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Electronic Supporting Information

for

Benzimidazole-based Ionic and Non-ionic Organoselenium Compounds: Innovative Synthetic Strategies, Structural Characterizations and Preliminary Anti-Proliferative Activities

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NMR Spectroscopic data of the synthesized compounds

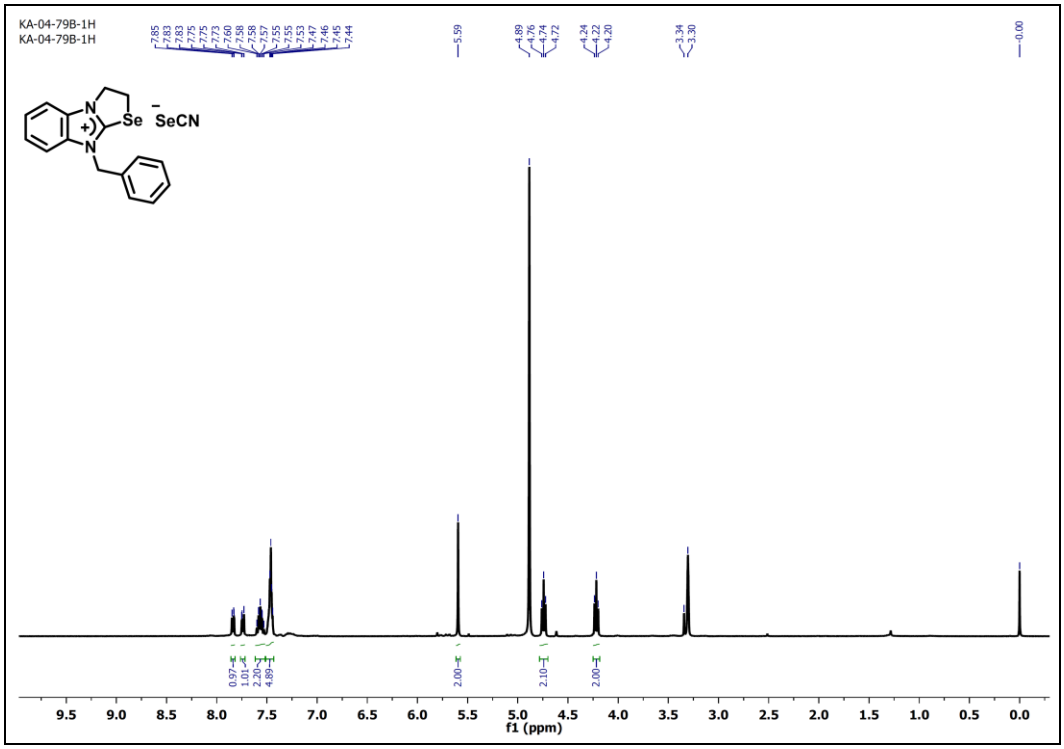


Figure S1. ^{1}H NMR spectrum (methanol-d_4, 400 MHz) of compound **7a**.

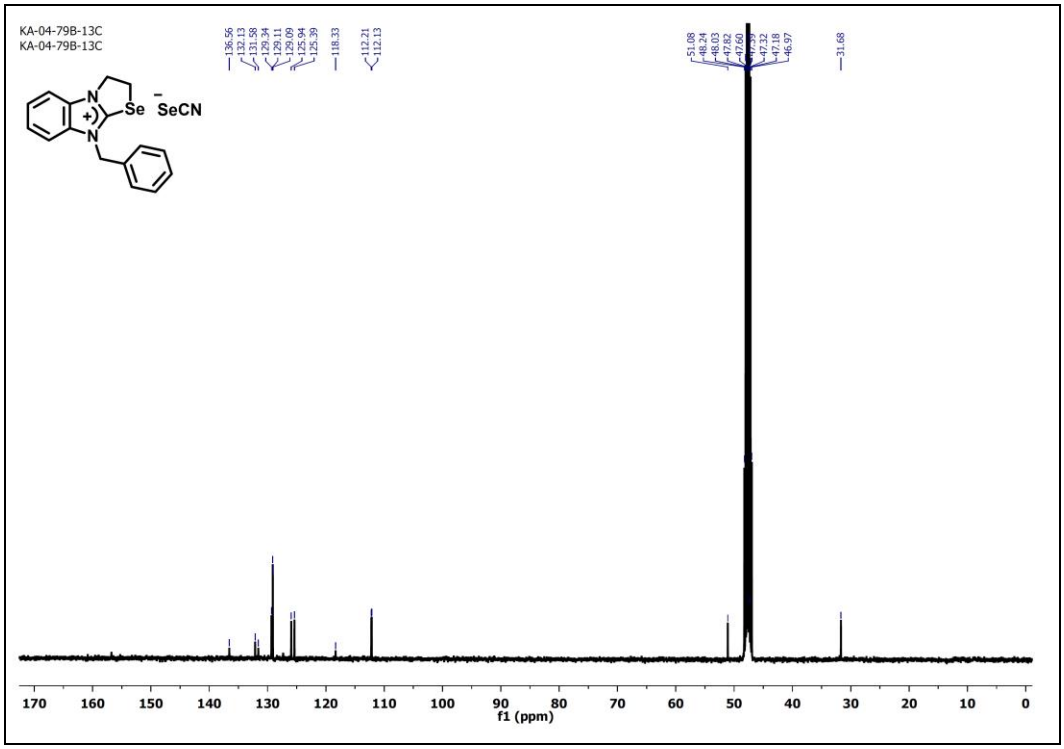


Figure S2. ^{13}C NMR spectrum (methanol-d_4, 100 MHz) of compound **7a**.

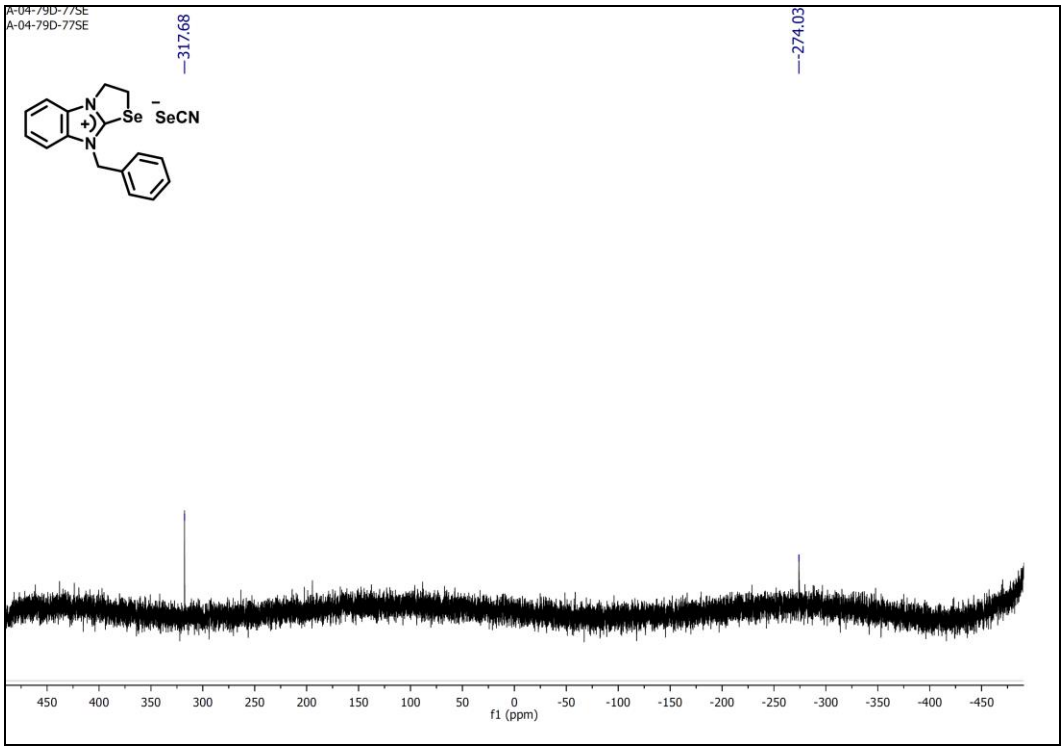


Figure S3. ^{77}Se NMR spectrum (DMSO-d_6, 76 MHz) of compound **7a**.

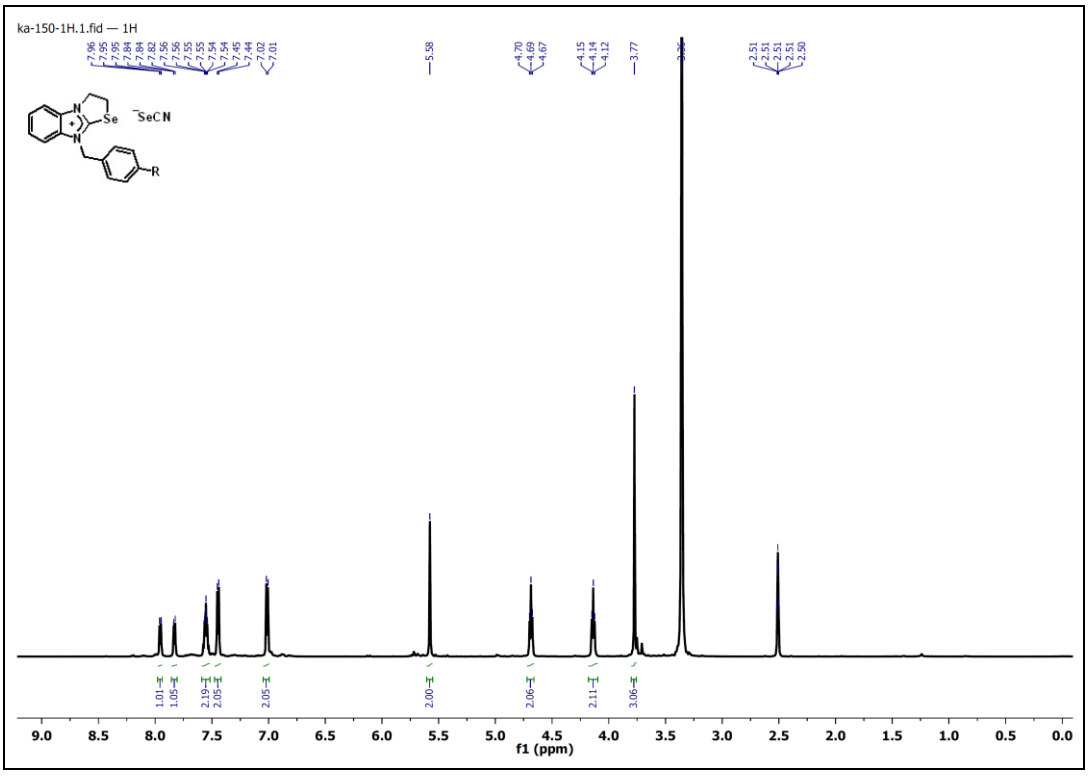


Figure S4. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **7b**.

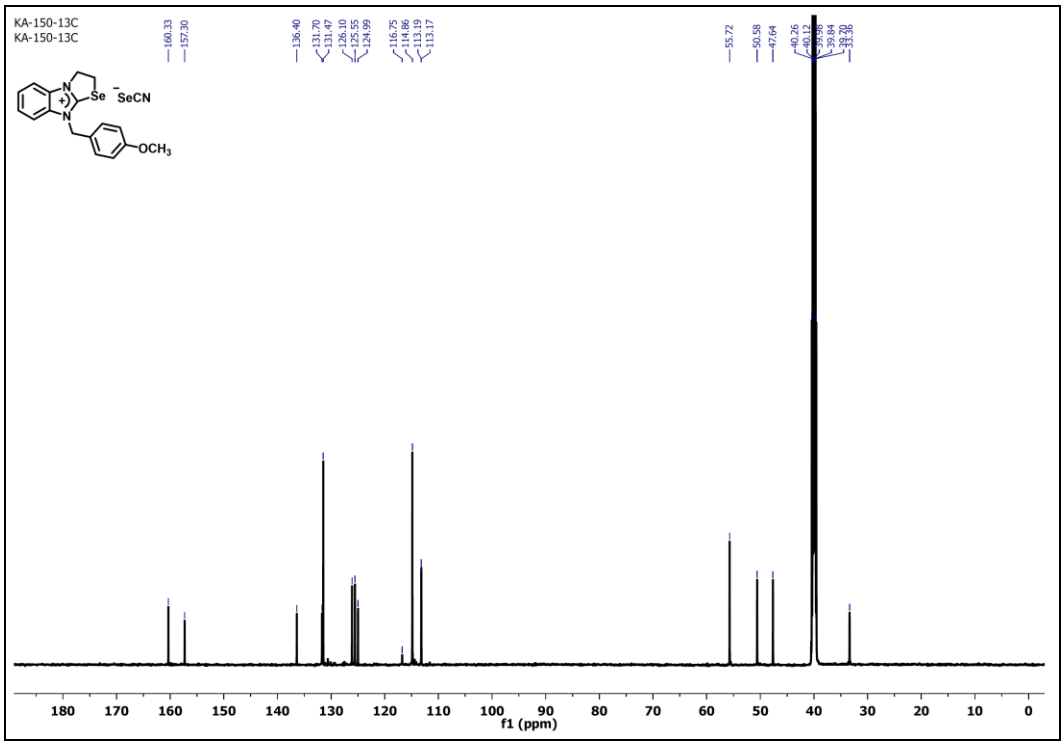


Figure S5. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **7b**.

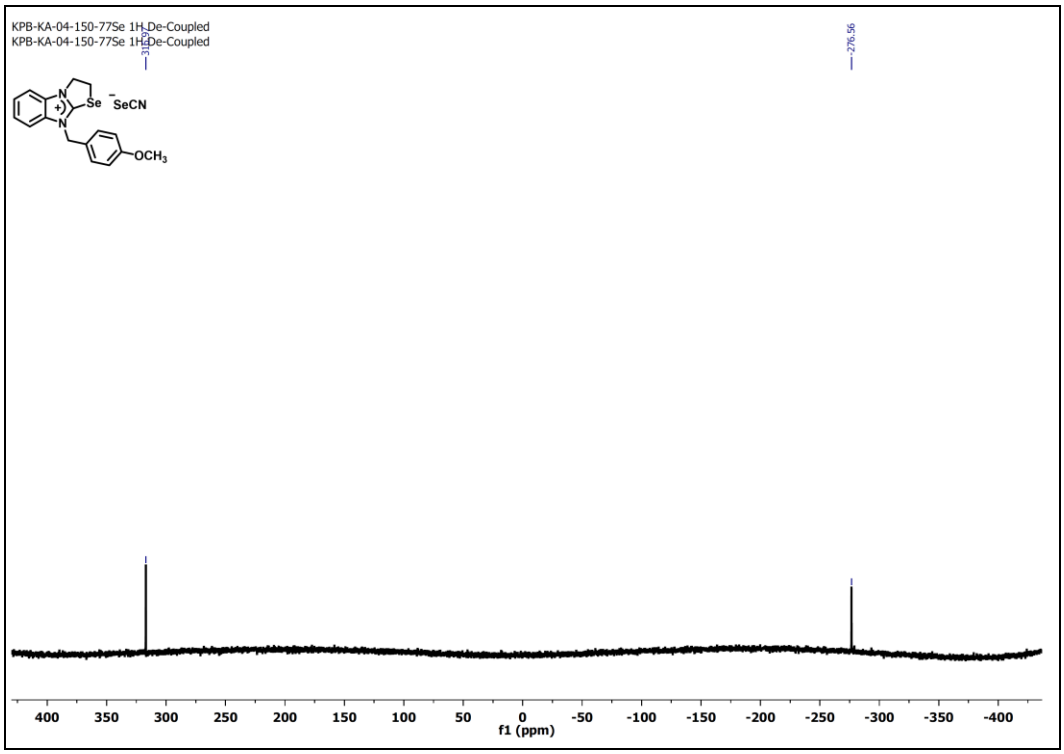


Figure S6. ^{77}Se NMR spectrum (DMSO-d_6, 76 MHz) of compound **7b**.

(Compound **7c** could not be purified and characterized)

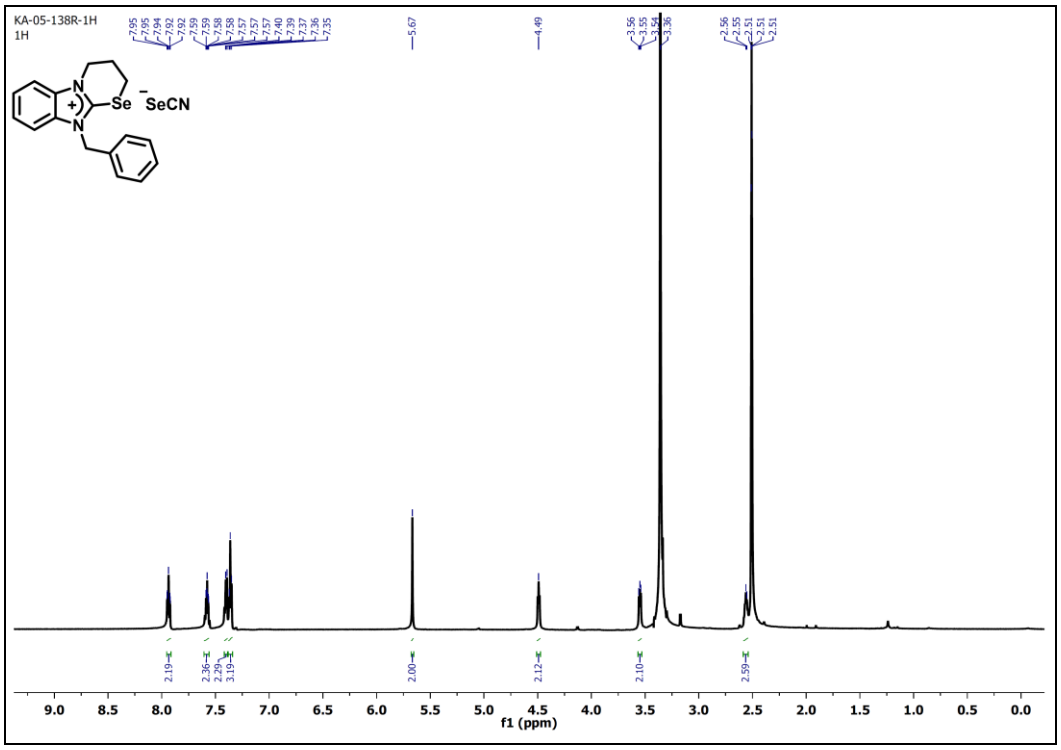


Figure S7. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **8a**.

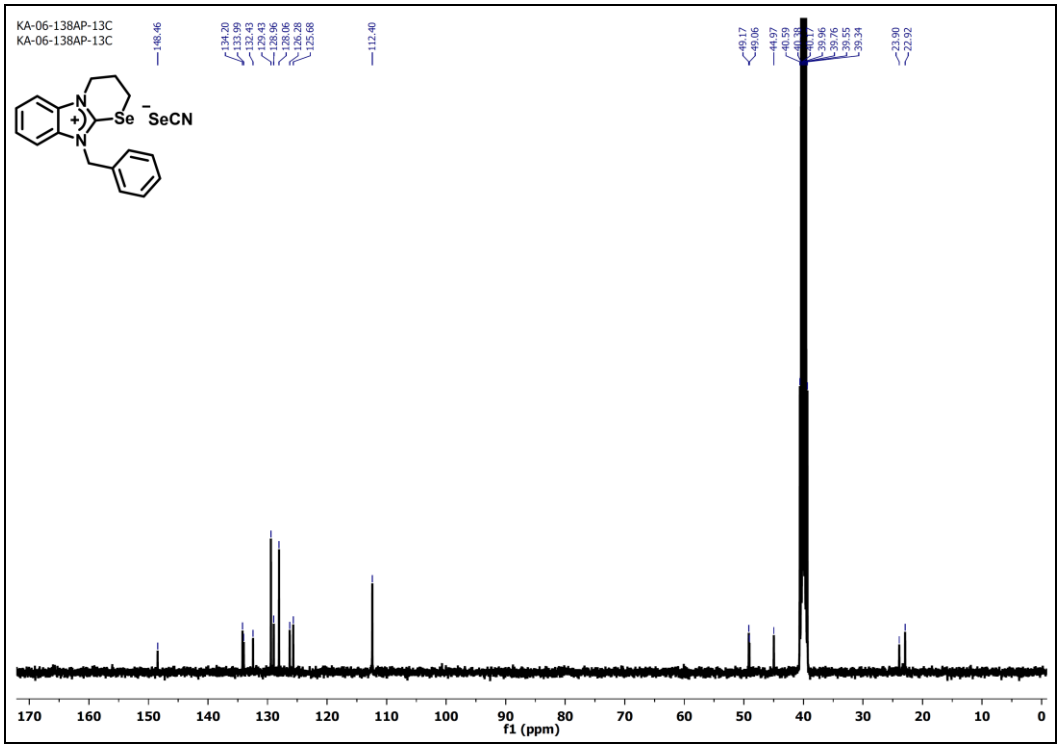


Figure S8. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **8a**.

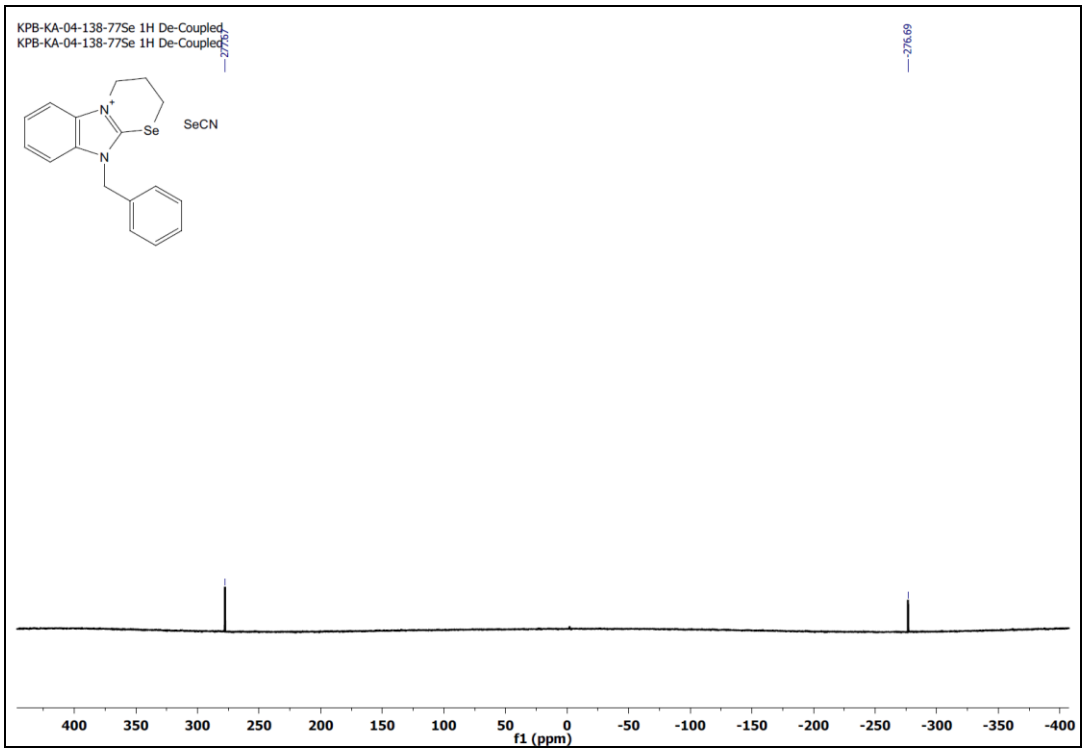


Figure S9. ^{77}Se NMR spectrum (DMSO-d_6, 114 MHz) of compound **8a**.

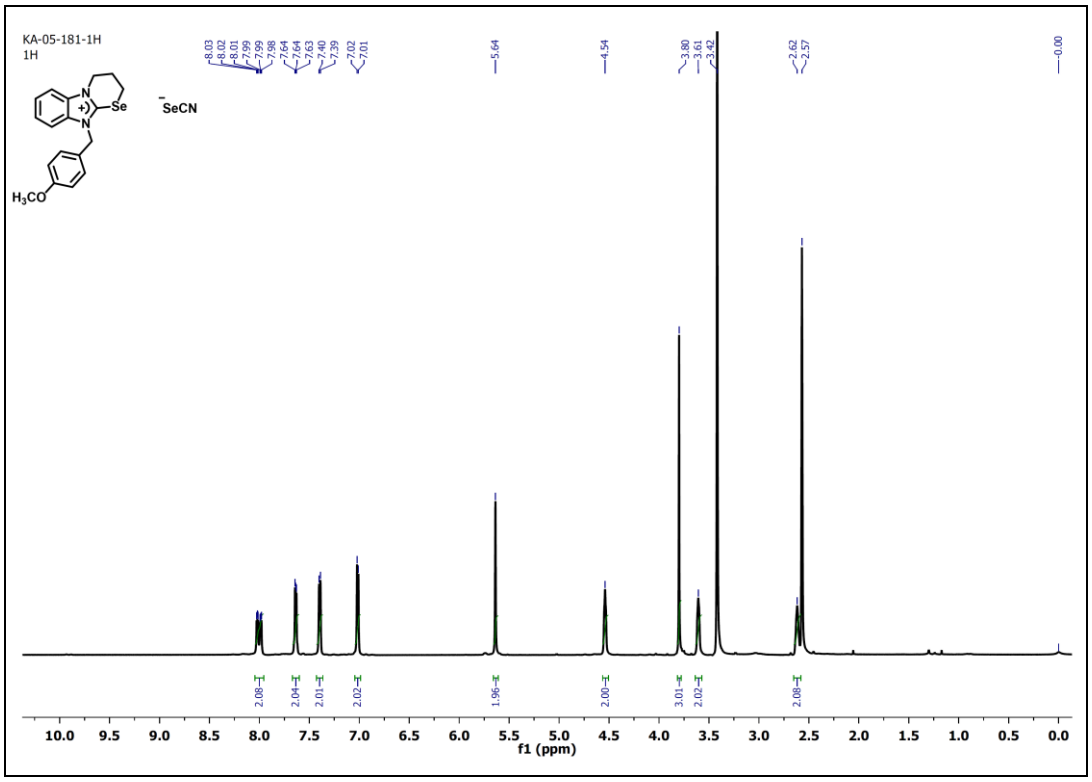


Figure S10. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **8b**.

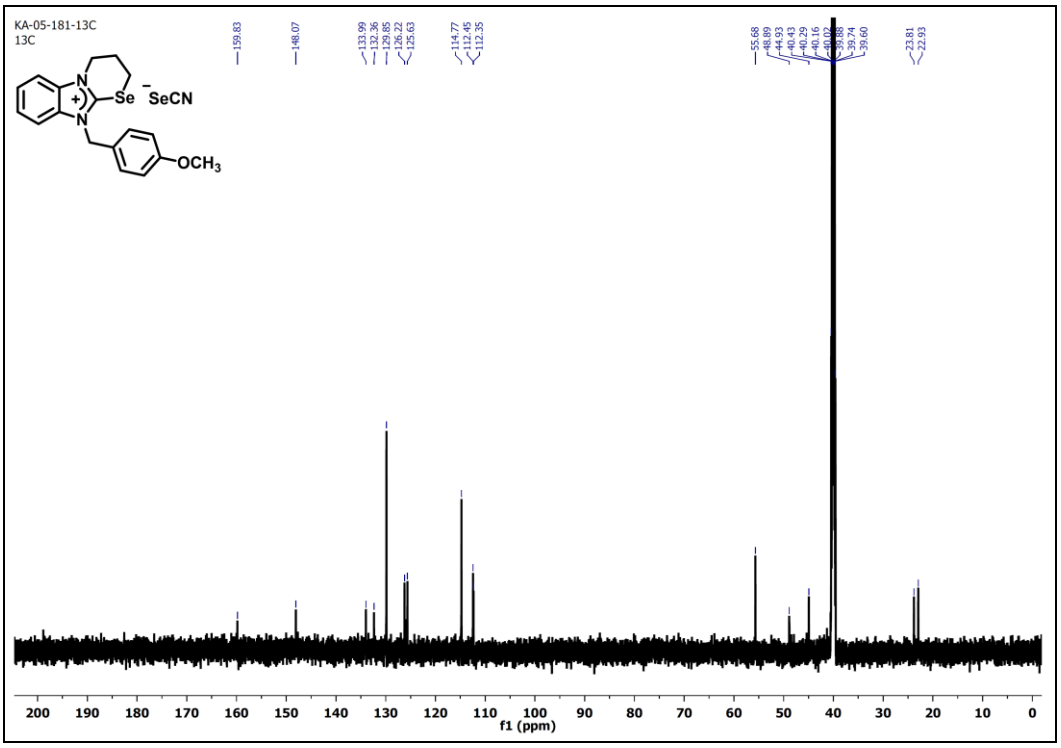


Figure S11. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **8b**.

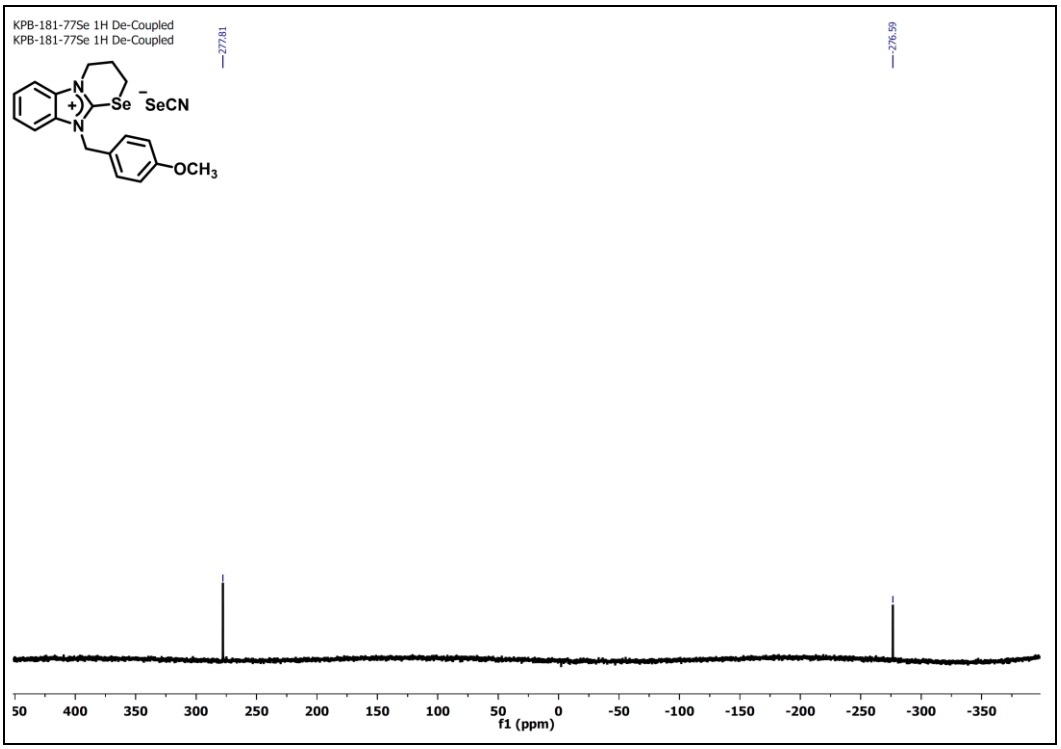


Figure S12. ^{77}Se NMR spectrum (DMSO-d_6, 76 MHz) of compound **8b**.

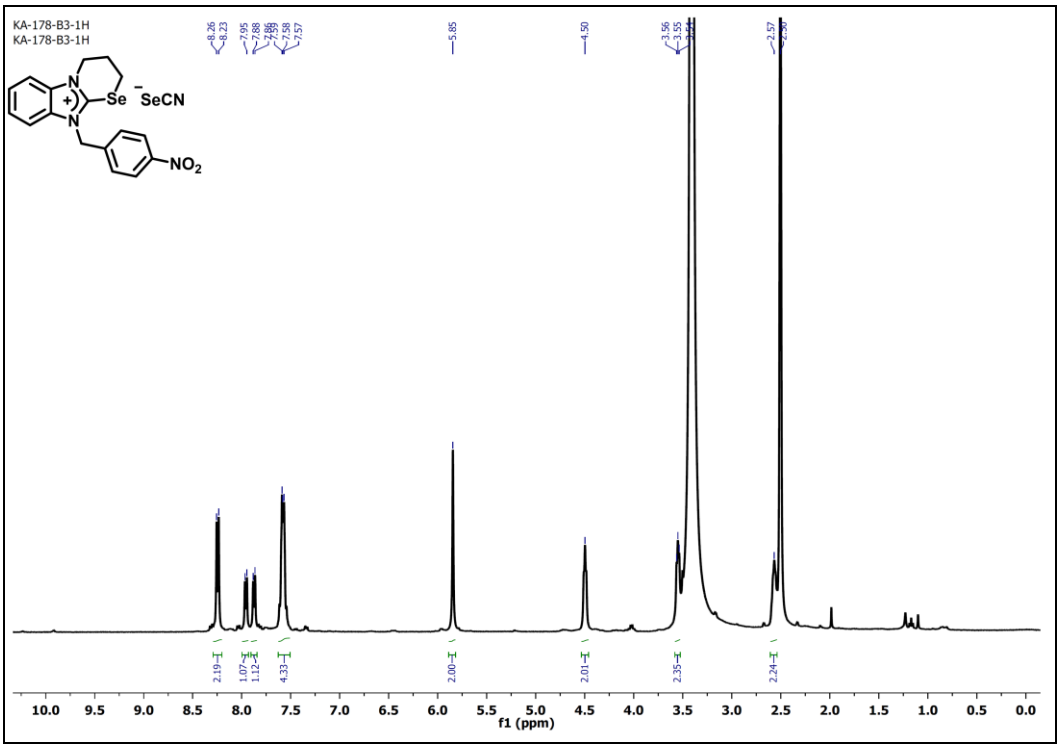


Figure S13. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound **8c**.

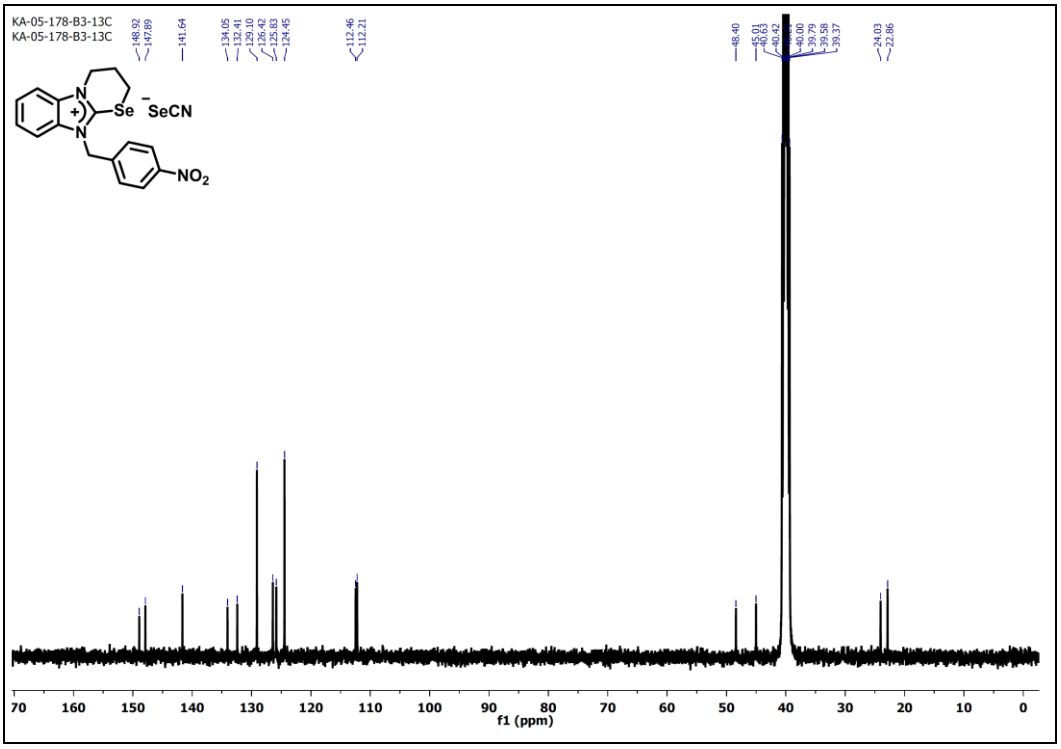


Figure S14. ^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound **8c**.

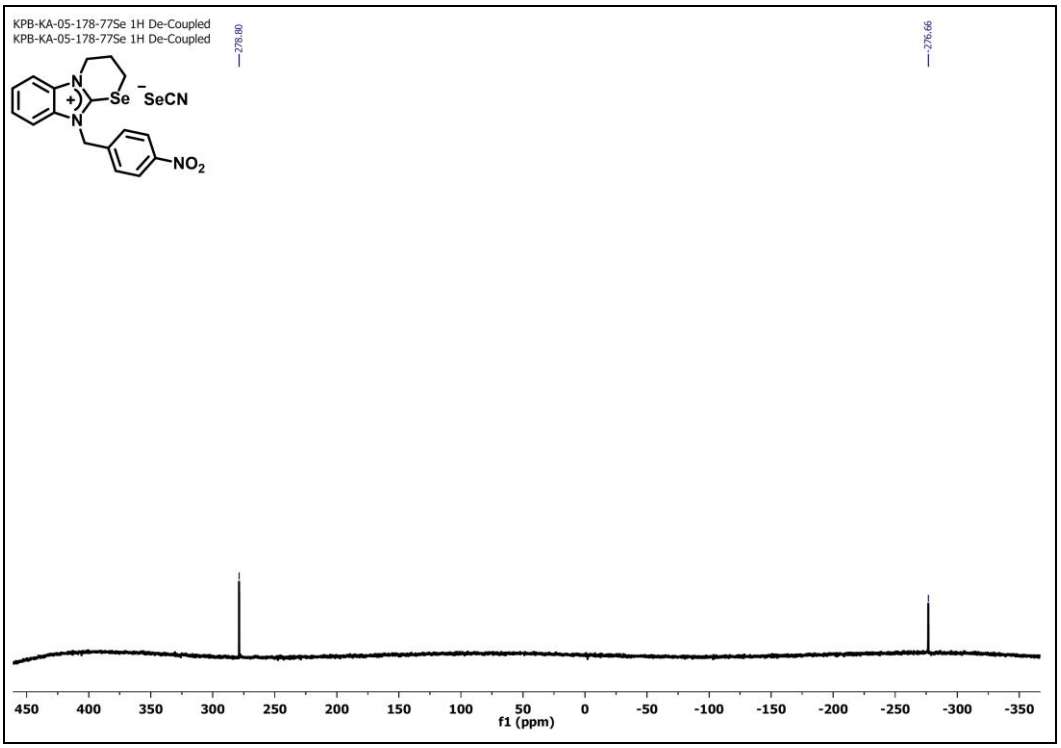


Figure S15. ^{77}Se NMR spectrum (DMSO-d_6, 76 MHz) of compound **8c**.

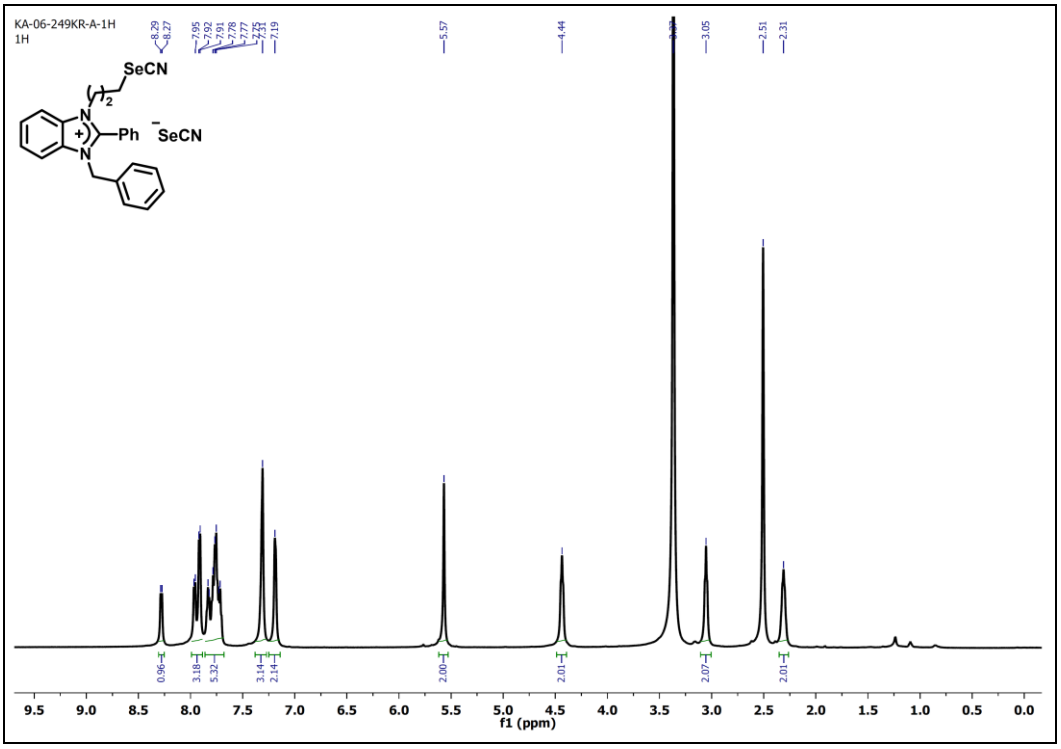


Figure S16. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **9a**.

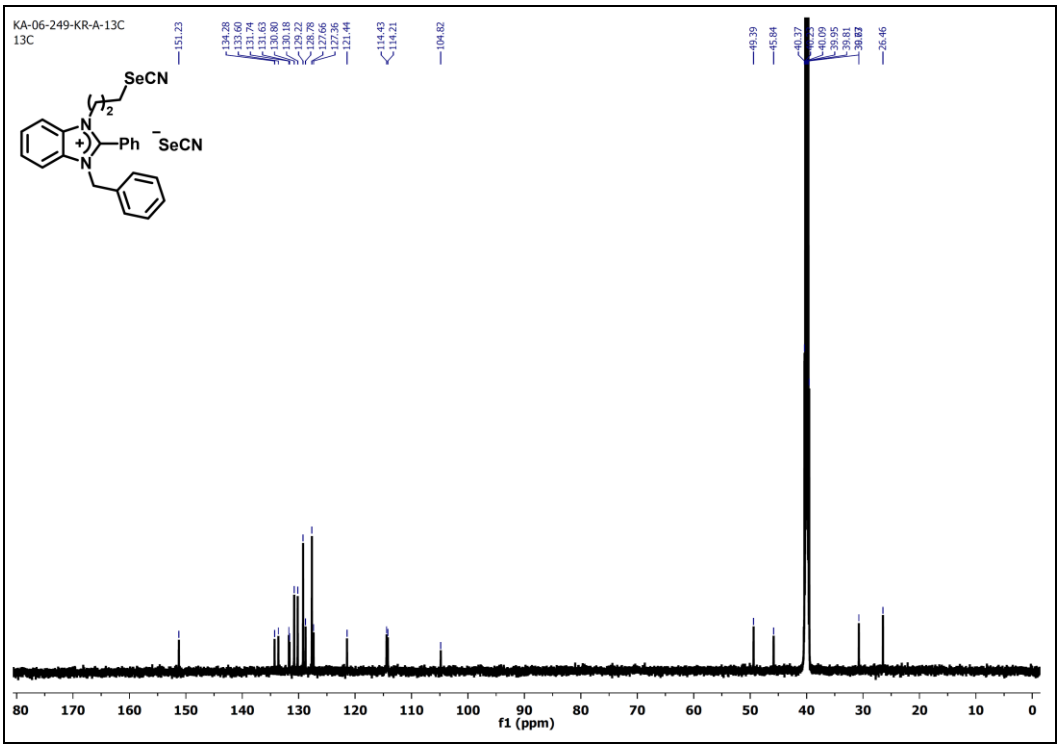


Figure S17. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **9a**.

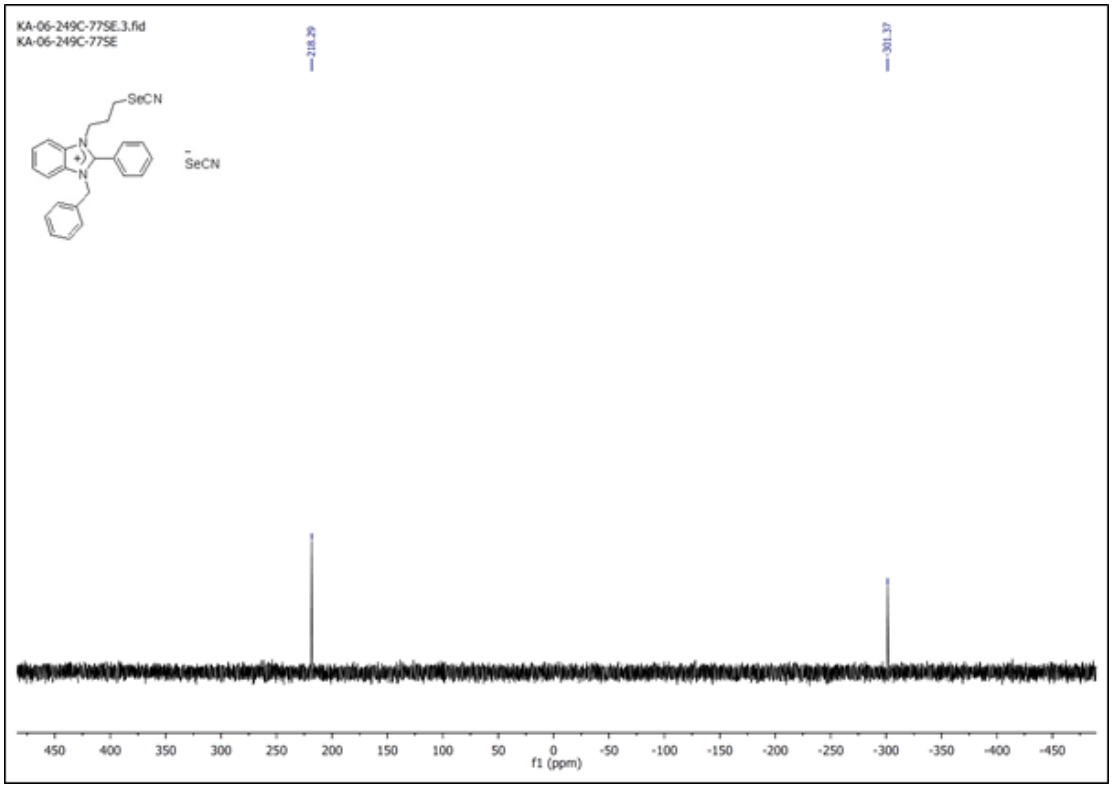


Figure S18. ^{77}Se NMR spectrum (DMSO-d_6, 150 MHz) of compound **9a**.

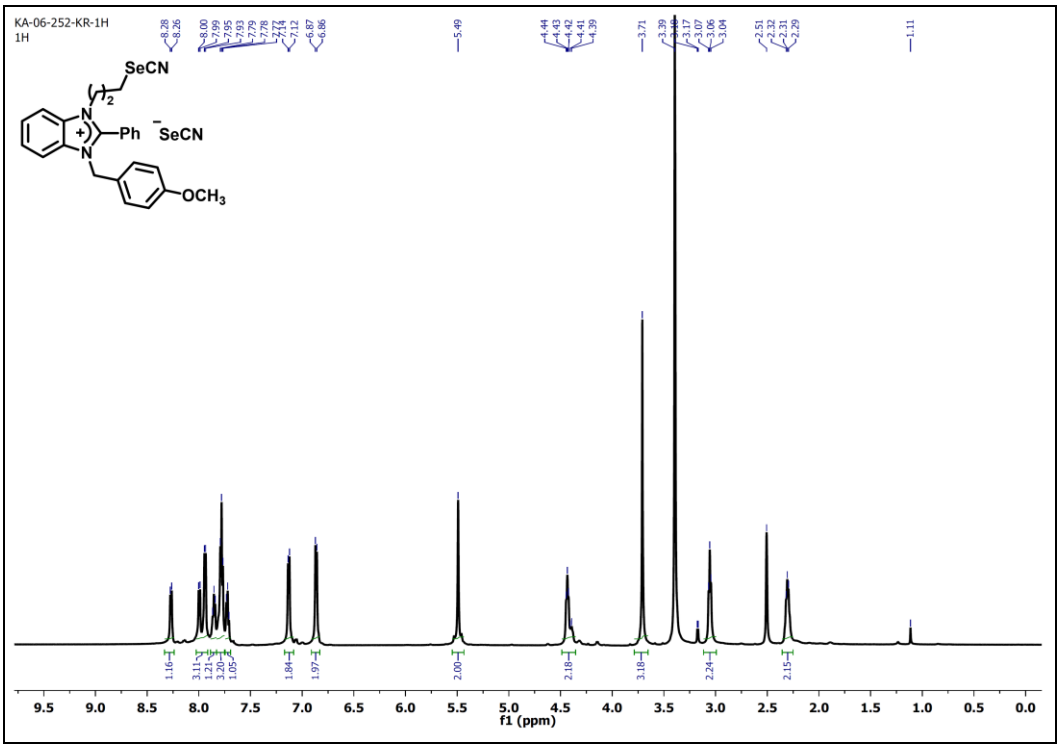


Figure S19. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **9b**.

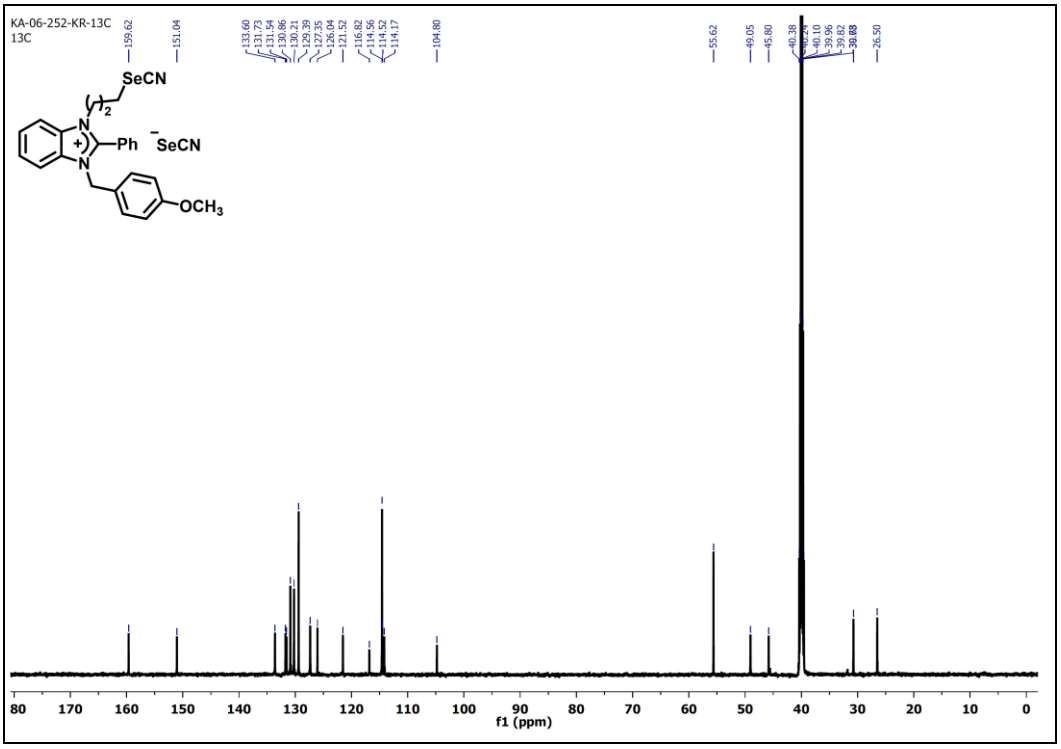


Figure S20. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **9b**.

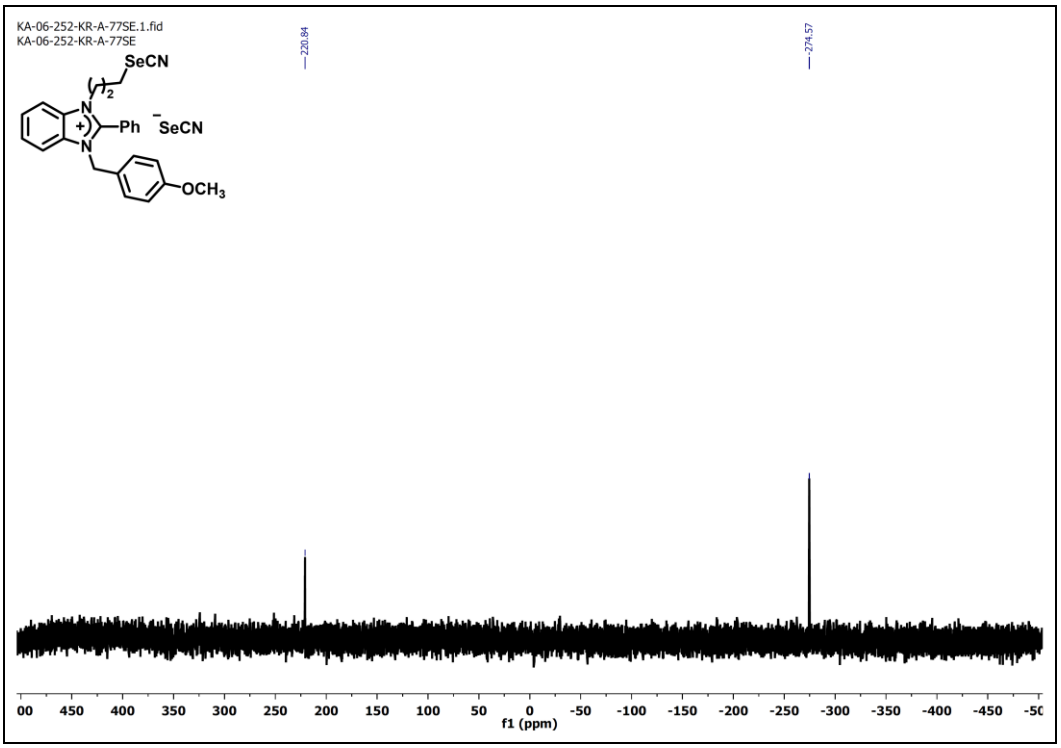


Figure S21. ^{77}Se NMR spectrum (DMSO-d_6, 95 MHz) of compound **9b**.

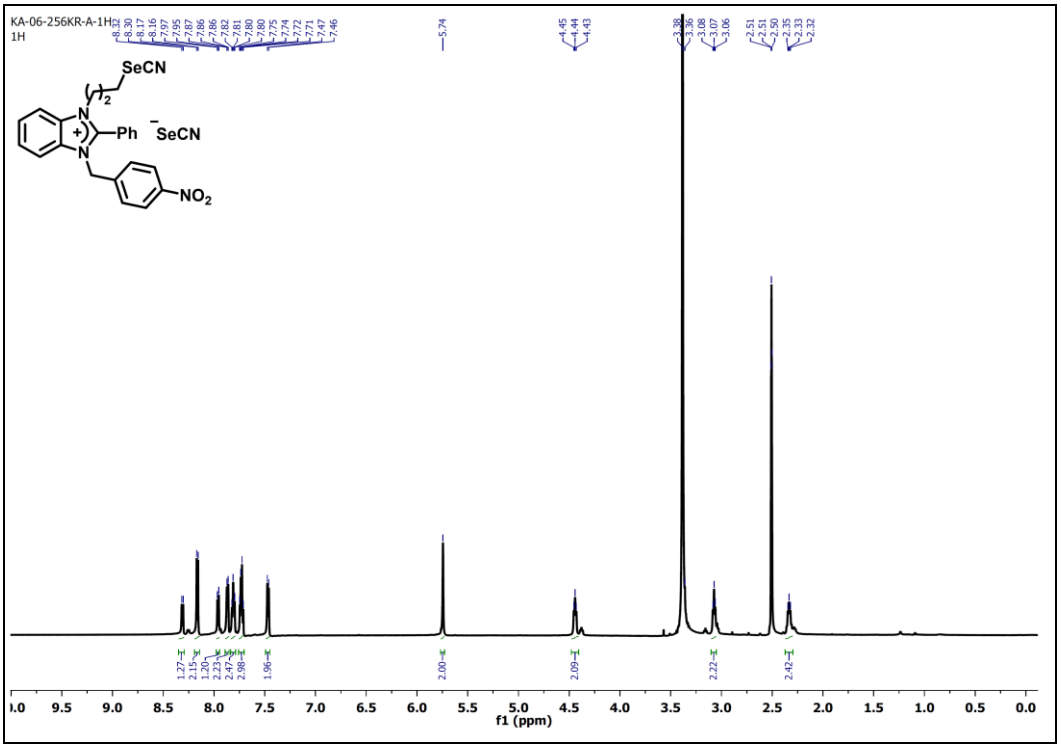


Figure S22. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **9c**.

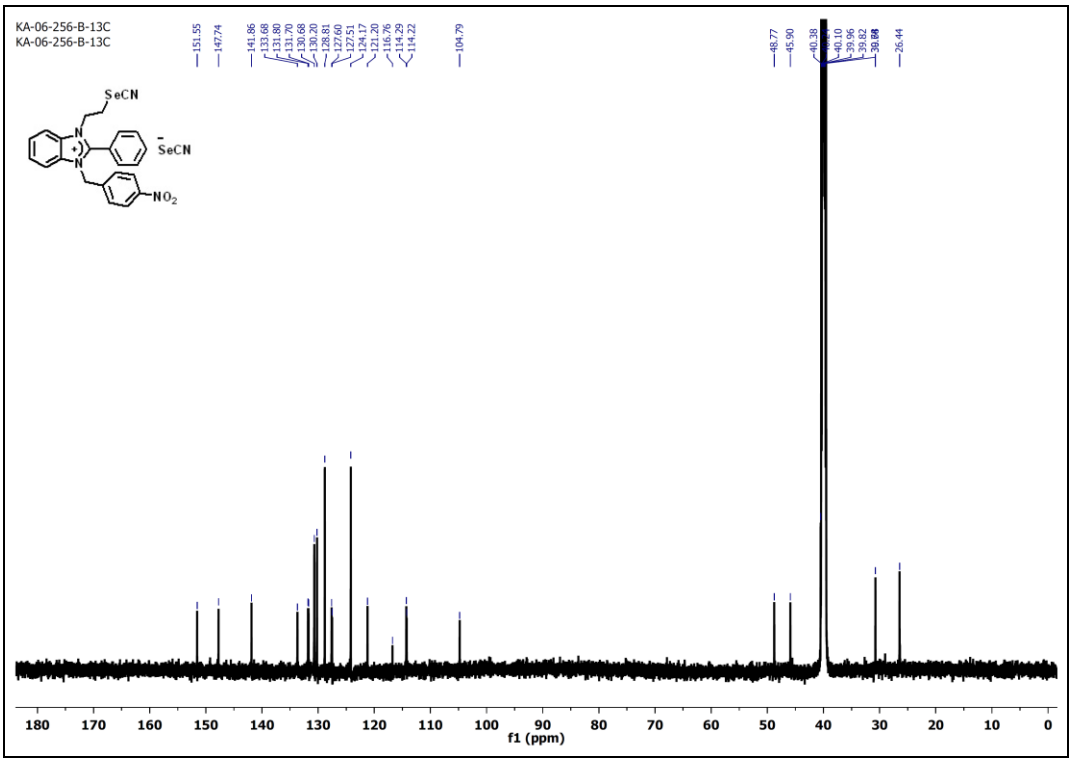


Figure S23. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **9c**.

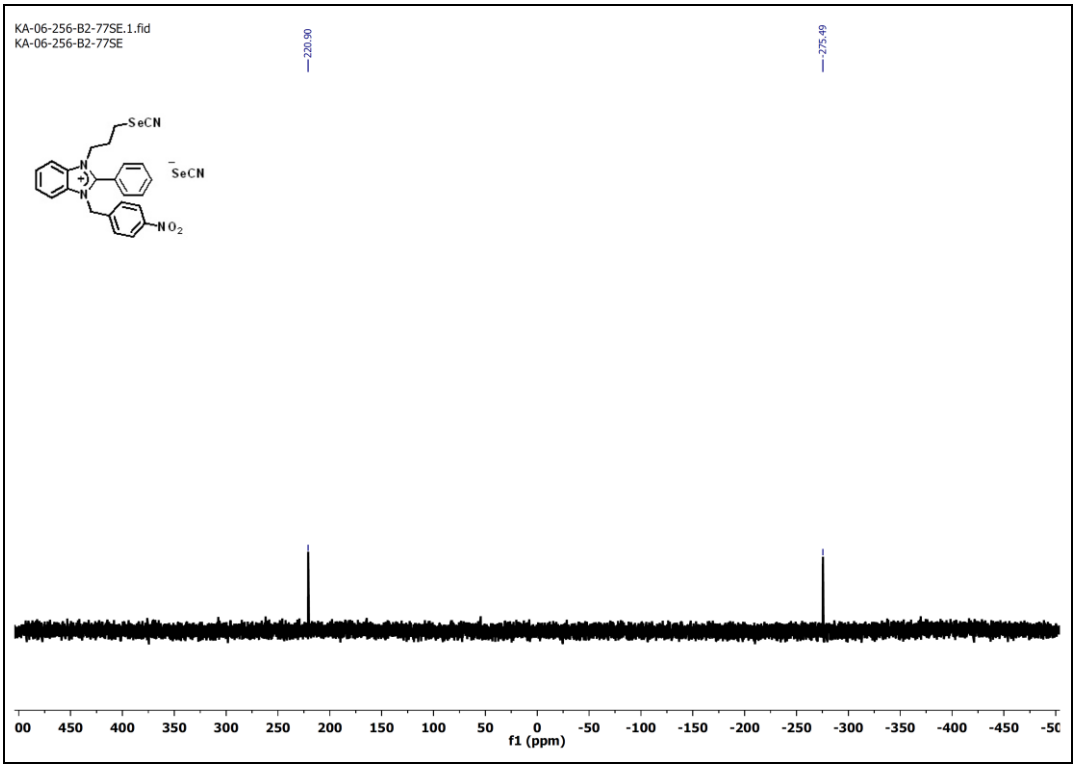
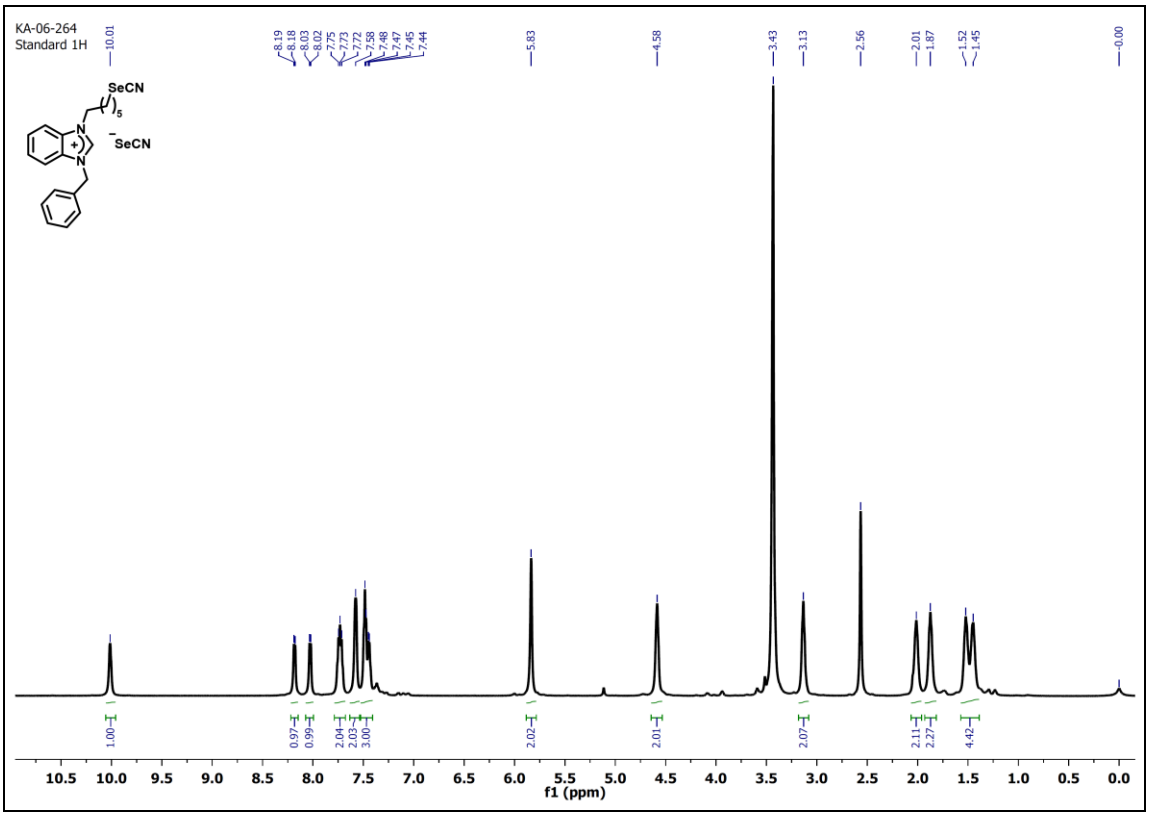


Figure S24. ^{77}Se NMR spectrum (DMSO-d_6, 95 MHz) of compound **9c**.



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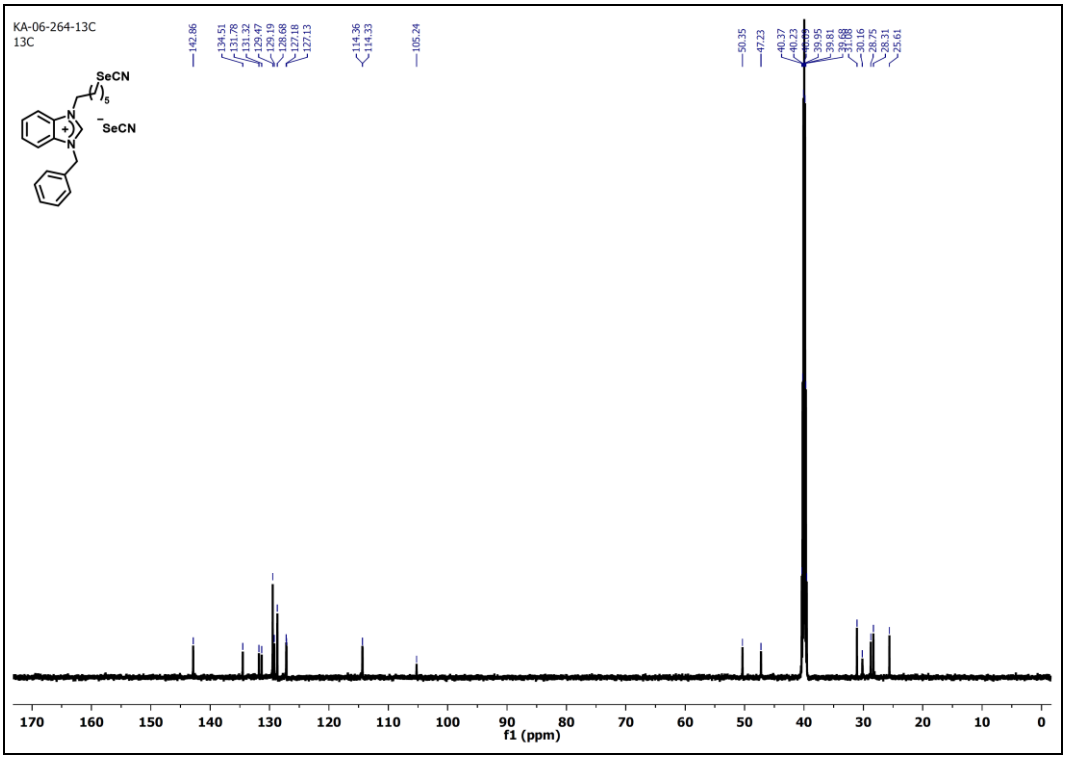

Figure S26. ^{13}C NMR (DMSO-d_6, 150 MHz) of compound **9d**.

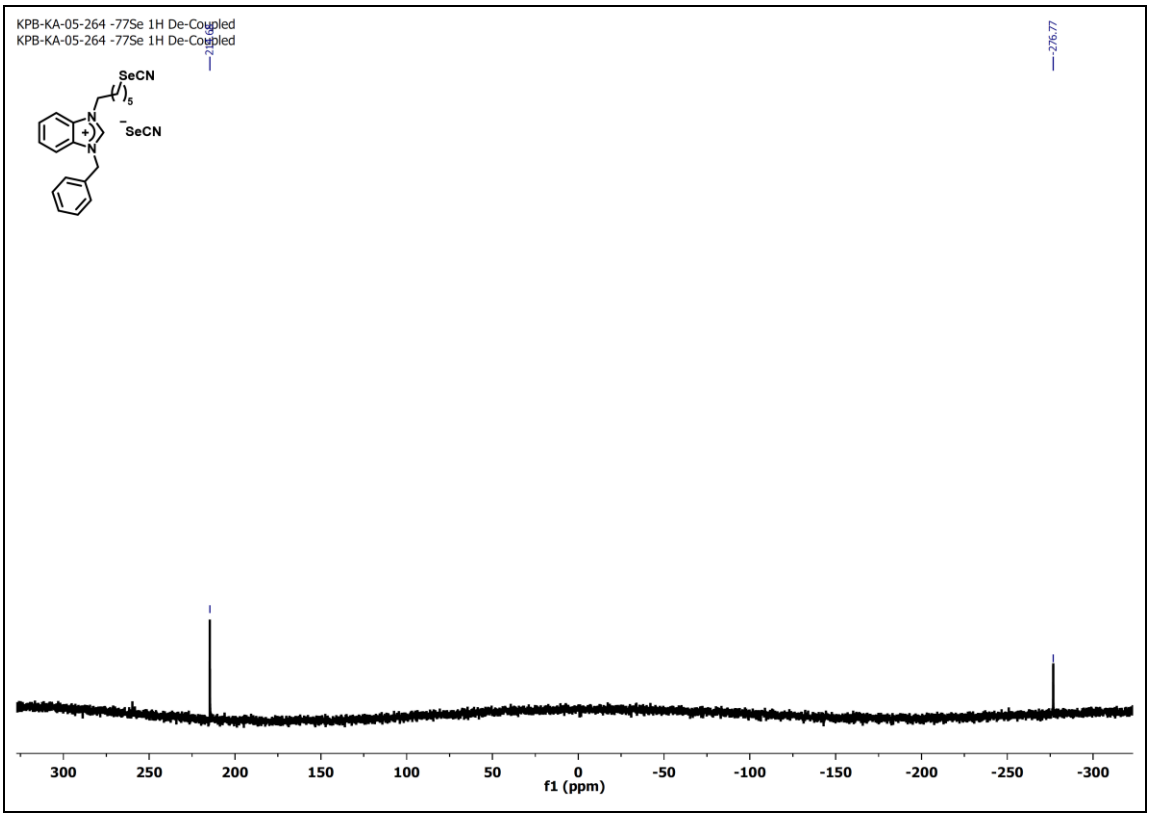

Figure S27. ^{77}Se NMR (DMSO-d_6, 76 MHz) of compound **9d**.

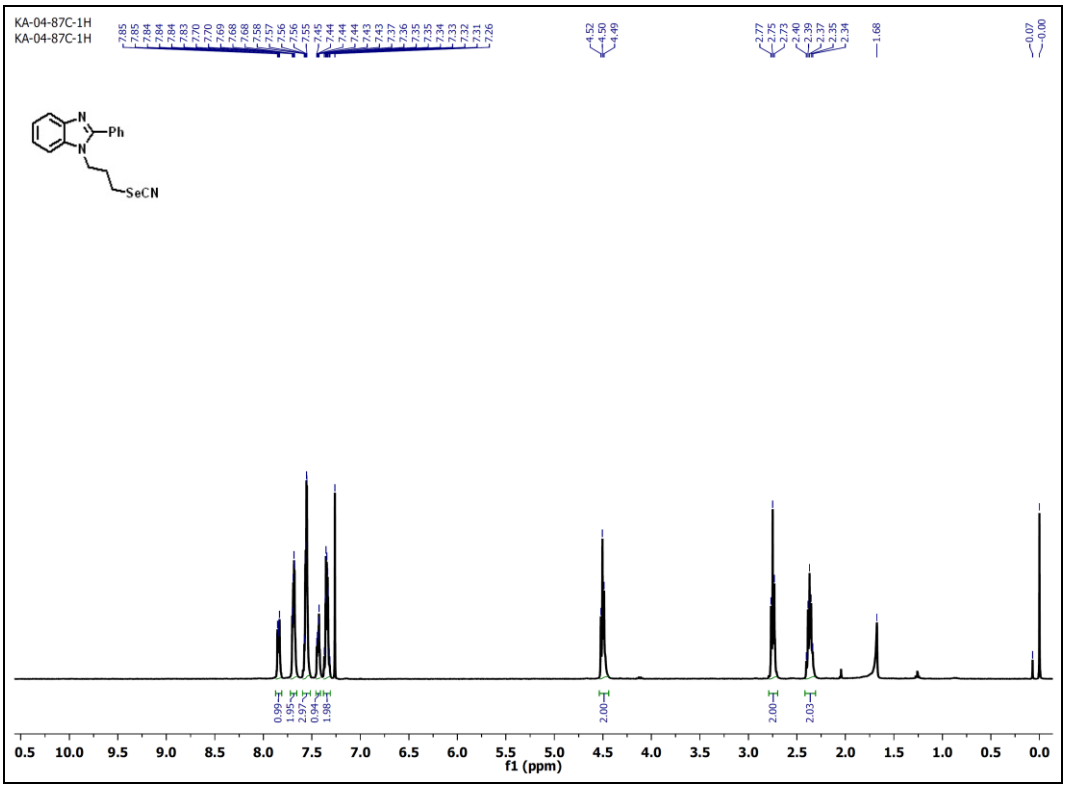

Figure S28. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **10a**.

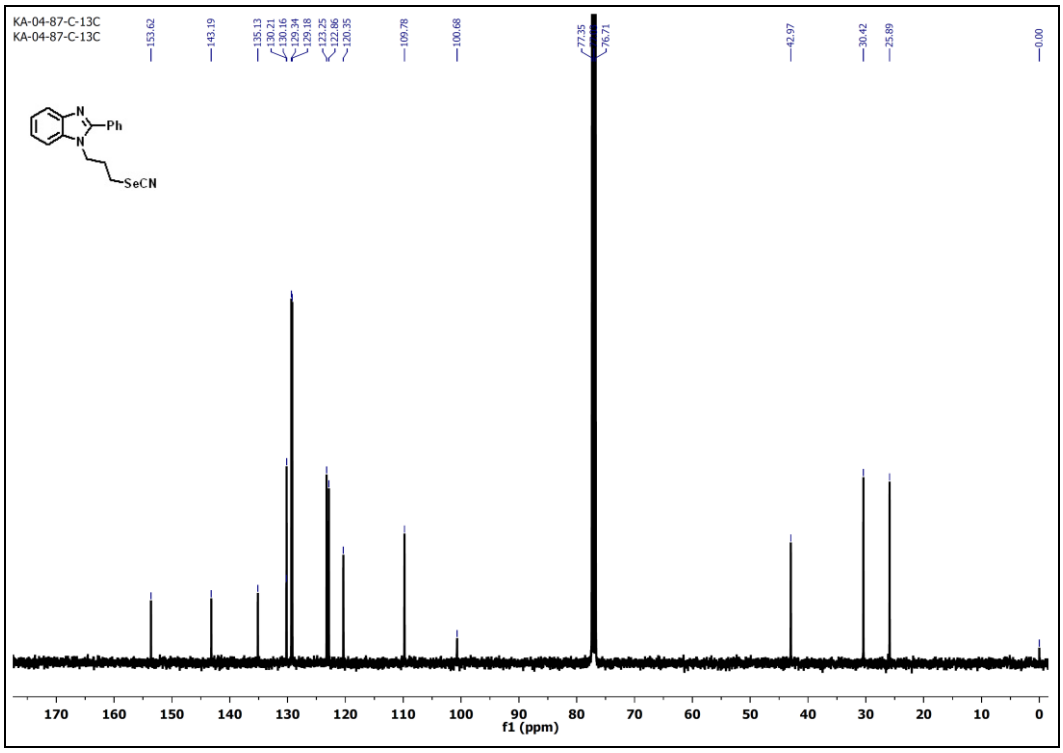

Figure S29. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound **10a**.

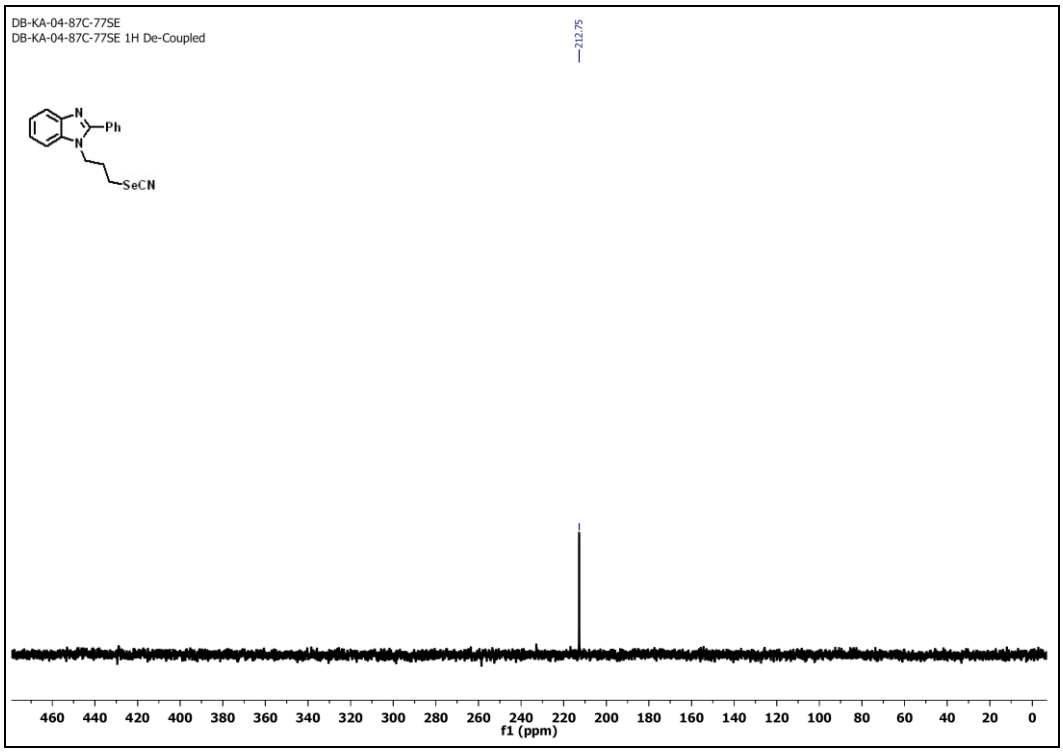

Figure S30. ^{77}Se NMR spectrum ($CDCl_3$, 76 MHz) of compound **10a**.

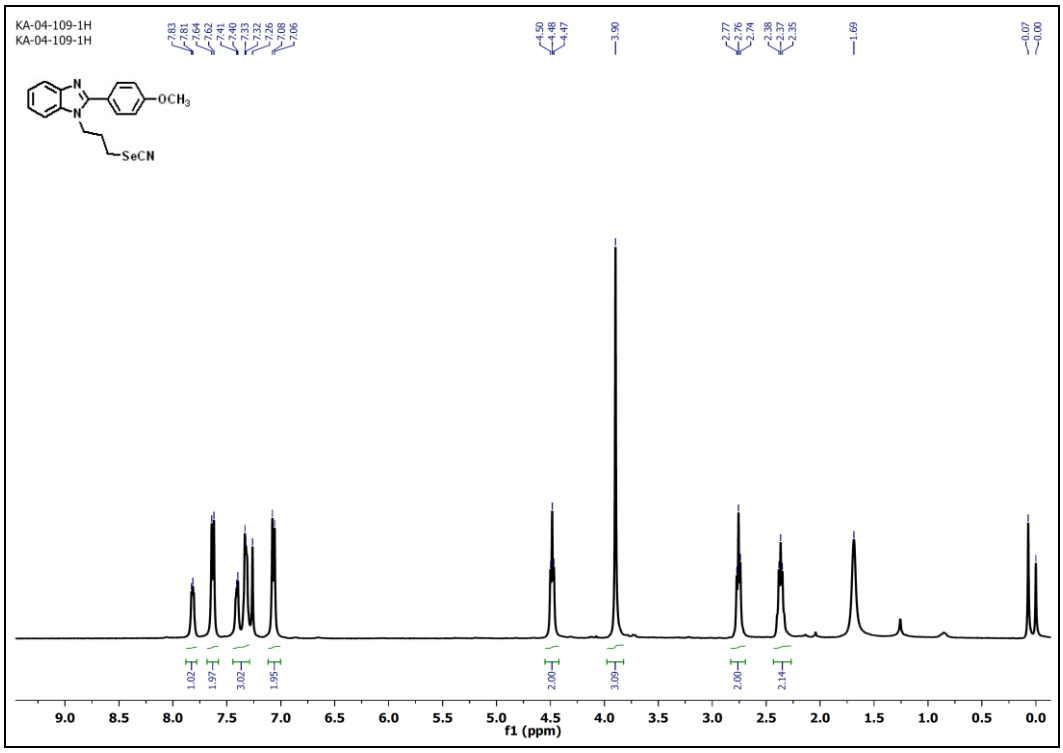

Figure S31. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **10b**.

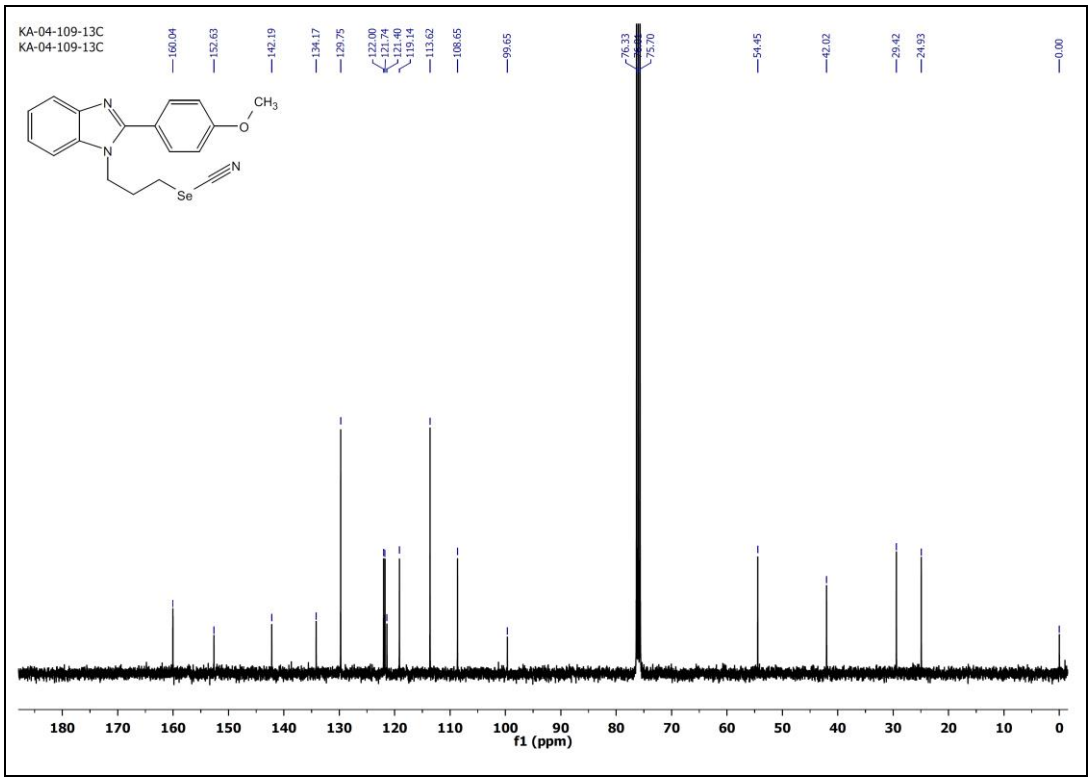

Figure S32. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound **10b**.

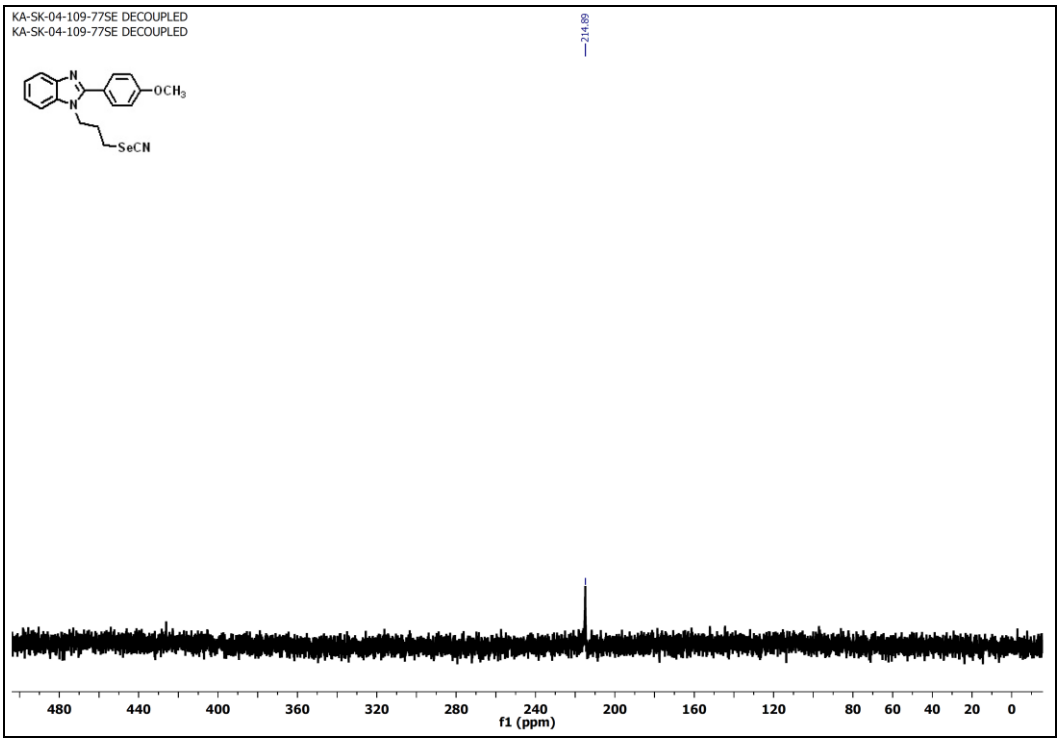

Figure S33. ^{77}Se NMR spectrum ($CDCl_3$, 76 MHz) of compound **10b**.

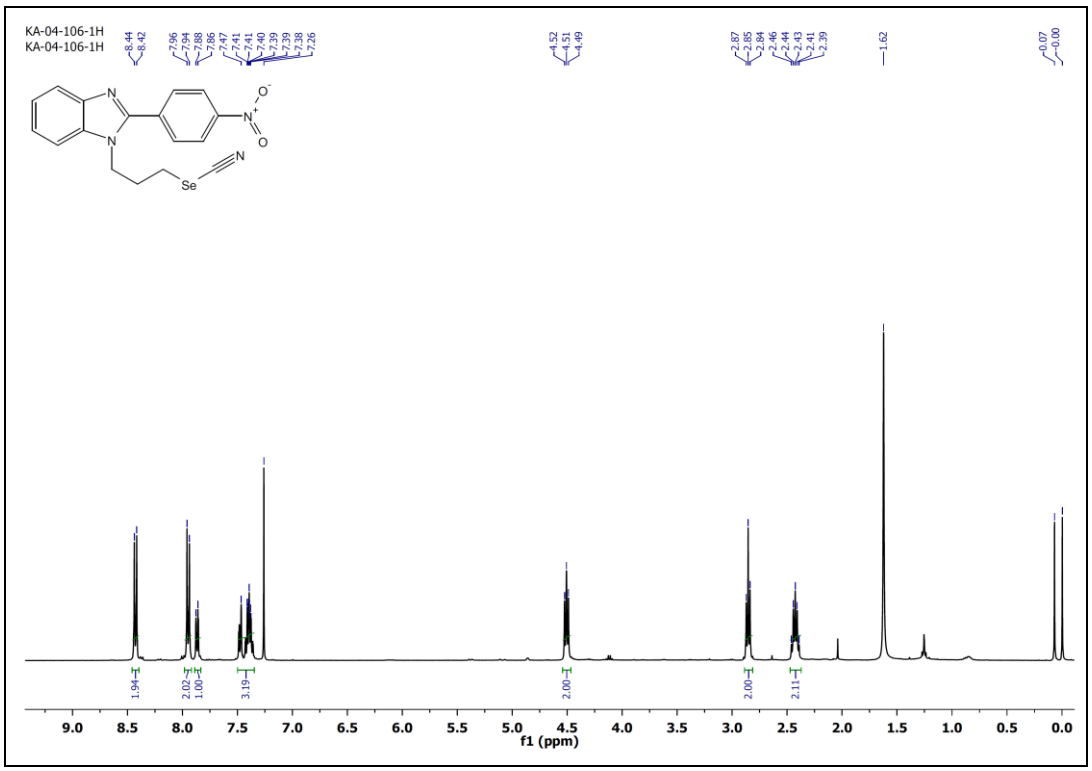

Figure S34. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **10c**.

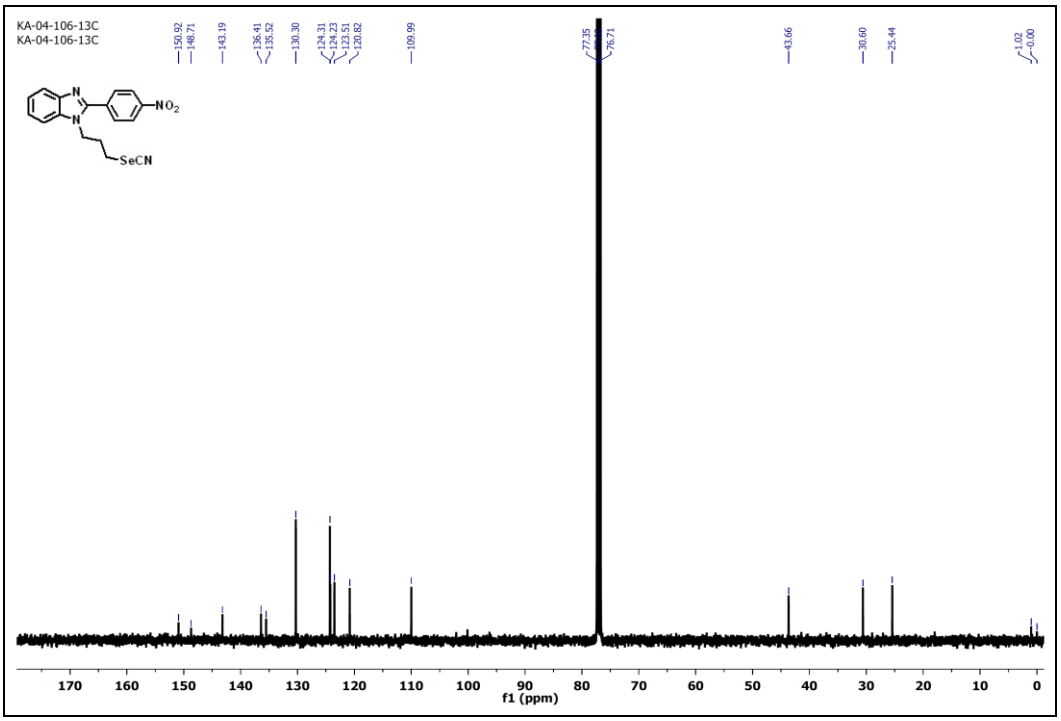

Figure S35. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound **10c**.

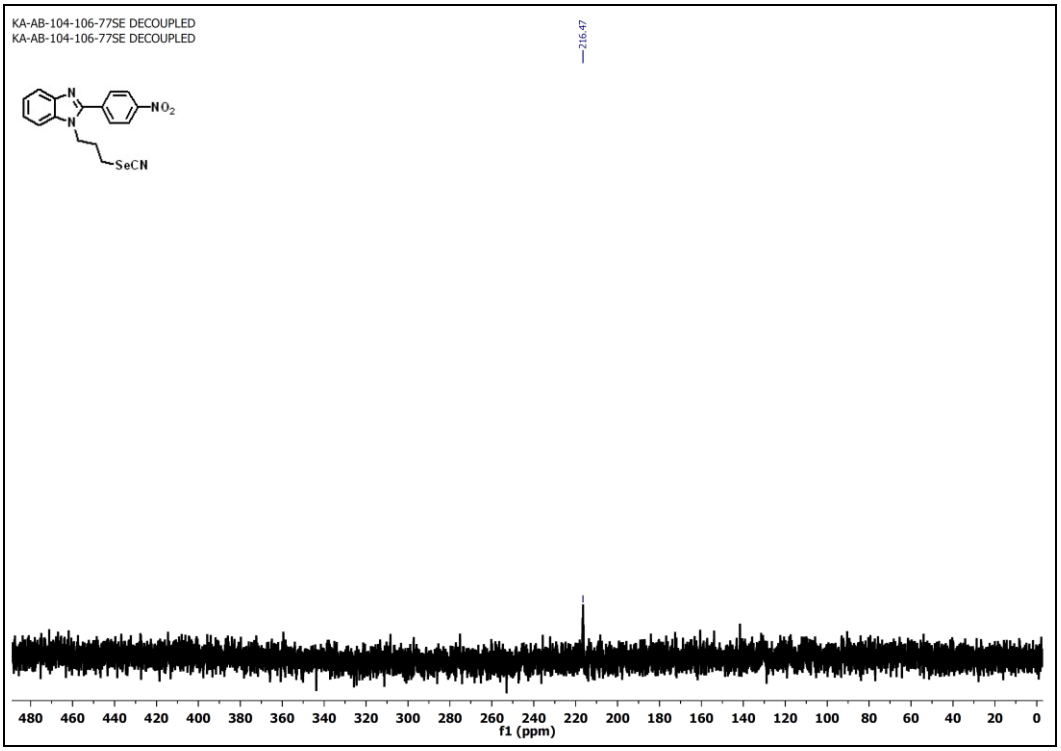

Figure S36. ^{77}Se NMR spectrum ($CDCl_3$, 76 MHz) of compound **10c**.

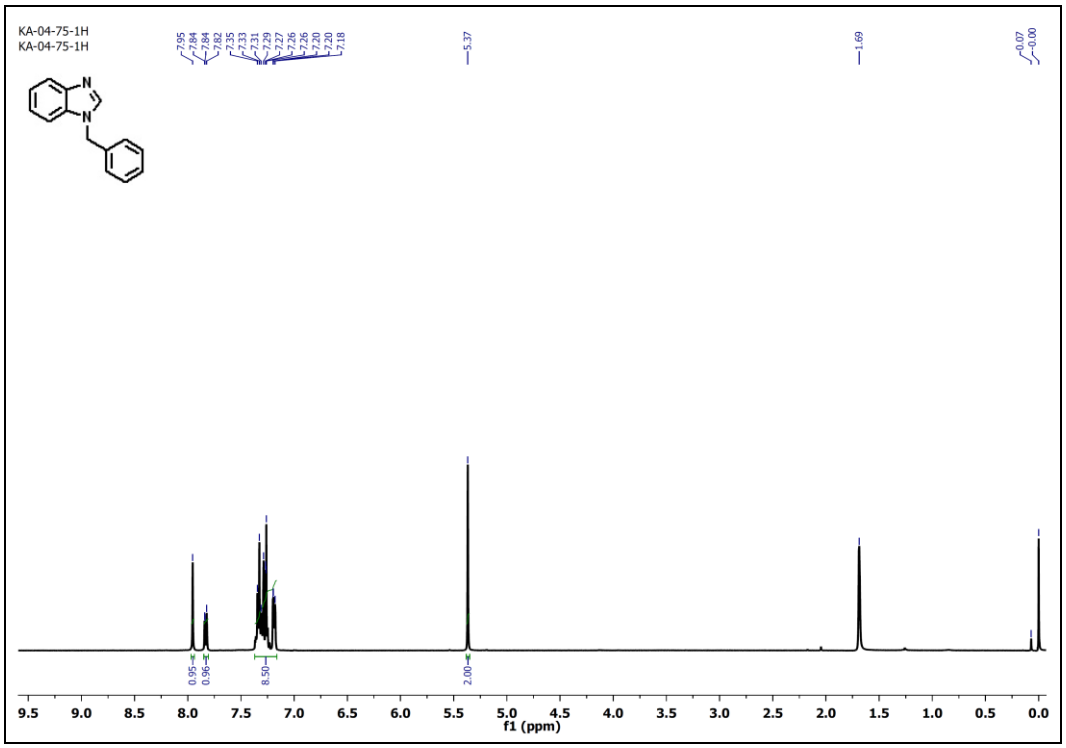

Figure S37. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **11a**.

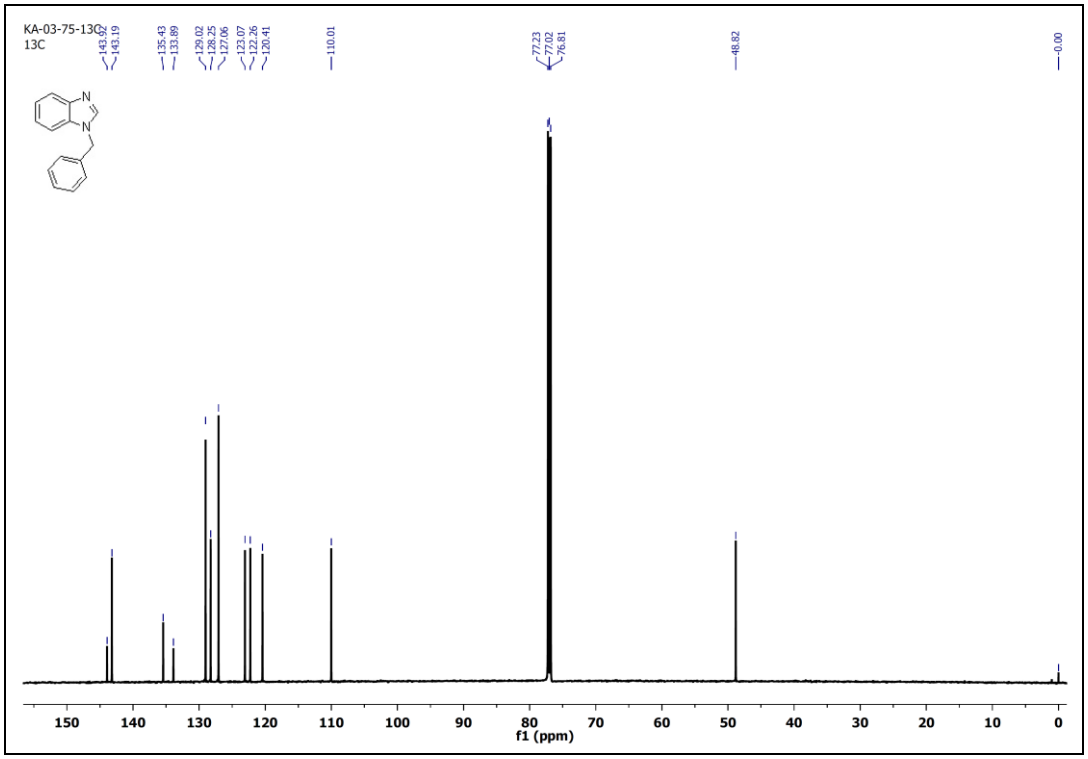

Figure S38. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of compound **11a**.

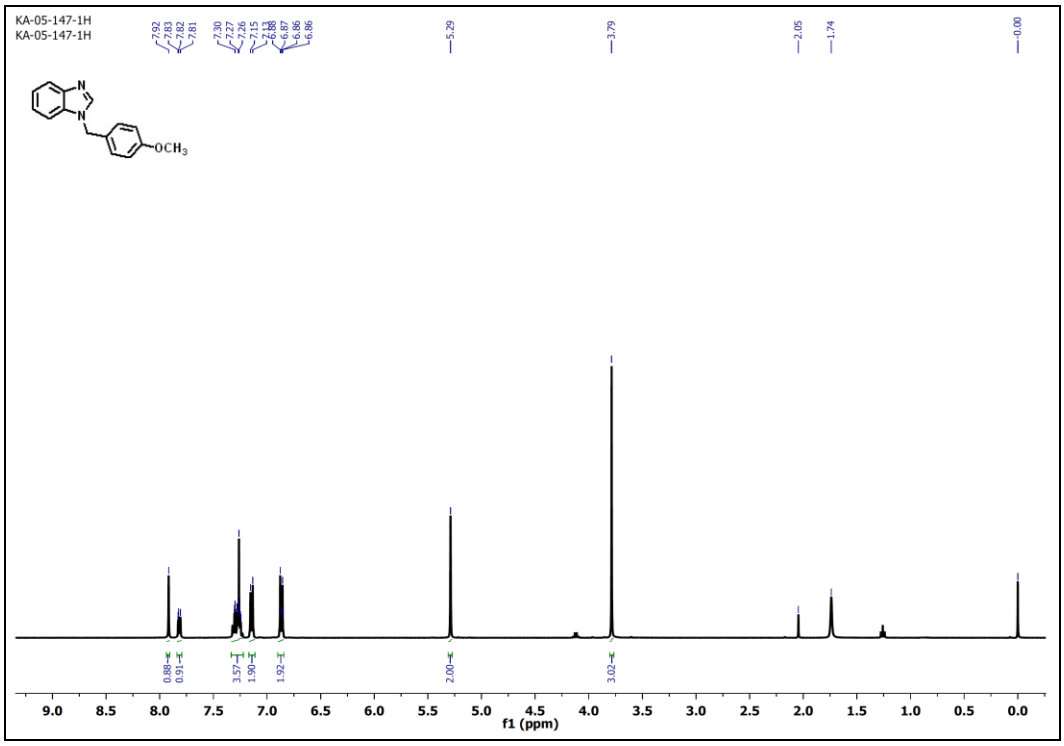

Figure S39. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **11b**.

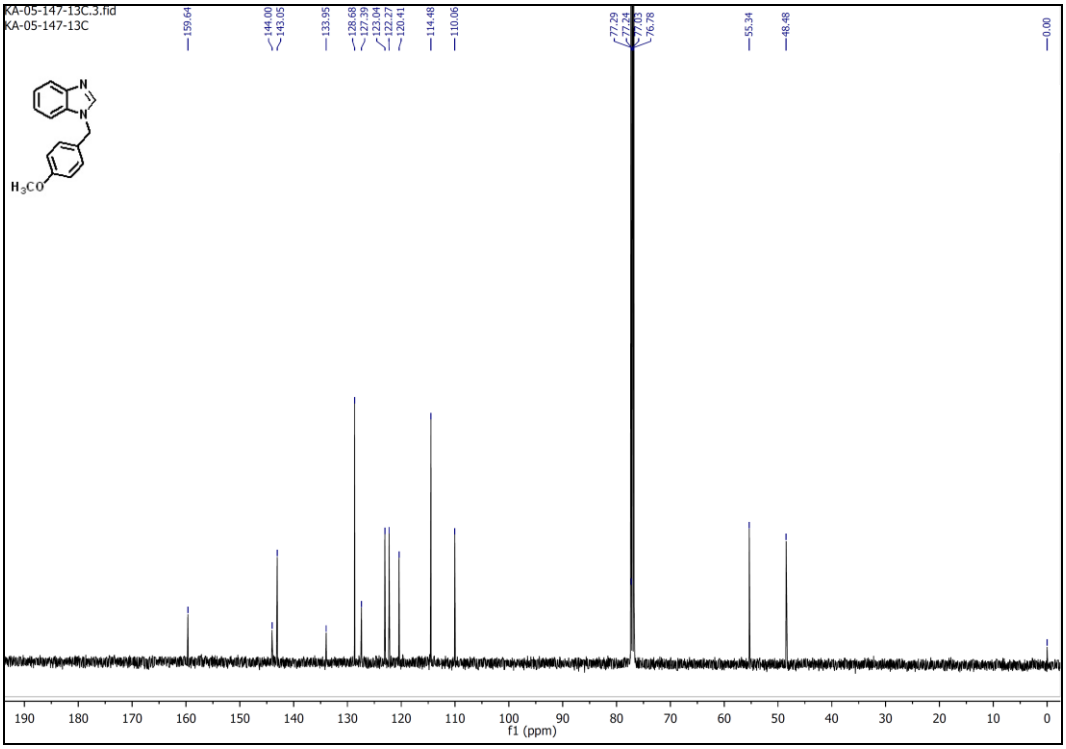

Figure S40. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **11b**.

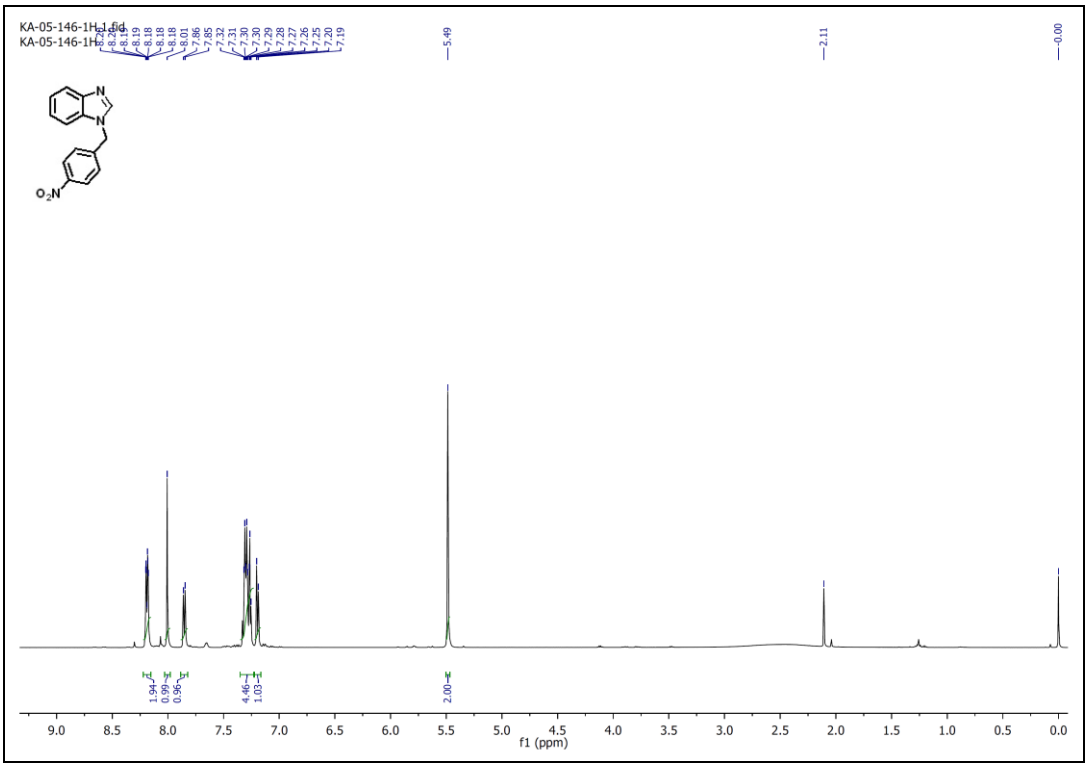

Figure S41. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **11c**.

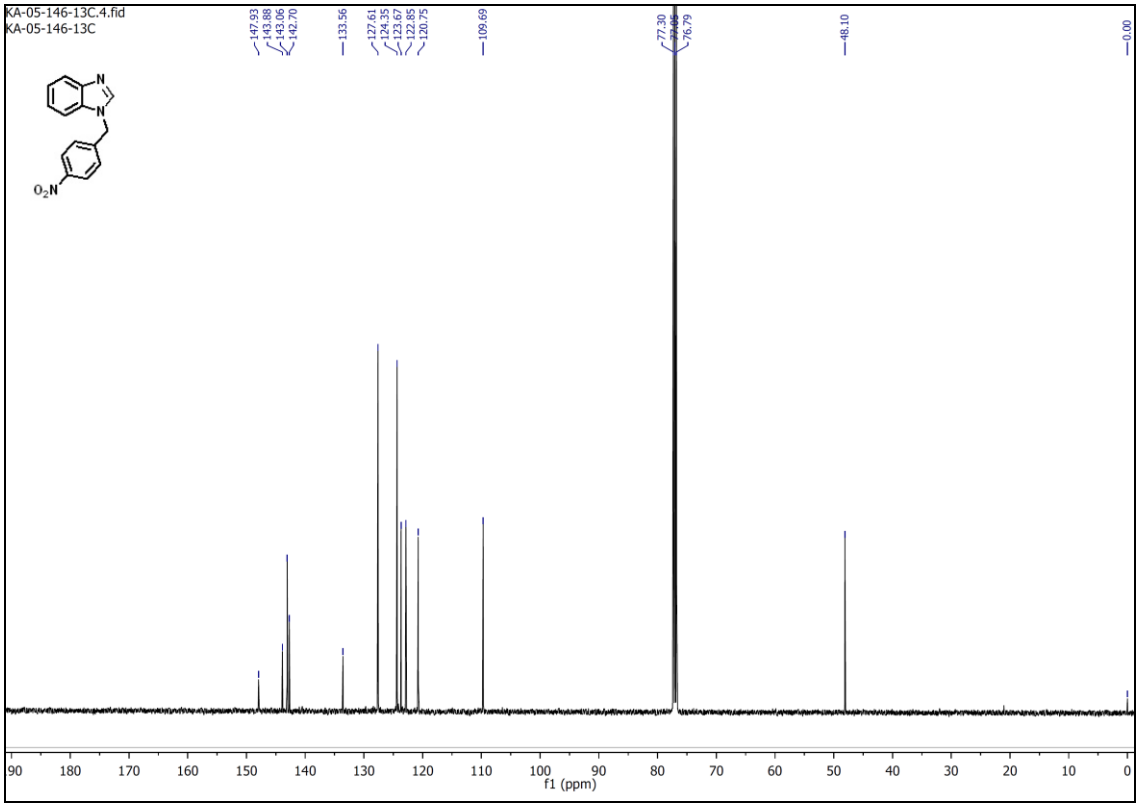

Figure S42. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **11c**.

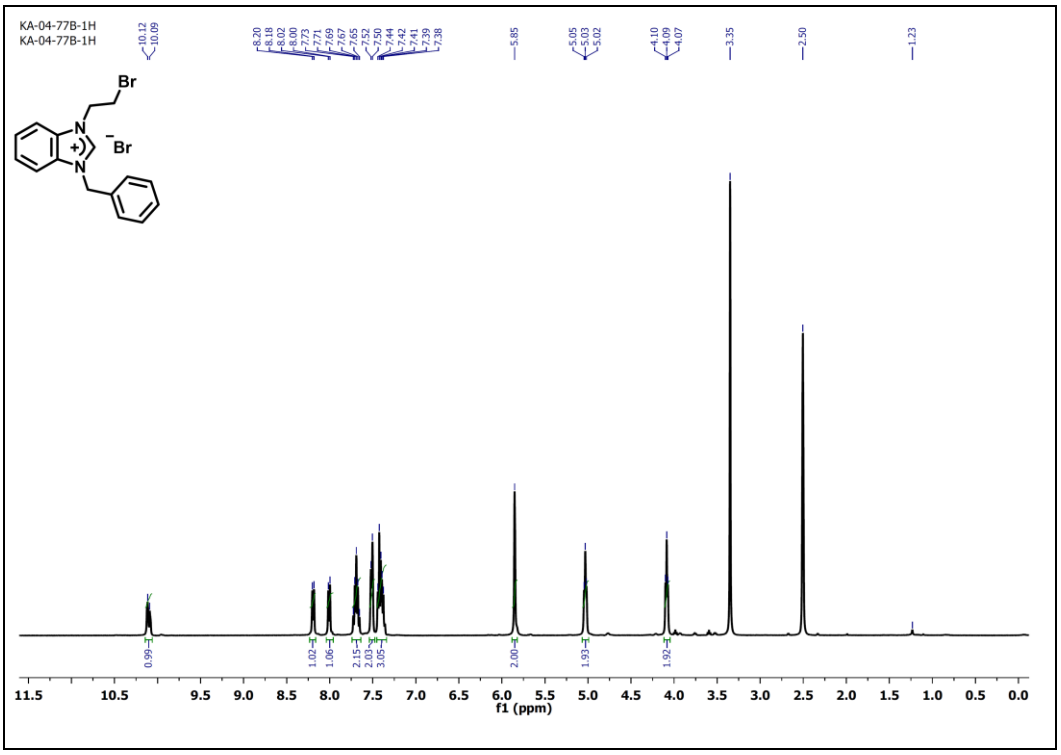

Figure S43. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound **11a-1**.

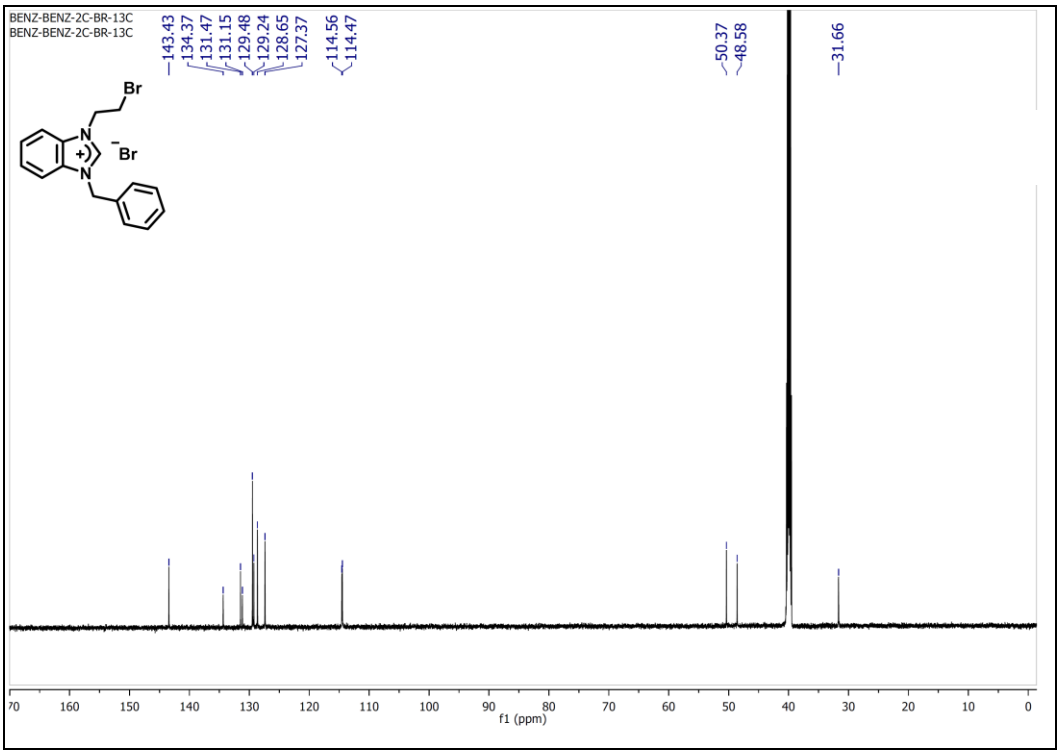

Figure S44. ^{13}C NMR spectrum (DMSO-d_6, 150 MHz) of compound **11a-1**.

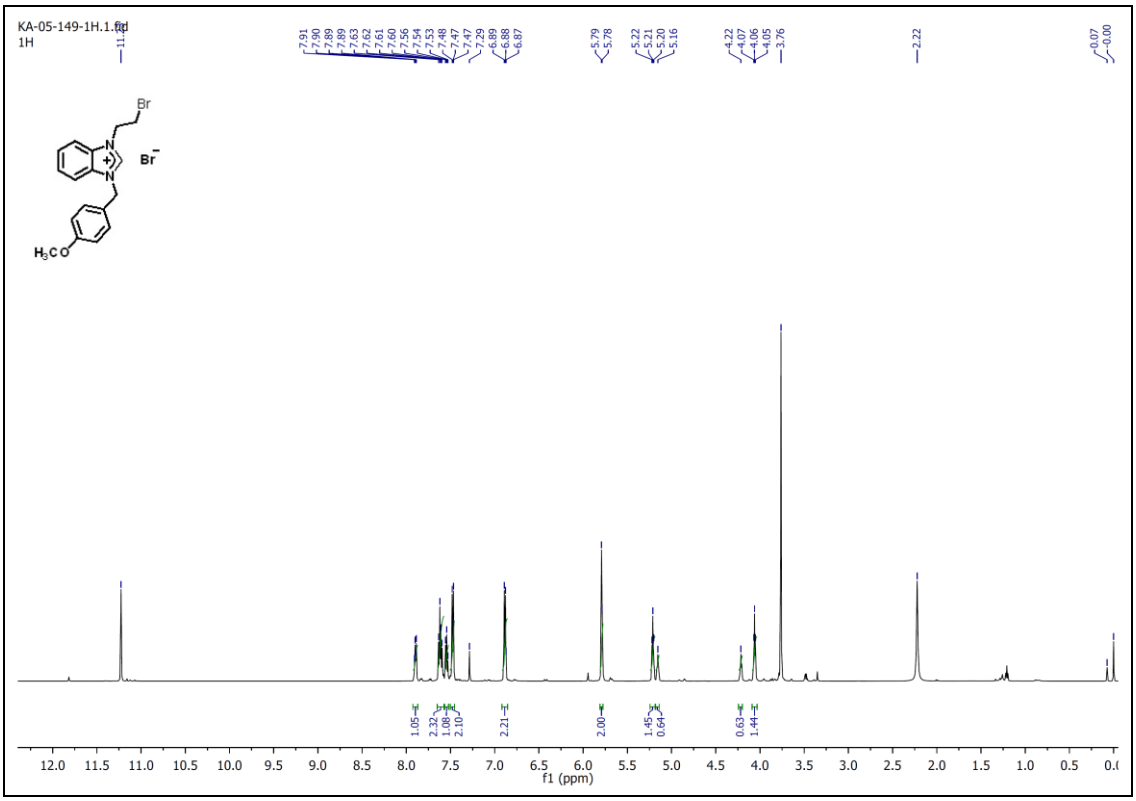

Figure S45. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of compound **11b-1**.

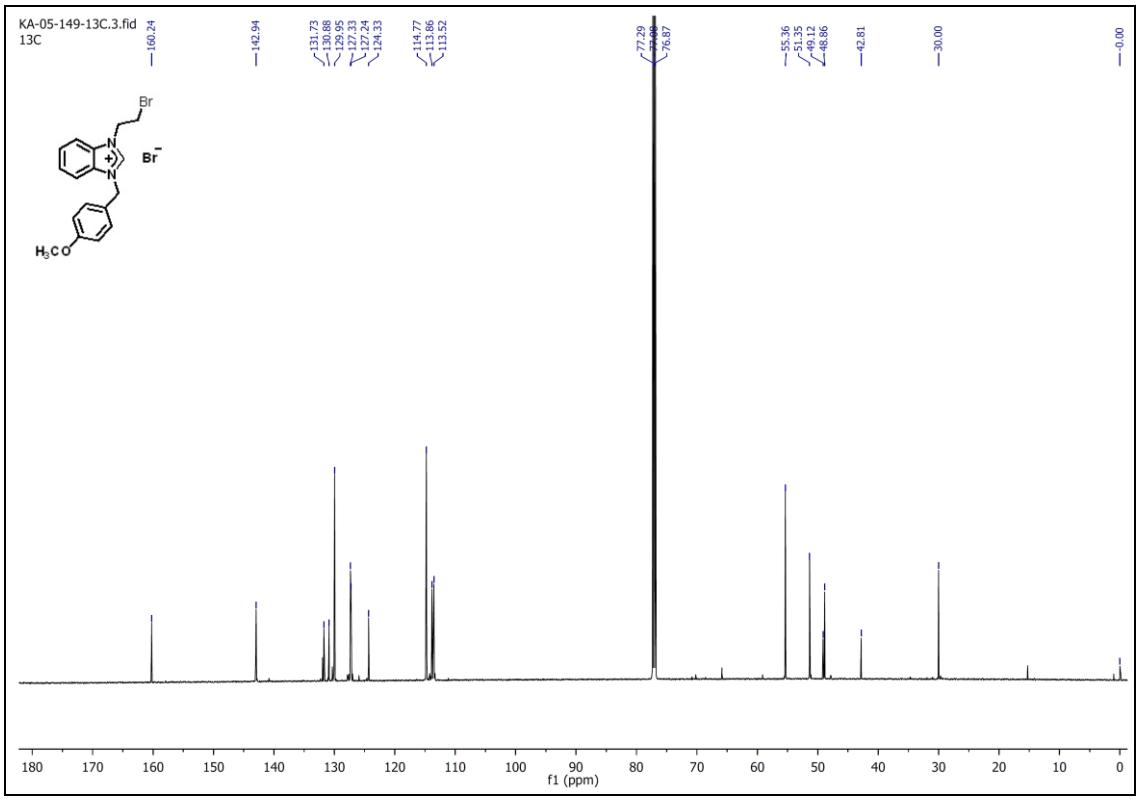

Figure S46. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **11b-1**.

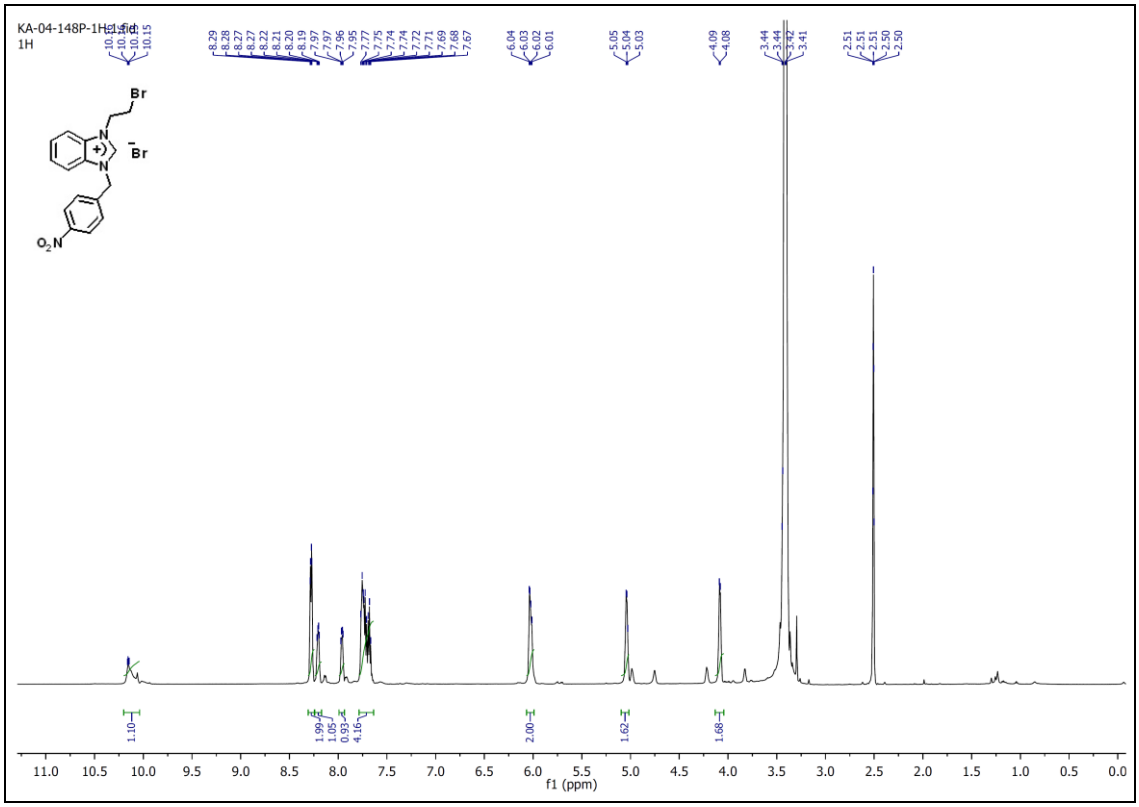

Figure S47. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of compound **11c-1**.

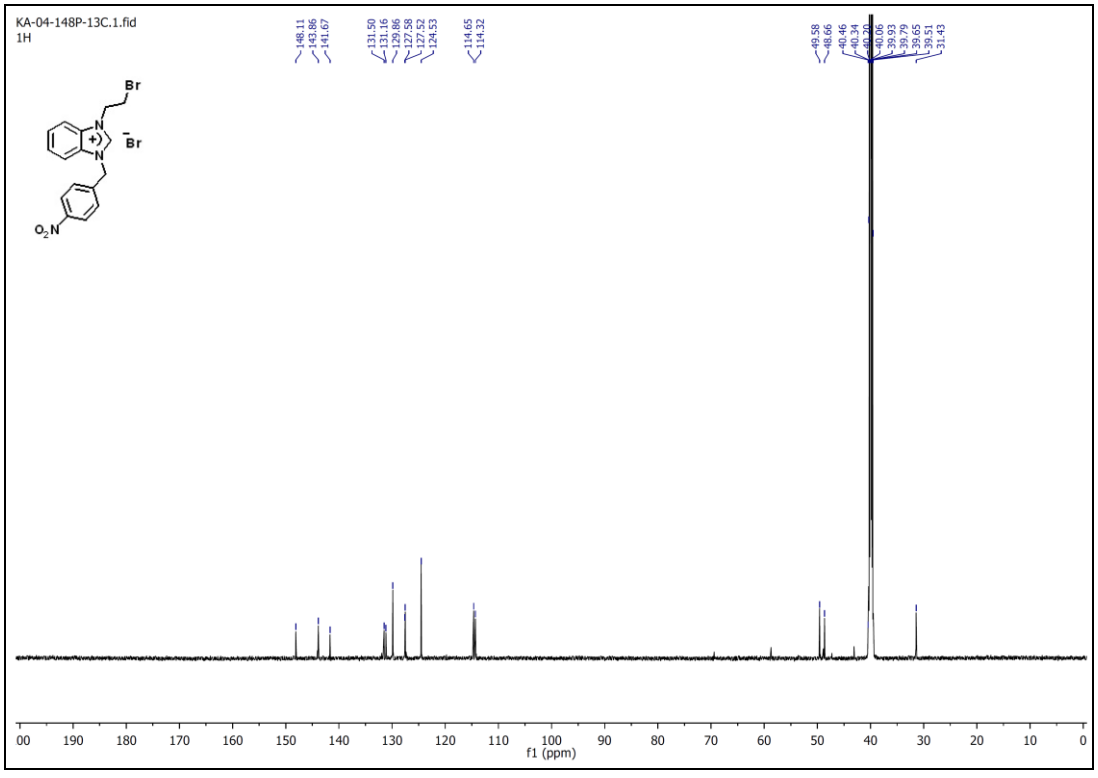

Figure S48. ^{13}C NMR (DMSO-d_6, 150 MHz) of compound **11c-1**.

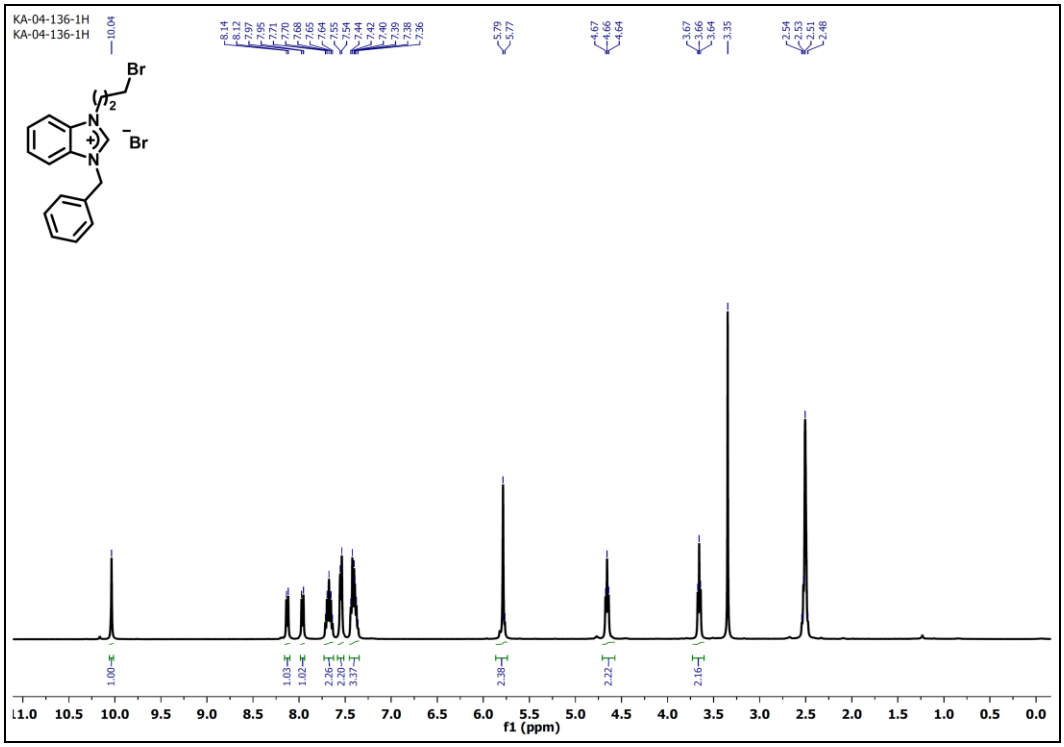

Figure S49. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound **11a-2**.

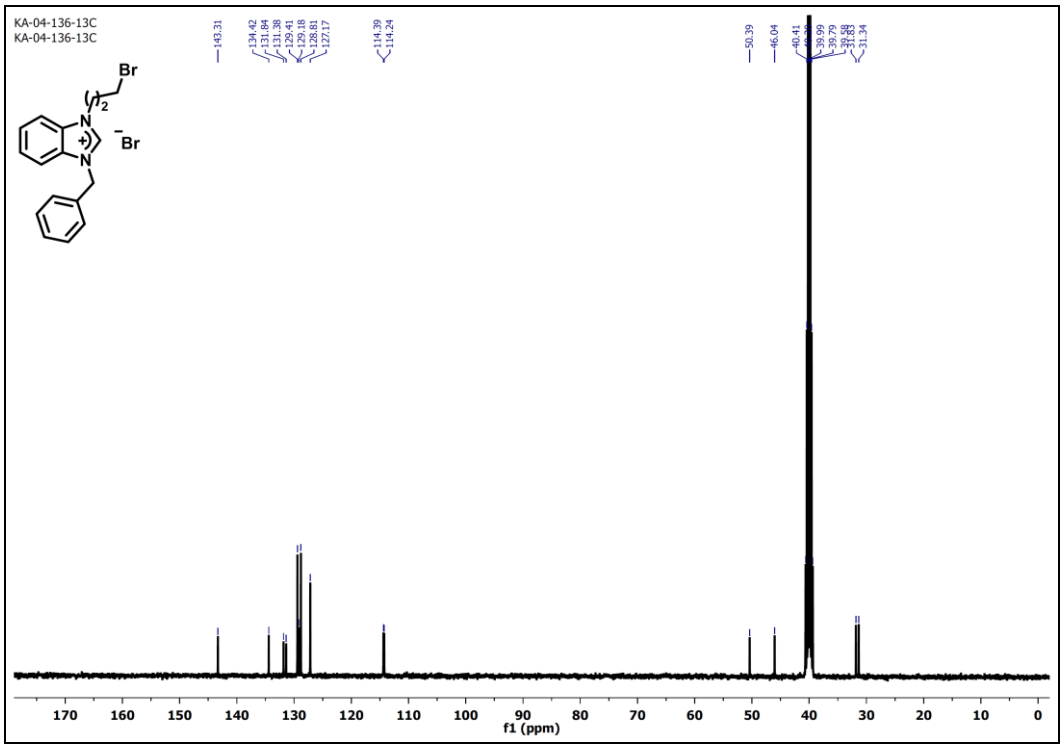

Figure S50. ^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound **11a-2**.

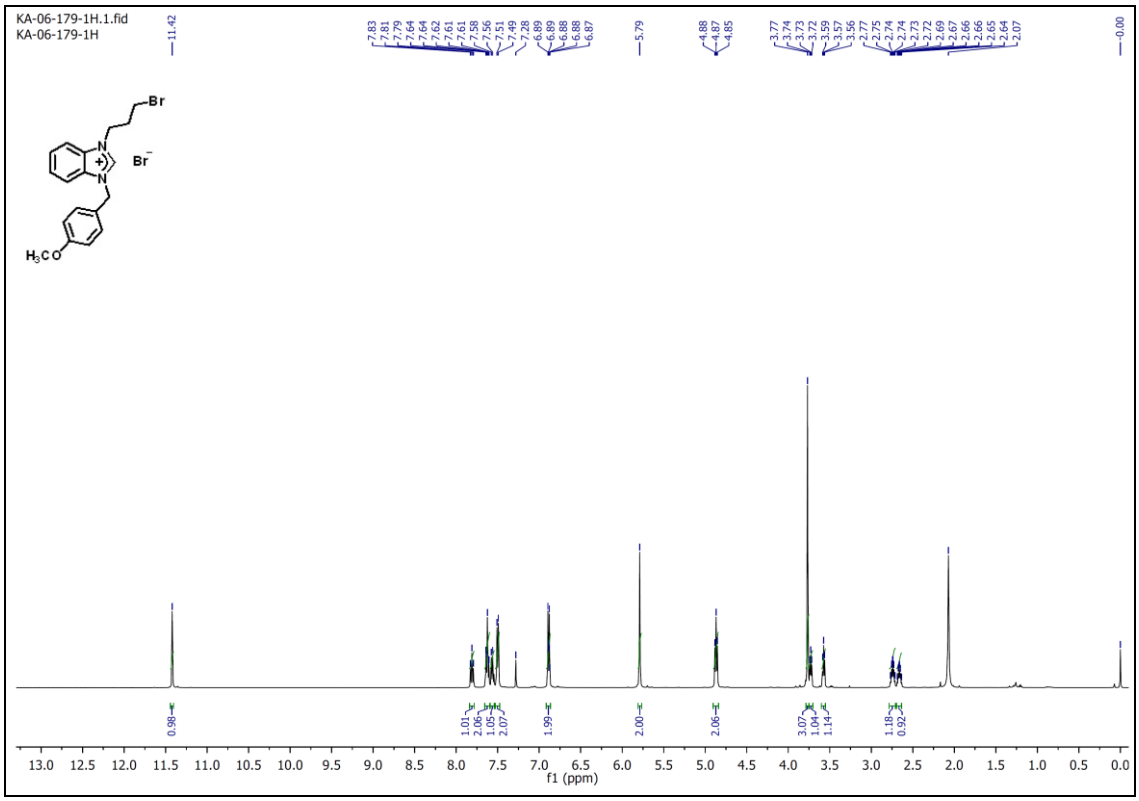

Figure S51. ^{1}H NMR ($CDCl_3$, 500 MHz) of compound **11b-2**.

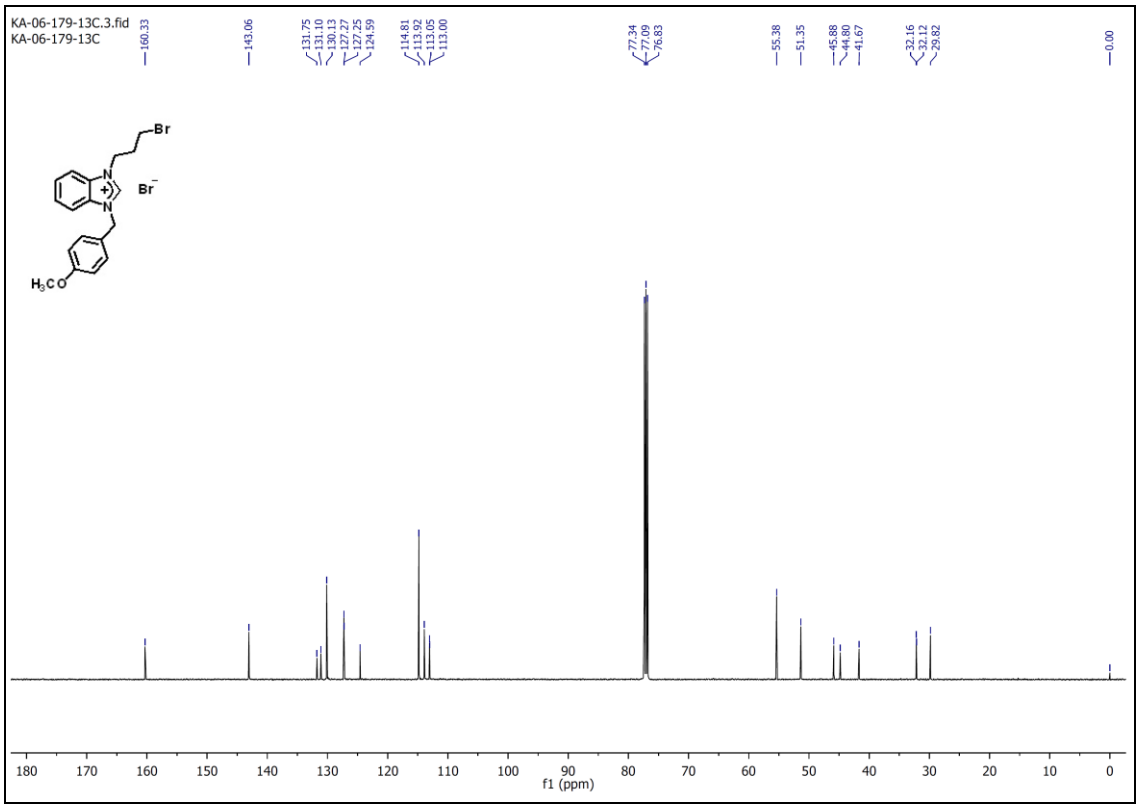

Figure S52. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **11b-2**.

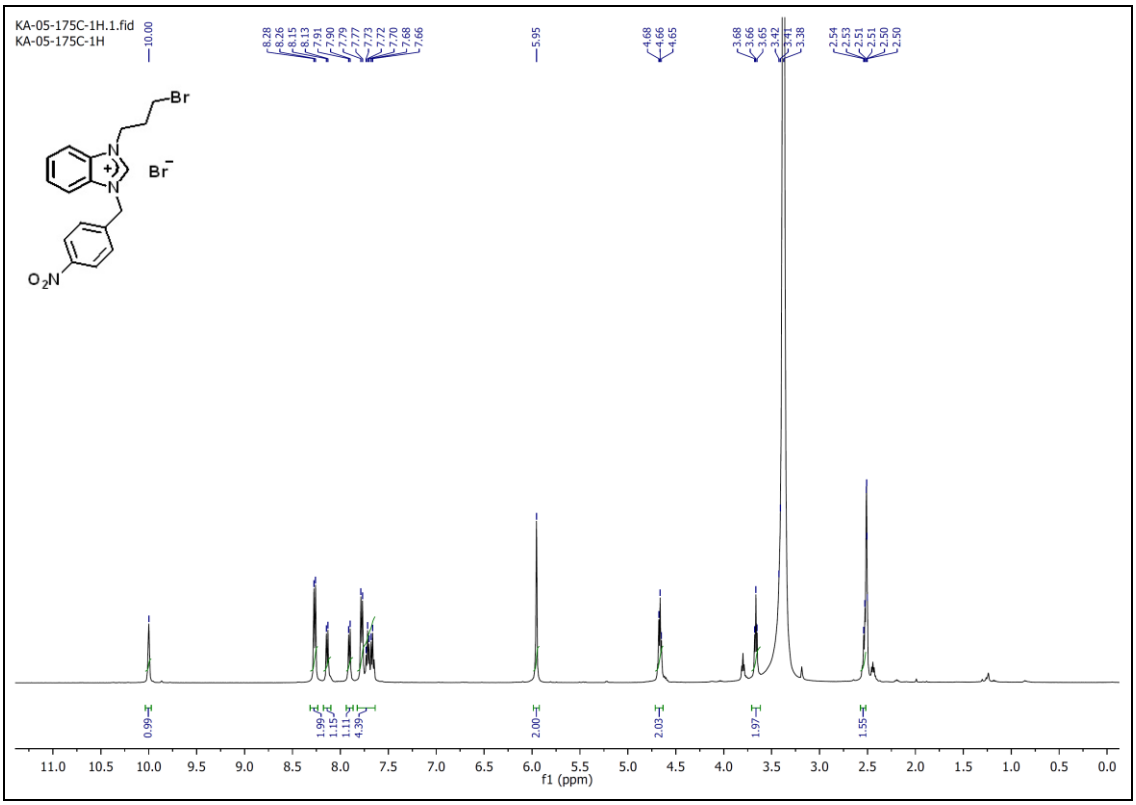

Figure S53. ^{1}H NMR spectrum (DMSO-d_6, 500 MHz) of compound **11c-2**.

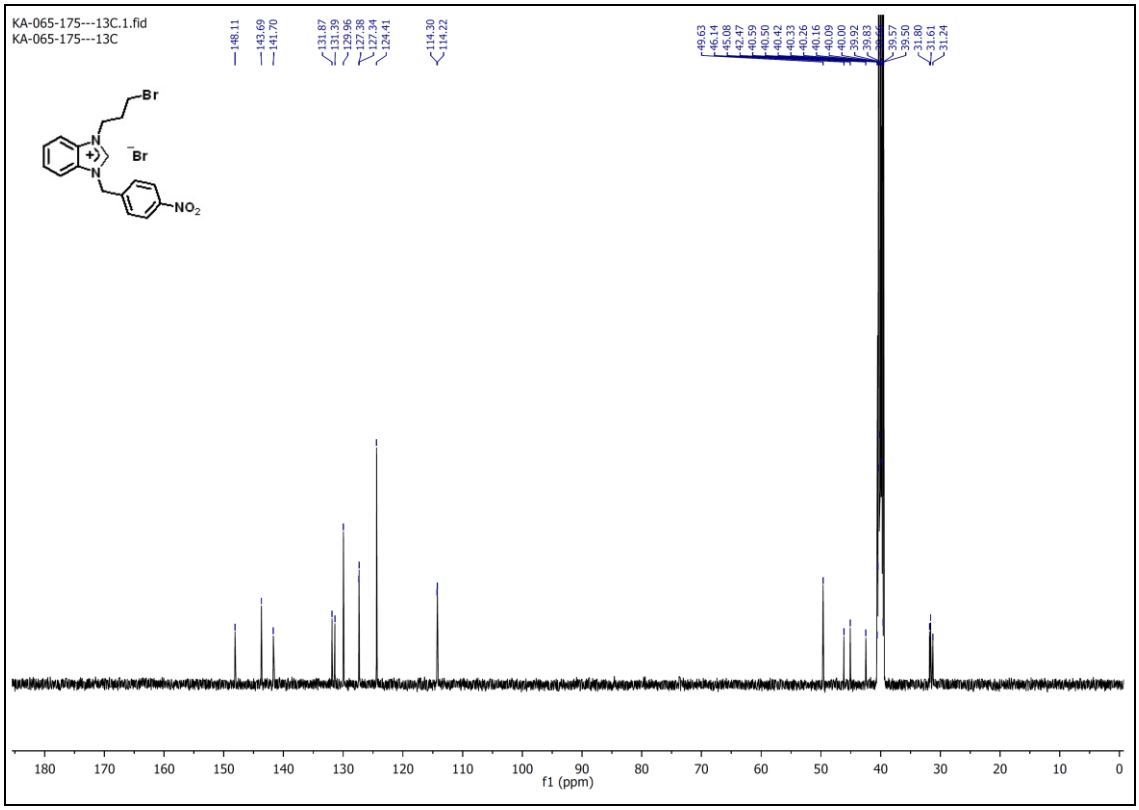

Figure S54. ^{13}C NMR (DMSO-d_6, 125 MHz) of compound **11c-2**.

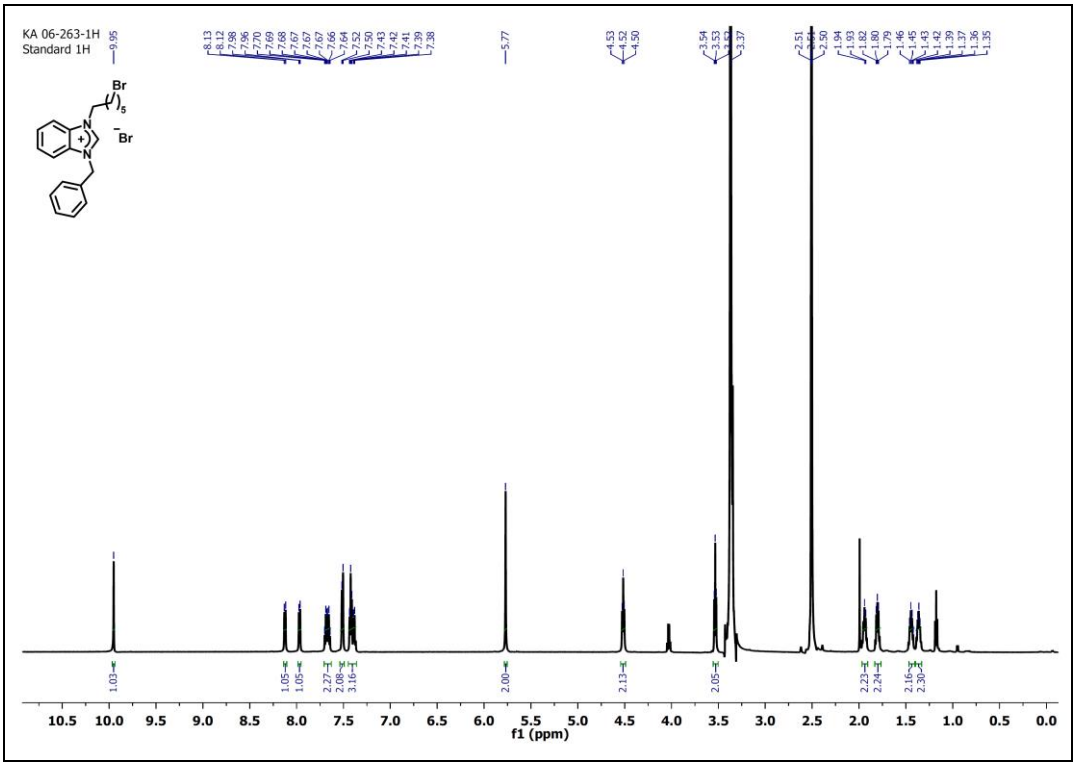

Figure S55. ^{1}H NMR (DMSO-d_6, 600 MHz) of compound **11a-5**.

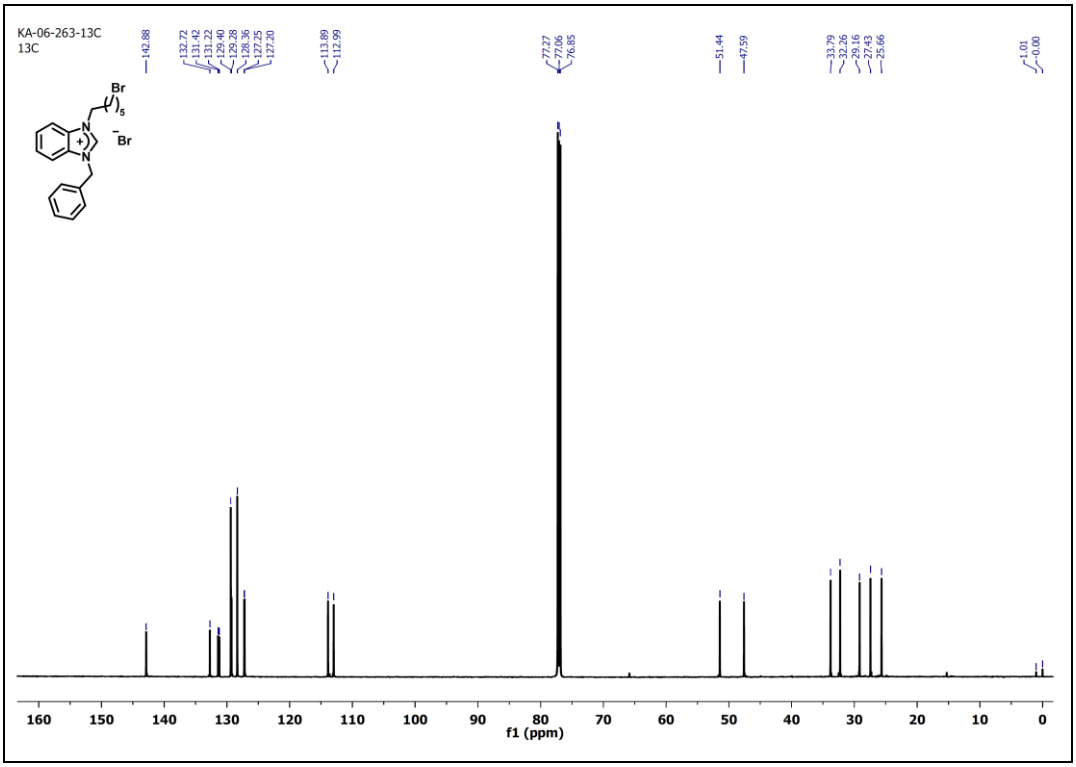

Figure S56. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **11a-5**.

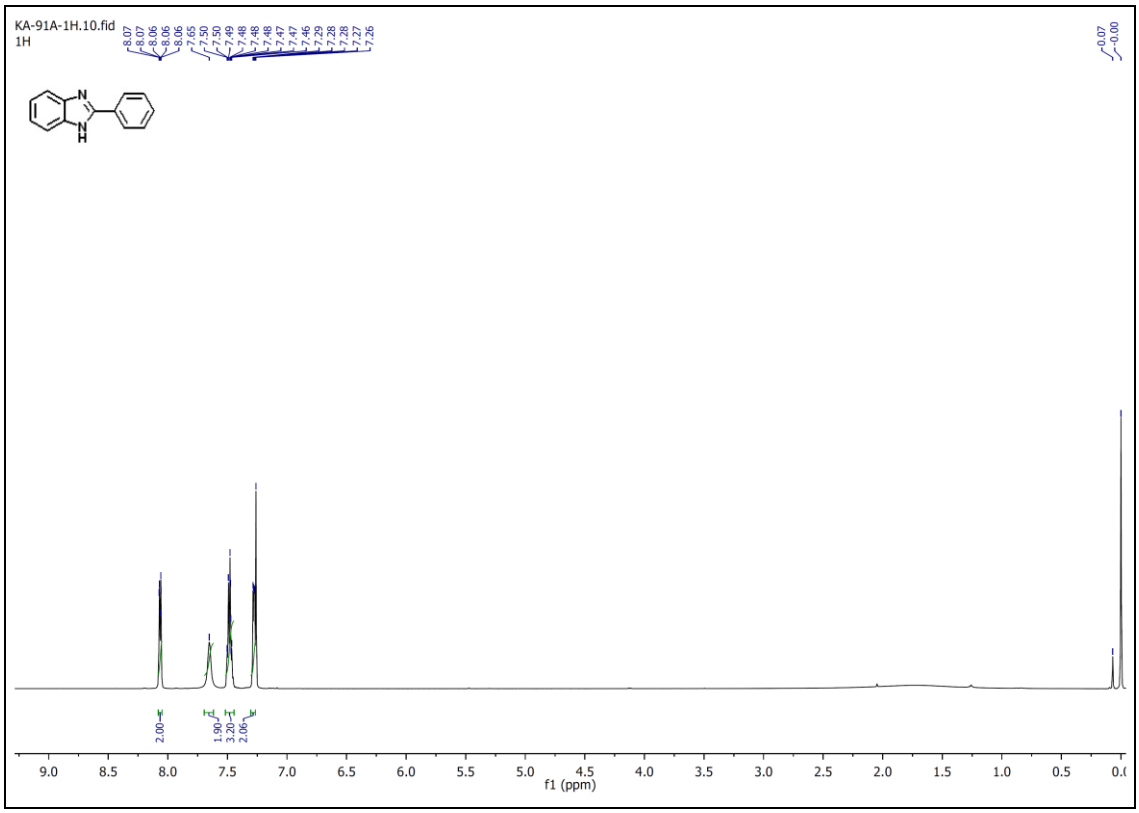

Figure S57. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of compound **13**.

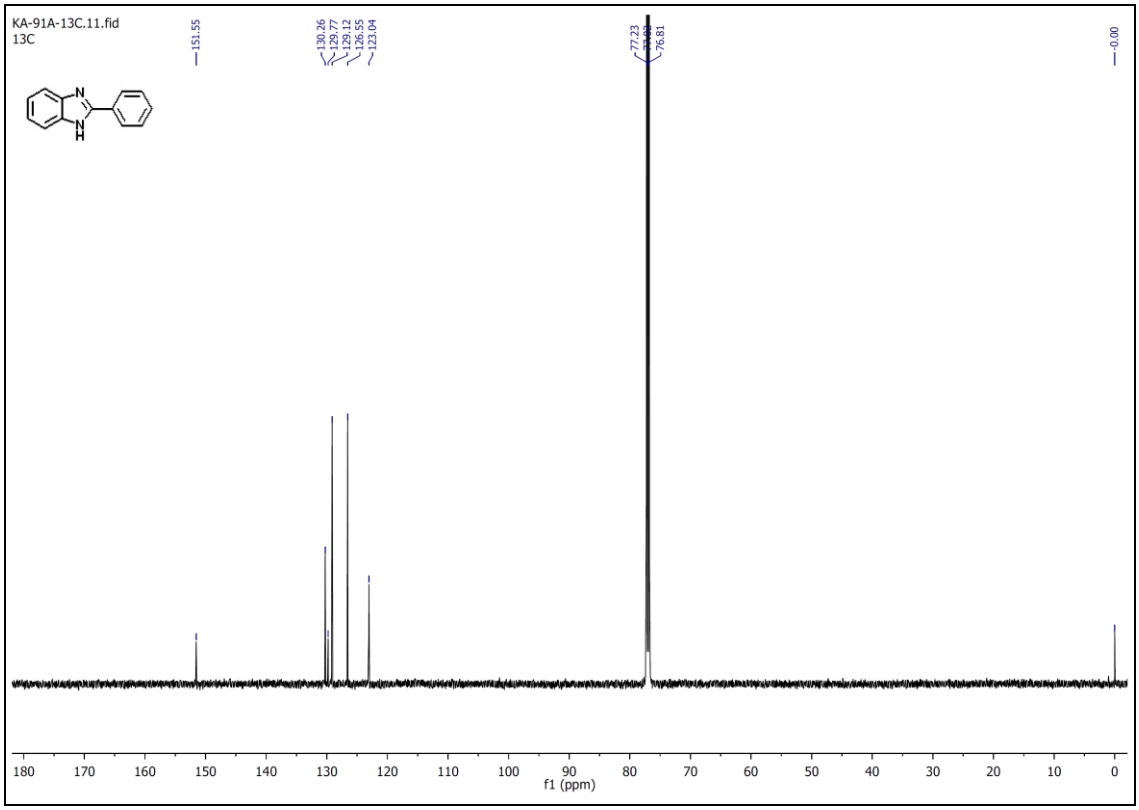

Figure S58. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **13**.

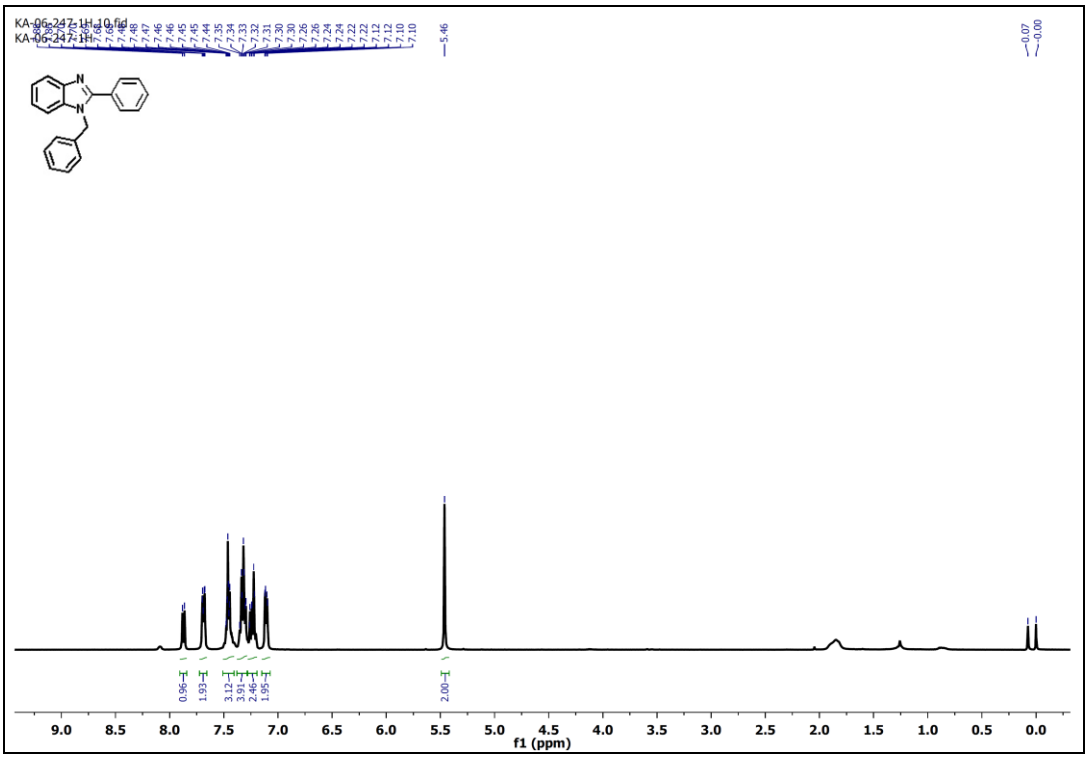

Figure S59. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **13a**.

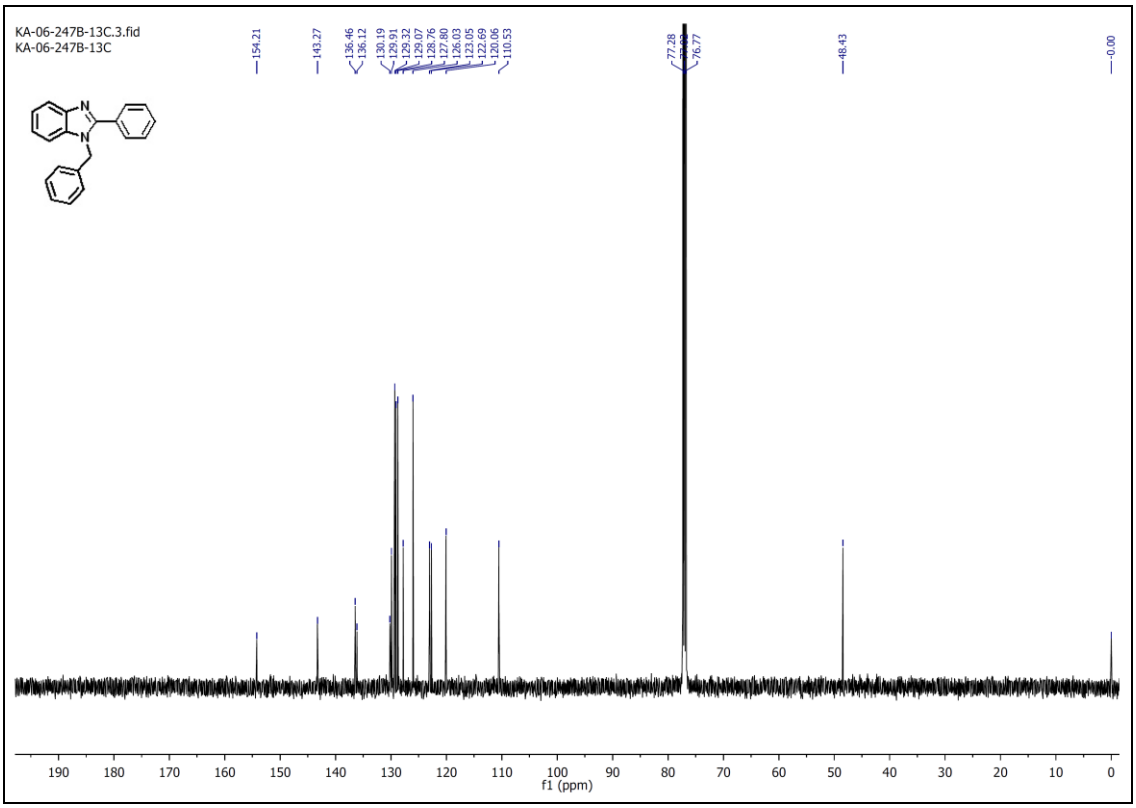

Figure S60. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **13a**.

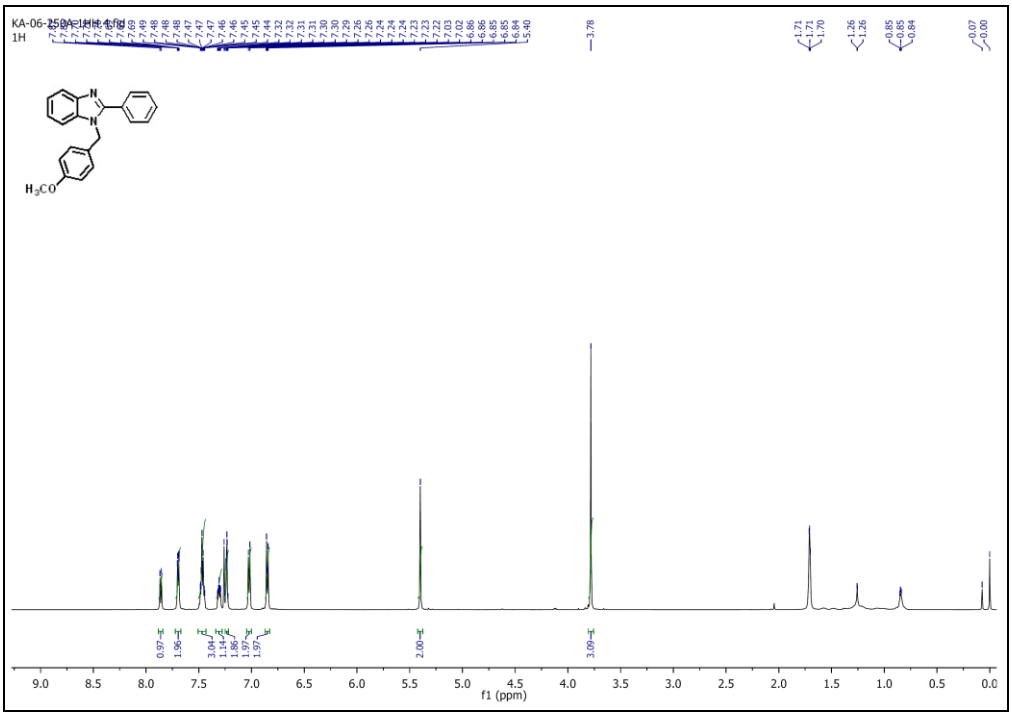

Figure S61. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of compound **13b**.

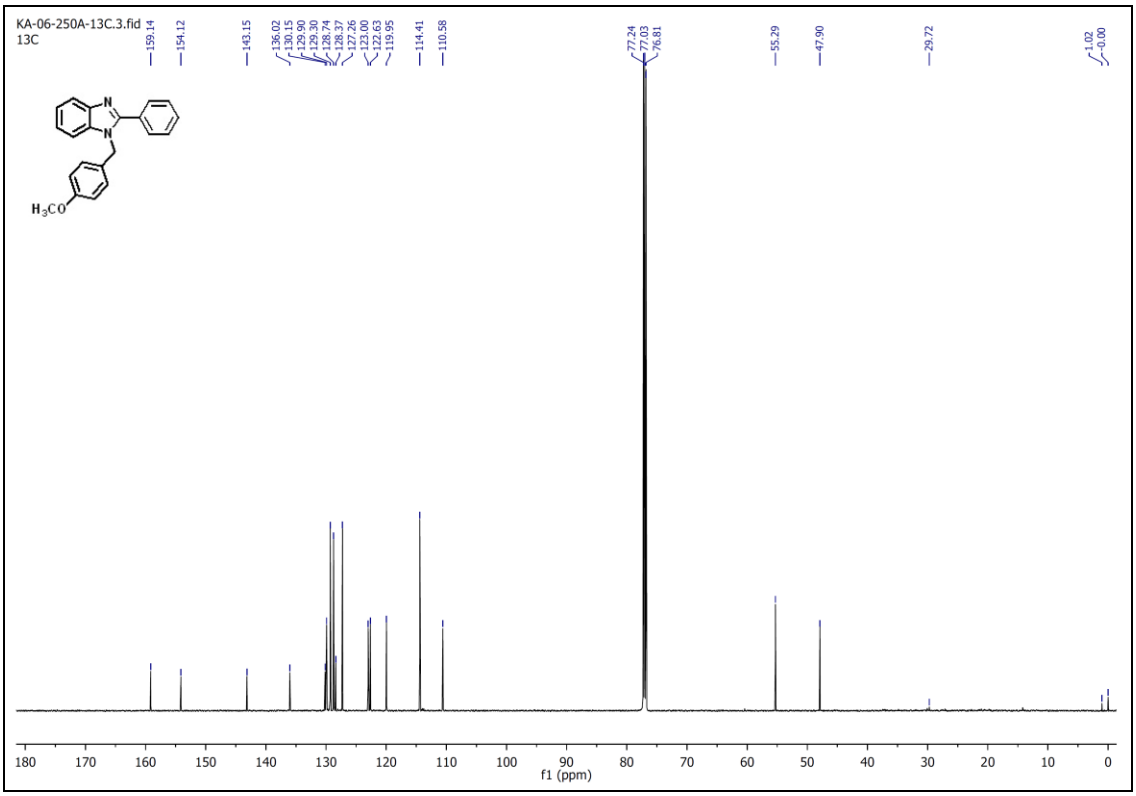

Figure S62. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **13b**.

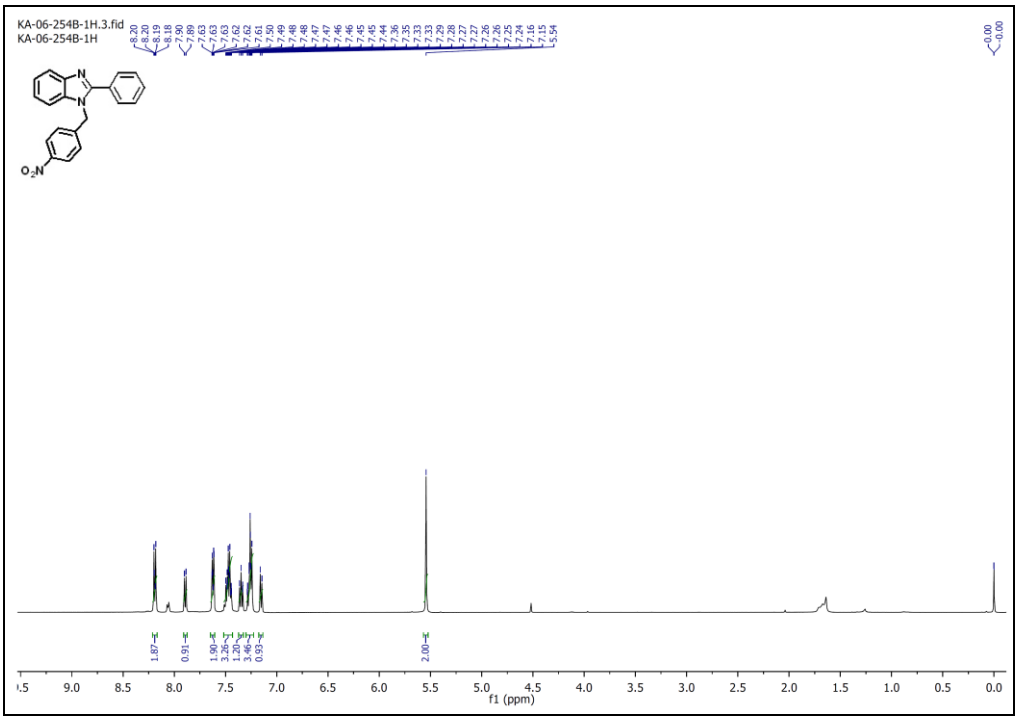

Figure S63. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of compound **13c**.

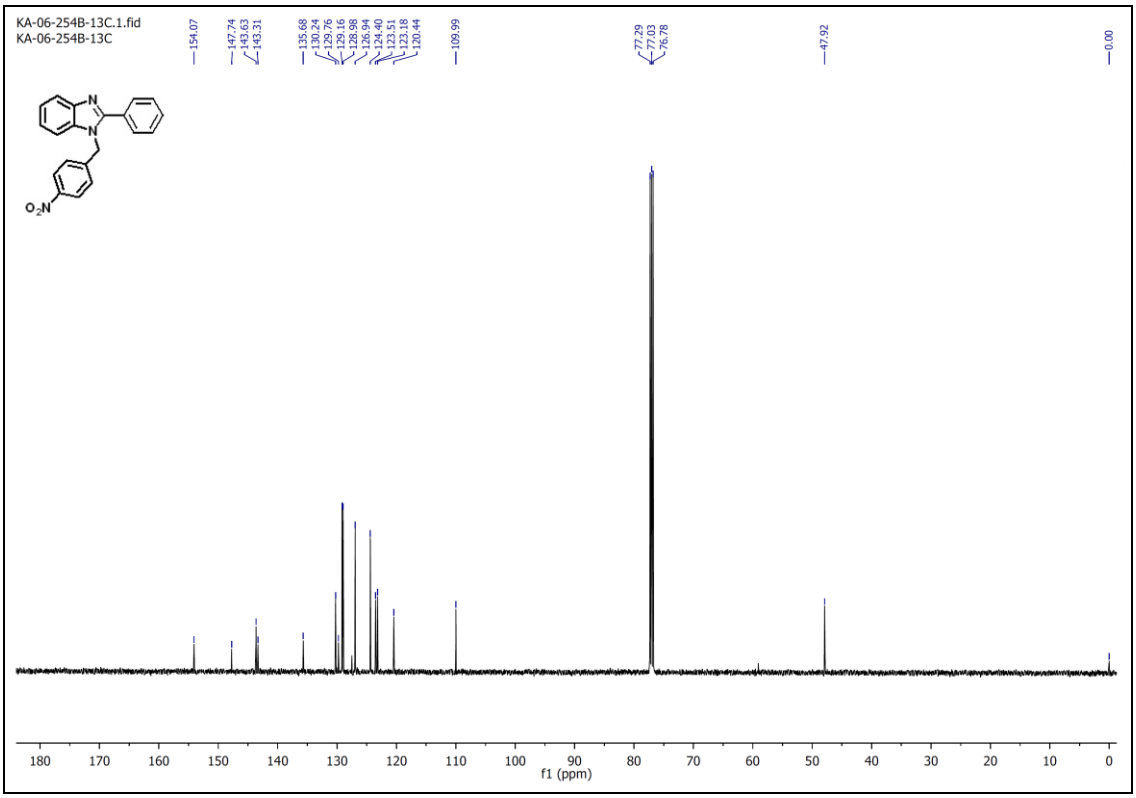

Figure S64. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **13c**.

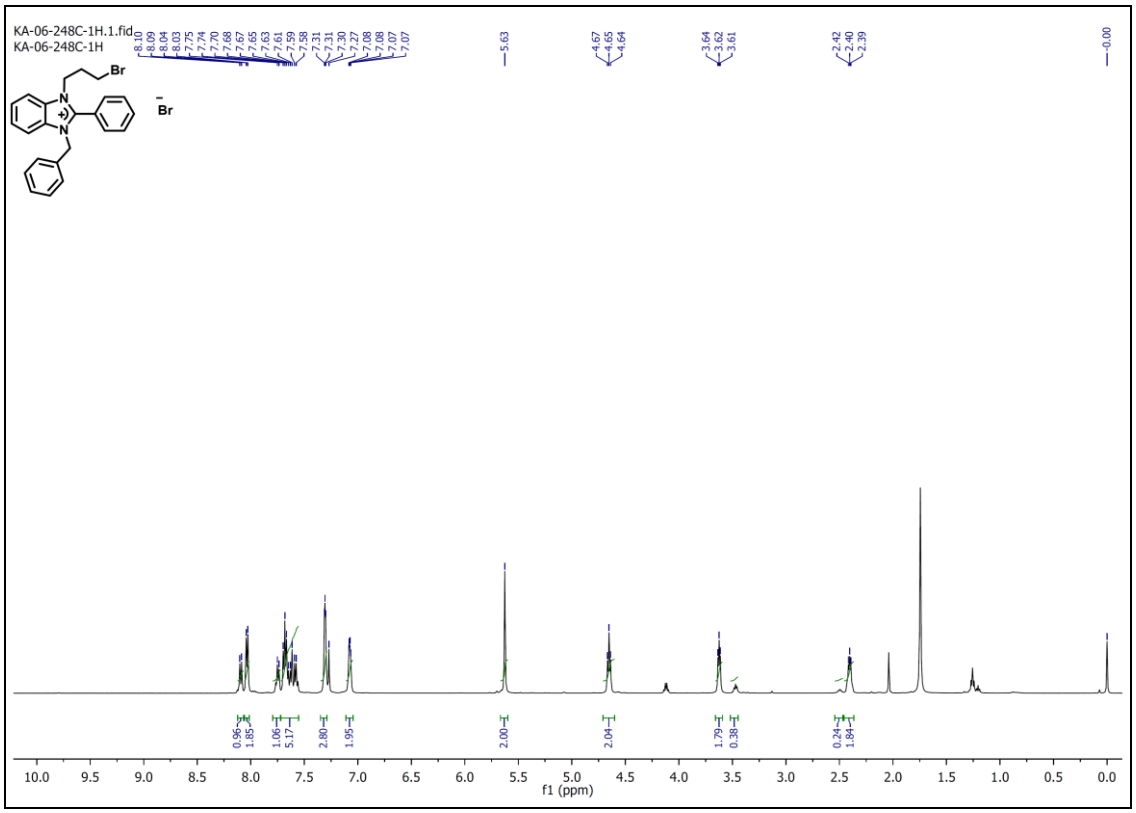

Figure S65. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of compound **13a-2**.

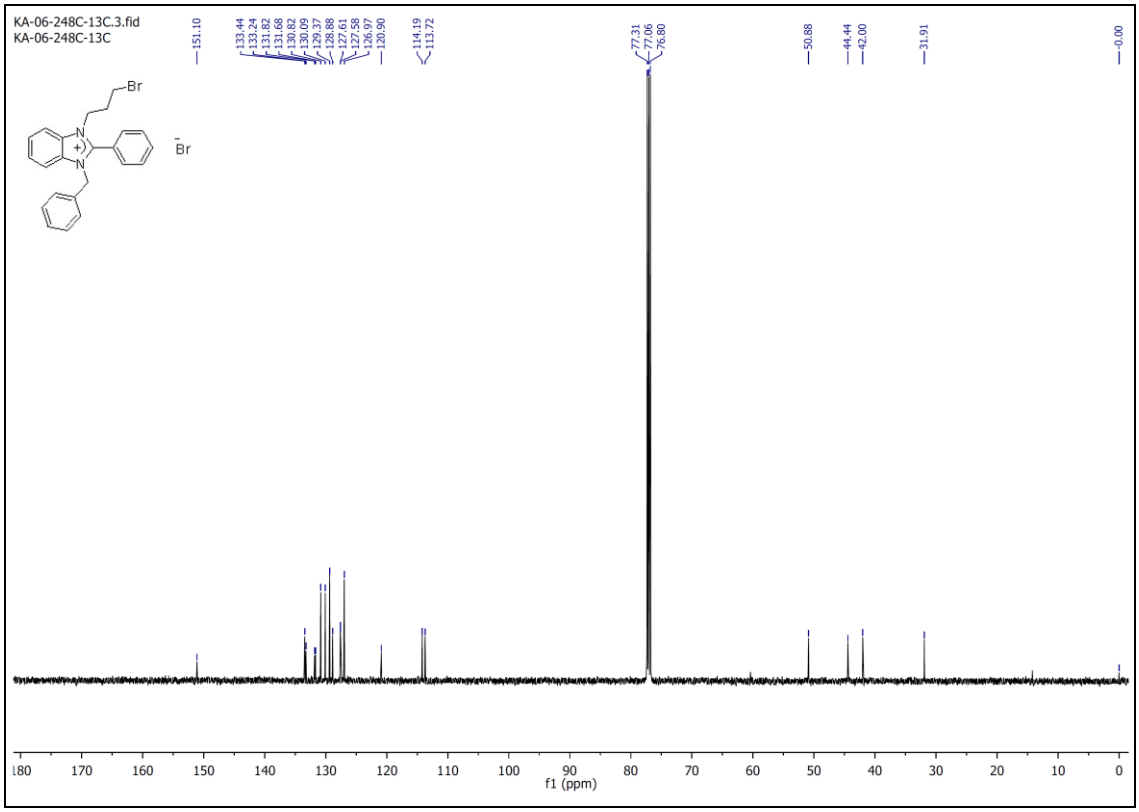

Figure S66. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **13a-2**.

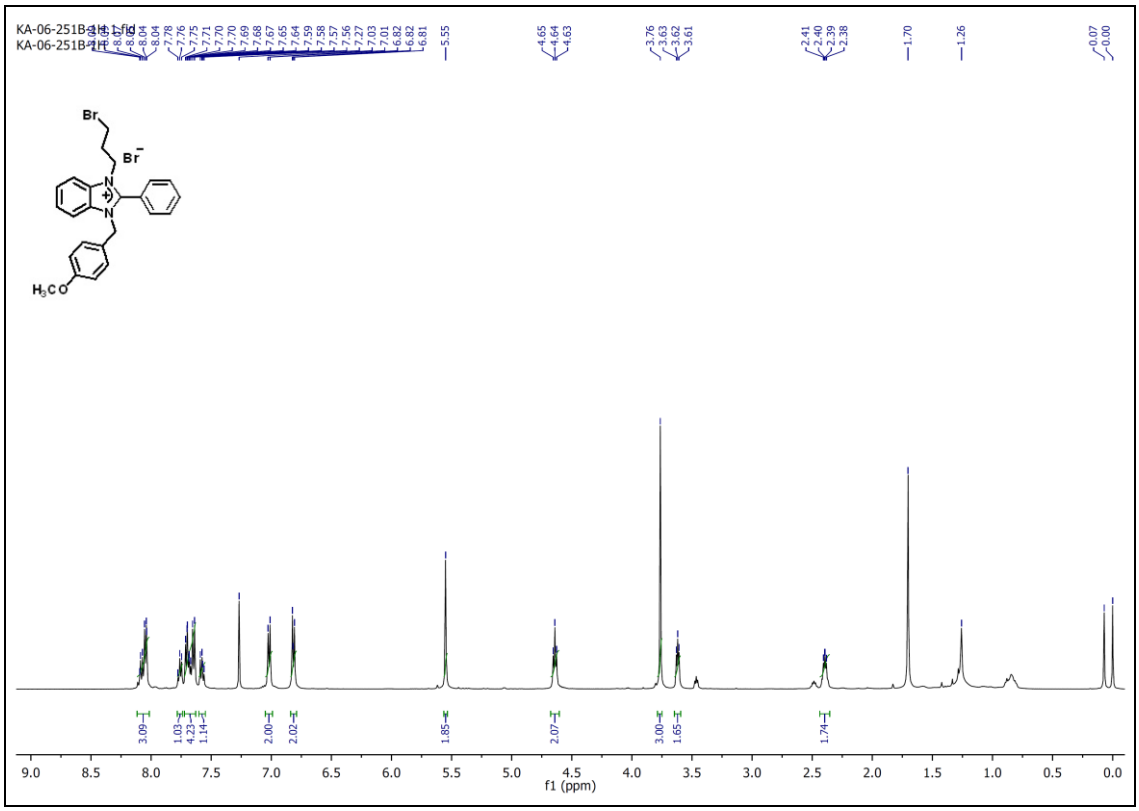

Figure S67. ^{1}H NMR ($CDCl_3$, 500 MHz) of compound **13b-2**.

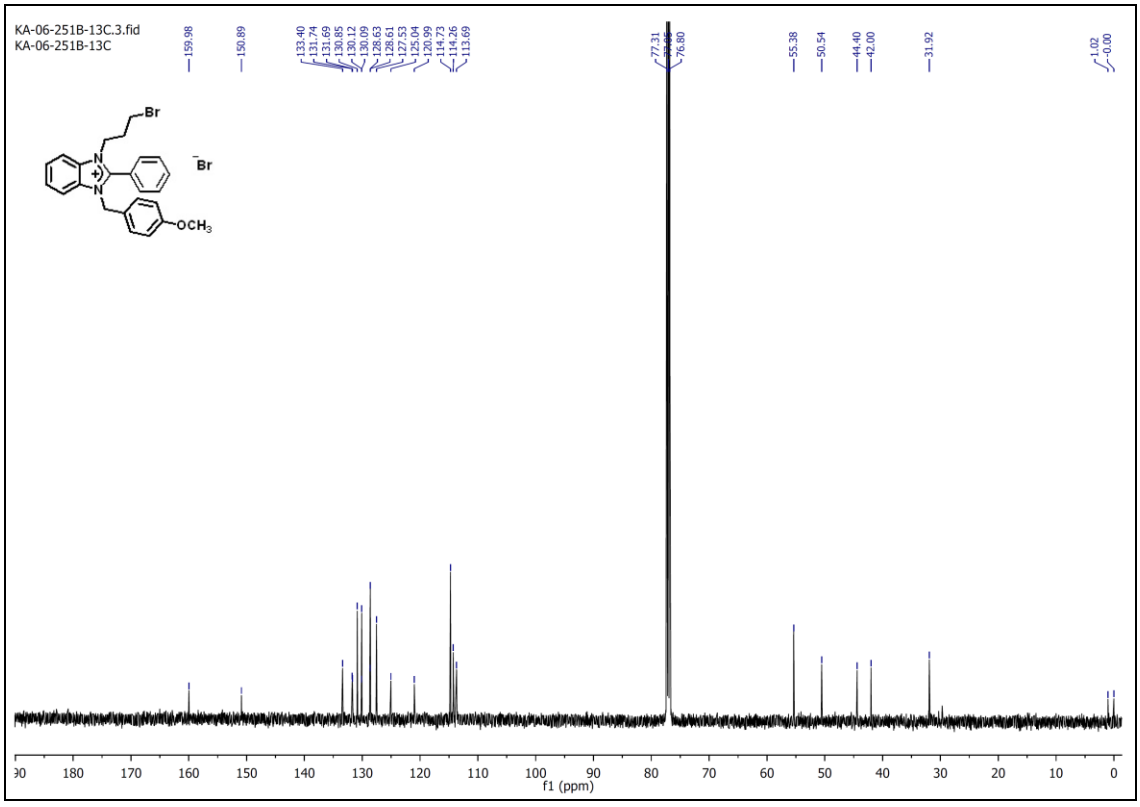

Figure S68. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **13b-2**.

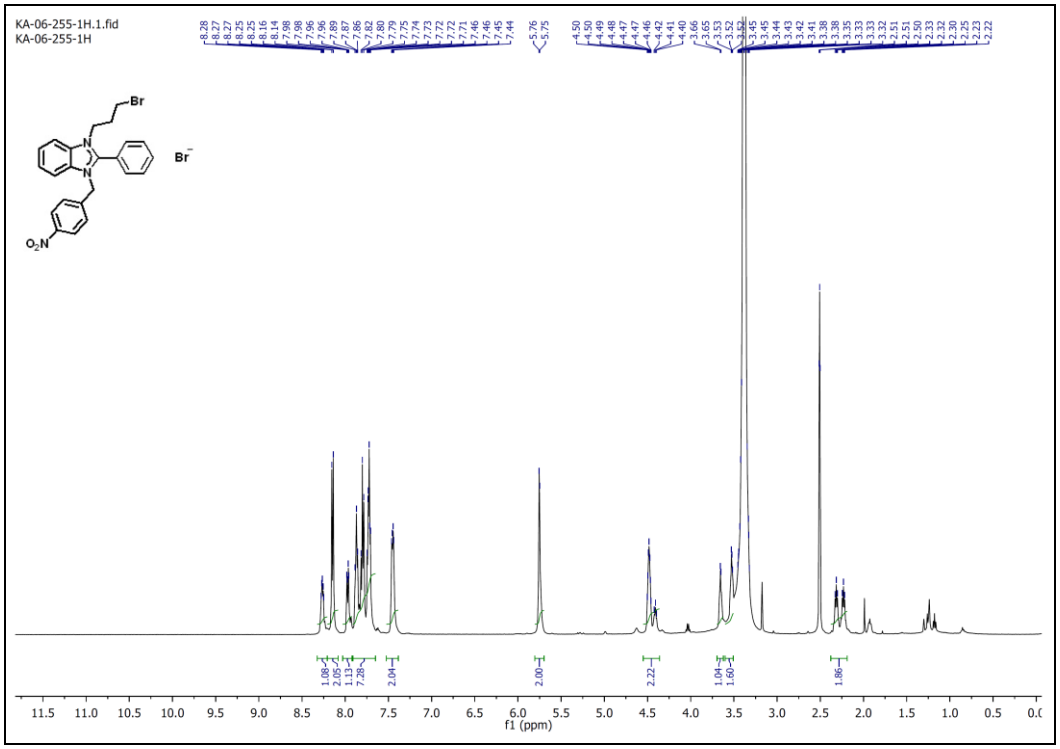

Figure S69. ^{1}H NMR spectrum (DMSO-d_6, 500 MHz) of compound **13c-2**.

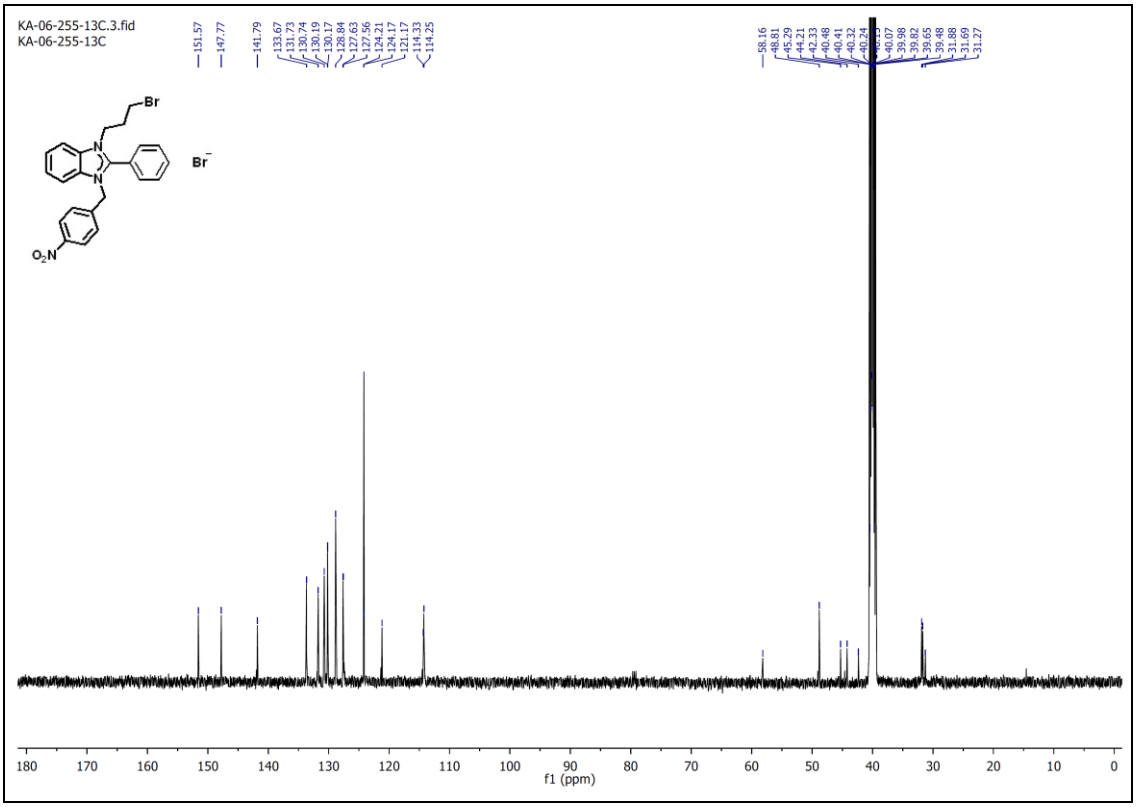

Figure S70. ^{13}C NMR (DMSO-d_6, 125 MHz) of compound **13c-2**.

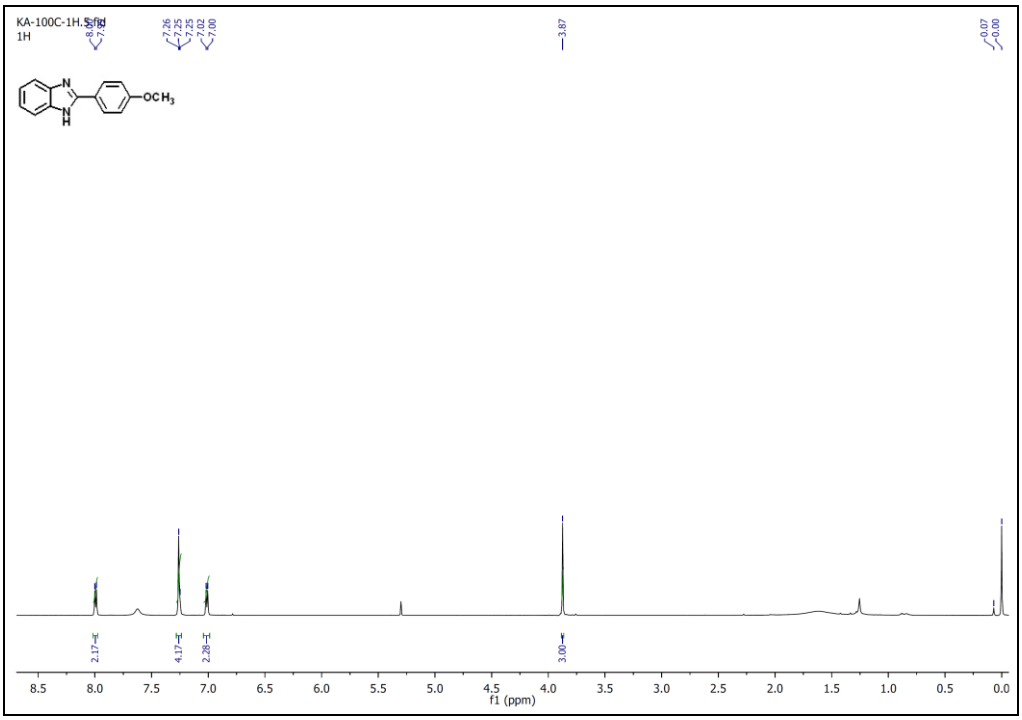

Figure S71. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of compound **14**.

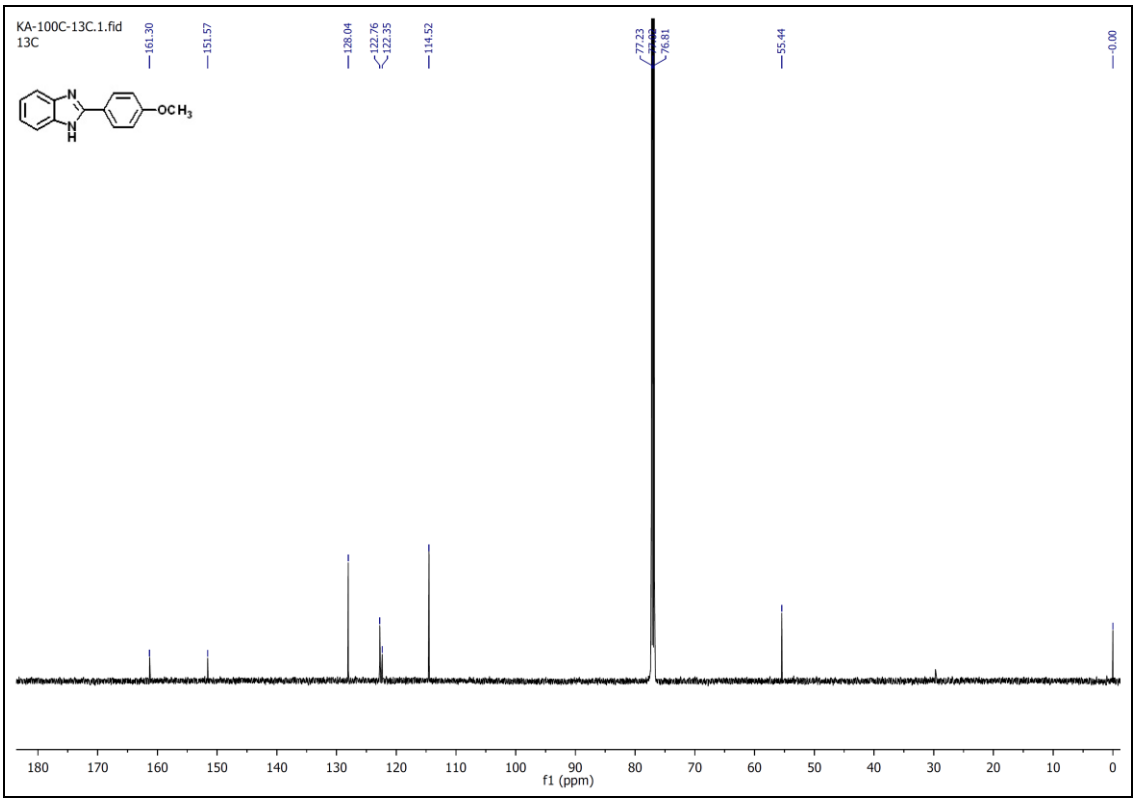

Figure S72. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **14**.

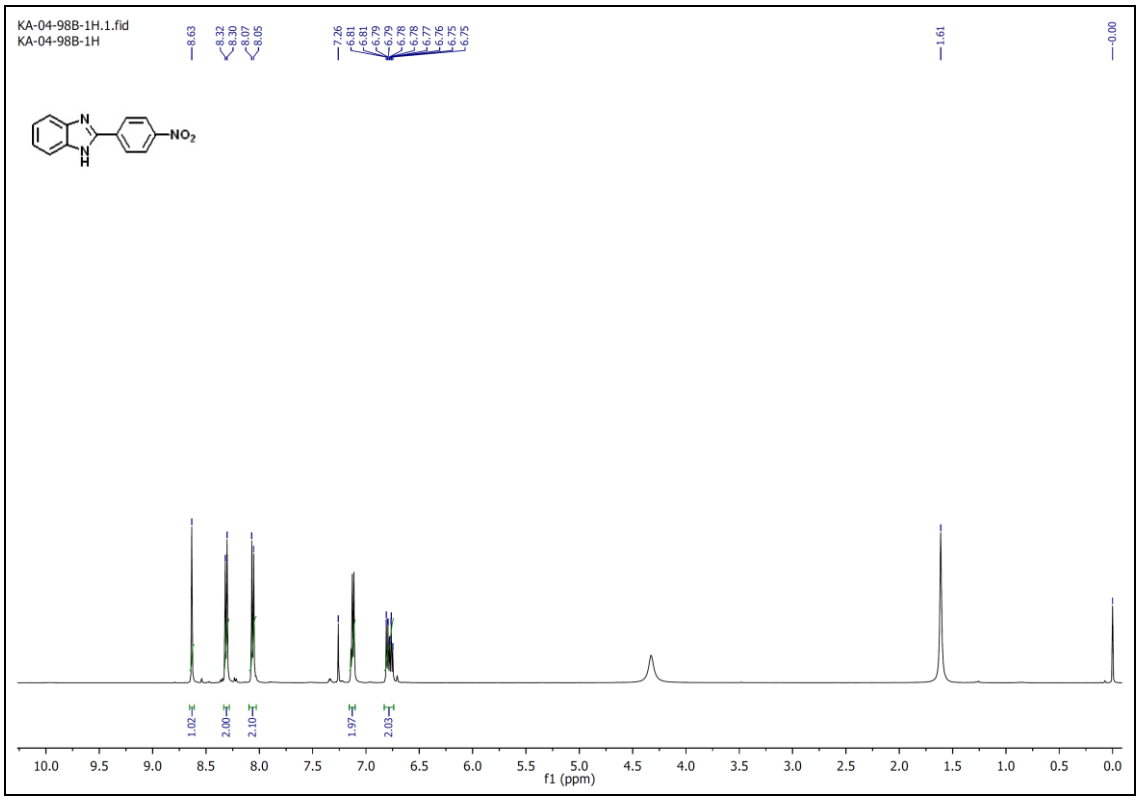

Figure S73. ^{1}H NMR ($CDCl_3$, 500 MHz) of compound **15**.

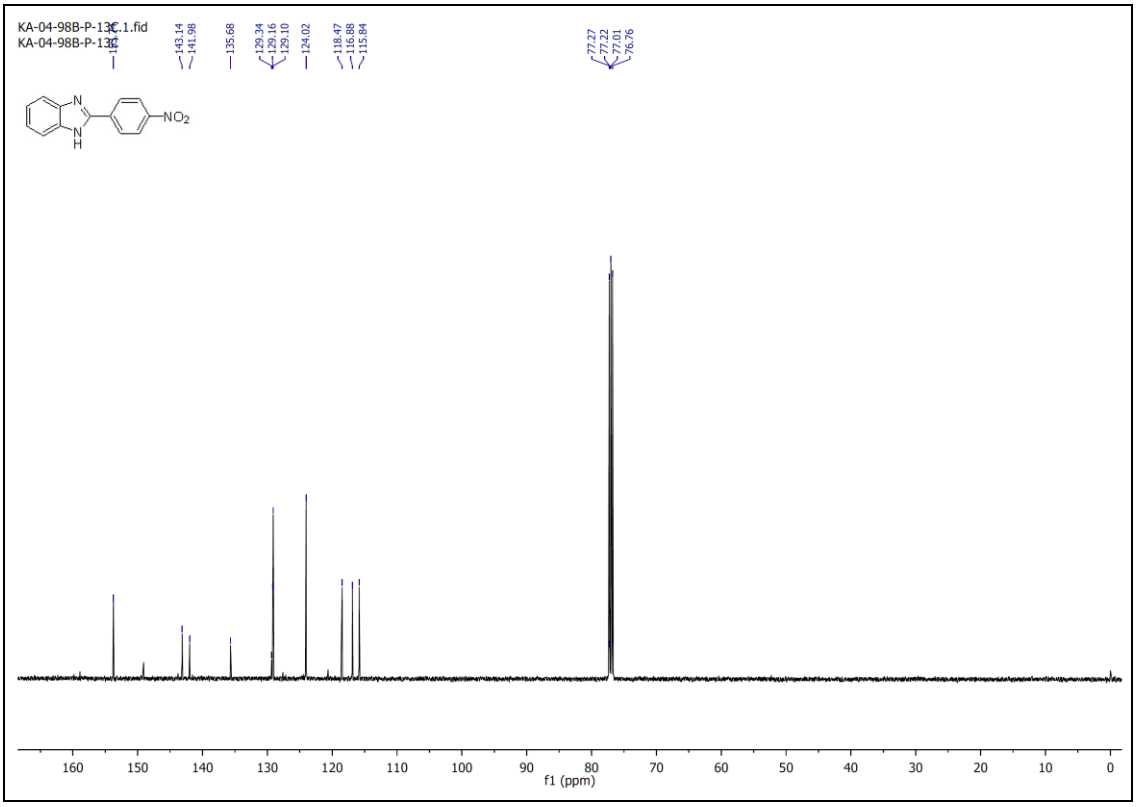

Figure S74. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **15**.

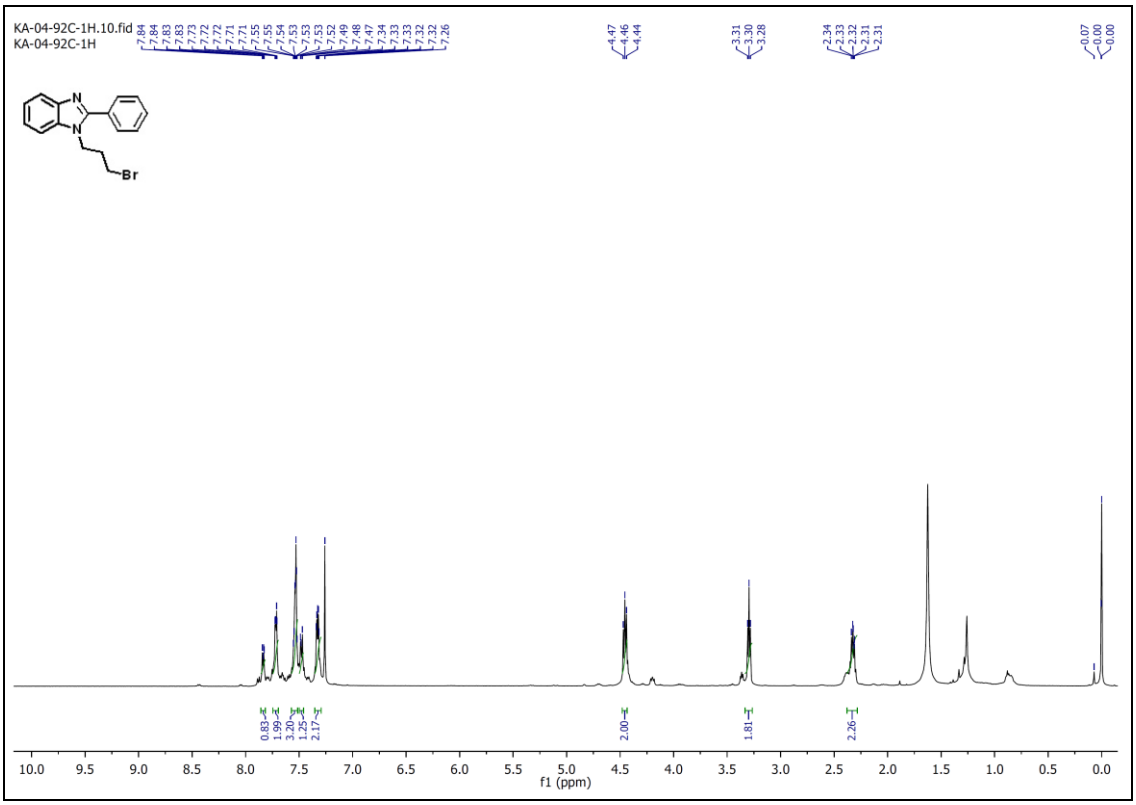

Figure S75. ^{1}H NMR ($CDCl_3$, 400 MHz) of compound **13-2**

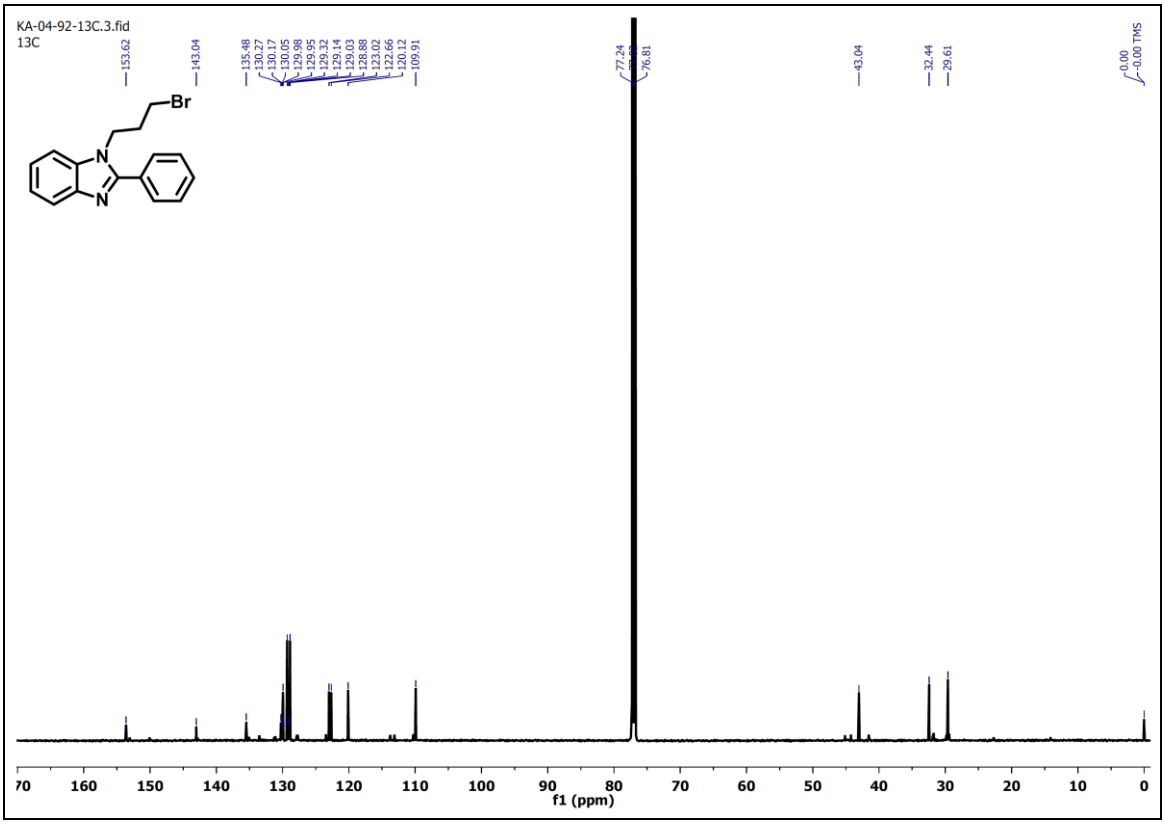

Figure S76. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **13-2**.

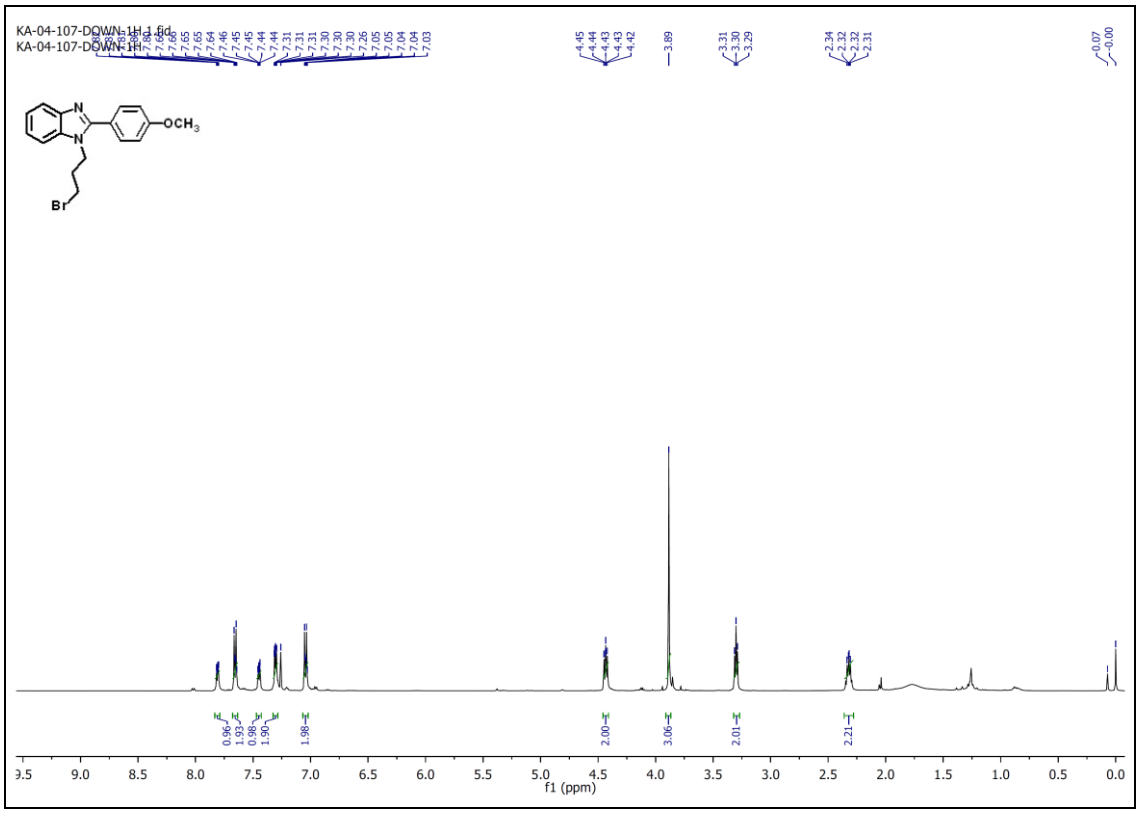

Figure S77. ^{1}H NMR ($CDCl_3$, 500 MHz) of compound **14-2**.

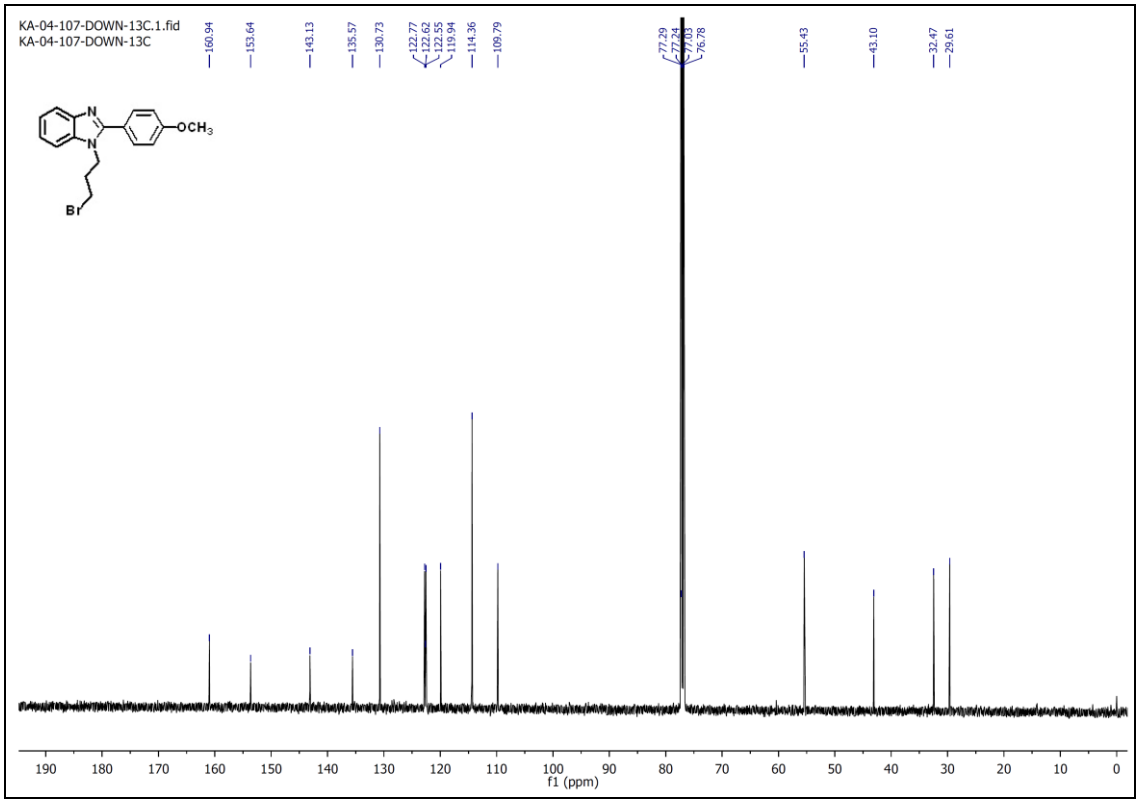

Figure S78. ^{13}C NMR ($CDCl_3$, 125 MHz) of compound **14-2**.

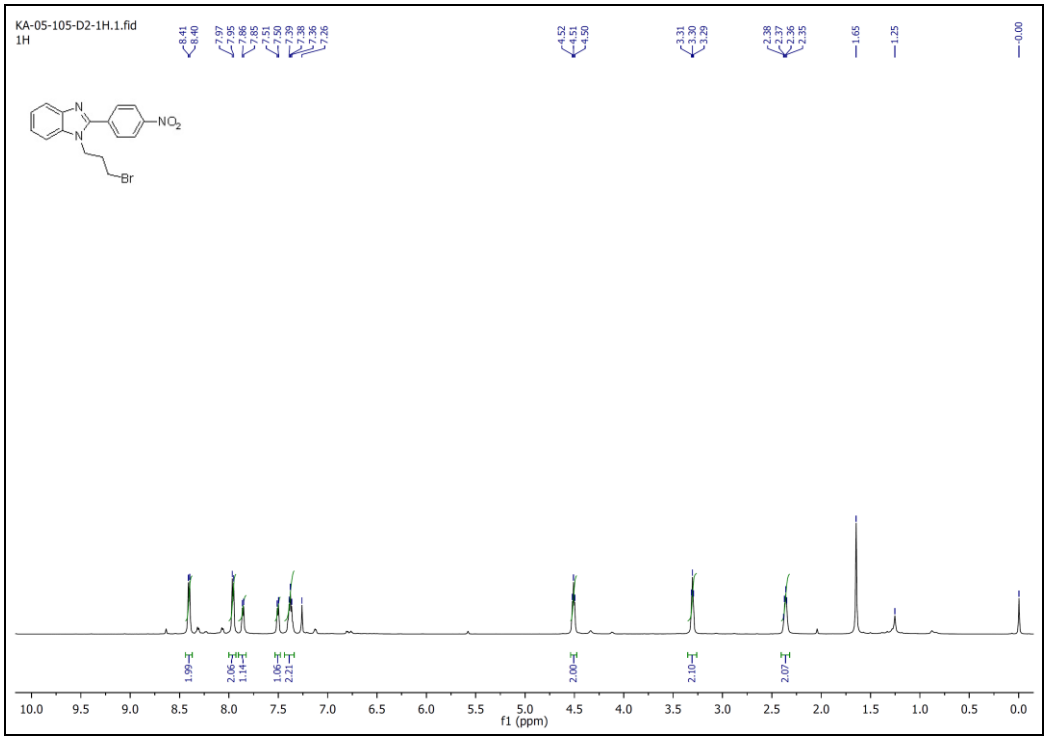

Figure S79. ^{1}H NMR ($CDCl_3$, 600 MHz) of compound **15-2**.

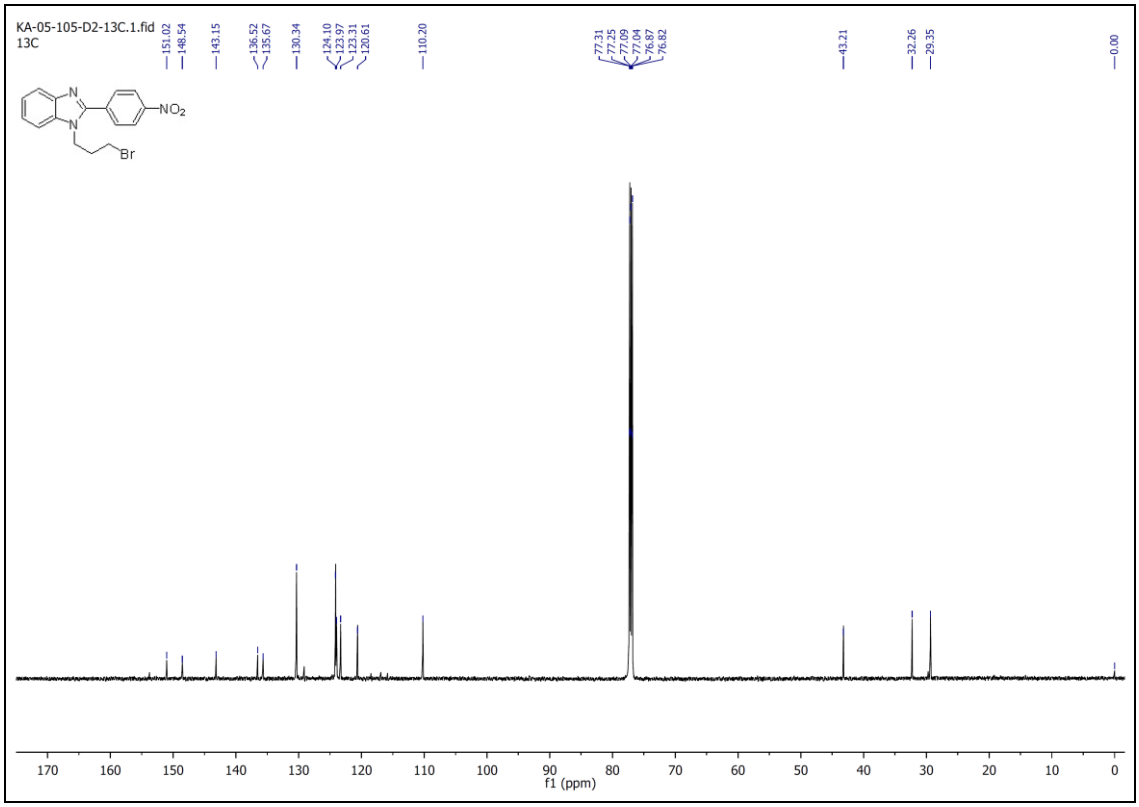

Figure S80. ^{13}C NMR ($CDCl_3$, 150 MHz) of compound **15-2**.

Table S1. Single Crystal X-Ray diffraction data for compound **7b**.

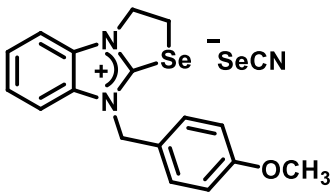	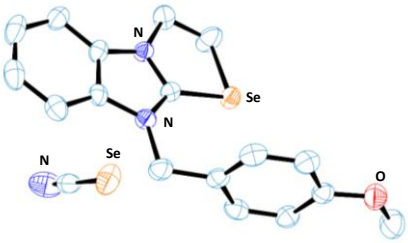
Crystal data and structure refinement for **7b**	
Empirical formula	$C_{18}H_{17}N_3OSe_2$
Formula Weight	449.26
Crystal habit, color	Rectangular, pale yellow
Crystal size	0.170 × 0.130 × 0.090
Temperature, *T* (K)	296(2)
Wavelength, λ (Å)	0.71073
Crystal System	Orthorhombic
Space Group	*'P 21'*
Unit cell dimension	*a* = 6.7765(10) Å *b* = 16.086(2) Å *c* = 16.129(2) Å α = 90.00°, β = 90.00° , γ =90.00°
Volume, *V*(Å^3)	1758.1(4)
Cell Formula units, Z	4
Absorption Coefficient, μ (mm^{-1})	4.216
F(000)	888
θ range for data collection	1.788° to 24.997°
Limiting Indices	$-8 \le h \le 8$, $-19 \le k \le 19$, $-19 \le l \le 19$
Reflection Collected / unique	89565 / 3090
Refinement method	'SHELXL-2018/3 (Sheldrick, 2018)'
Data / Restraints / Parameters	3090 / 0 / 217
Goodness-of-fit on F^2	1.095
Largest diff. peak and hole	0.687 and -0.700

Table S2. Binding interaction of compound **10c** with target proteins as predicted by docking studies

Sl no.	Target	Gibbs free Energy (Kcal/mol)	Interactions
1	Bcl2	-6.6	R105
2	COX-2	-9.6	S530, Y385, H90, F518, I517
3	Survivin	-4.7	T97, K91
