Supplementary Information

Isostructural Re(I)/^{99m}Tc(I) Tricarbonyl Complexes Functionalized with Benzothiazole Derivatives for Cancer Theranostics

Patrique Nunes,[1] Goreti Ribeiro Morais,[1] Elisa Palma,[1] Francisco Silva,[1] Maria Cristina Oliveira, [1] Vera F. C. Ferreira,[1] Filipa Mendes,[1] Lurdes Gano,[1] Hugo Vicente Miranda,[2] Tiago F. Outeiro,[2,3,4] Isabel Santos,[1] António Paulo[1*]

[1]*Centro de Ciências e Tecnologias e Nucleares, IST, Universidade de Lisboa, Estrada Nacional 10, 2695-066 Bobadela LRS, Portugal*

[2]*Cell and Molecular Neuroscience Unit, Instituto de Medicina Molecular, Av. Prof. Egas Moniz, 1649-028 Lisboa, Portugal;*

[3]*Instituto de Fisiologia, Faculdade de Medicina da Universidade de Lisboa, Lisboa, Portugal*

[4]*Department of NeuroDegeneration and Restorative Research, University Medical Center Göttingen, Waldweg 33, 37073 Göttingen, Germany*

NMR data

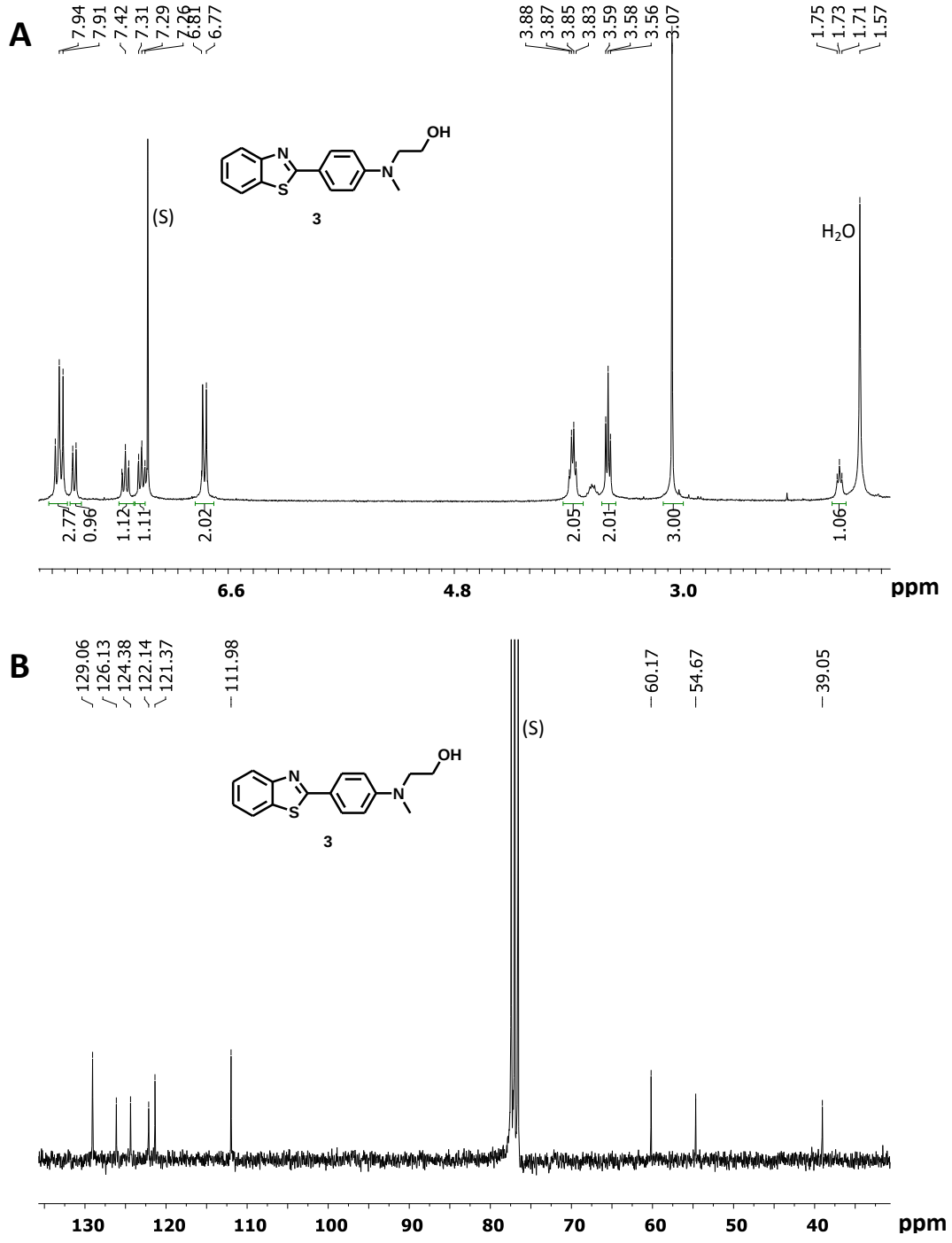

Figure S1. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**3**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons. Peak from residual water is also assigned.

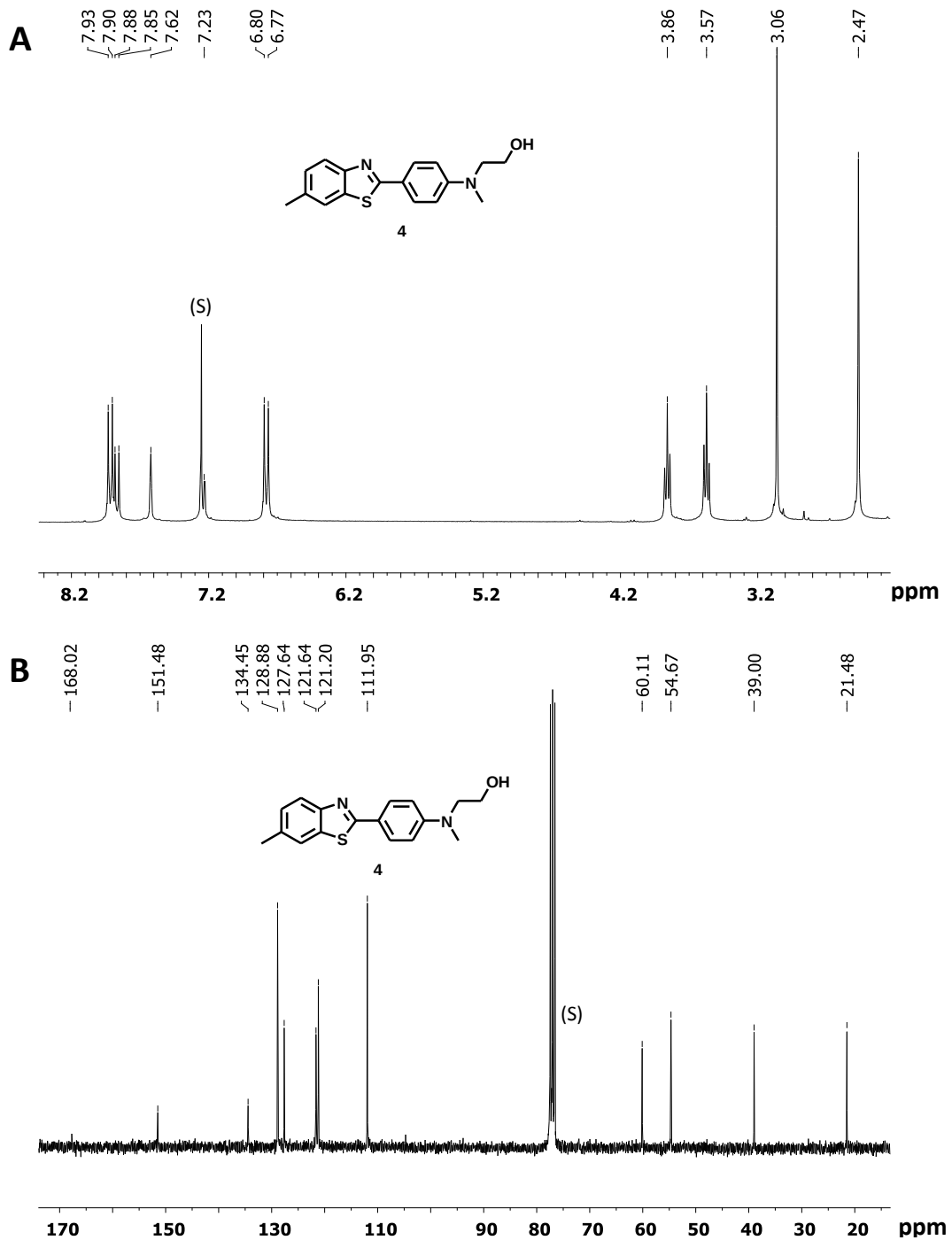

Figure S2. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**4**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

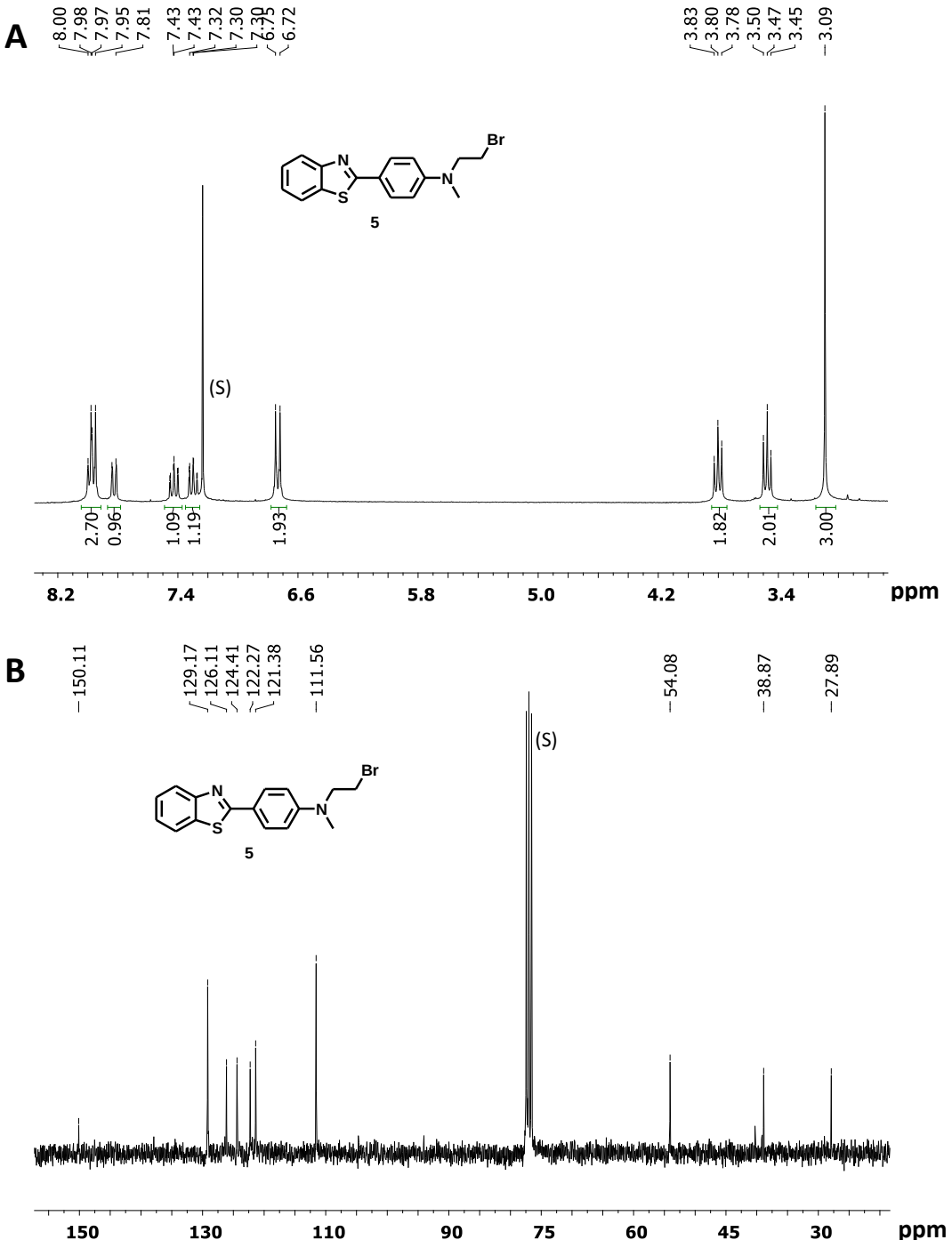

Figure S3. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**5**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

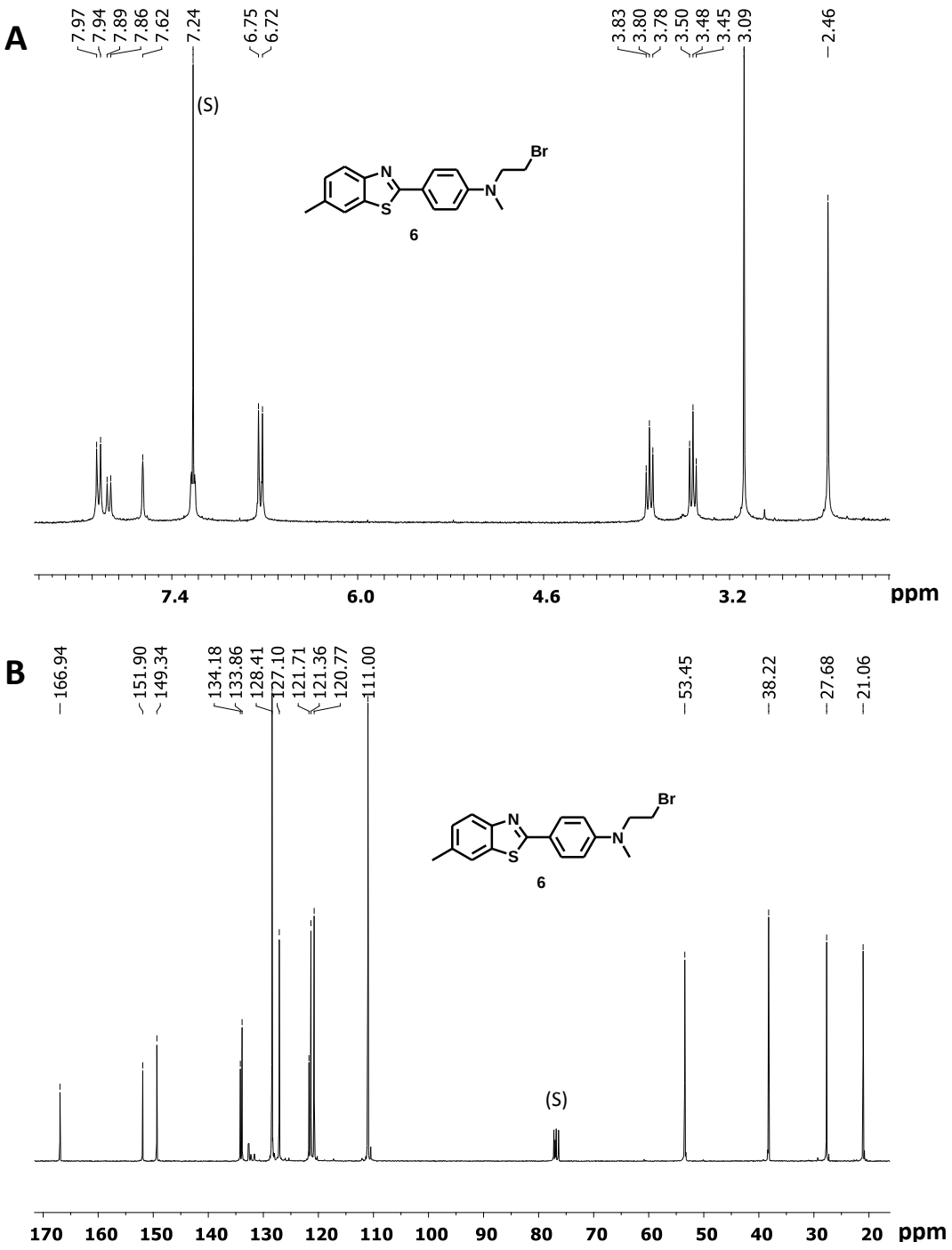

Figure S4. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**6**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

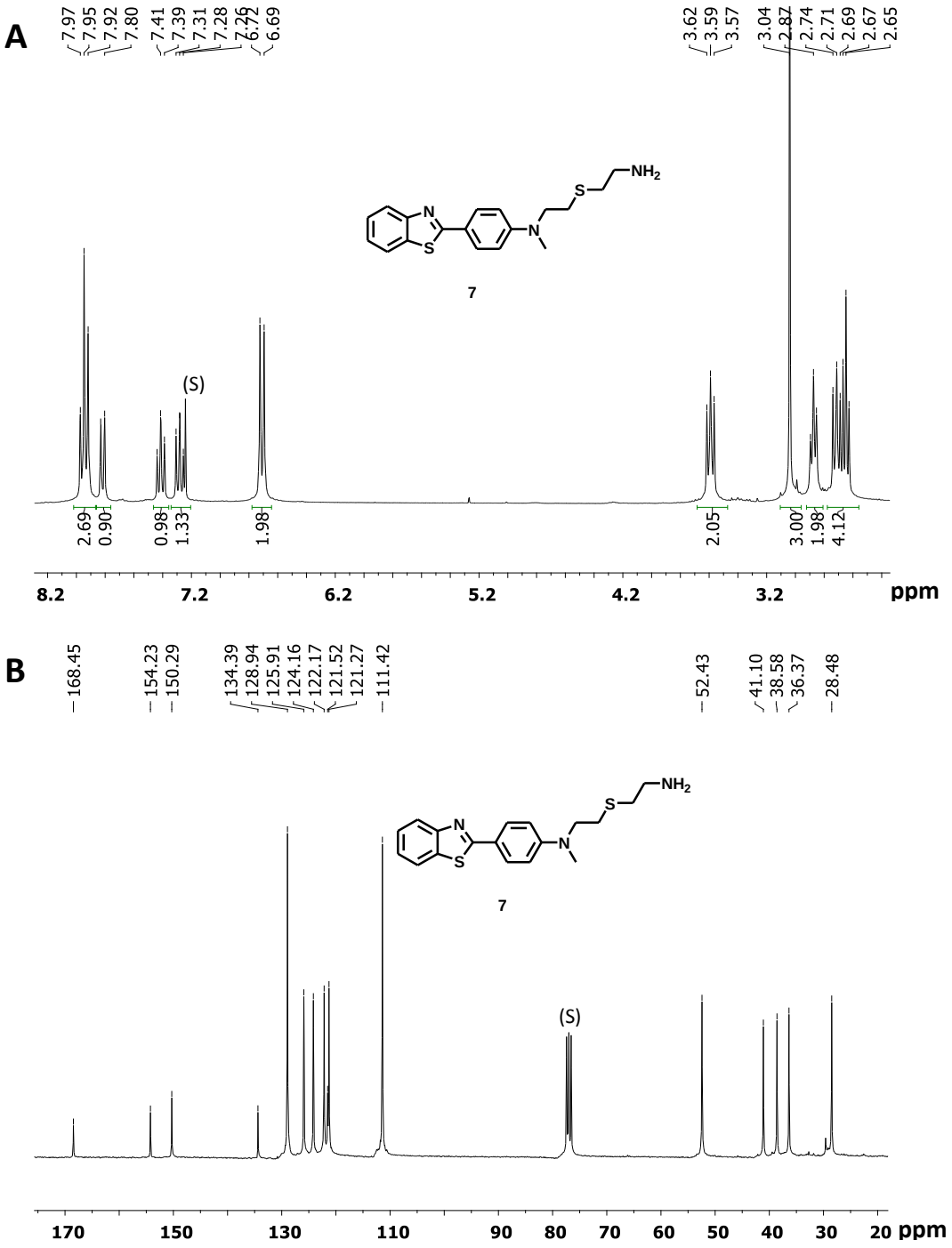

Figure S5. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**7**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

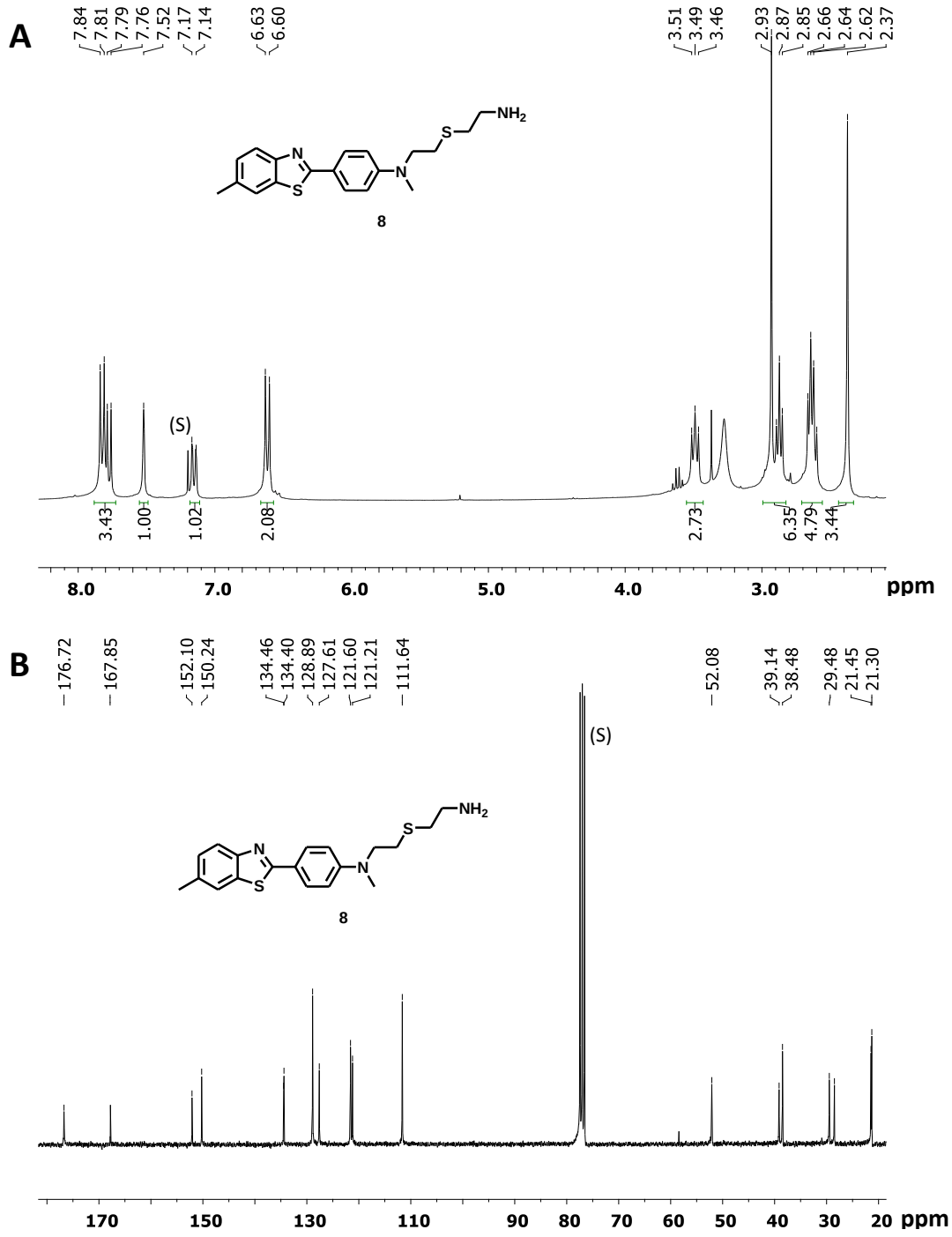

Figure S6. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**8**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

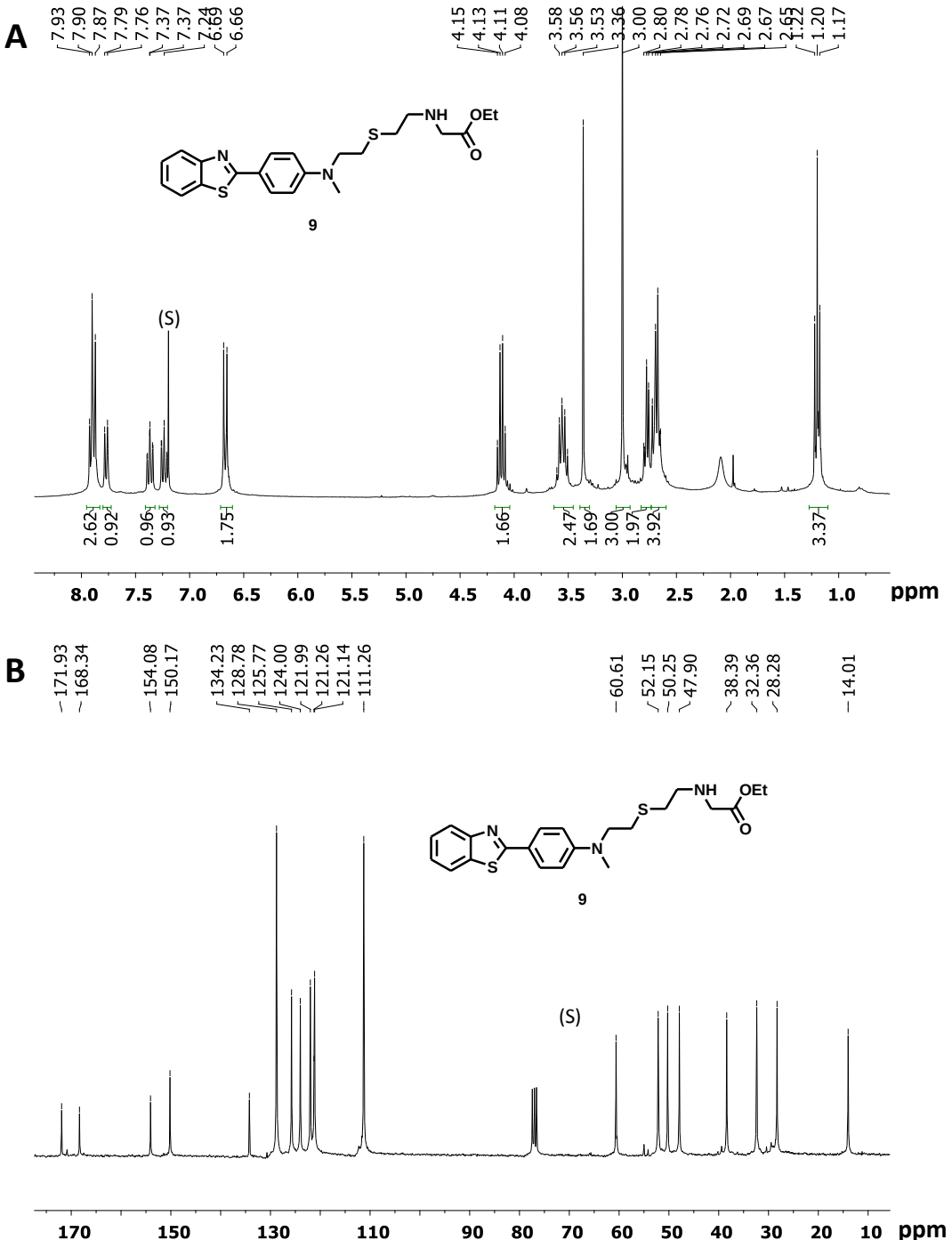

Figure S7. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**9**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

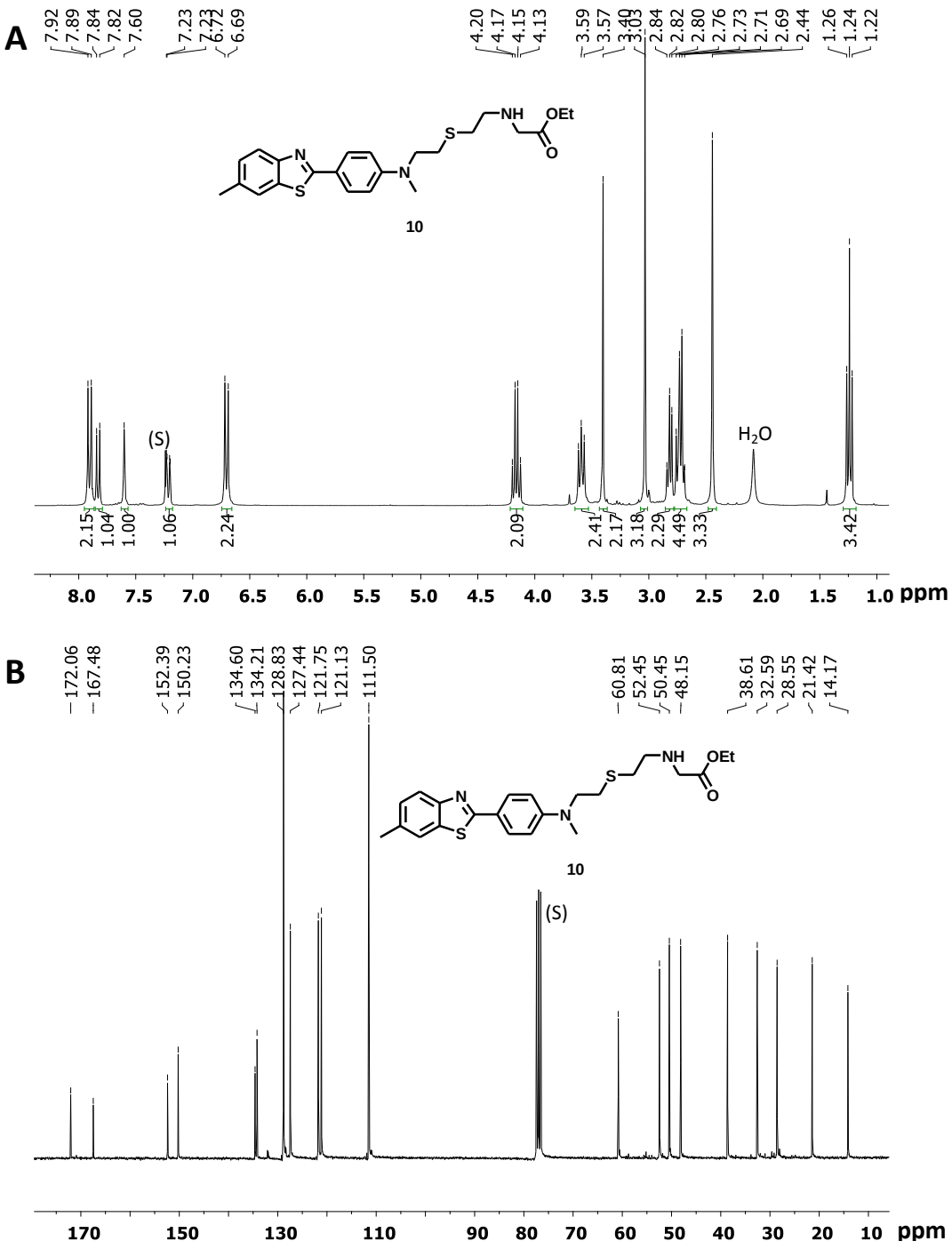

Figure S8. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**10**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons. Peak from residual water is also assigned.

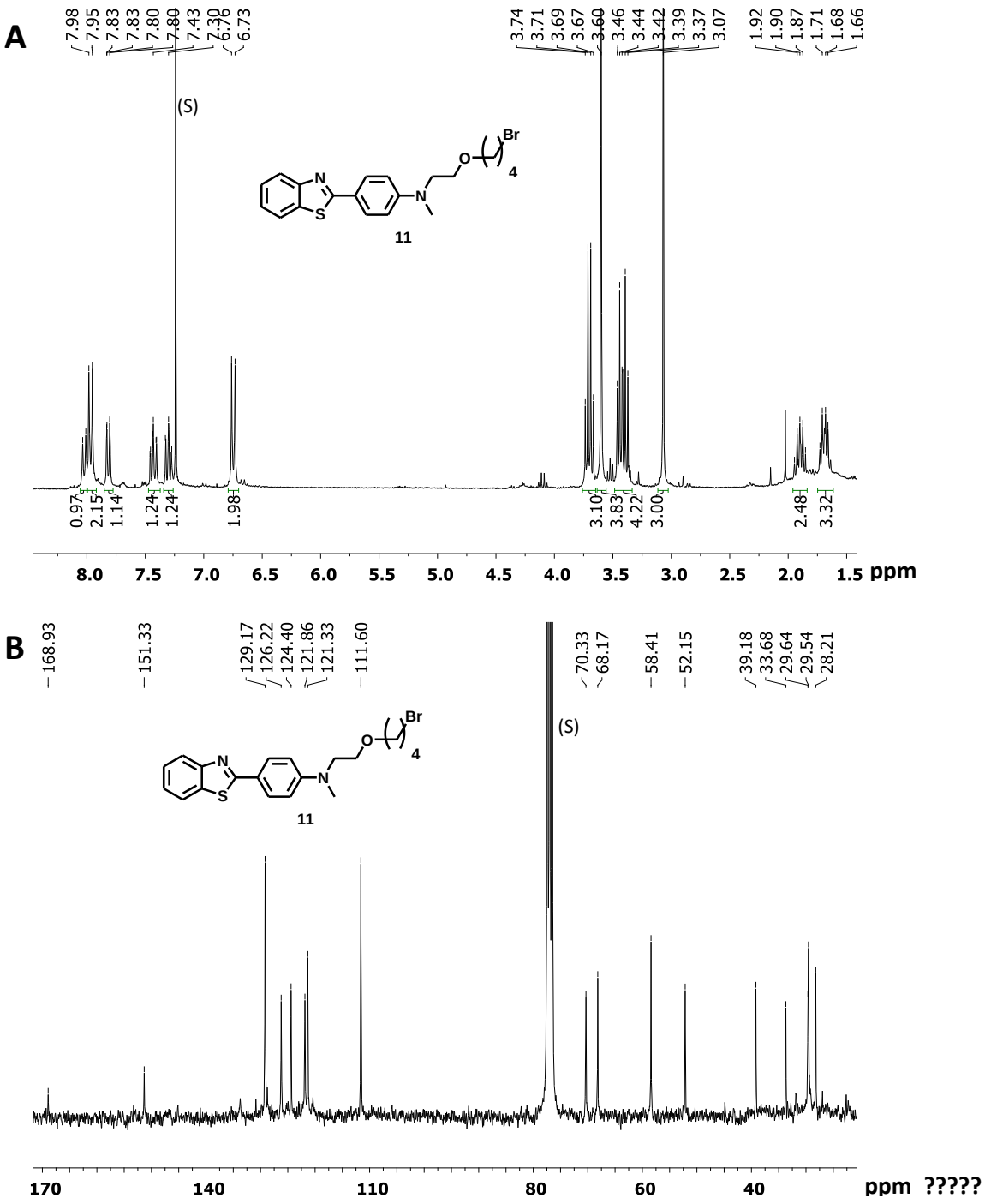

Figure S9. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**11**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

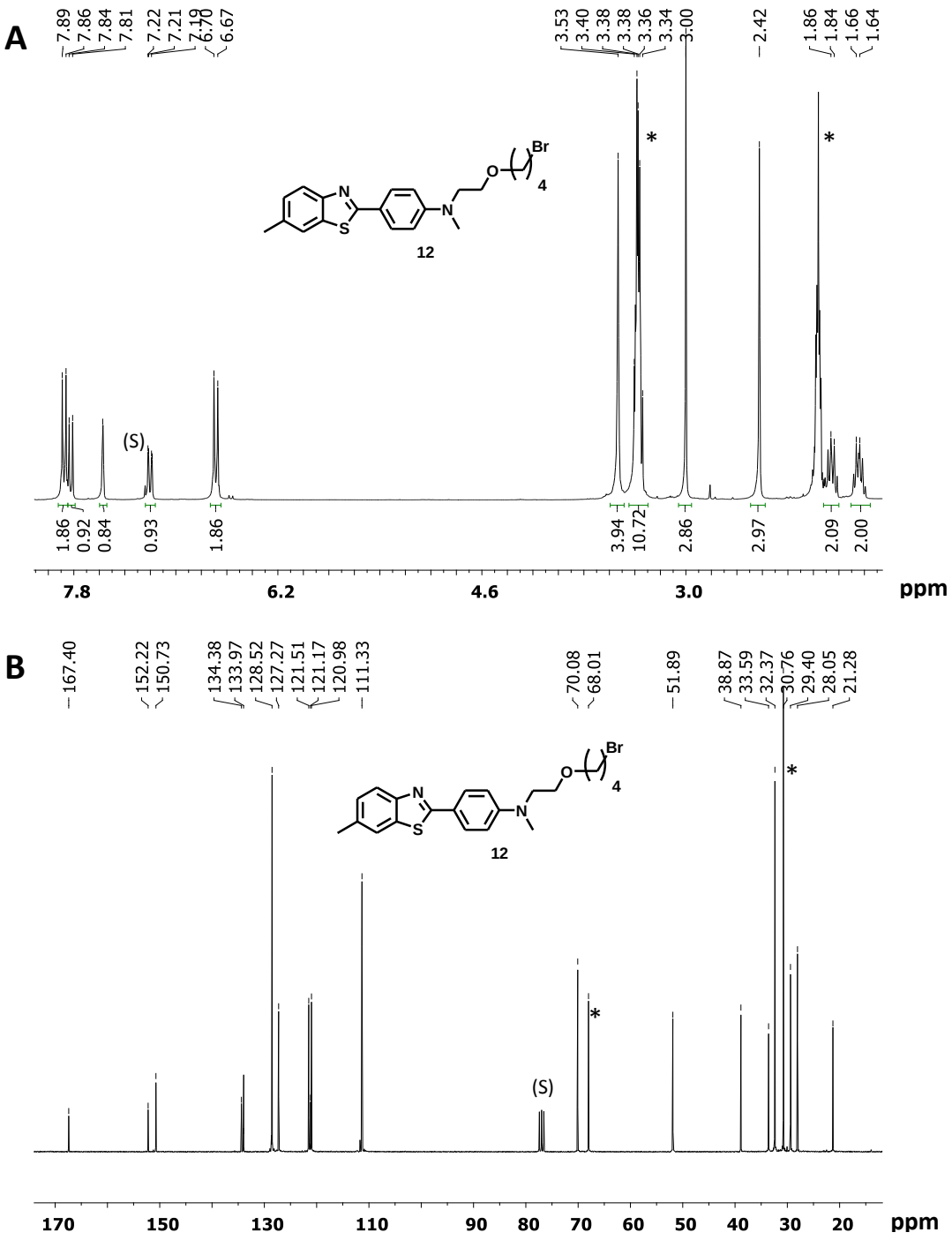

Figure S10. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**12**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons. Peaks from residual THF (*) are also assigned.

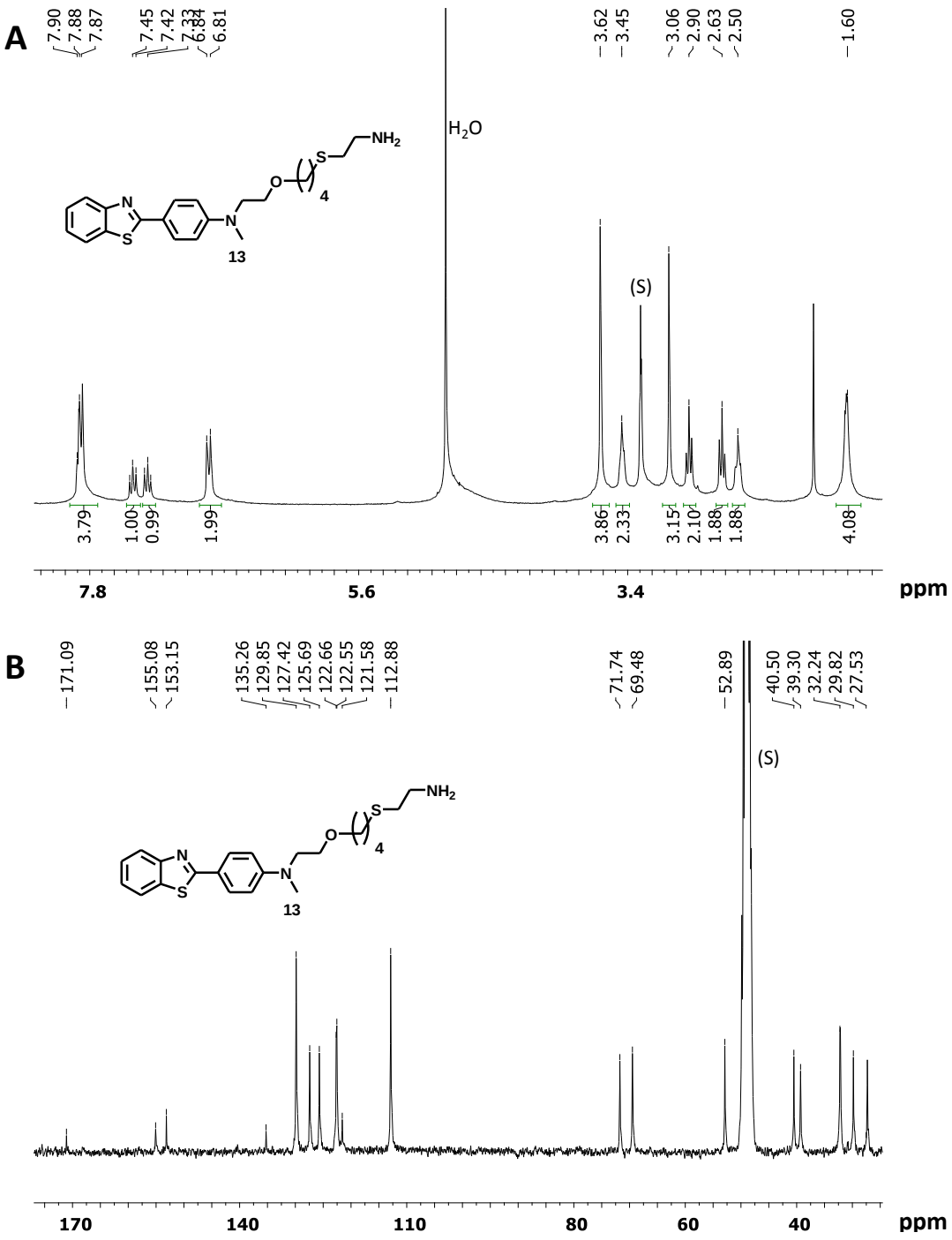

Figure S11. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**13**) in CD_3OD (S) showing the integration of aromatic and aliphatic protons. Peak from residual water is also assigned.

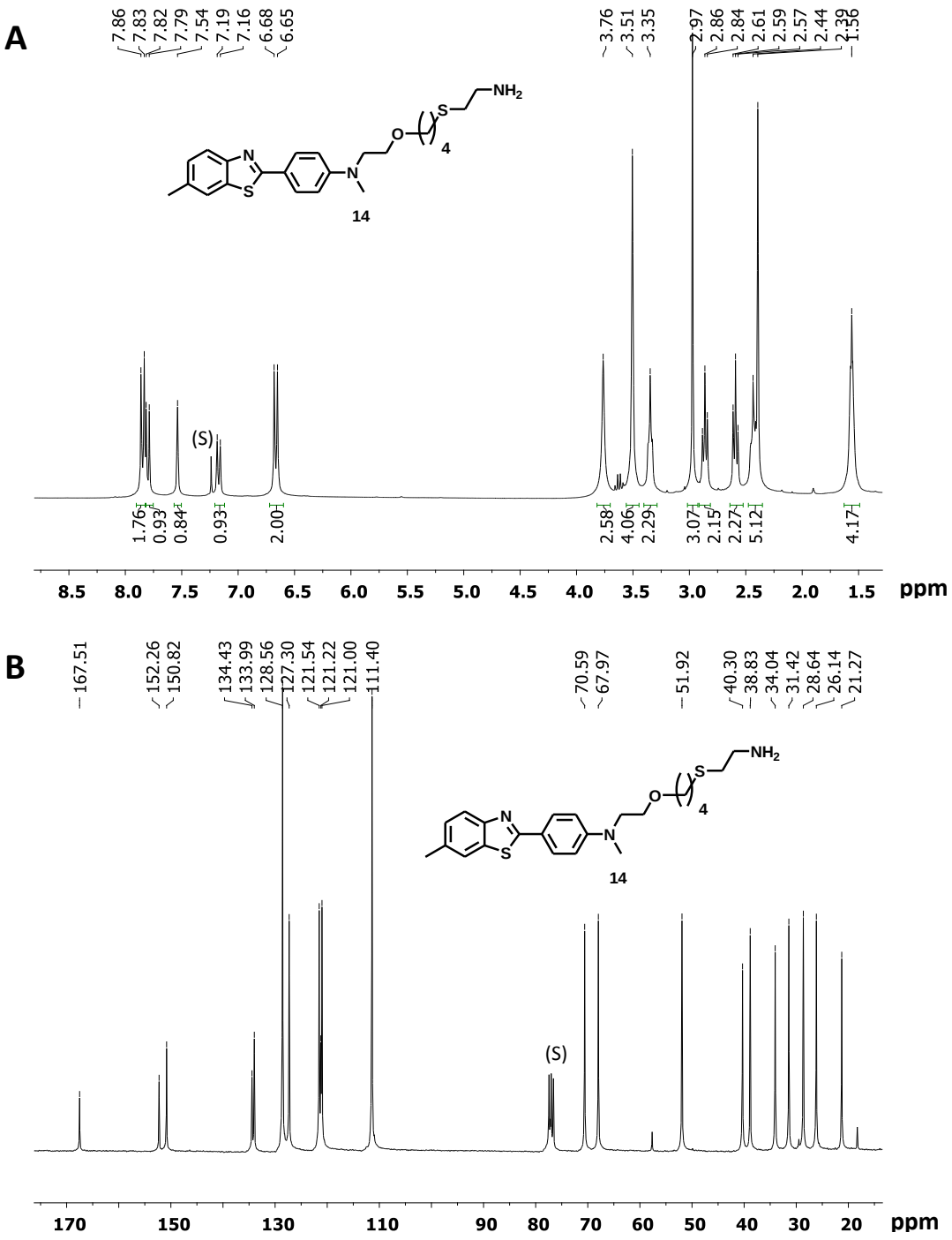

Figure S12. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**14**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

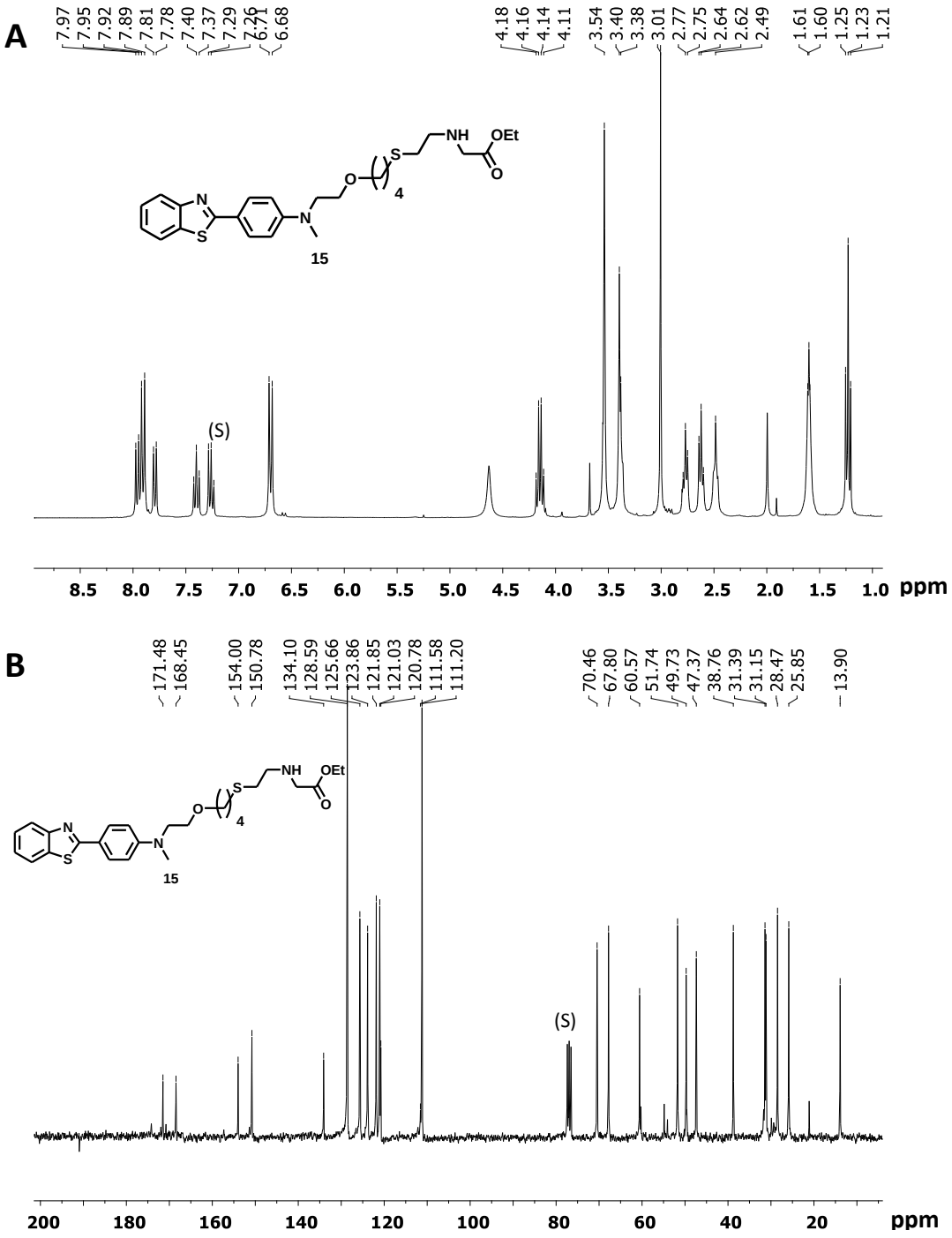

Figure S13. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**15**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

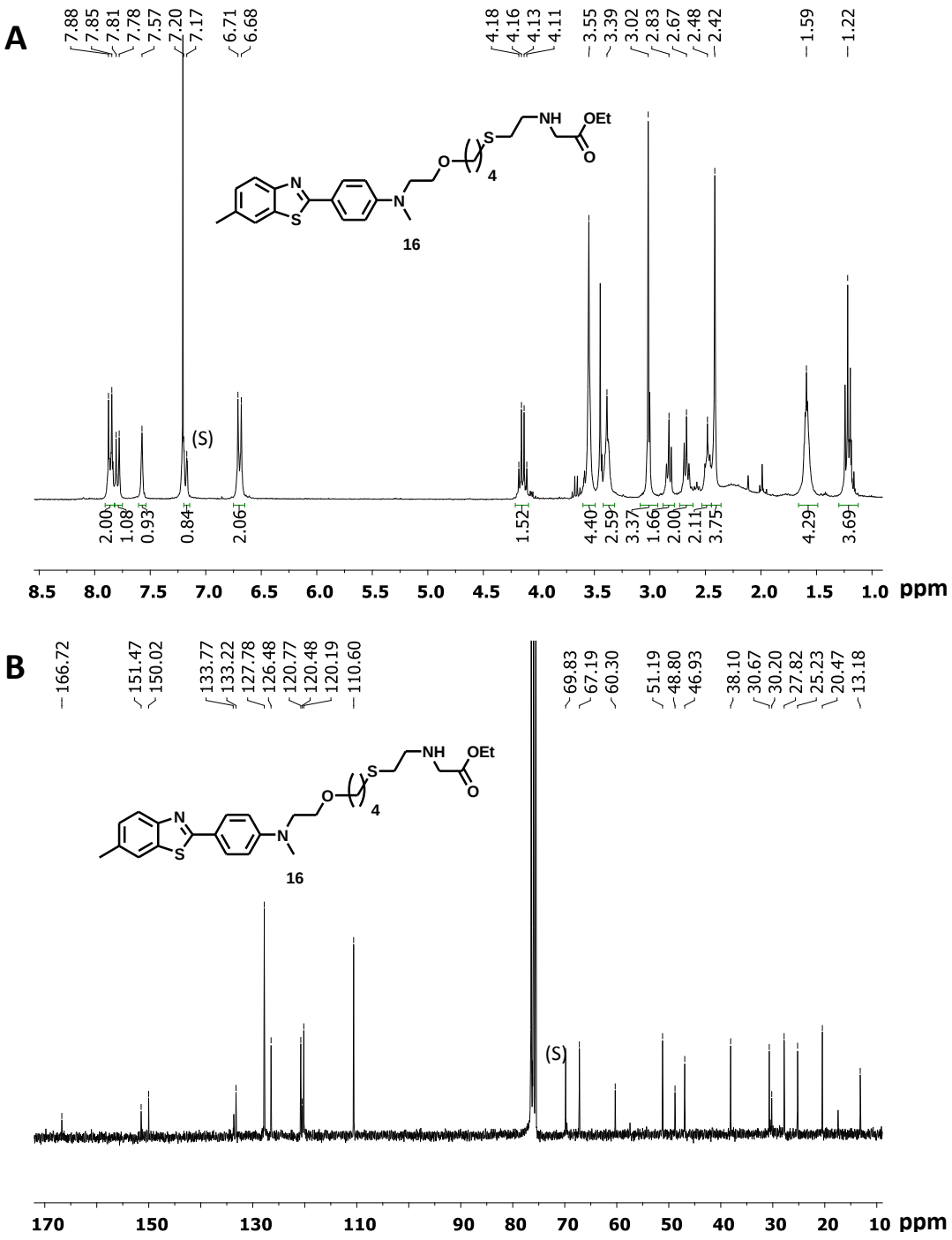

Figure S14. (**A**) ^{1}H and (**B**) ^{13}C spectrum of (**16**) in $CDCl_3$ (S) showing the integration of aromatic and aliphatic protons.

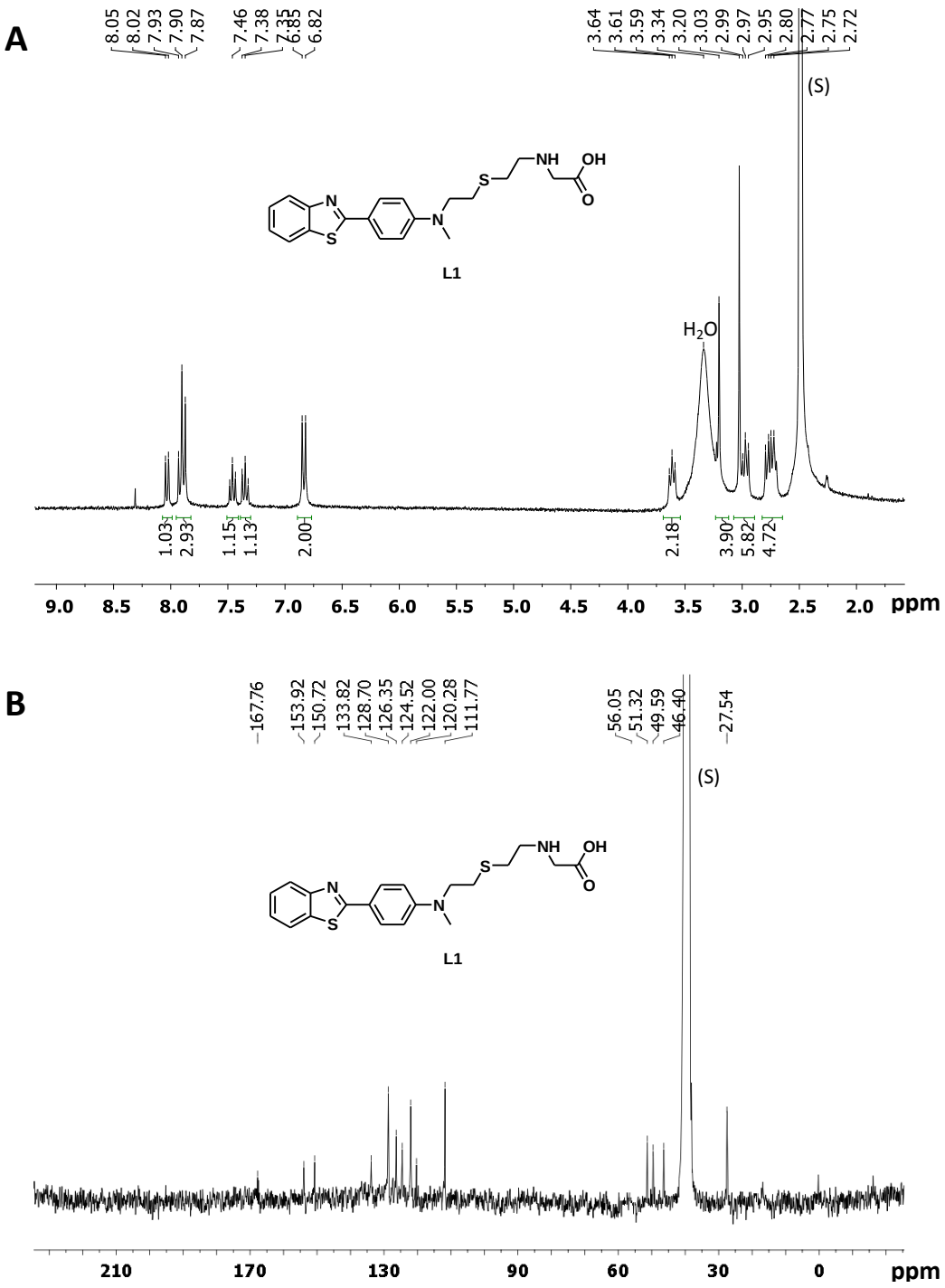

Figure S15. (**A**) ^{1}H and (**B**) ^{13}C spectrum of **2-[(2-((2``-((4``–(benzo[*d*]thiazol–2-yl)phenyl)(methyl)amino)ethyl)thio]ethyl)amino) acetic acid** (**L1**) in DMSO-*d6* (S) showing the integration of aromatic and aliphatic protons.

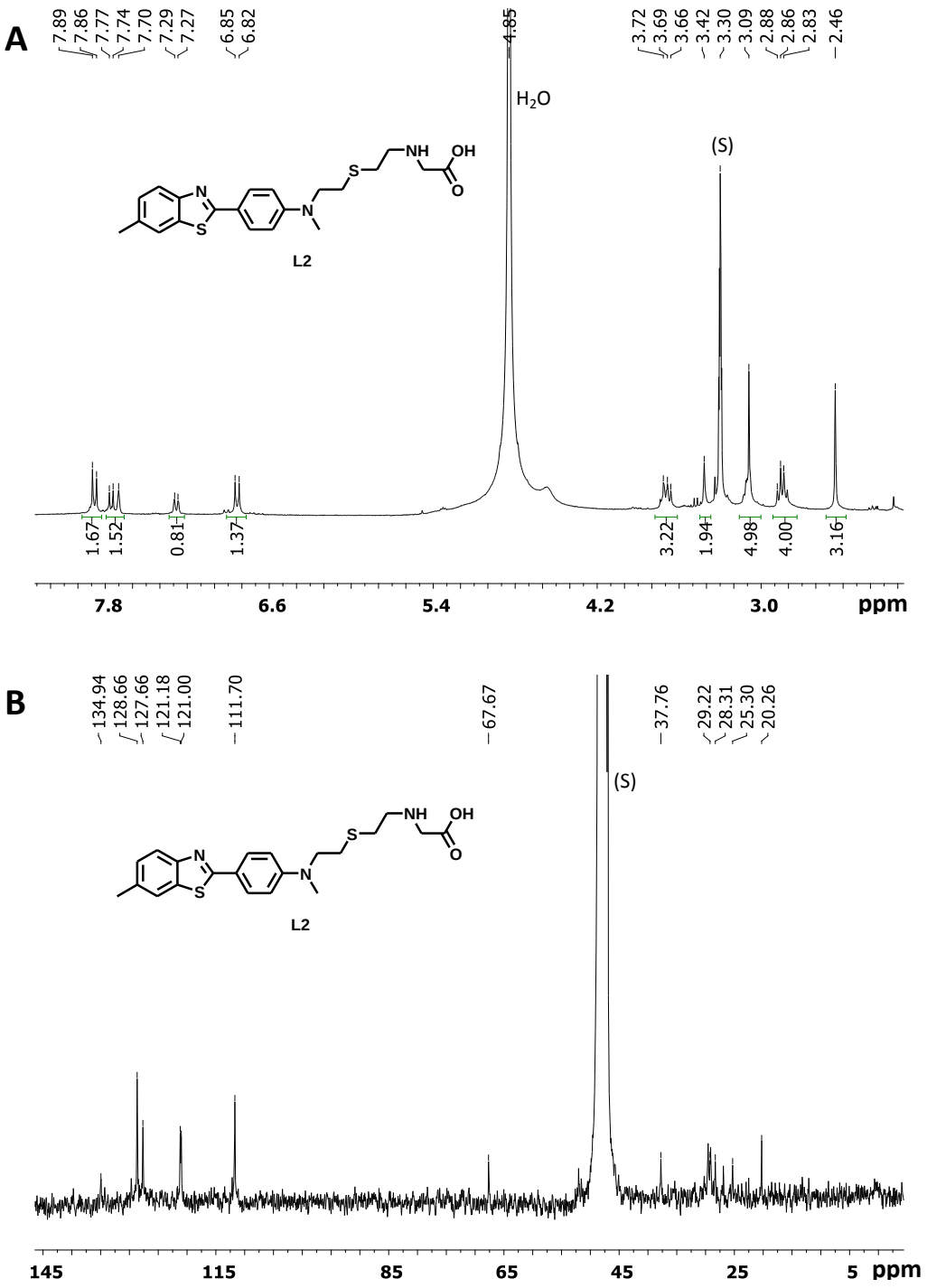

Figure S16. (**A**) ^{1}H and (**B**) ^{13}C spectrum of **2-[2`-(2``-((4```-(6````-methylbenzo[*d*]thiazol–2-yl)phenyl)(methyl)amino)ethylthio)ethylamino] acetic acid (L2)** in CD_3OD (S). Peak from residual water is also assigned.

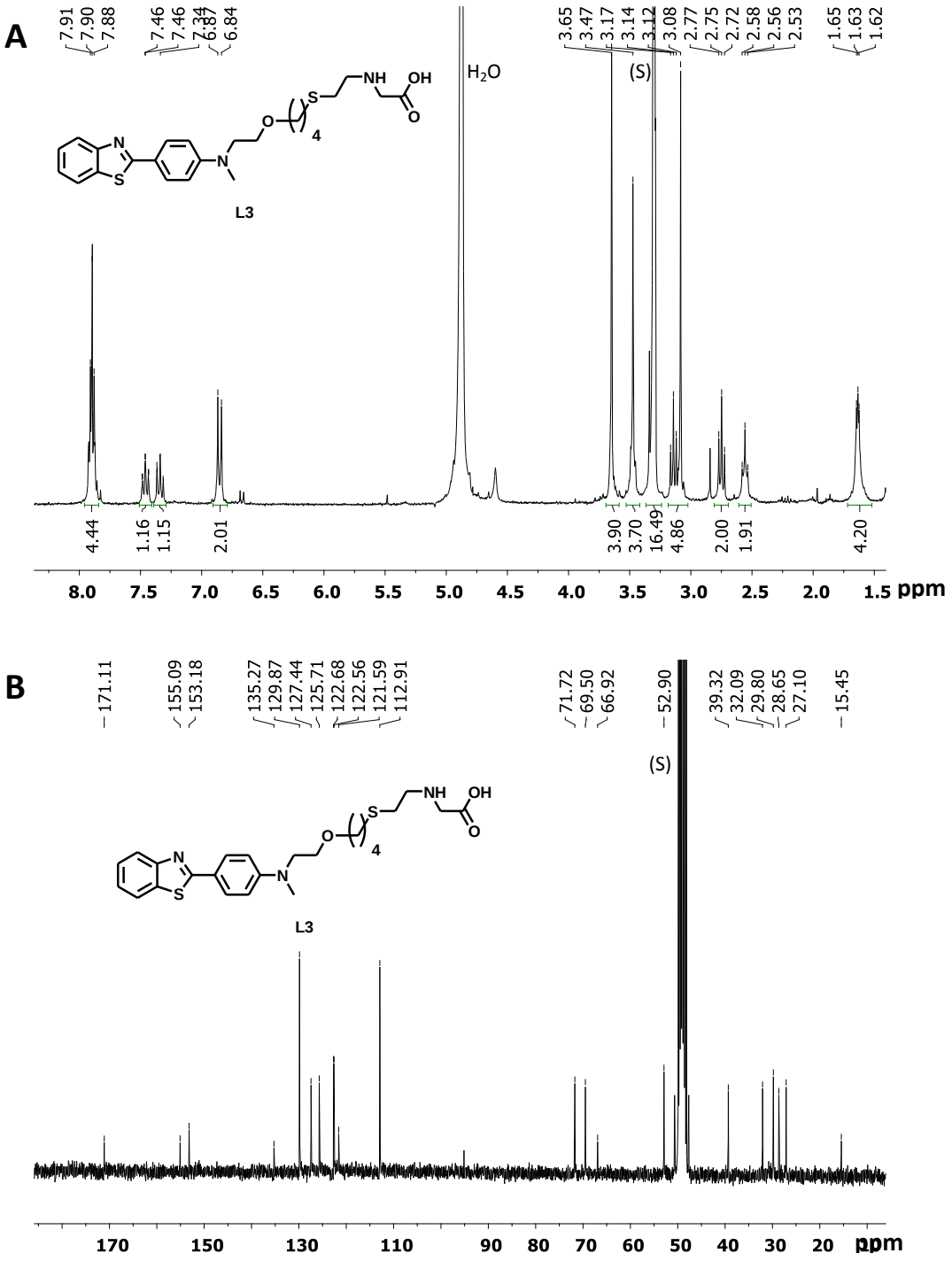

Figure S17. (**A**) ^{1}H and (**B**) ^{13}C spectrum of [4-(benzo[*d*]thiazol–2-yl)phenyl]–5–oxa–10–thia-2,13–diazapentadecan–15-oic acid **(L3)** in CD_3OD (S). Peak from residual water is also assigned.

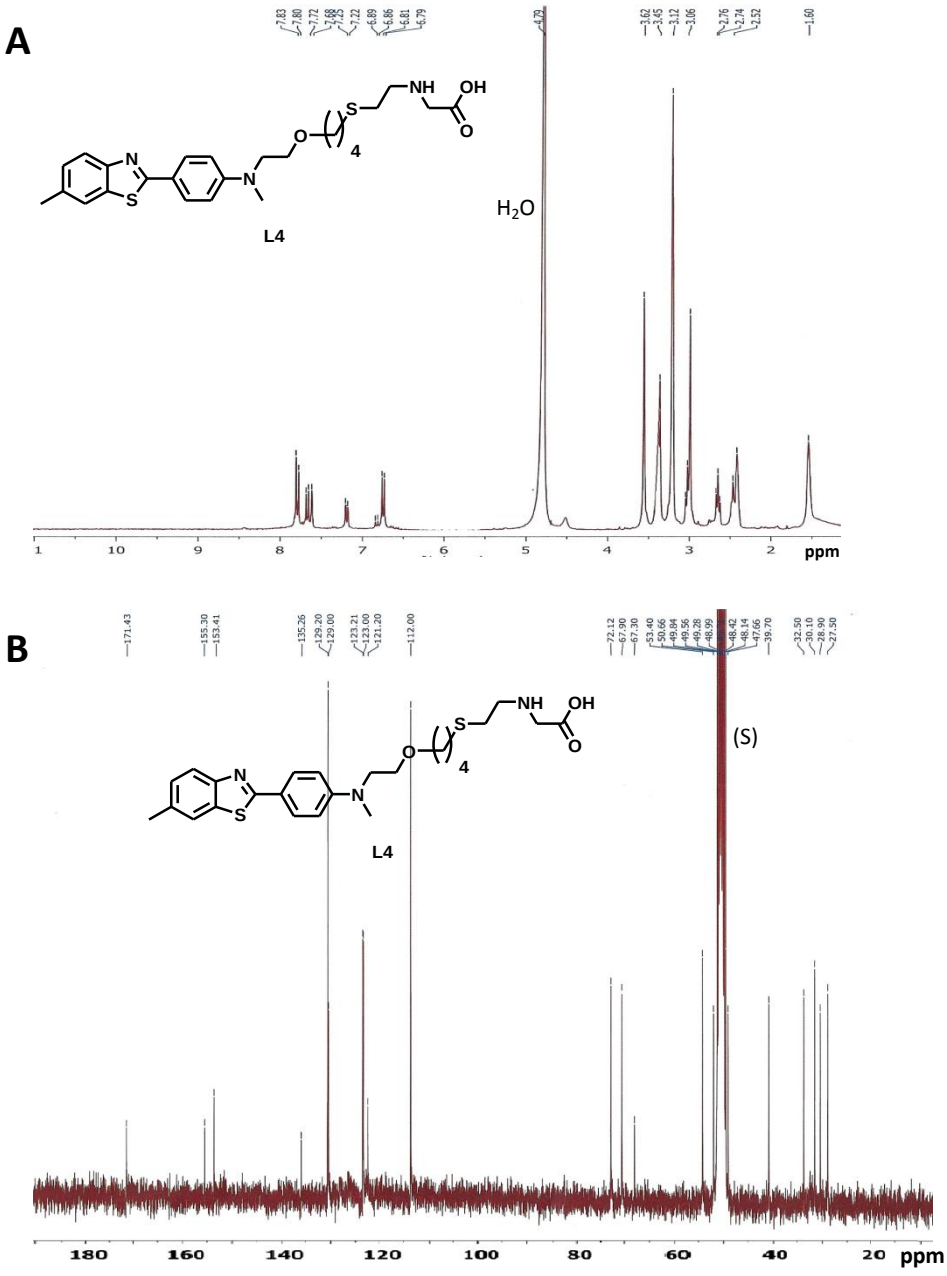

Figure S18. (**A**) ^{1}H and (**B**) ^{13}C spectrum of 2-[4`-((6``–methyl)benzo[*d*]thiazol–2-yl)phenyl]–5–oxa–10-thia-2,13–diazapentadecan-15-oic acid **(L4)** in CD_3OD (S). Peak from residual water is also assigned.

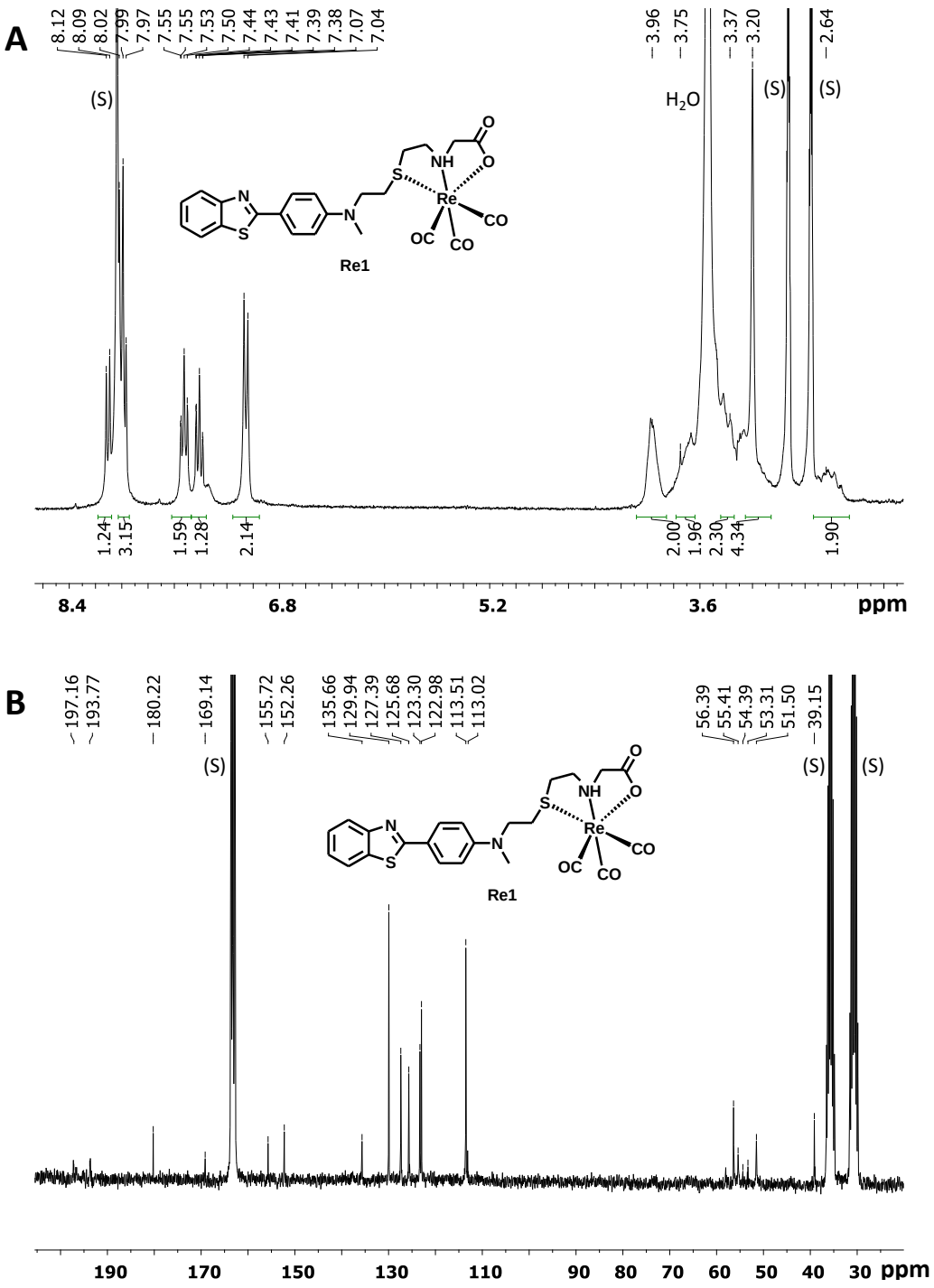

Figure S19. (**A**) ^{1}H and (**B**) ^{13}C spectrum of **Re1** in DMF-d_7 (S) and 20 ºC.

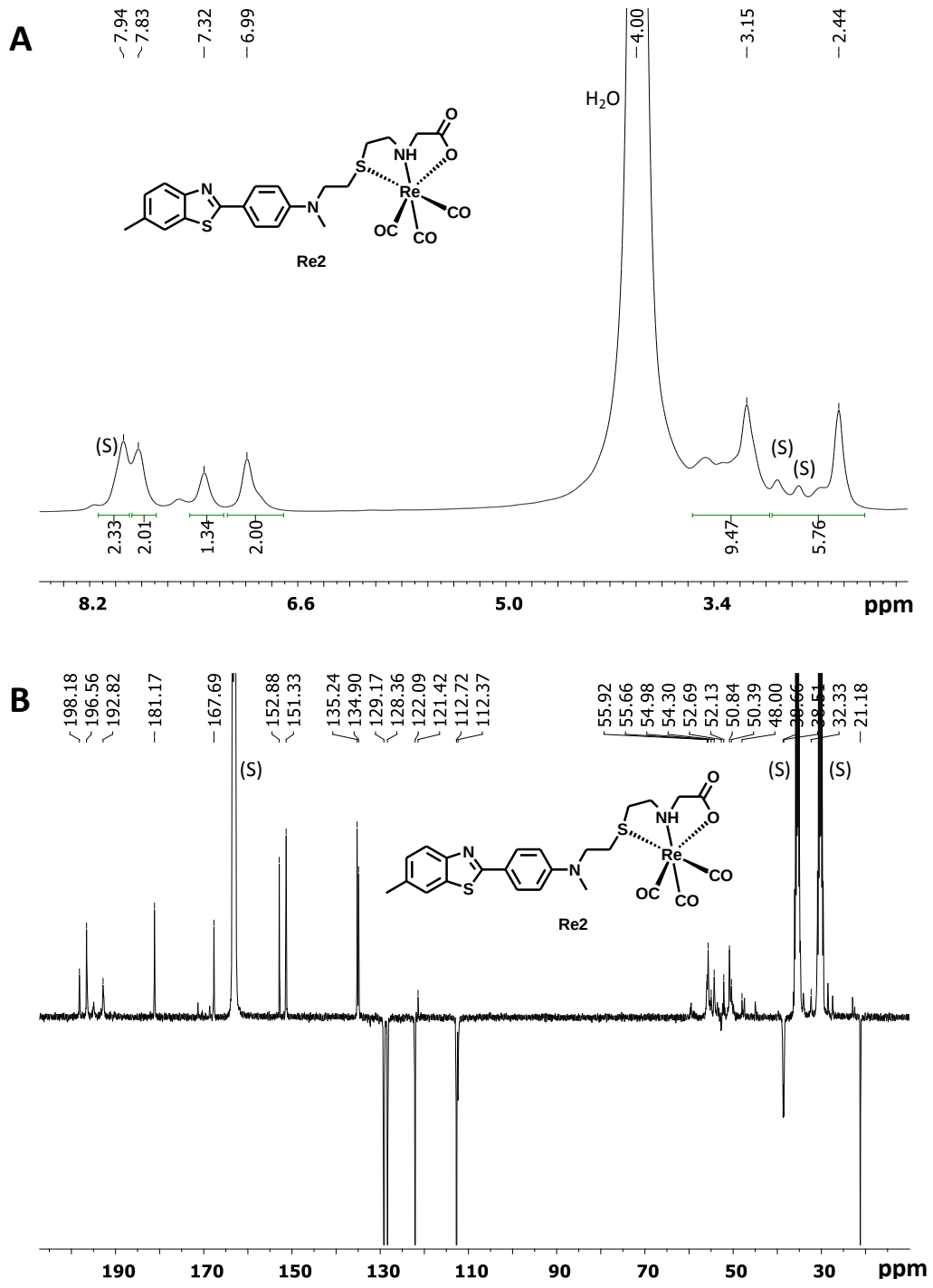

Figure S20. (**A**) ^{1}H and (**B**) DEPT spectrum of **Re2** in DMF-d_7 (S) and 20 ºC. Peak from residual water is also assigned.

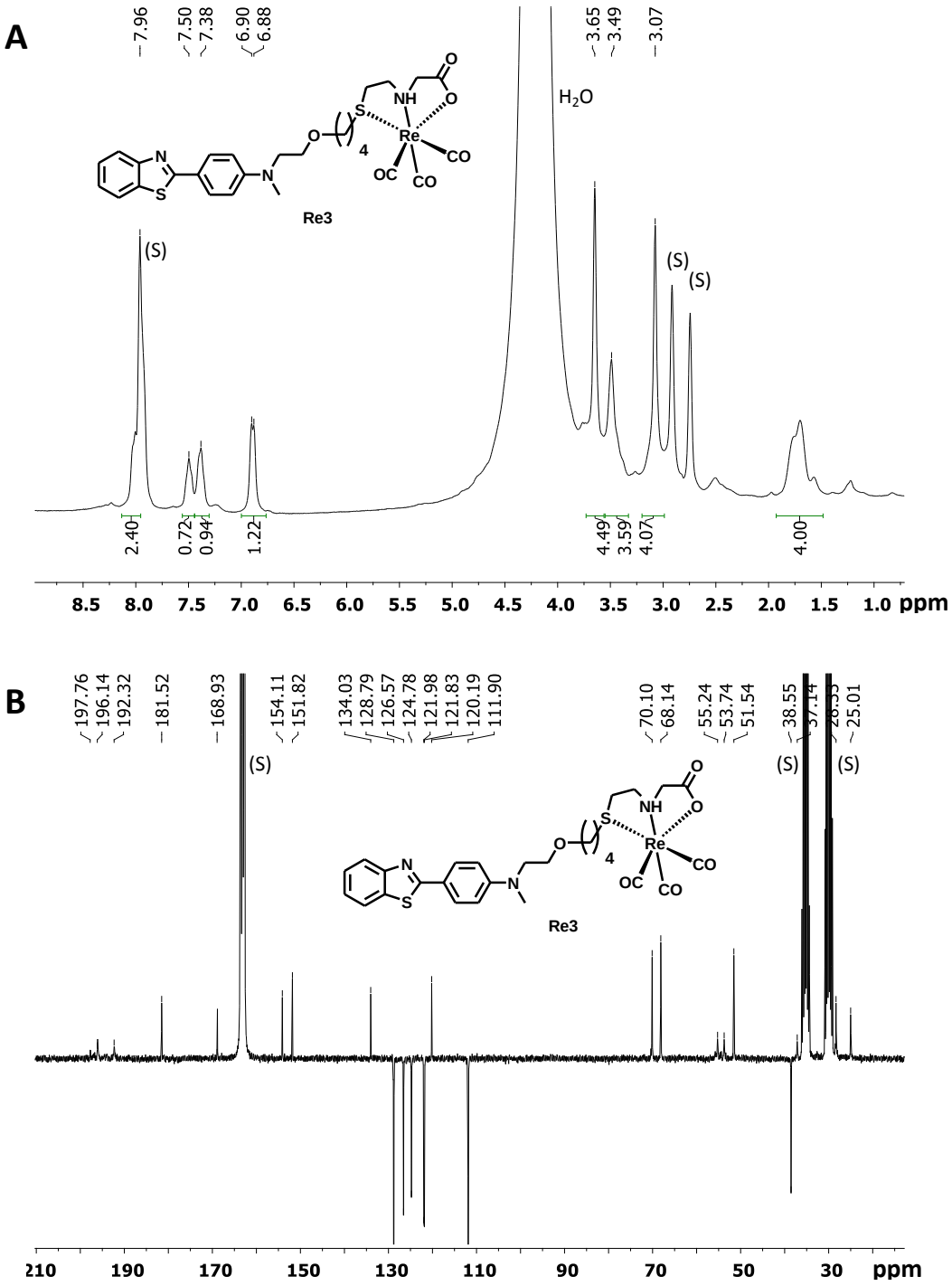

Figure S21. (**A**) ^{1}H and (**B**) DEPT spectrum of **Re3** in DMF-*d*7 (S) and 20 ºC. Peak from residual water is also assigned.

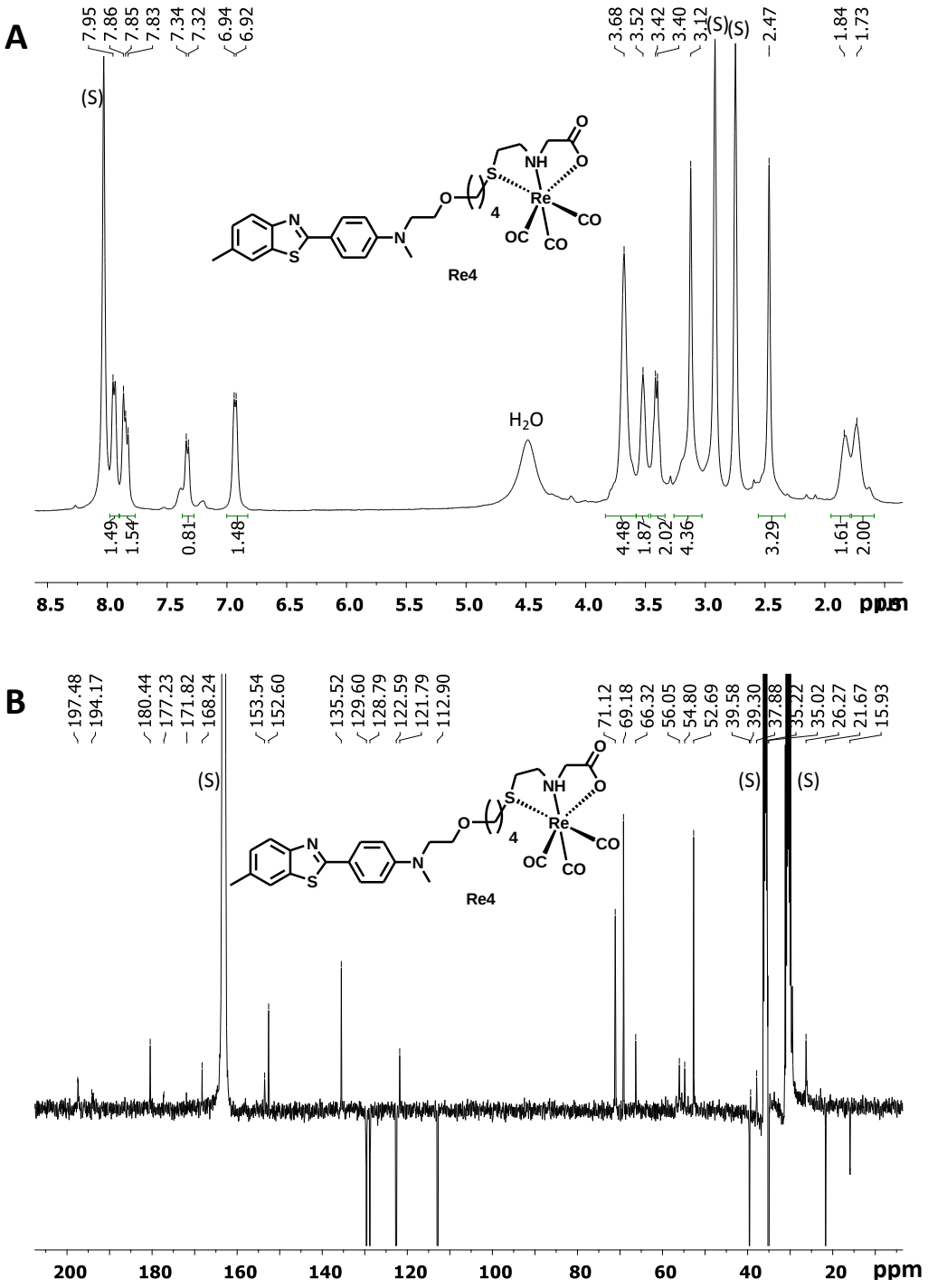

Figure S22. (**A**) ^{1}H and (**B**) DEPT spectrum of **Re4** in DMF-d_7 (S) and 20 ºC. Peak from residual water is also assigned.