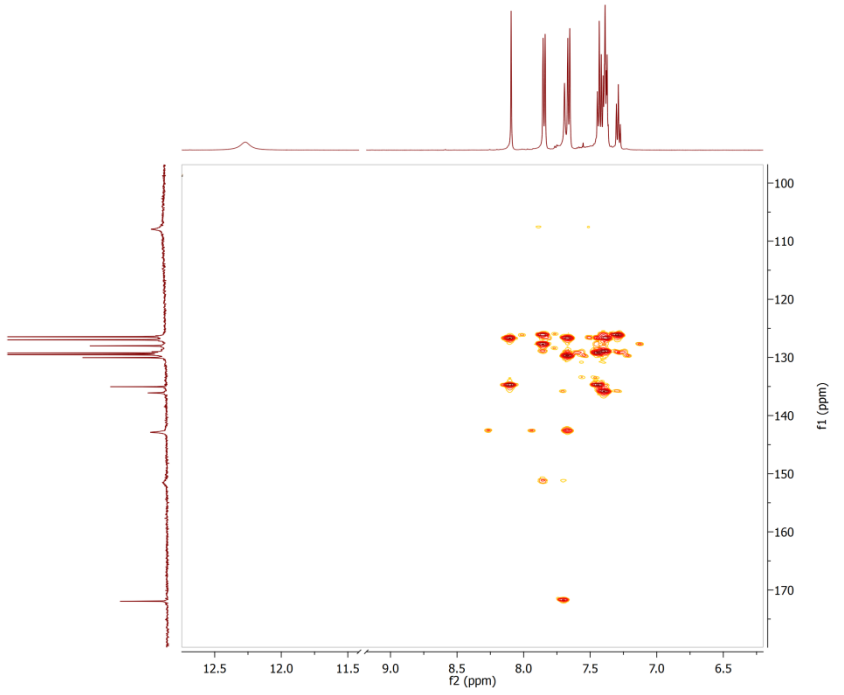
Supplementary Figure S4. COSY spectrum of **1** in DMSO-d_6.



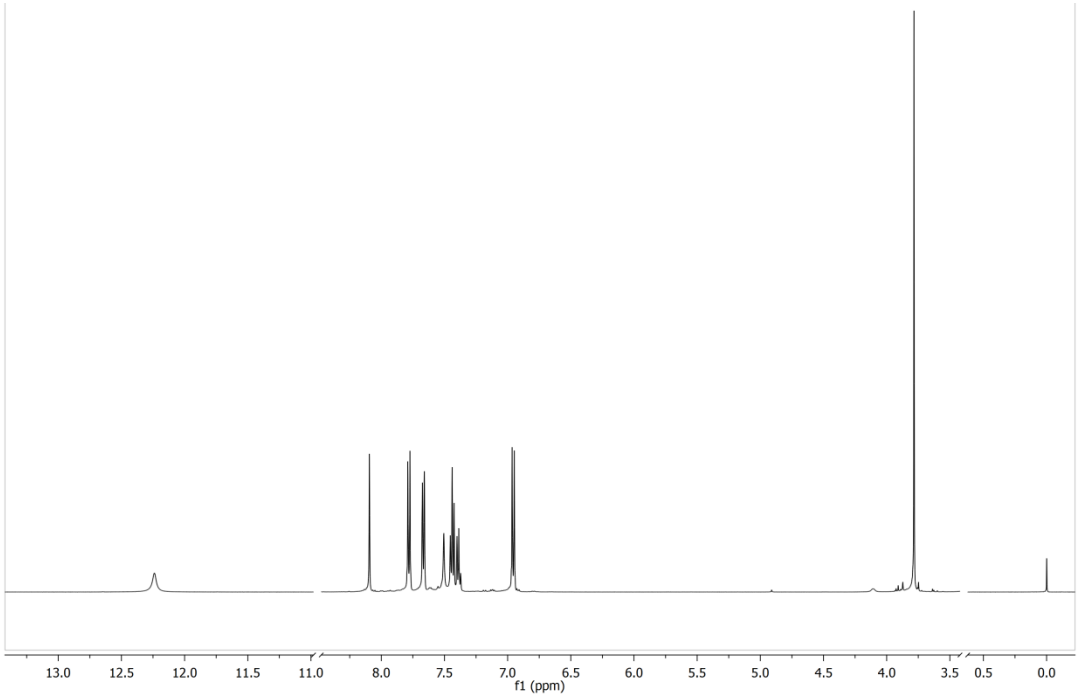
Supplementary Figure S5. NOESY spectrum of **1** in DMSO-d_6.



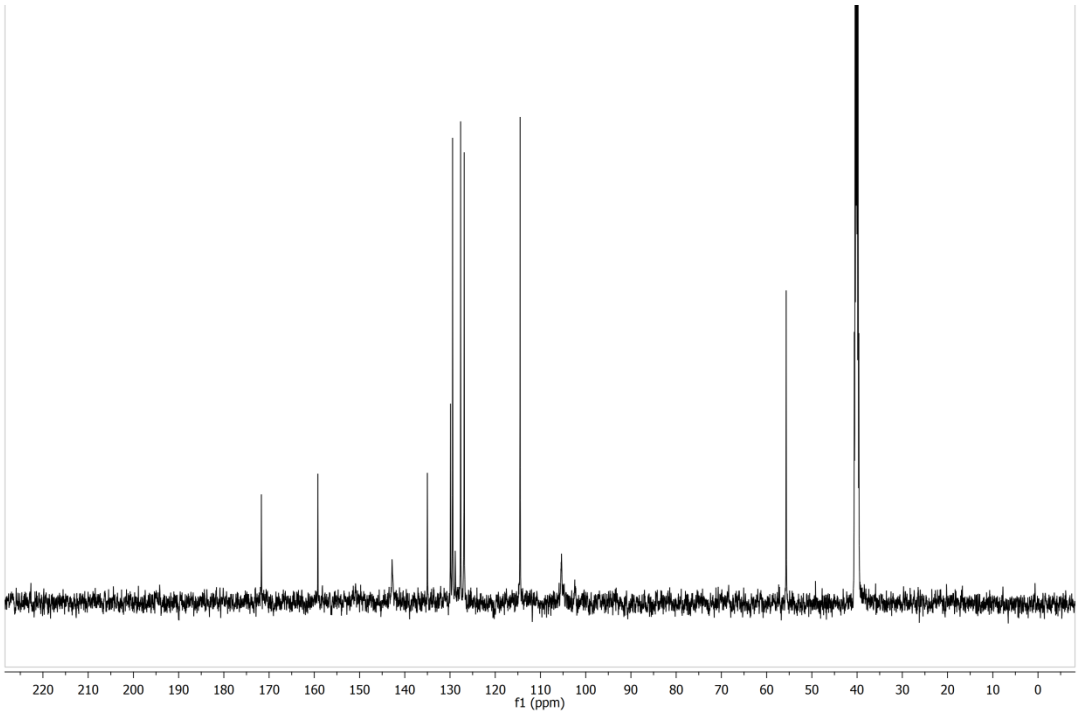
Supplementary Figure S6. $^{1}H–^{13}C$ HSQC NMR spectrum of **1** in DMSO-d_6.



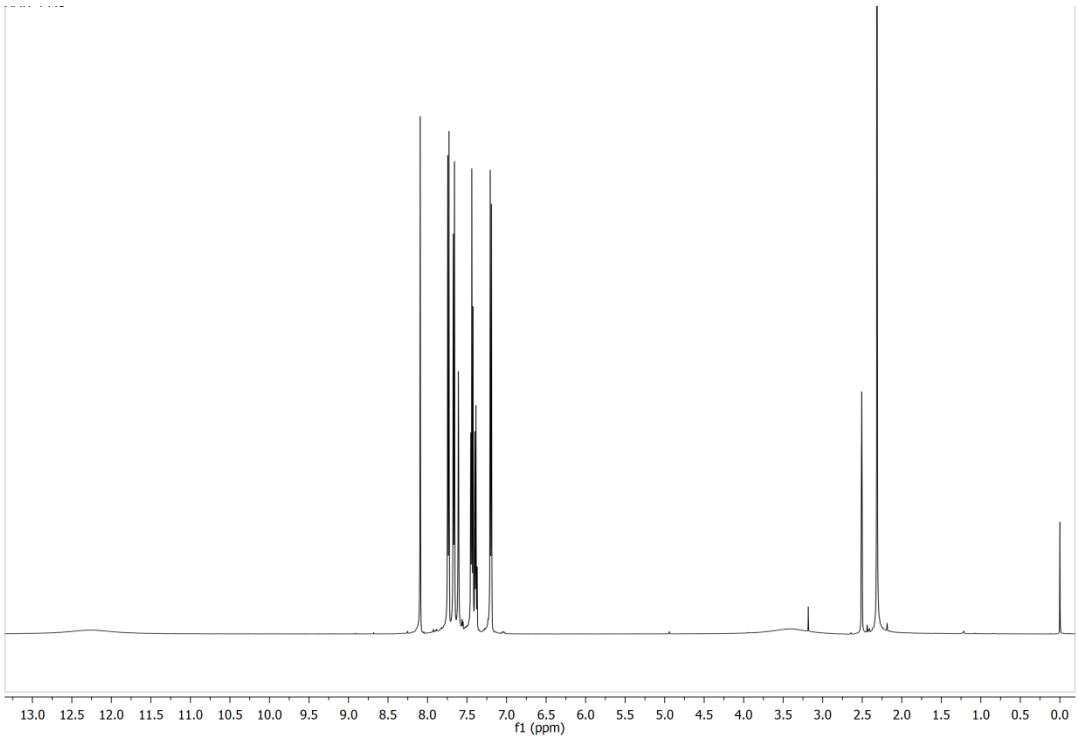
Supplementary Figure S7. $^{1}H–^{13}C$ HMBC NMR spectrum of **1** in DMSO-d_6.



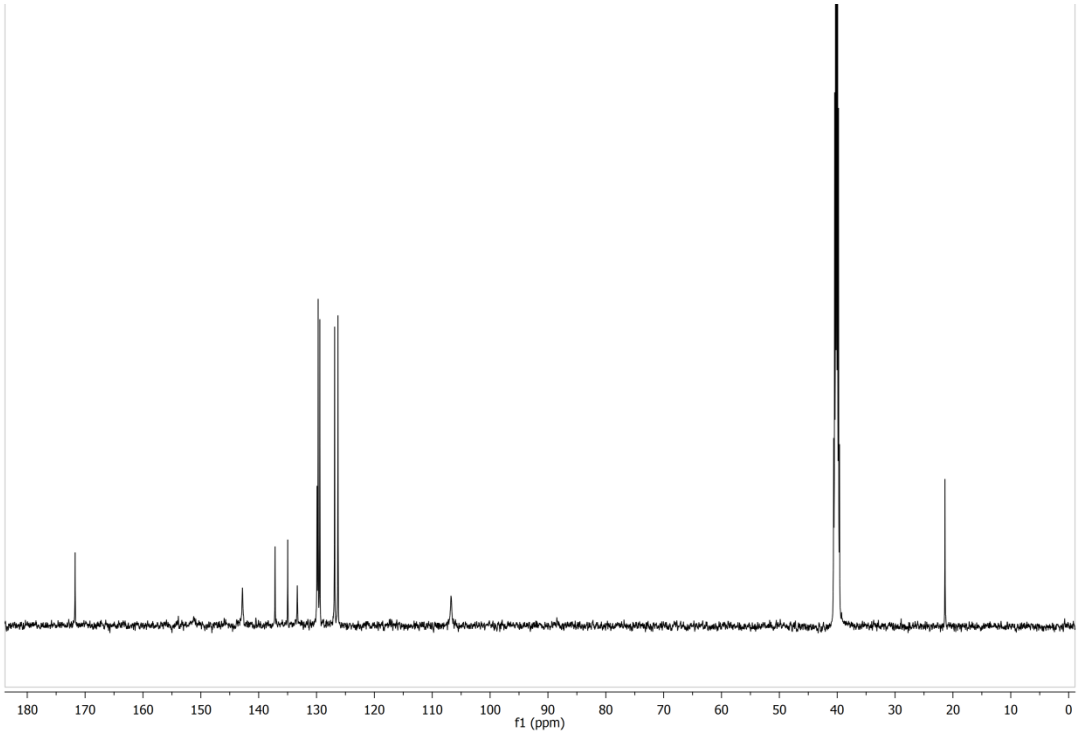
Supplementary Figure S8. ^{1}H NMR spectrum of **1-OMe** in DMSO-d_6.



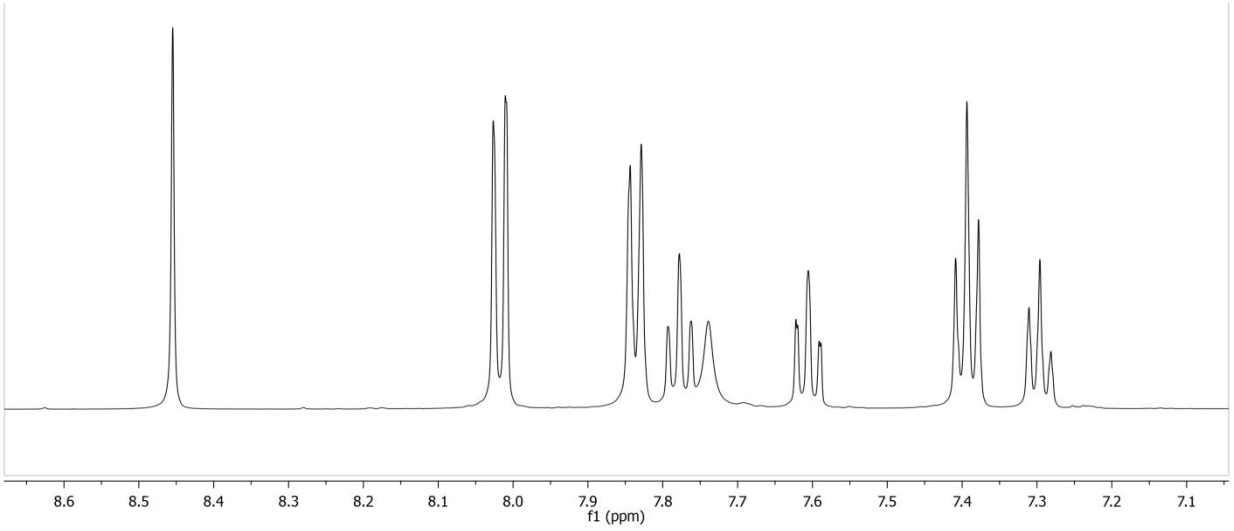
Supplementary Figure S9. ^{13}C NMR spectrum of **1-OMe** in DMSO-d_6.



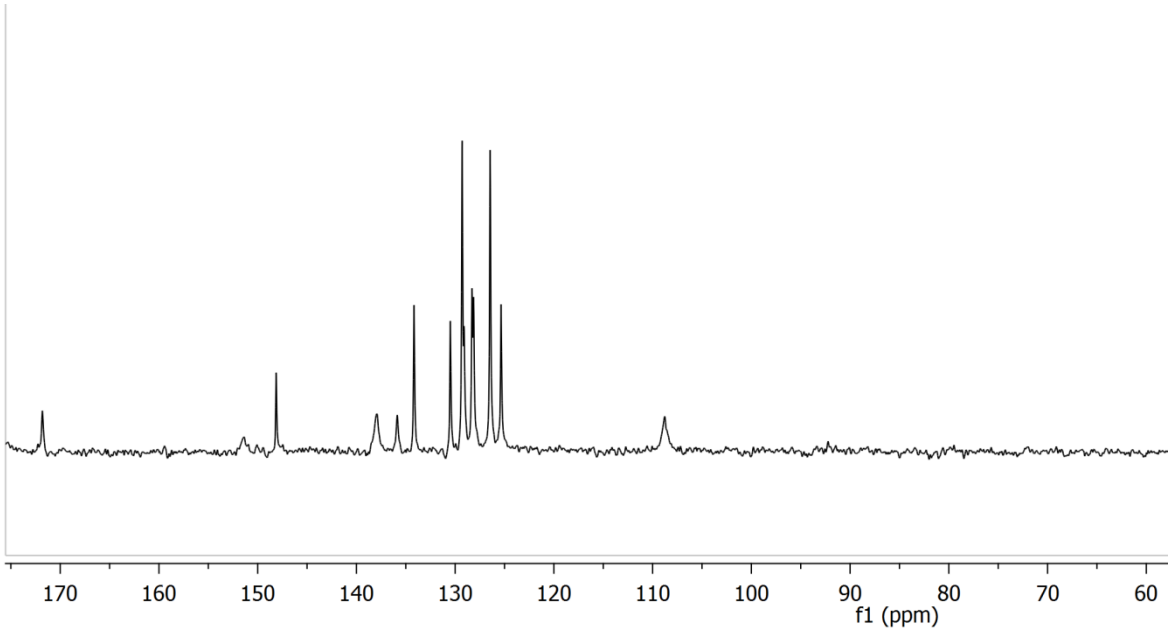
Supplementary Figure S10. ^{1}H NMR spectrum of **1-Me** in DMSO-d_6.



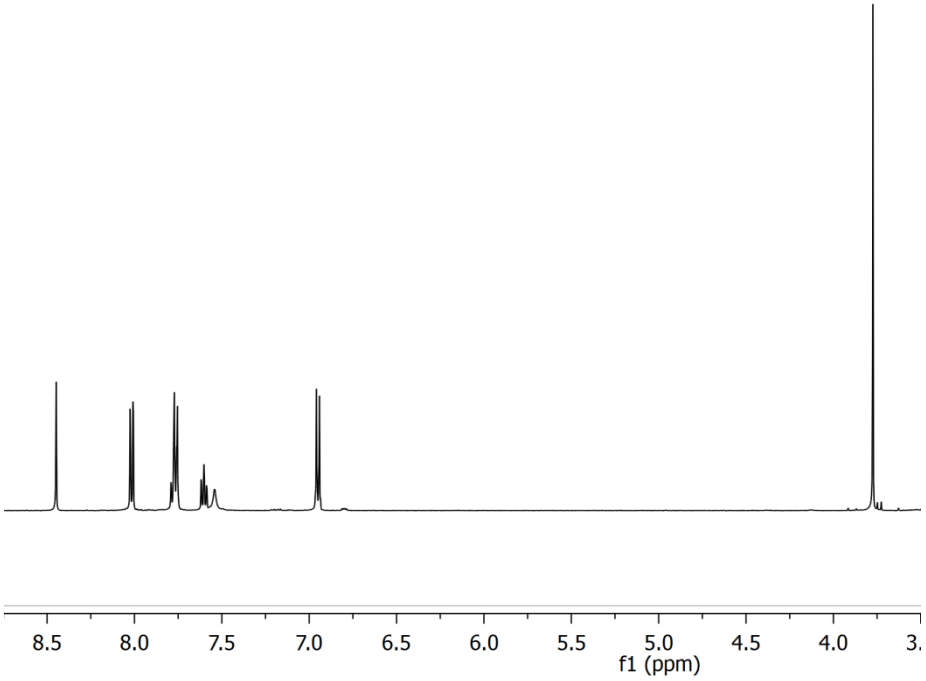
Supplementary Figure S11. ^{13}C NMR spectrum of **1-Me** in DMSO-d_6.



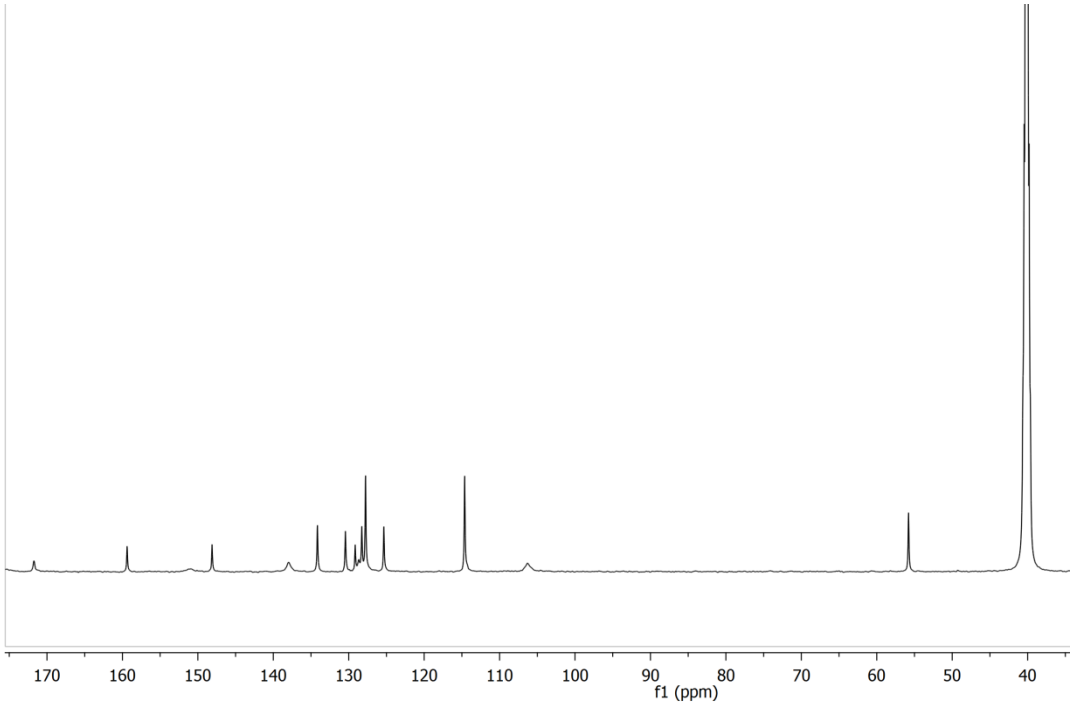
Supplementary Figure S12. ^{1}H NMR spectrum of **2** in DMSO-d_6.



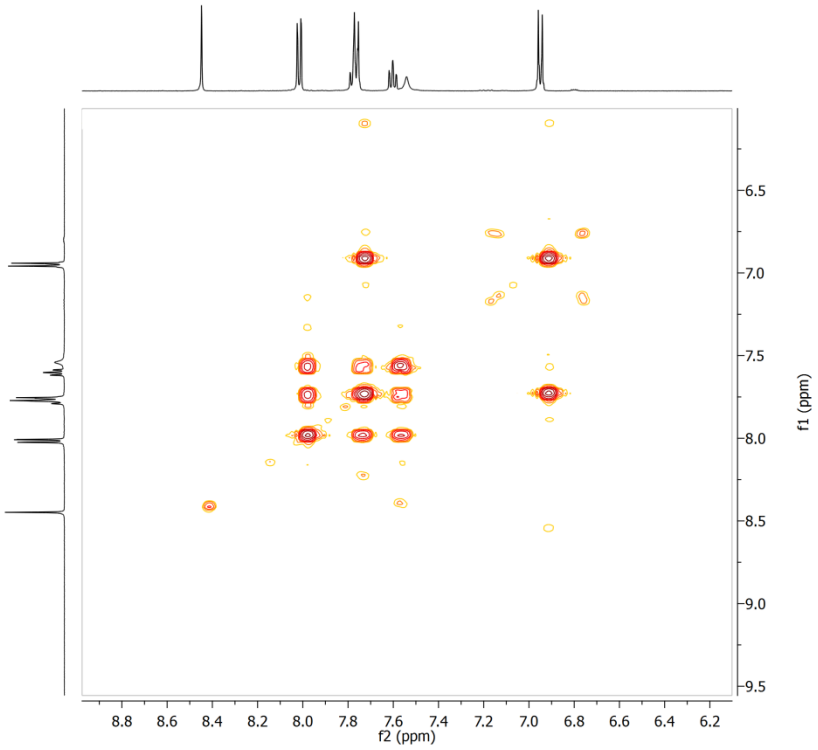
Supplementary Figure S13. ^{13}C NMR spectrum of **2** in DMSO-d_6.



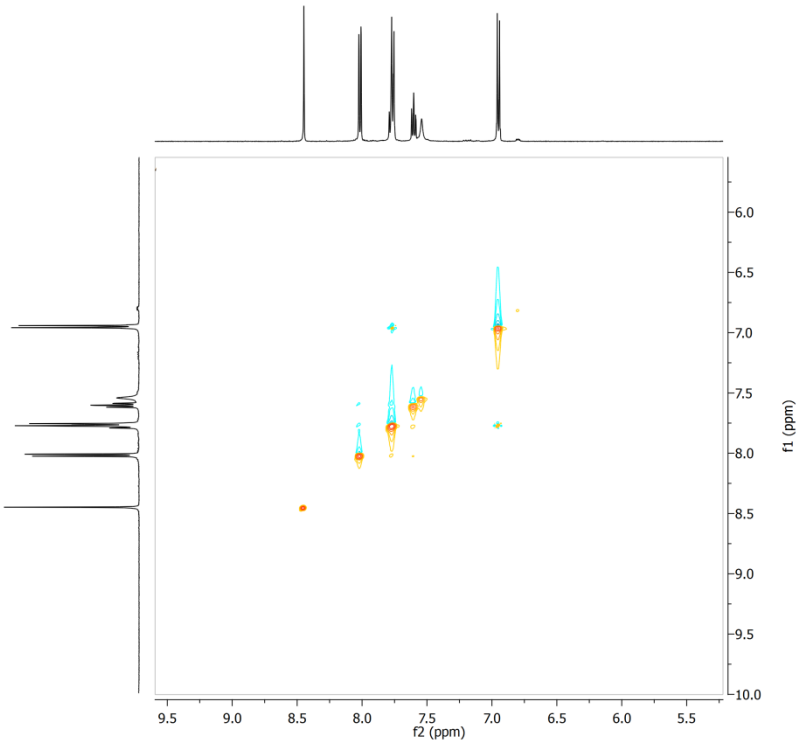
Supplementary Figure S14. ^{1}H NMR spectrum of **2-OMe** in DMSO-d_6.



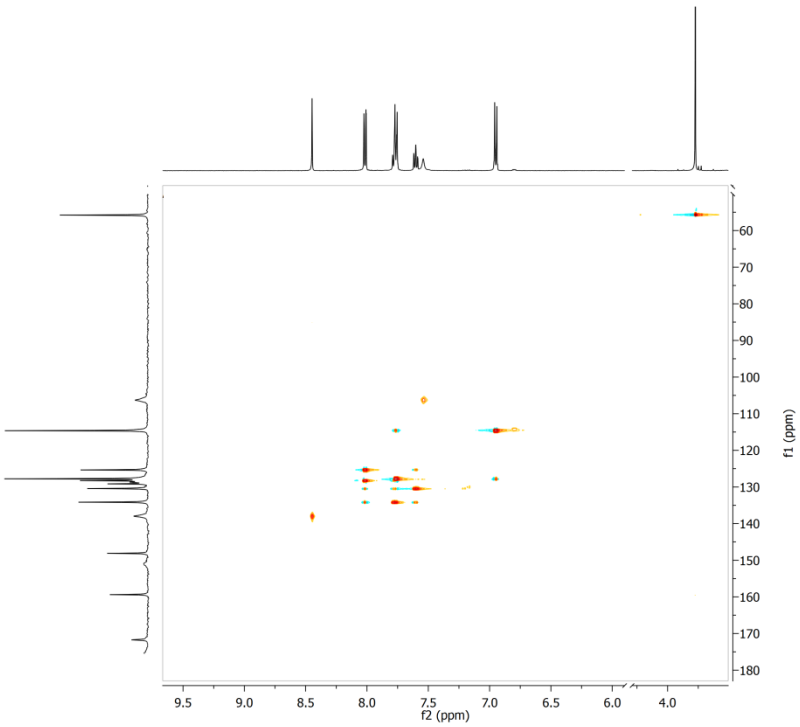
Supplementary Figure S15. ^{13}C NMR spectrum of **2-OMe** in DMSO-d_6.



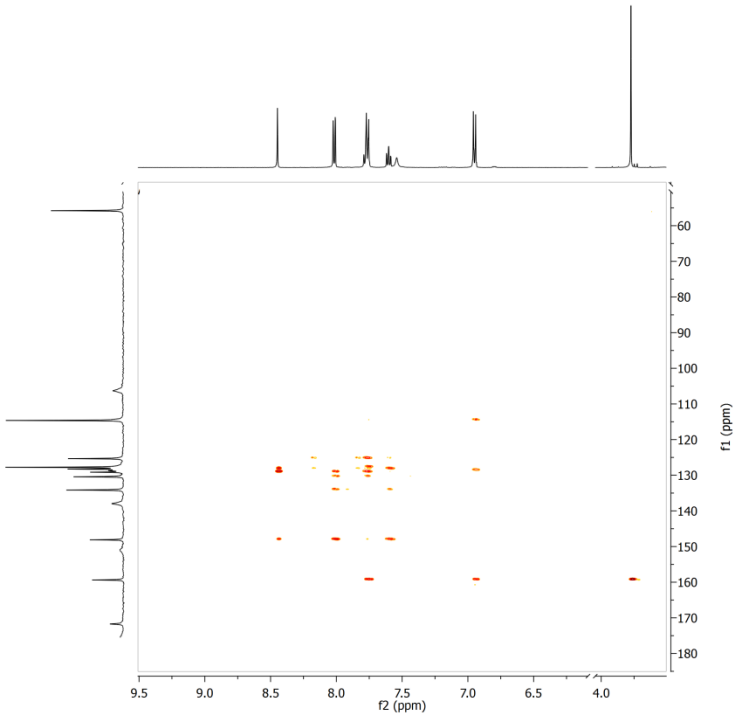
Supplementary Figure S16. COSY spectrum of **2-OMe** in DMSO-d_6.



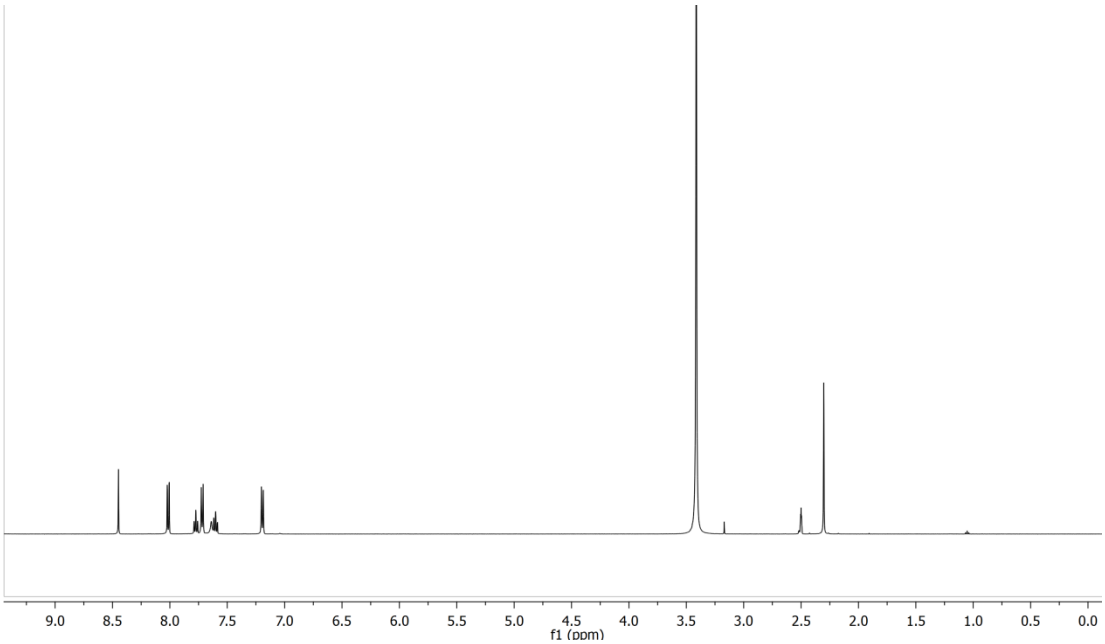
Supplementary Figure S17. NOESY spectrum of **2-OMe** in DMSO-d_6.



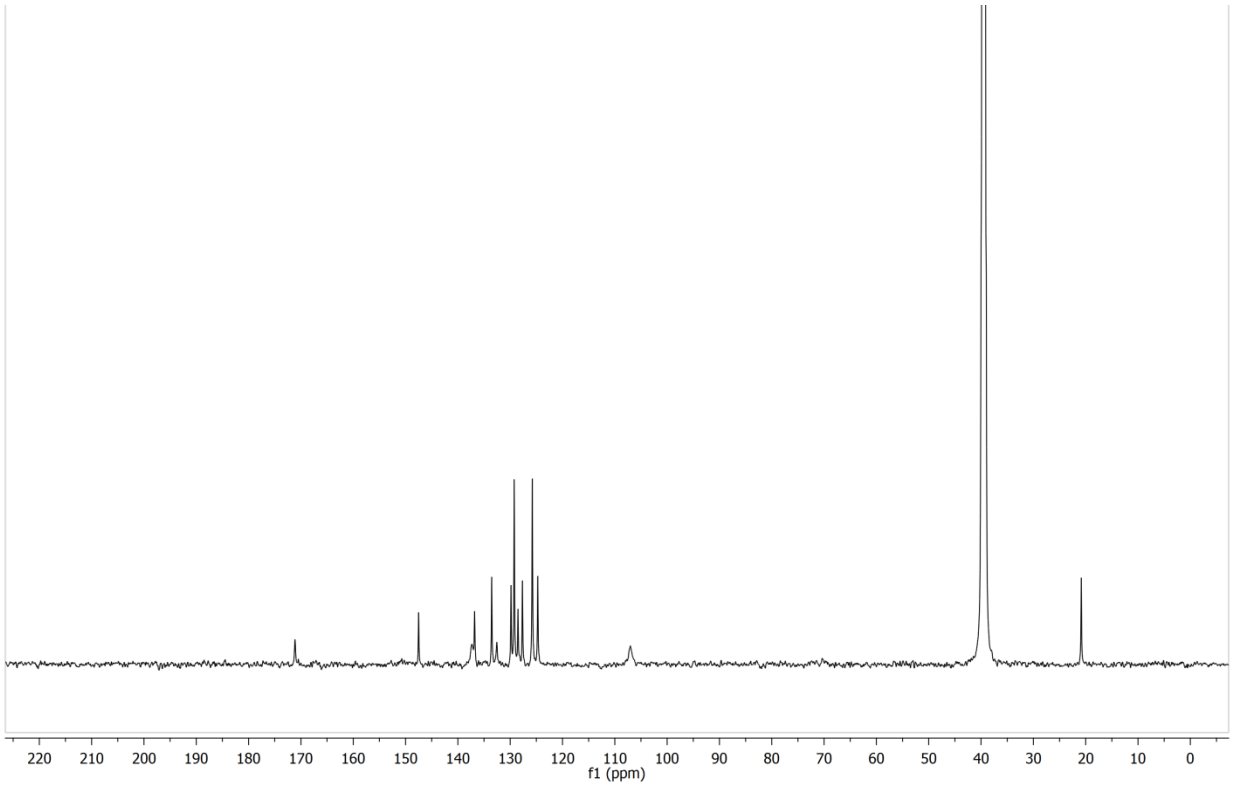
Supplementary Figure S18. $^{1}H–^{13}C$ HSQC NMR spectrum of **2-OMe** in DMSO-d_6.



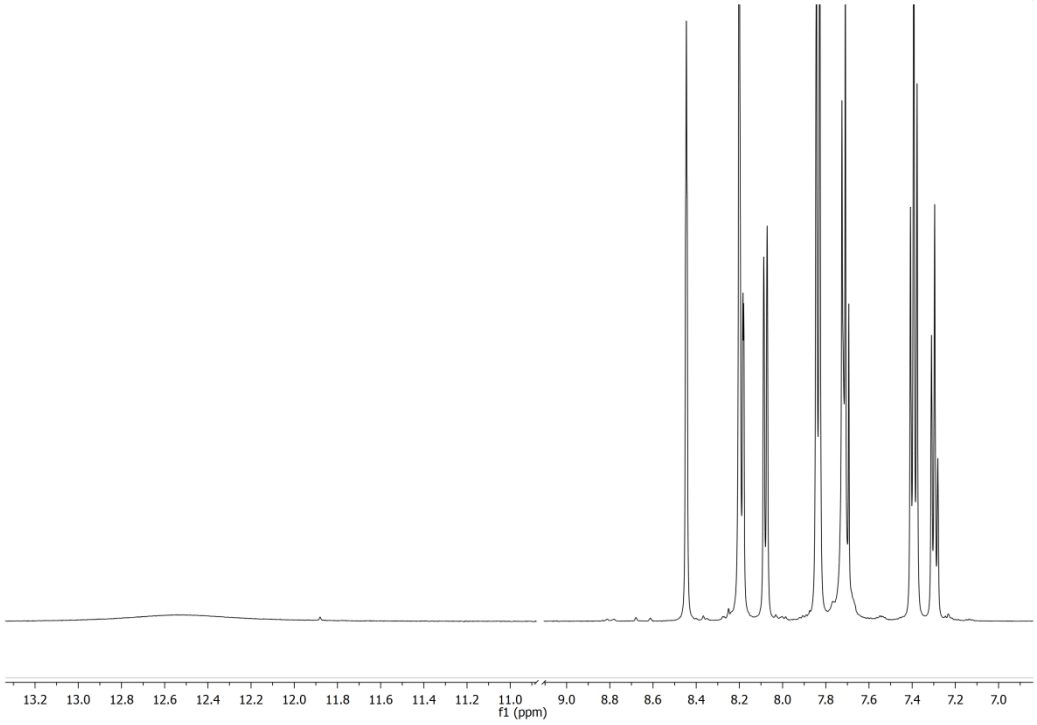
Supplementary Figure S19. $^{1}H–^{13}C$ HMBC NMR spectrum of **2-OMe** in DMSO-d_6.



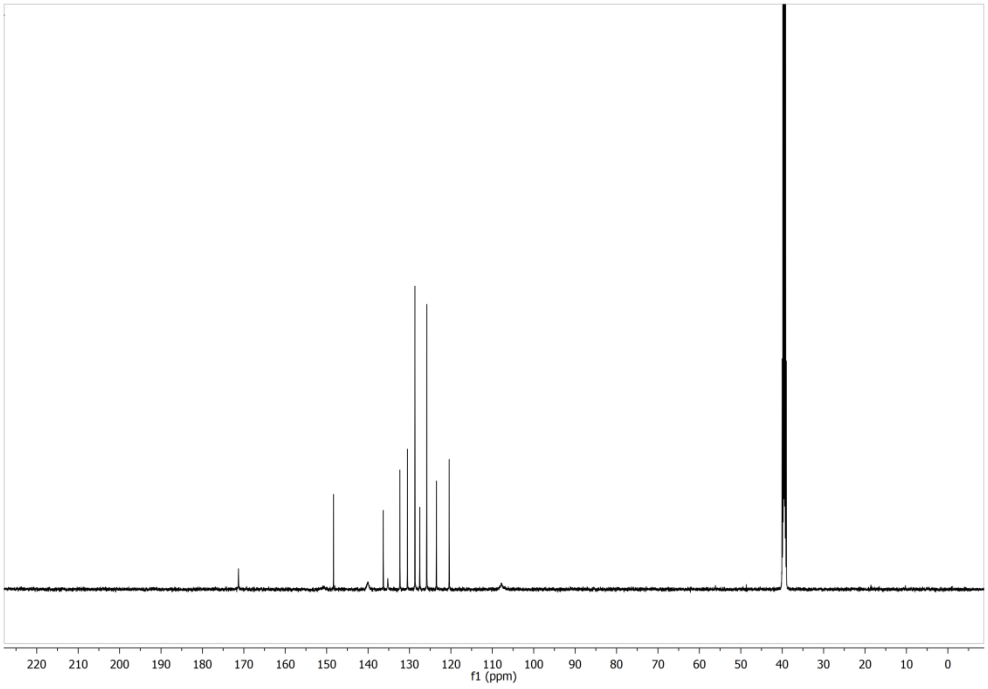
Supplementary Figure S20. ^{1}H NMR spectrum of **2-Me** in DMSO-d_6.



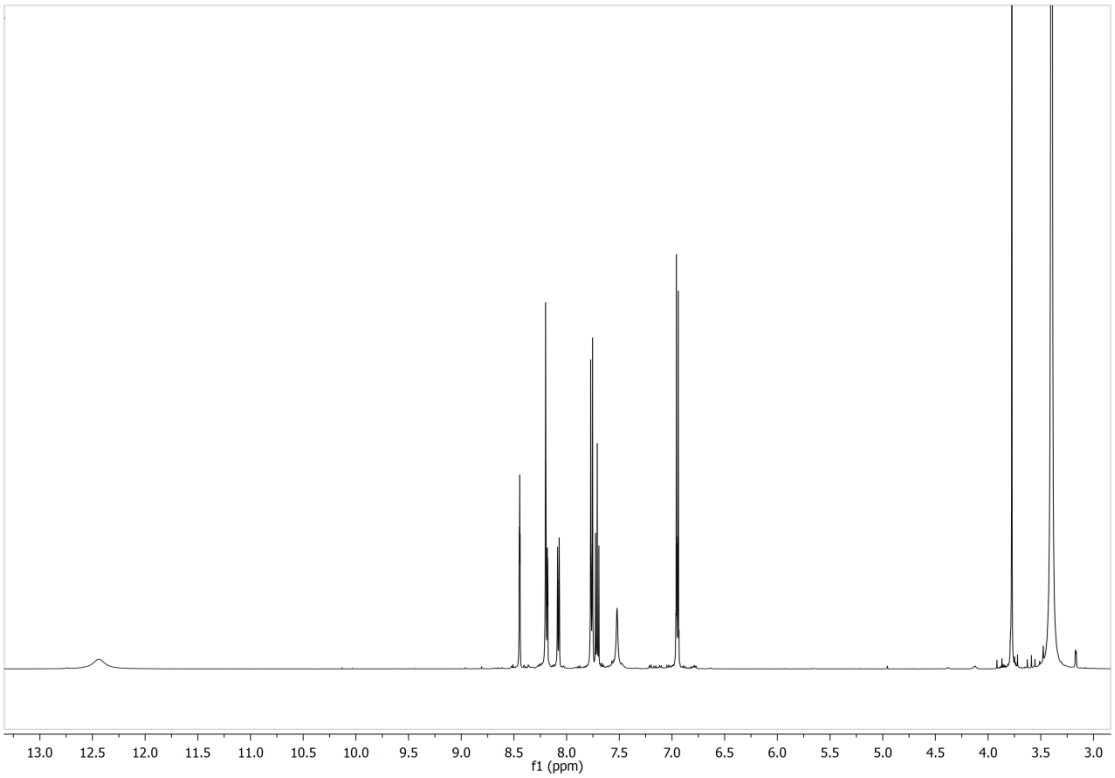
Supplementary Figure S21. ^{13}C NMR spectrum of **2-Me** in DMSO-d_6.



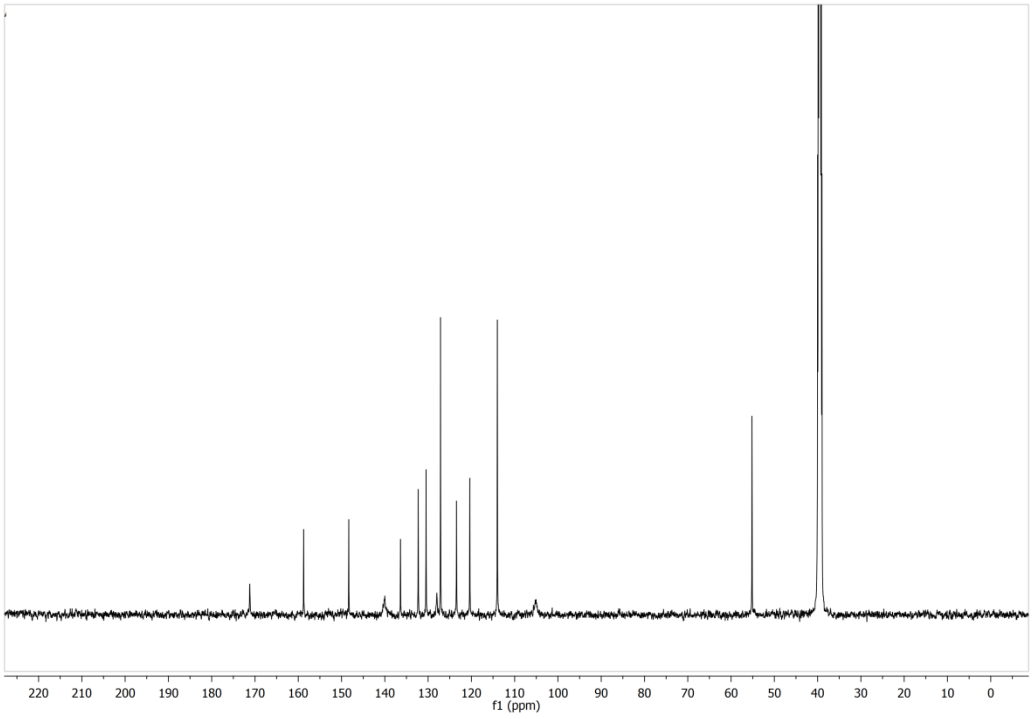
Supplementary Figure S22. ^{1}H NMR spectrum of **3** in DMSO-d_6.



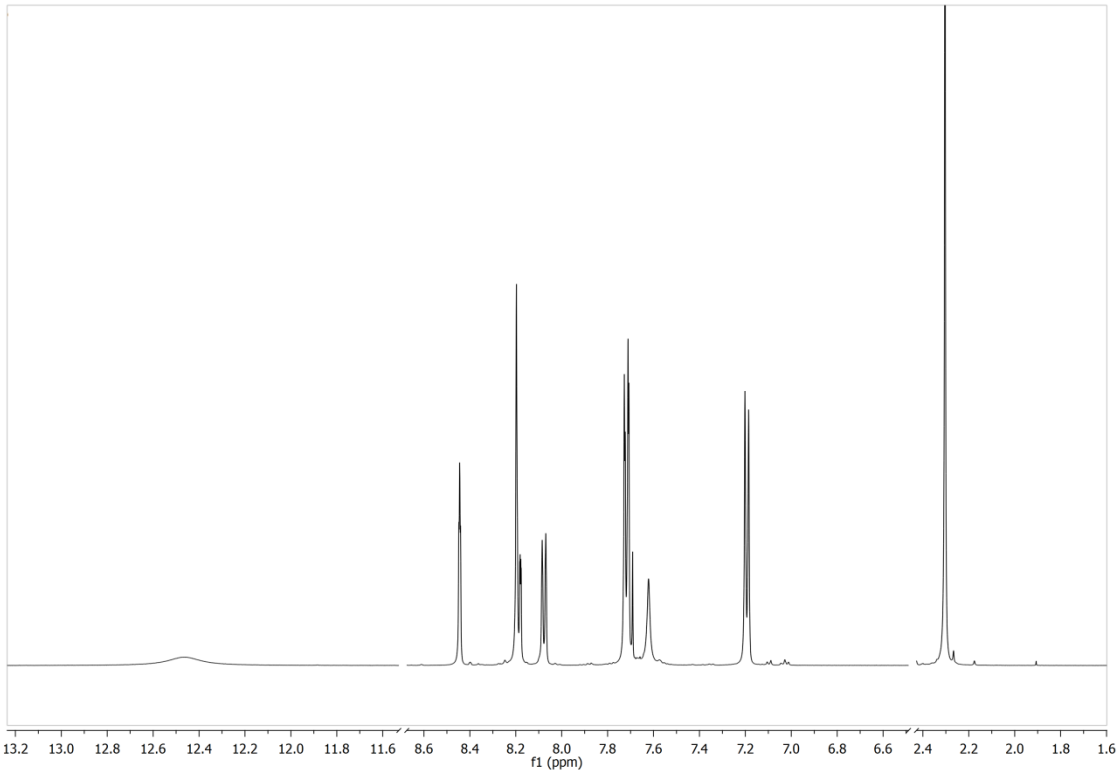
Supplementary Figure S23. ^{13}C NMR spectrum of **3** in DMSO-d_6.



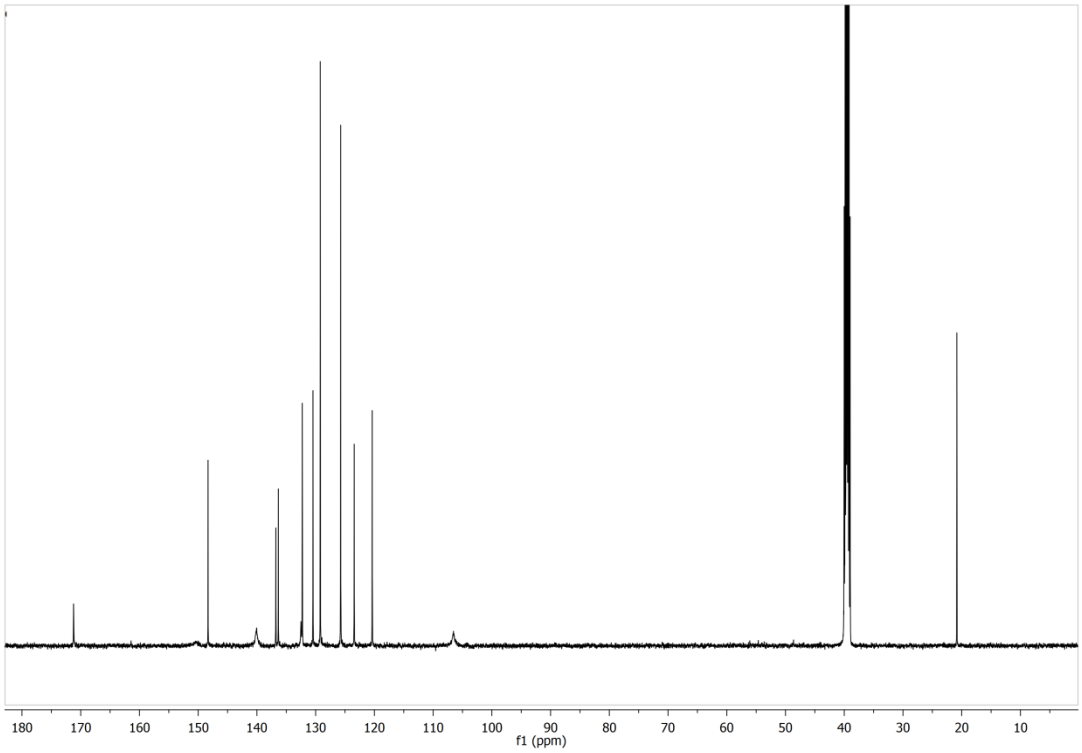
Supplementary Figure S24. ^{1}H NMR spectrum of **3-OMe** in DMSO-d_6.



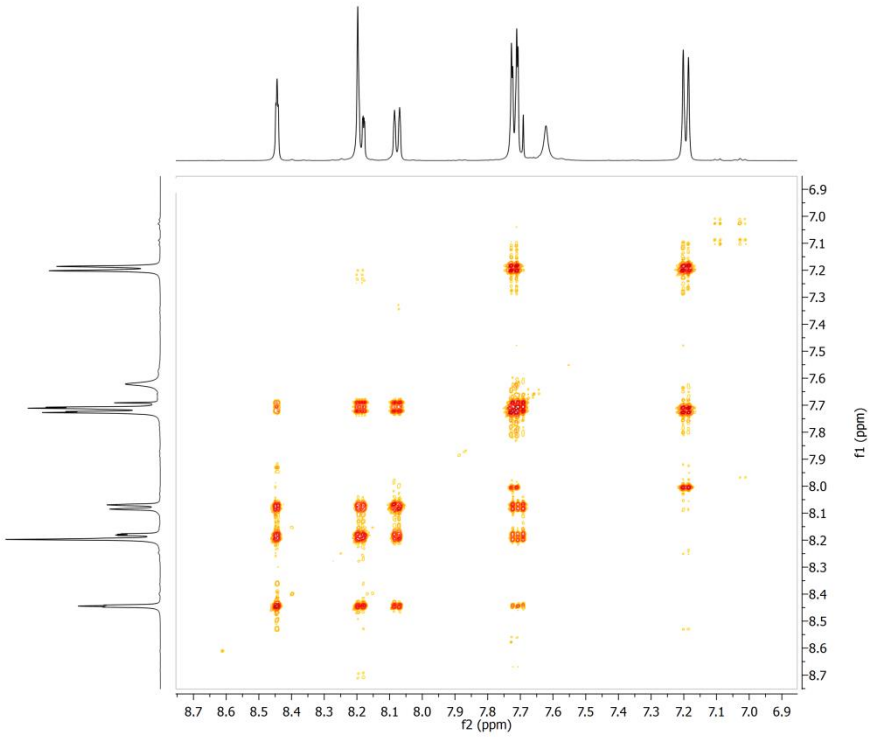
Supplementary Figure S25. ^{13}C NMR spectrum of **3-OMe** in DMSO-d_6.



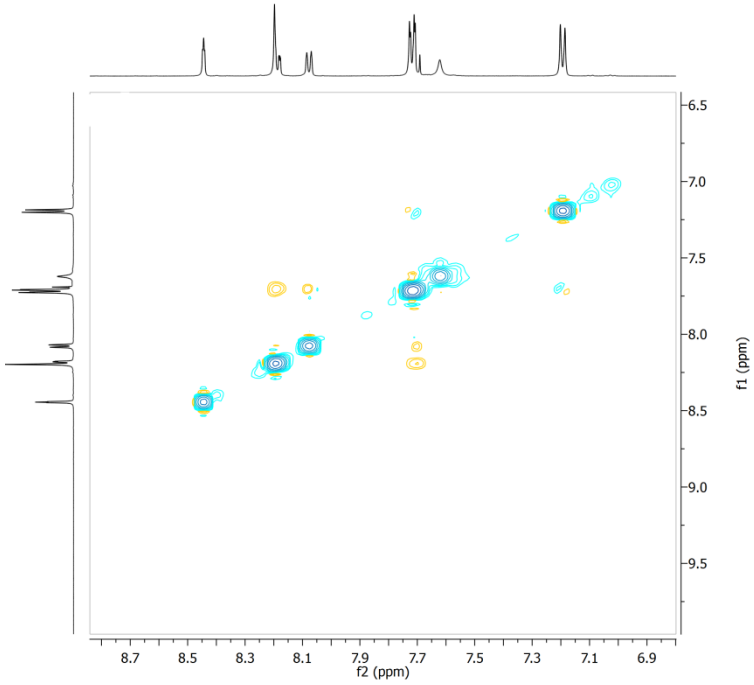
Supplementary Figure S26. ^{1}H NMR spectrum of **3-Me** in DMSO-d_6.



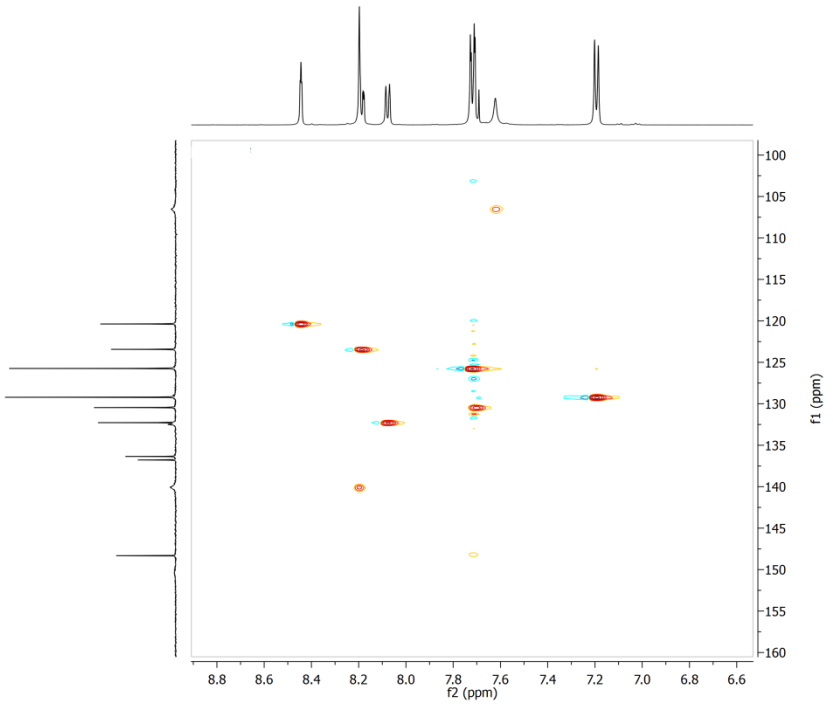
Supplementary Figure S27. ^{13}C NMR spectrum of **3-Me** in DMSO-d_6.



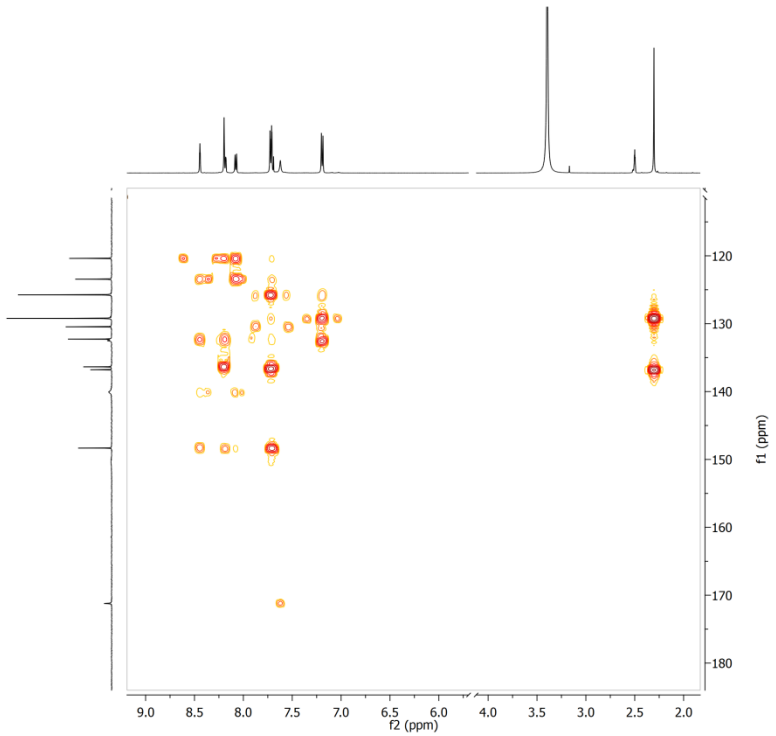
Supplementary Figure S28. COSY spectrum of **3-Me** in DMSO-d_6.



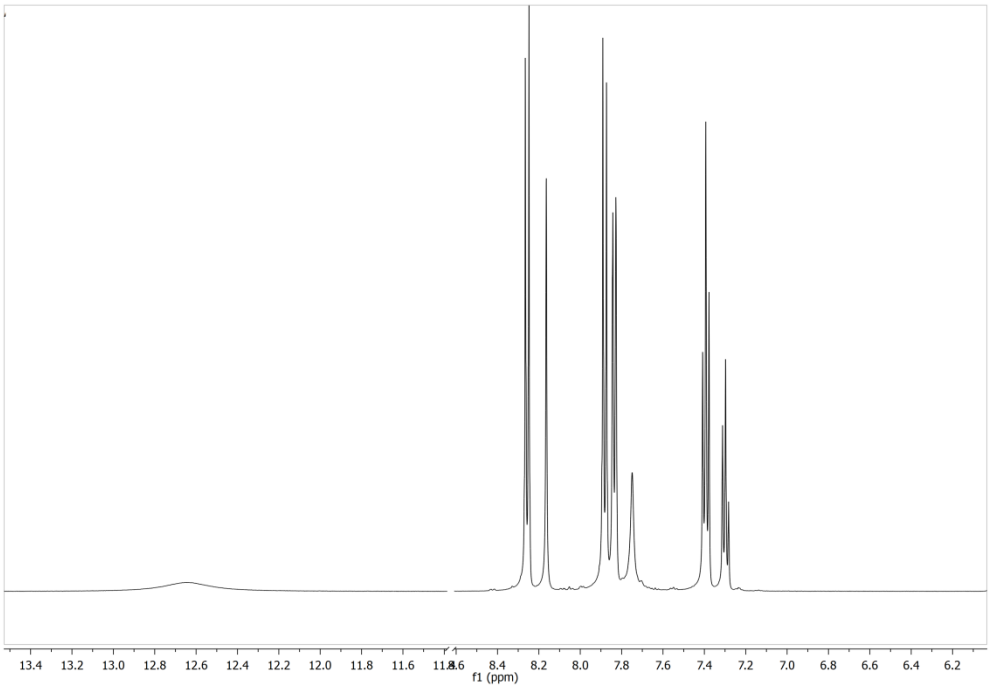
Supplementary Figure S29. NOESY spectrum of **3-Me** in DMSO-d_6.



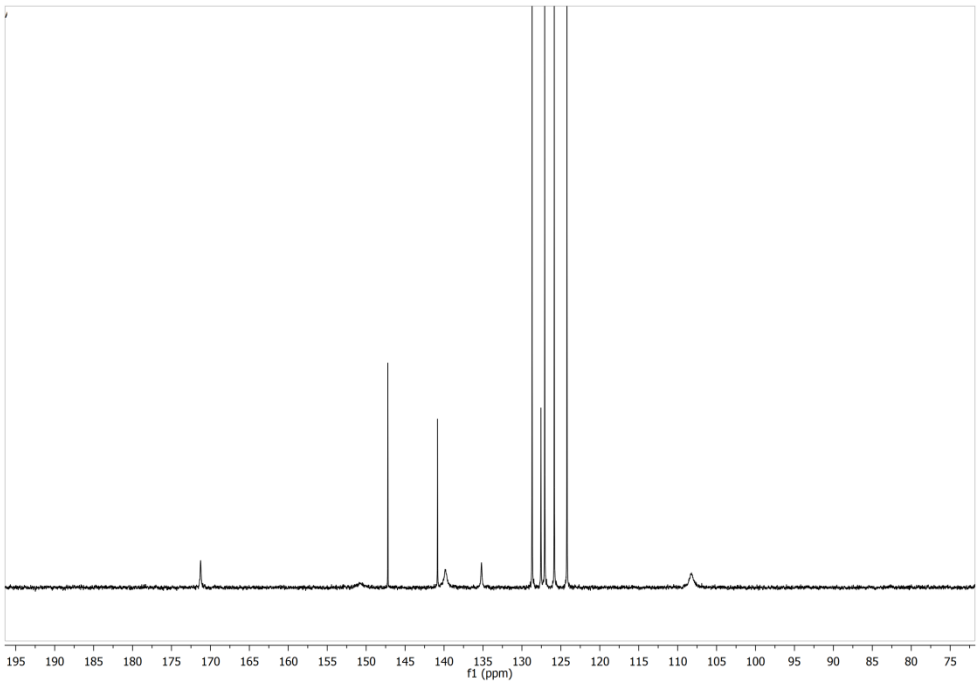
Supplementary Figure S30. $^{1}H–^{13}C$ HSQC NMR spectrum of **3-Me** in DMSO-d_6.



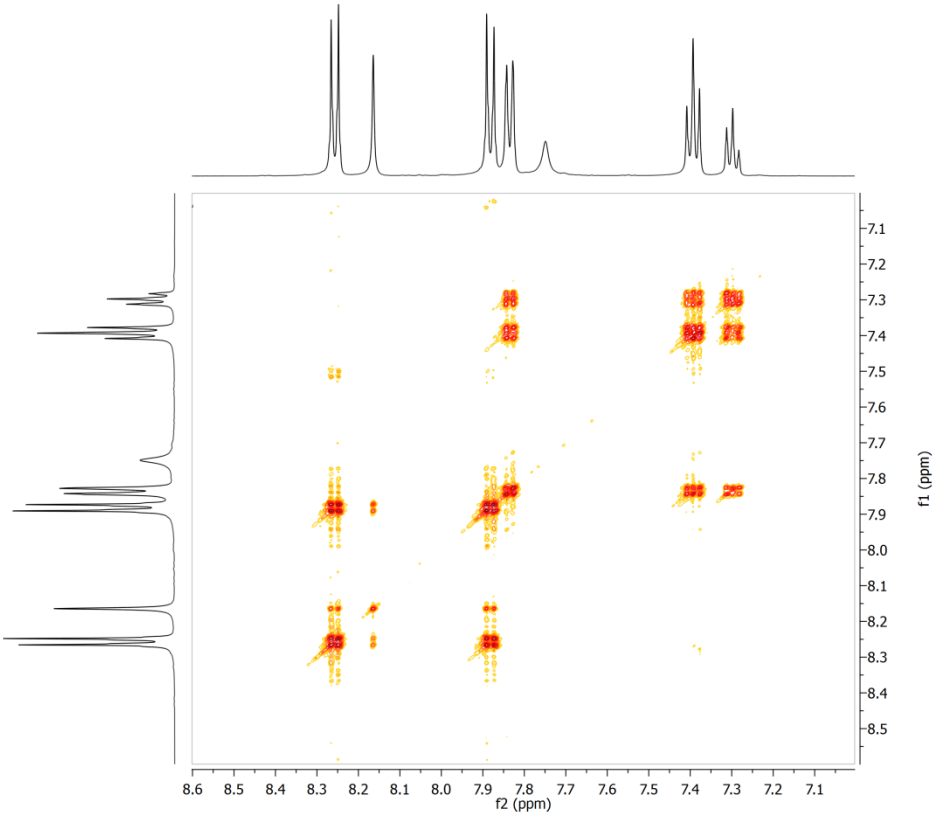
Supplementary Figure S31. $^{1}H–^{13}C$ HMBC NMR spectrum of **3-Me** in DMSO-d_6.



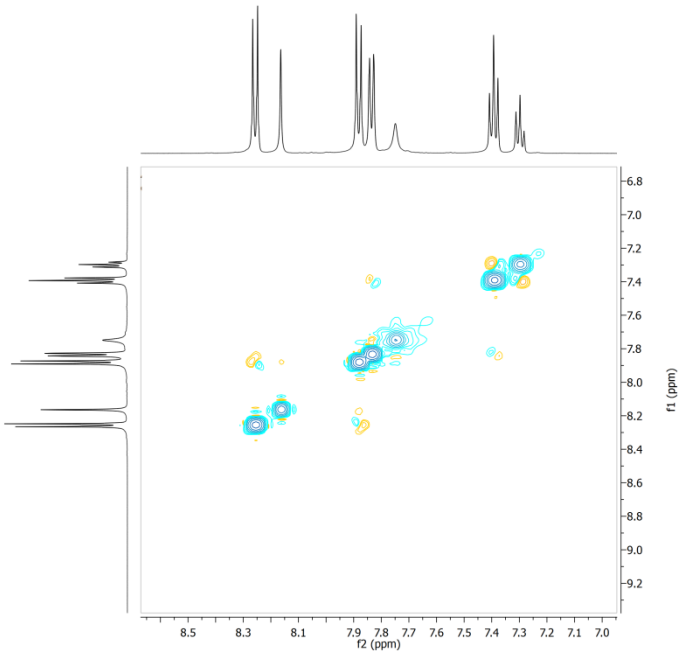
Supplementary Figure S32. ^{1}H NMR spectrum of **4** in DMSO-d_6.



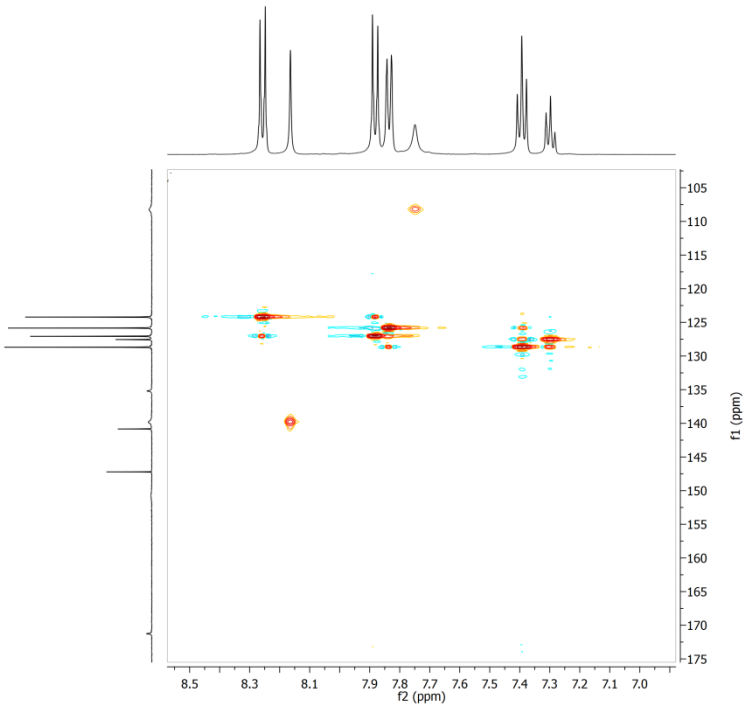
Supplementary Figure S33. ^{13}C NMR spectrum of **4** in DMSO-d_6.



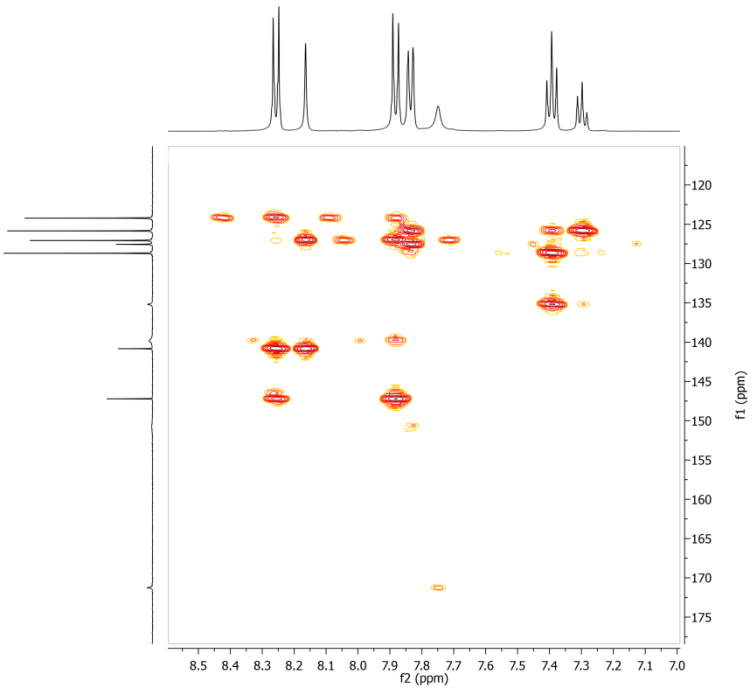
Supplementary Figure S34. COSY spectrum of **4** in DMSO-d_6.



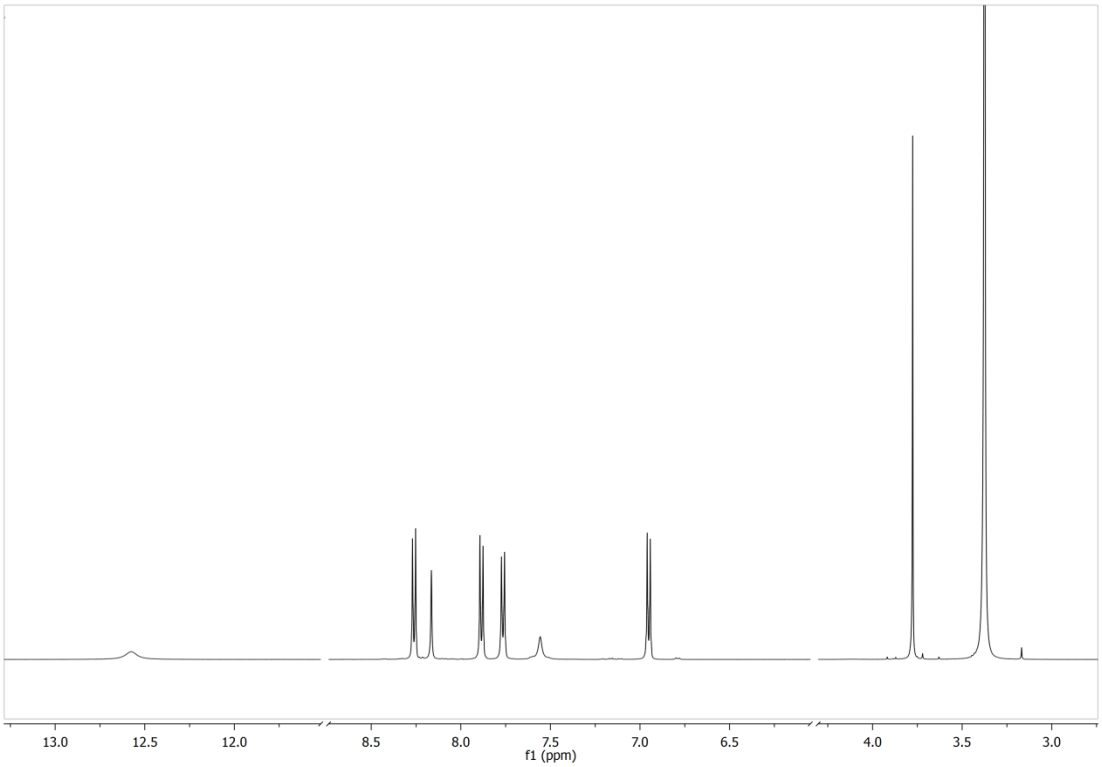
Supplementary Figure S35. NOESY spectrum of **4** in DMSO-d_6.



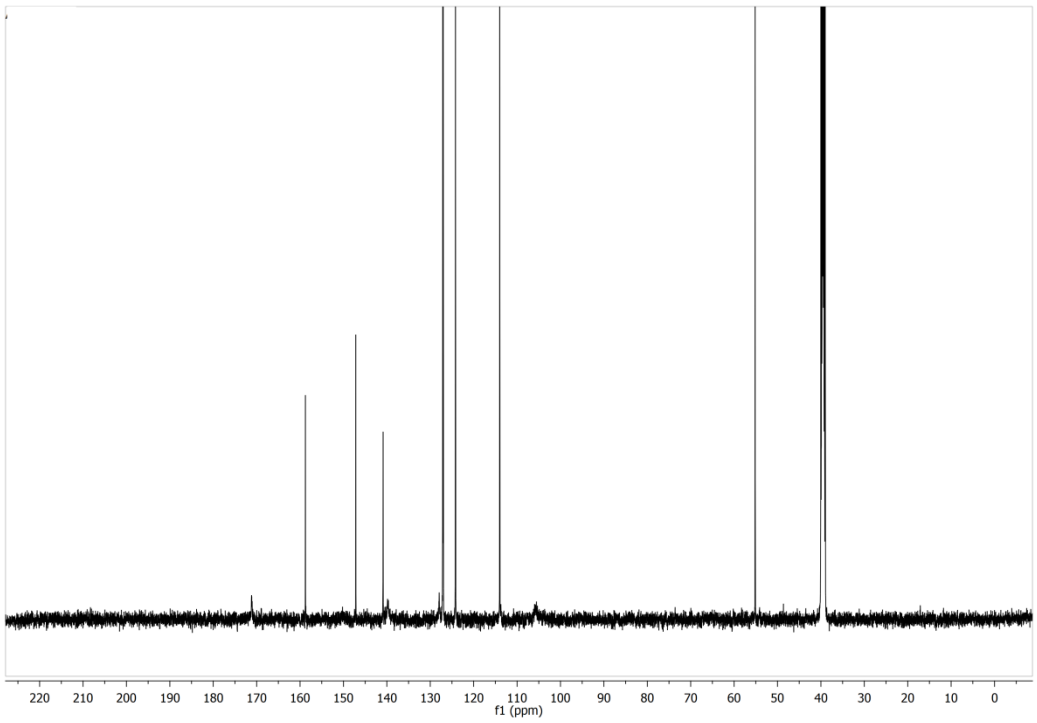
Supplementary Figure S36. $^{1}H–^{13}C$ HSQC NMR spectrum of **4** in DMSO-d_6.



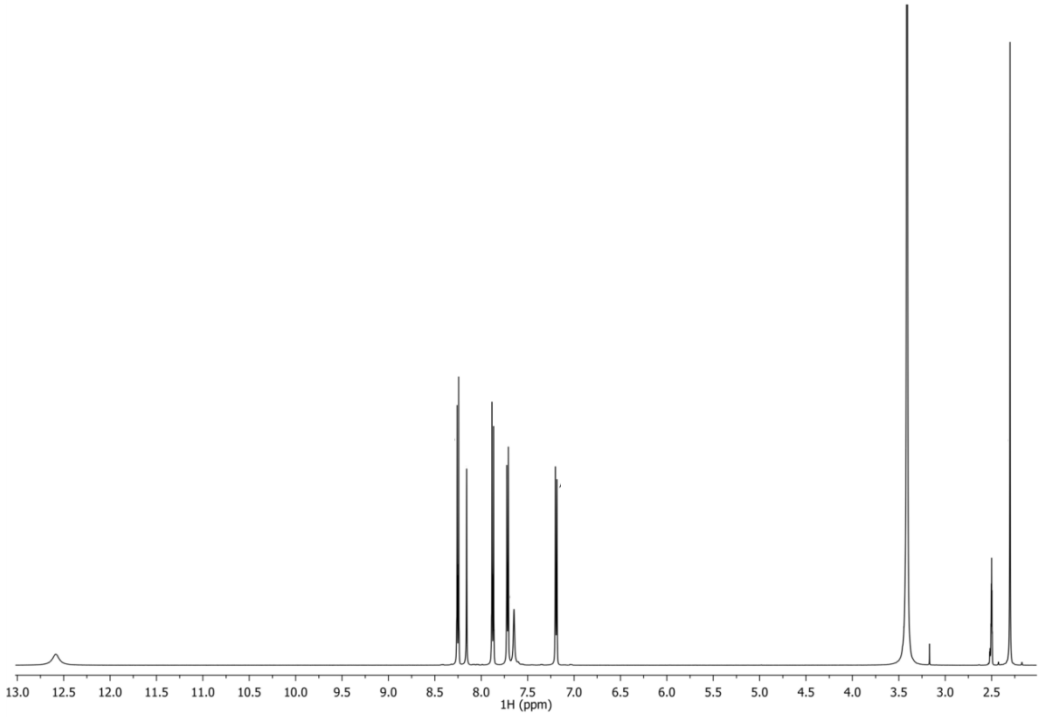
Supplementary Figure S37. $^{1}H–^{13}C$ HMBC NMR spectrum of **4** in DMSO-d_6.



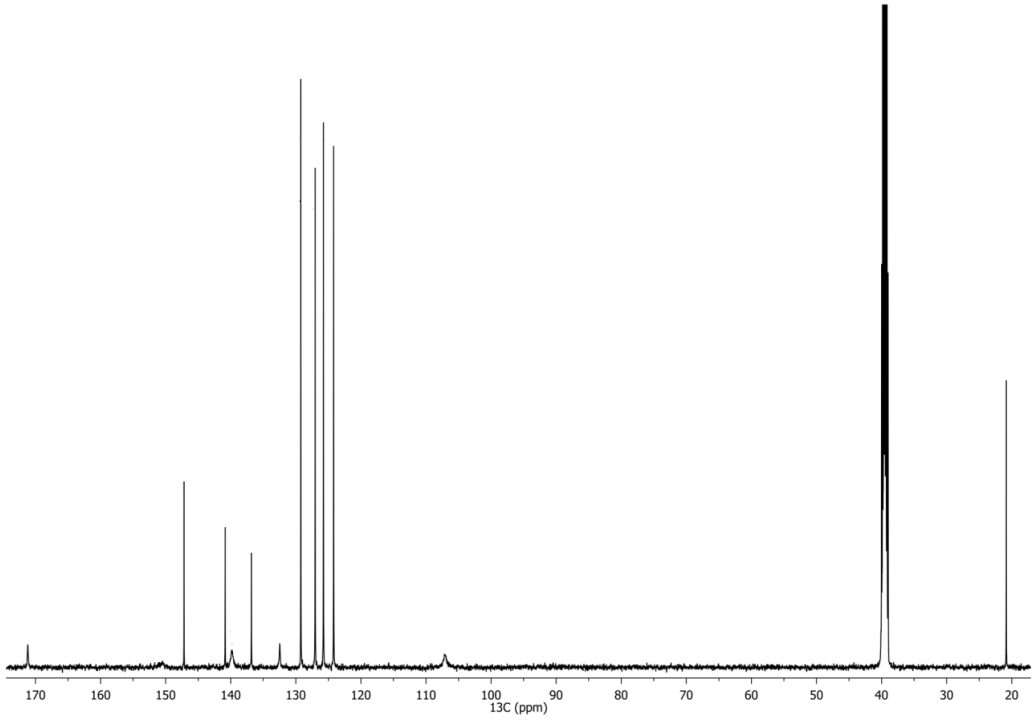
Supplementary Figure S38. ^{1}H NMR spectrum of **4-OMe** in DMSO-d_6.



Supplementary Figure S39. ^{13}C NMR spectrum of **4-OMe** in DMSO-d_6.



Supplementary Figure S40. ^{1}H NMR spectrum of **4-Me** in DMSO-d_6.



Supplementary Figure S41. ^{13}C NMR spectrum of **4-Me** in DMSO-d_6.

Supplementary Table S1. Crystallographic data for **4-Me** and **4-OMe**.

Structure	**4-Me**	**4-OMe**
Brutto formula	$C_{17}H_{14}N_4O_2Se$	$C_{17}H_{14}N_4O_3Se$
Formula weight ($gmol^{-1}$)	385.28	401.28
Crystal color and habit	Orange prism	Brown prism
Crystal dimensions (mm)	0.33 × 0.26 × 0.21	0.30 × 0.21 × 0.20
Space group	*Pbcn*	*Pbca*
a (Å)	11.4924(3)	11.8767(6)
b (Å)	7.9189(4)	13.5795(7)
c (Å)	35.9317(19)	20.3707(11)
V ($Å^3$)	3270.0(3)	3285.4(3)
Z	8	8
μ (CuK_α) (mm^{-1})	3.263	3.218
Absorption correction	Multi-scan	Multi-scan
F(000)	1552	1616
θ max (°)	74.000	76.014
No. refl. measured	7934	9975
No. refl. unique	3212	3383
No. refl. observed [$I>2\sigma(I)$]	2562	2912
R_{int}	0.0395	0.0229
R_σ	0.0601	0.0315
Parameters	227	239
R_1 [$I>2\sigma(I)$]	0.0461	0.0319
wR_2, all	0.1414	0.0964
S	1.054	1.044
ρ_{max}, ρ_{min} ($eÅ^{-3}$)	0.46, –0.68	0.25, –0.34

Supplementary Table S2. Angles between the selenazole ring least square plane and phenyl rings least square planes.

Se1–C8–C9–N10–C11	**4-Me** (º)	**4-OMe** (º)
C2–C3–C4–C5–C6–C7	30.18 (15)	4.94 (10)
C15–C16–C17–C18–C19–C20	24.86 (15)	6.03 (11)