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Supporting Information

Synthesis of sp²-iminosugar selenoglycolipids as multitarget drug candidates with antiproliferative, leishmanicidal and anti-inflammatory properties

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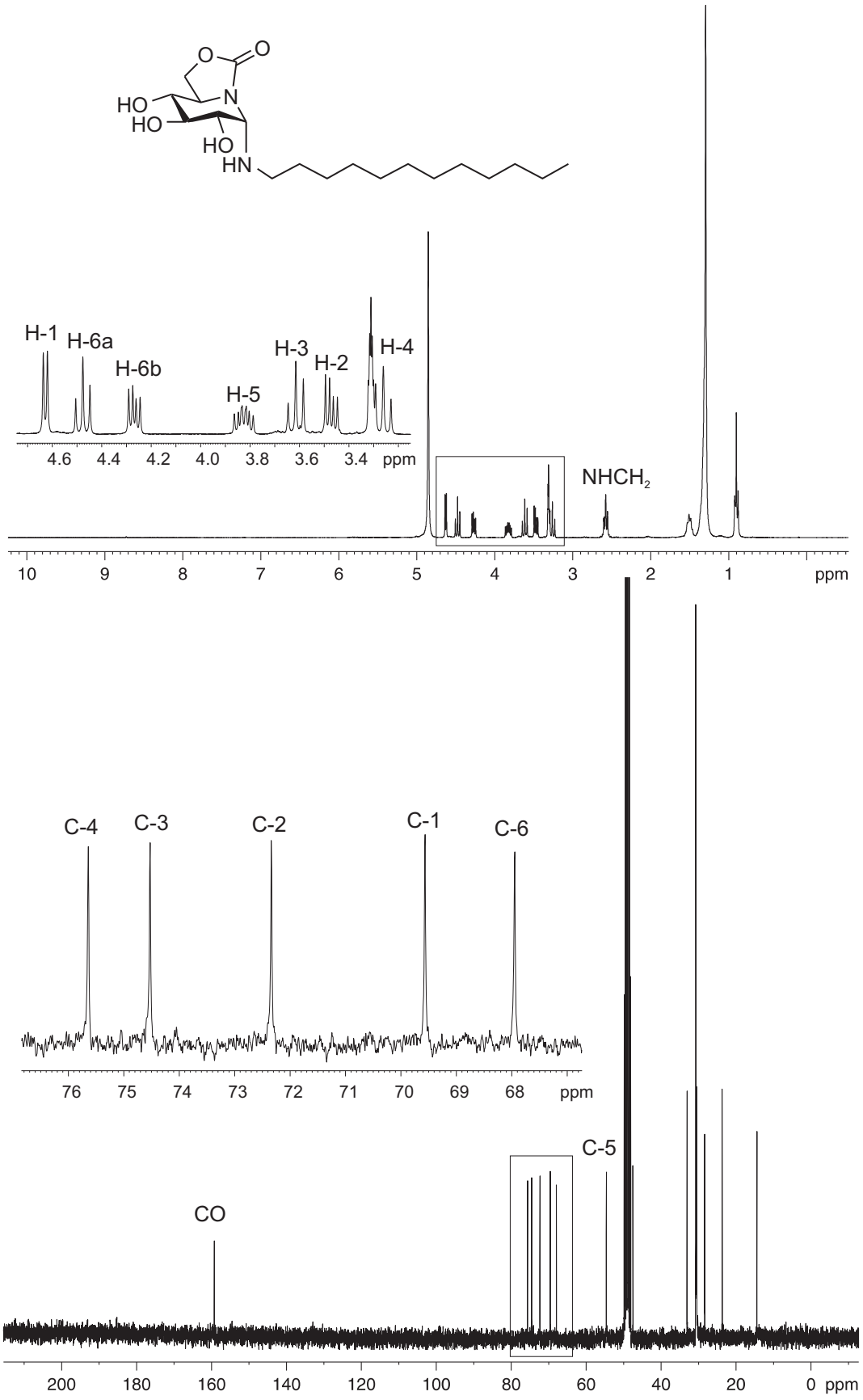

Figure S1. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, CD_3OD) of **12**.

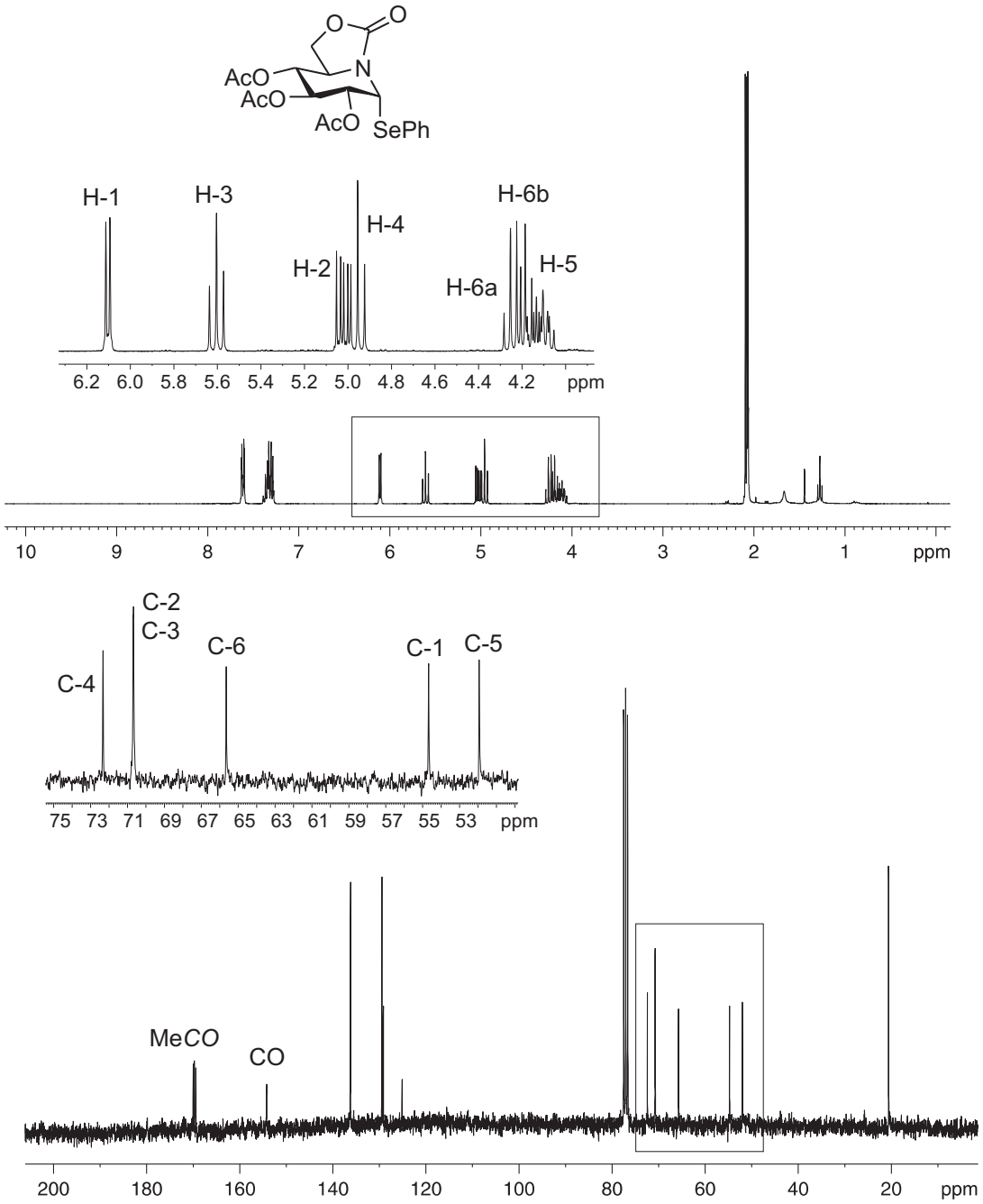

Figure S2. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, $CDCl_3$) of **17**.

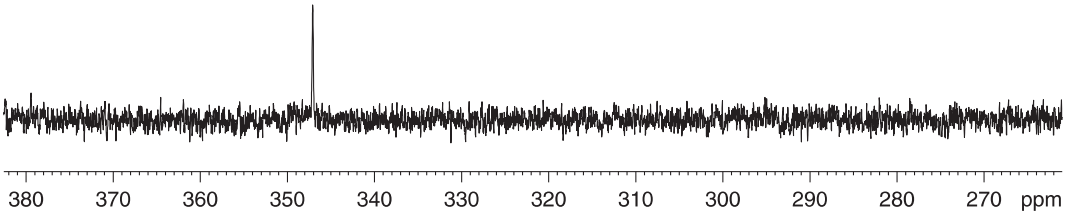

Figure S3. ^{77}Se NMR spectrum (95.4 MHz, $CDCl_3$) of **17**.

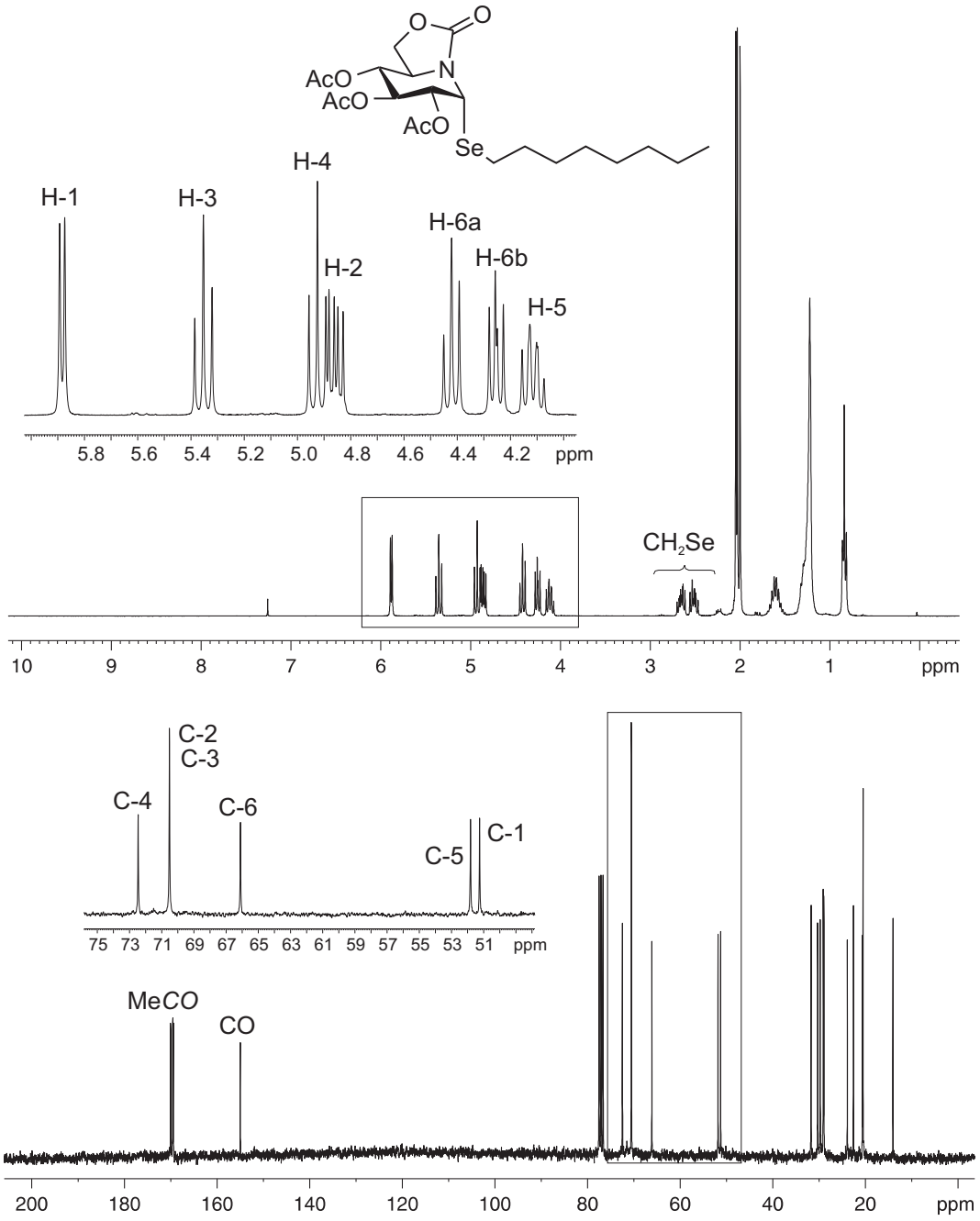

Figure S4. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, $CDCl_3$) of **18**.

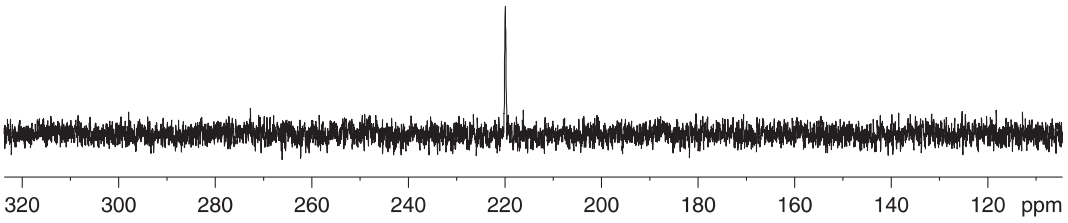

Figure S5. ^{77}Se NMR spectrum (95.4 MHz, $CDCl_3$) of **18**.

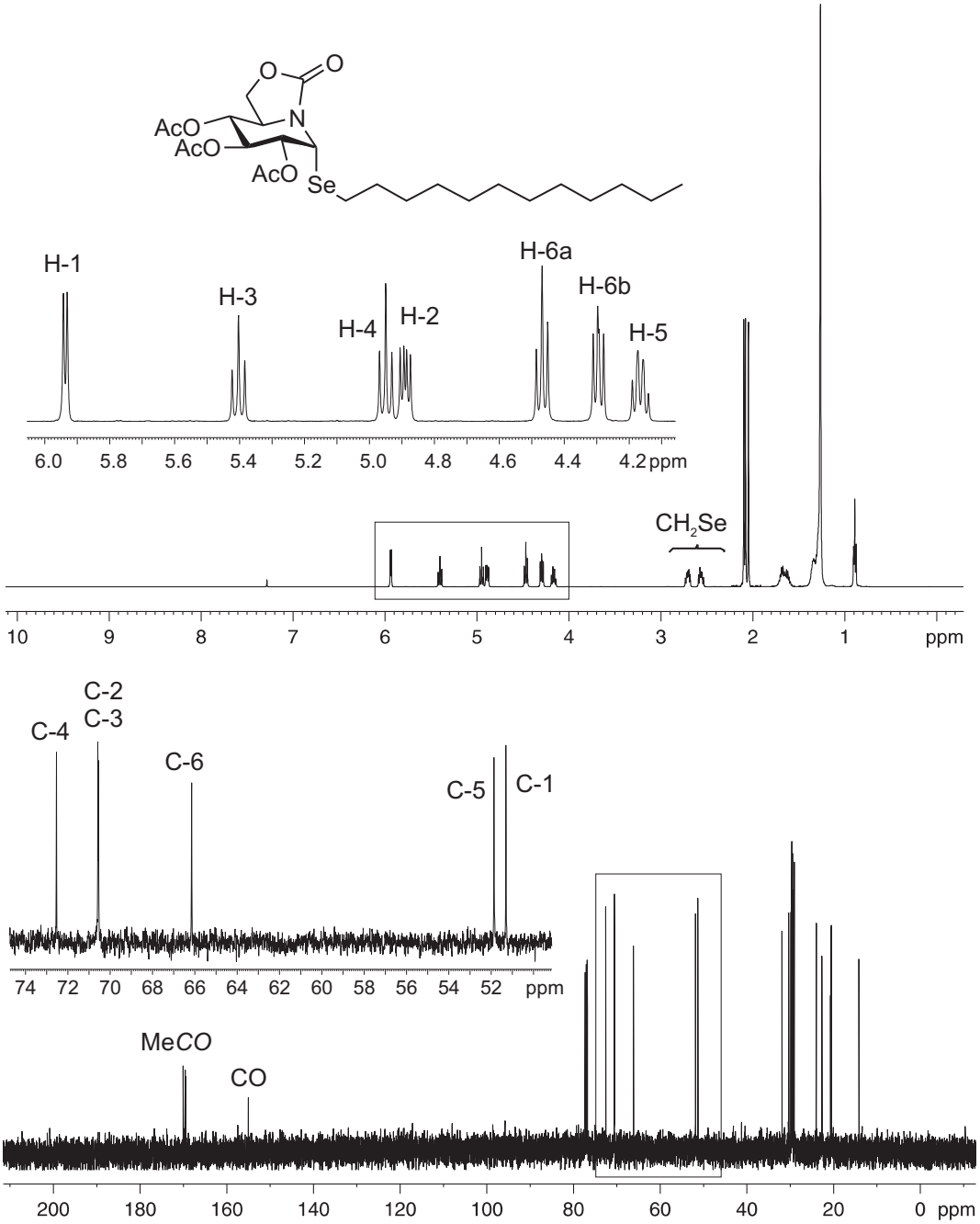

Figure S6. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, $CDCl_3$) of **19**.

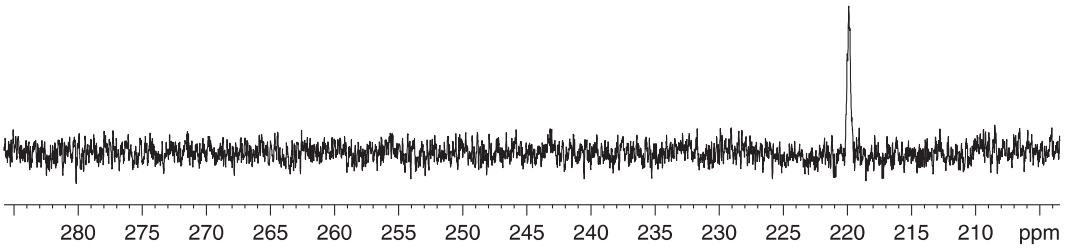

Figure S7. ^{77}Se NMR spectrum (95.4 MHz, $CDCl_3$) of **19**.

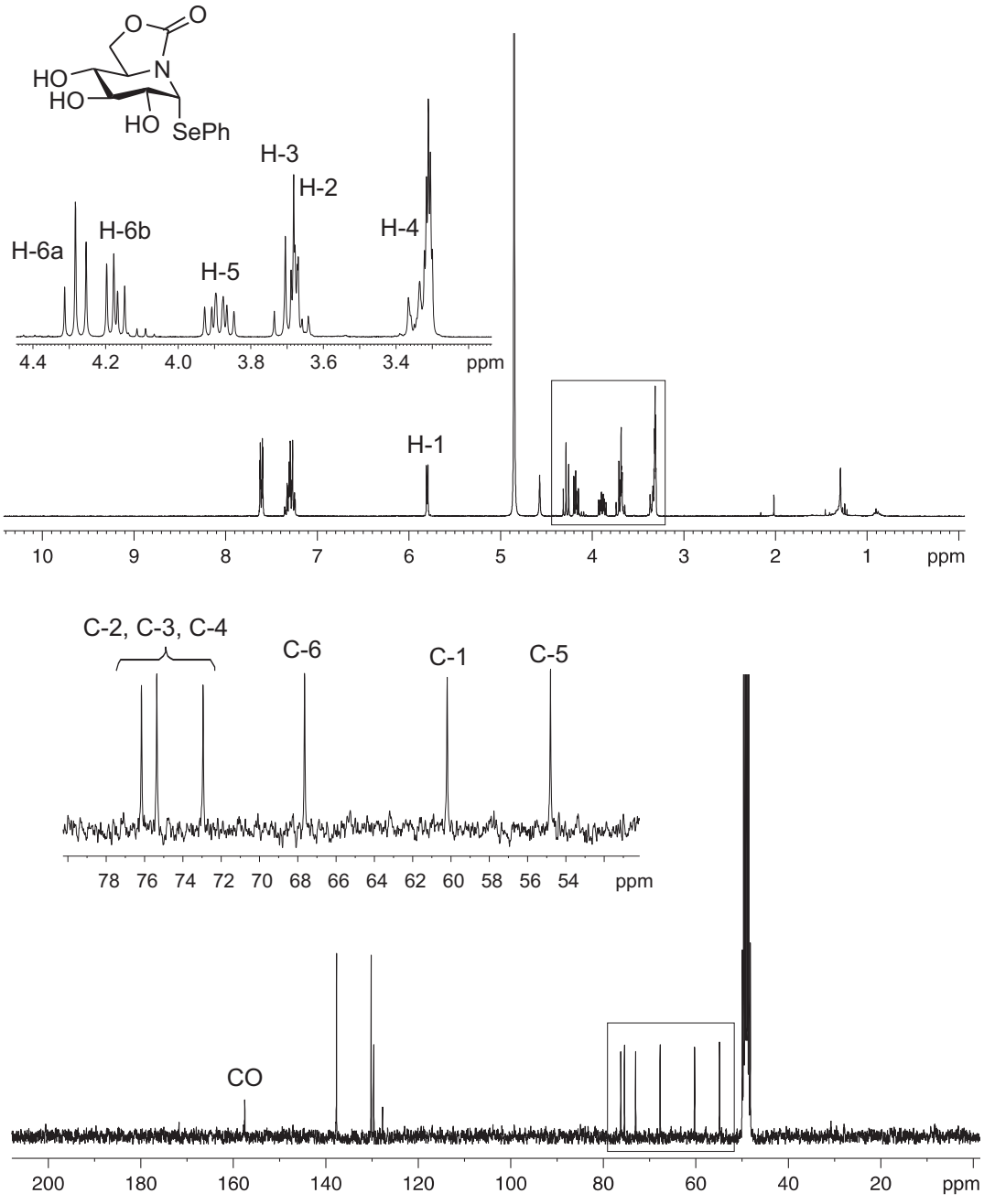

Figure S8. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, CD_3OD) of **8**.

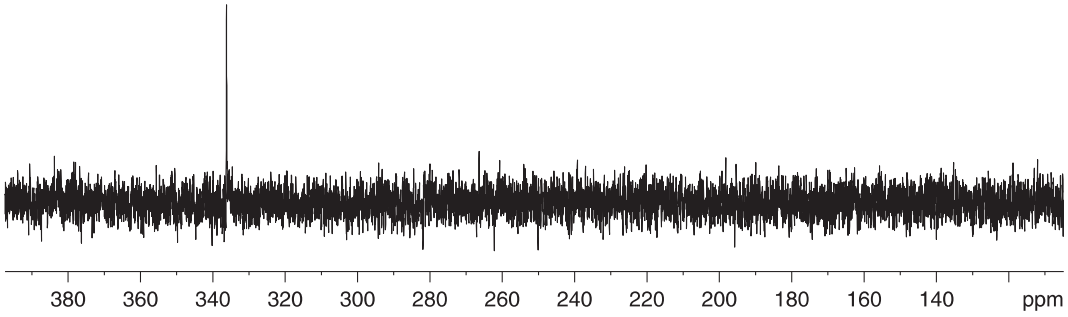

Figure S9. ^{77}Se NMR spectrum (95.4 MHz, CD_3OD) of **8**.

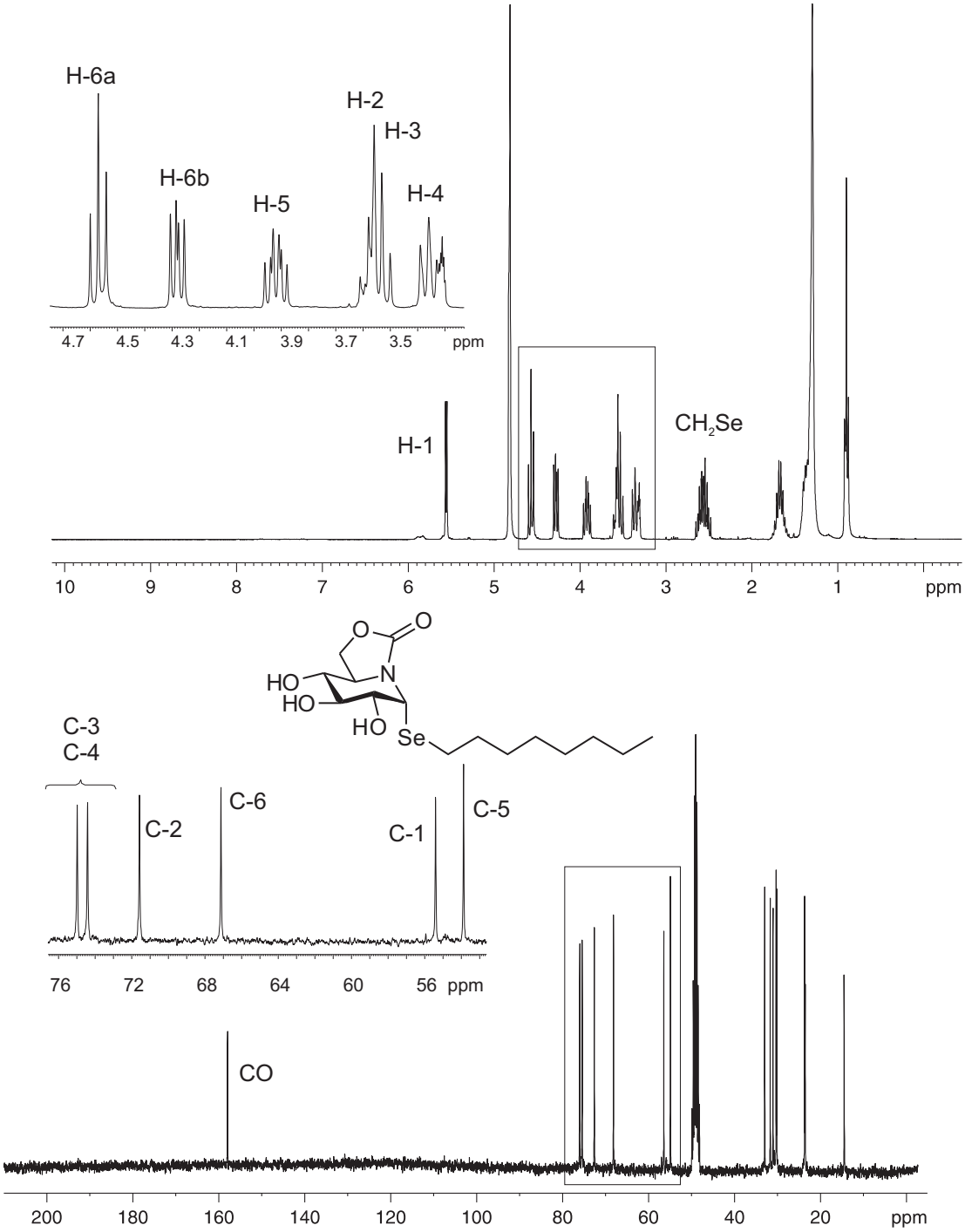

Figure S10. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, CD_3OD) of **9**.

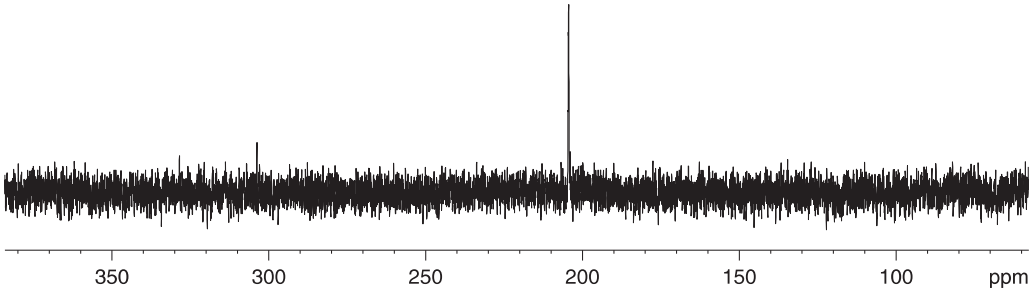

Figure S11. ^{77}Se NMR spectrum (95.4 MHz, CD_3OD) of **9**.

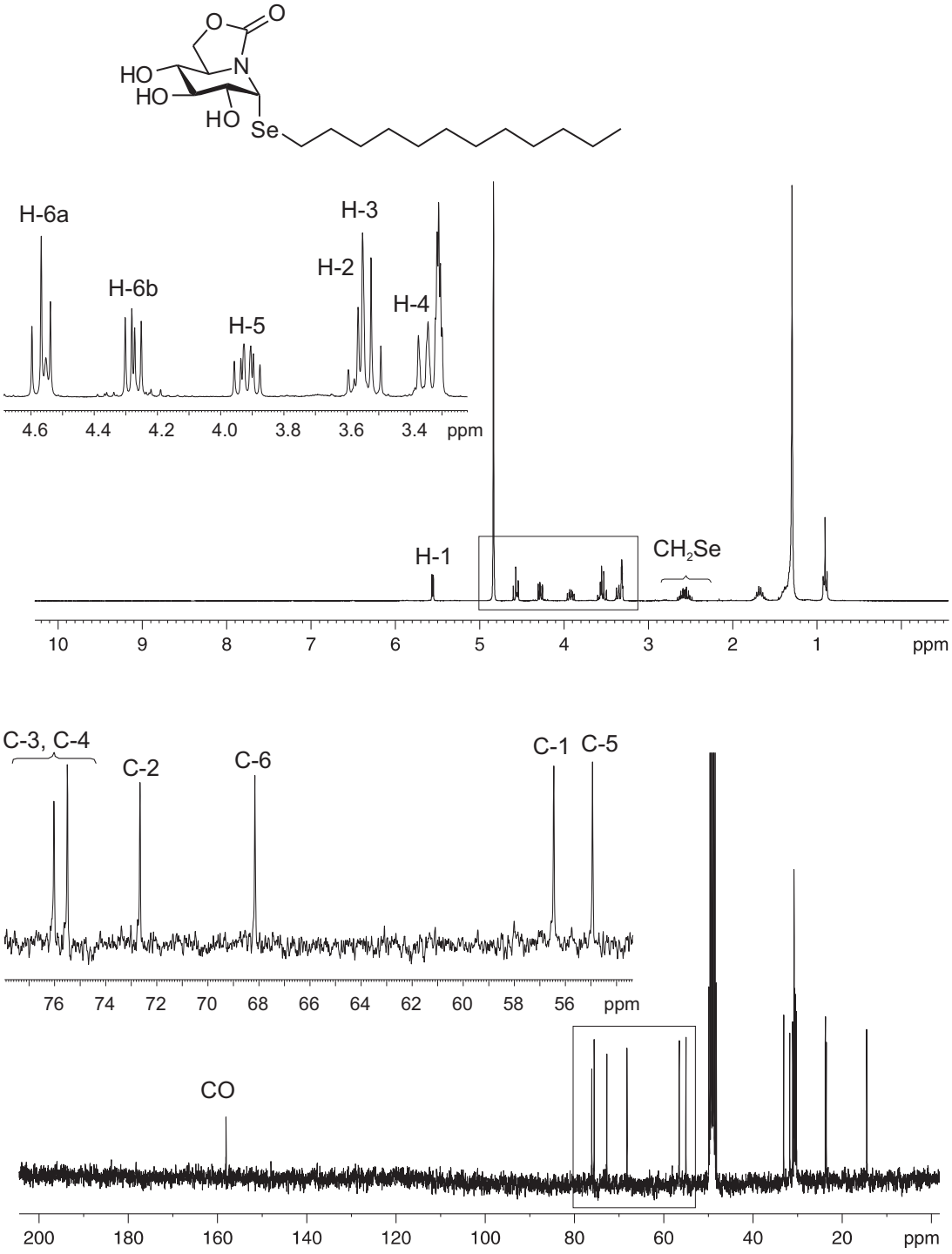

Figure S12. ^{1}H and ^{13}C NMR spectra (300 MHz and 75.5 MHz, CD_3OD) of **10**.

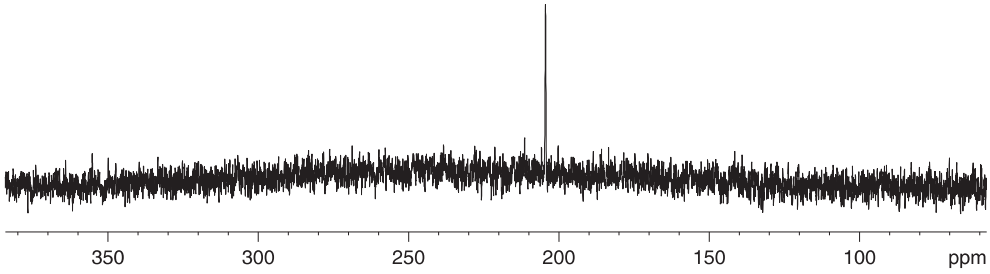

Figure S13. ^{77}Se NMR spectrum (95.4 MHz, CD_3OD) of **10**.

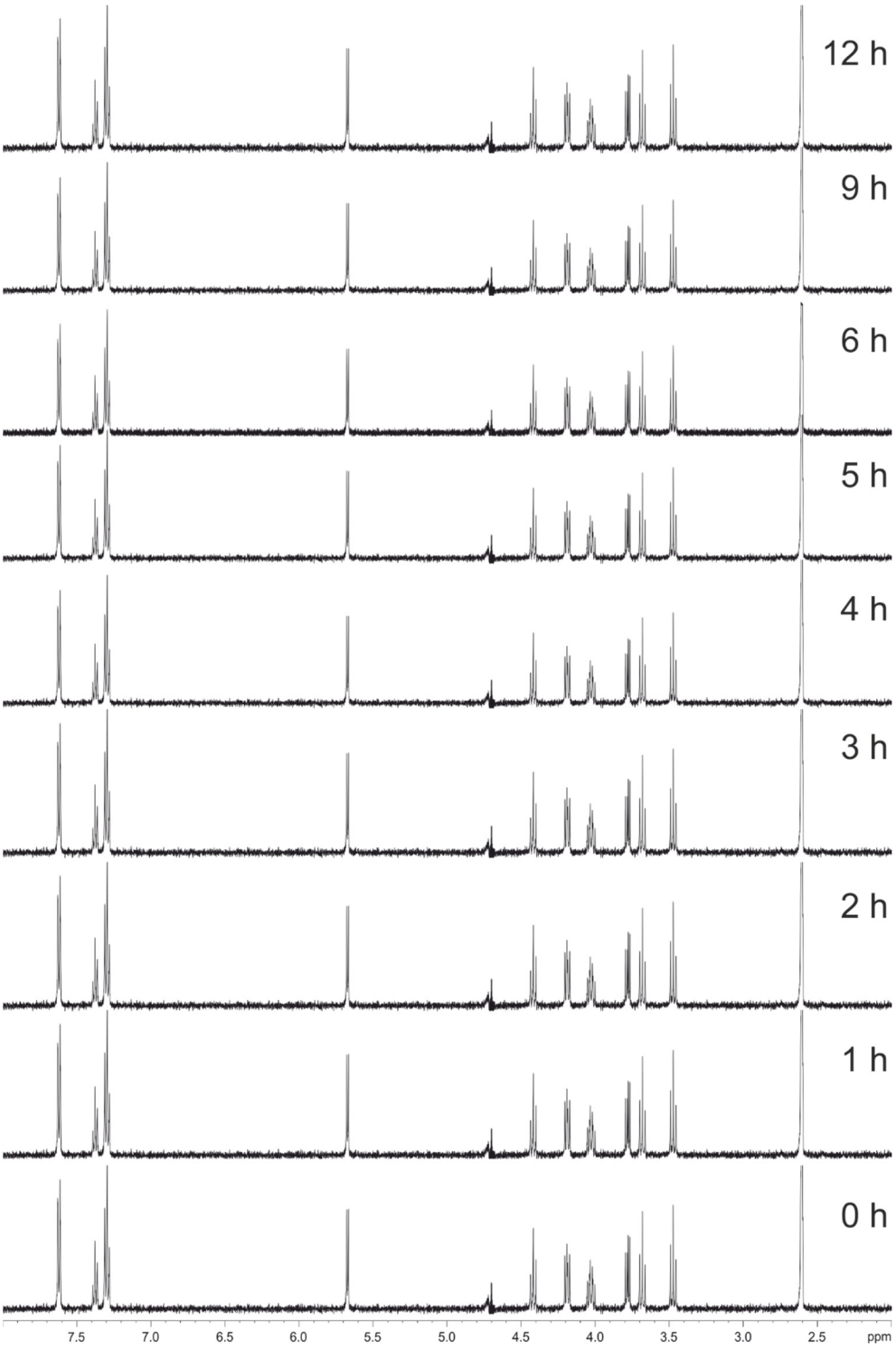

Figure S14. ^{1}H-NMR-monitored kinetic evaluation of the stability of **8** (1 mM) in 9:1 D_2O-DMSO-d_6 at pH 4.4 (10 mM formate buffer).

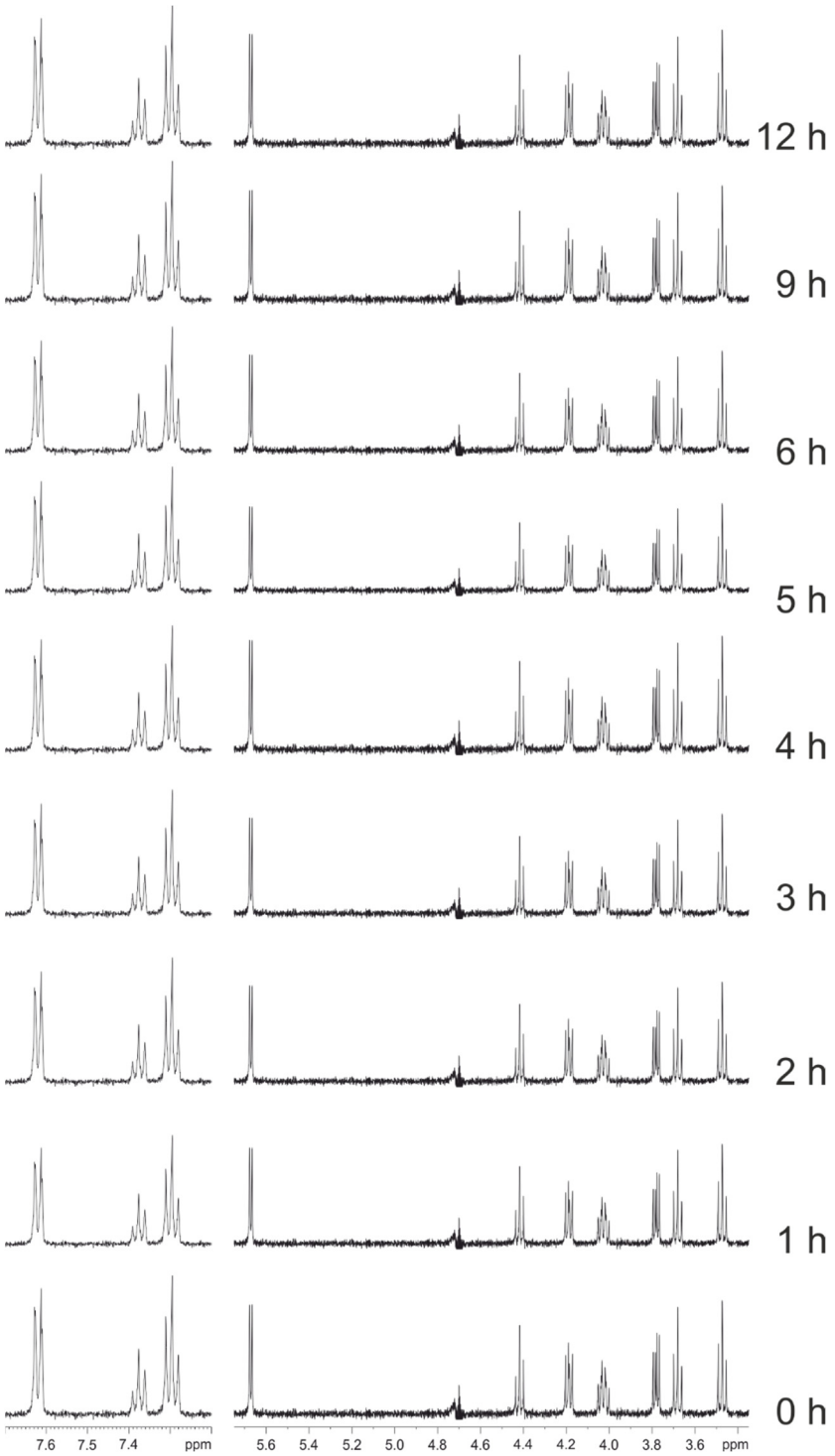

Figure S15. ^{1}H-NMR-monitored (selected regions) kinetic evaluation of the stability of **8** (1 mM) in 9:1 D_2O-DMSO-d_6 at pH 4.4 (10 mM formate buffer).

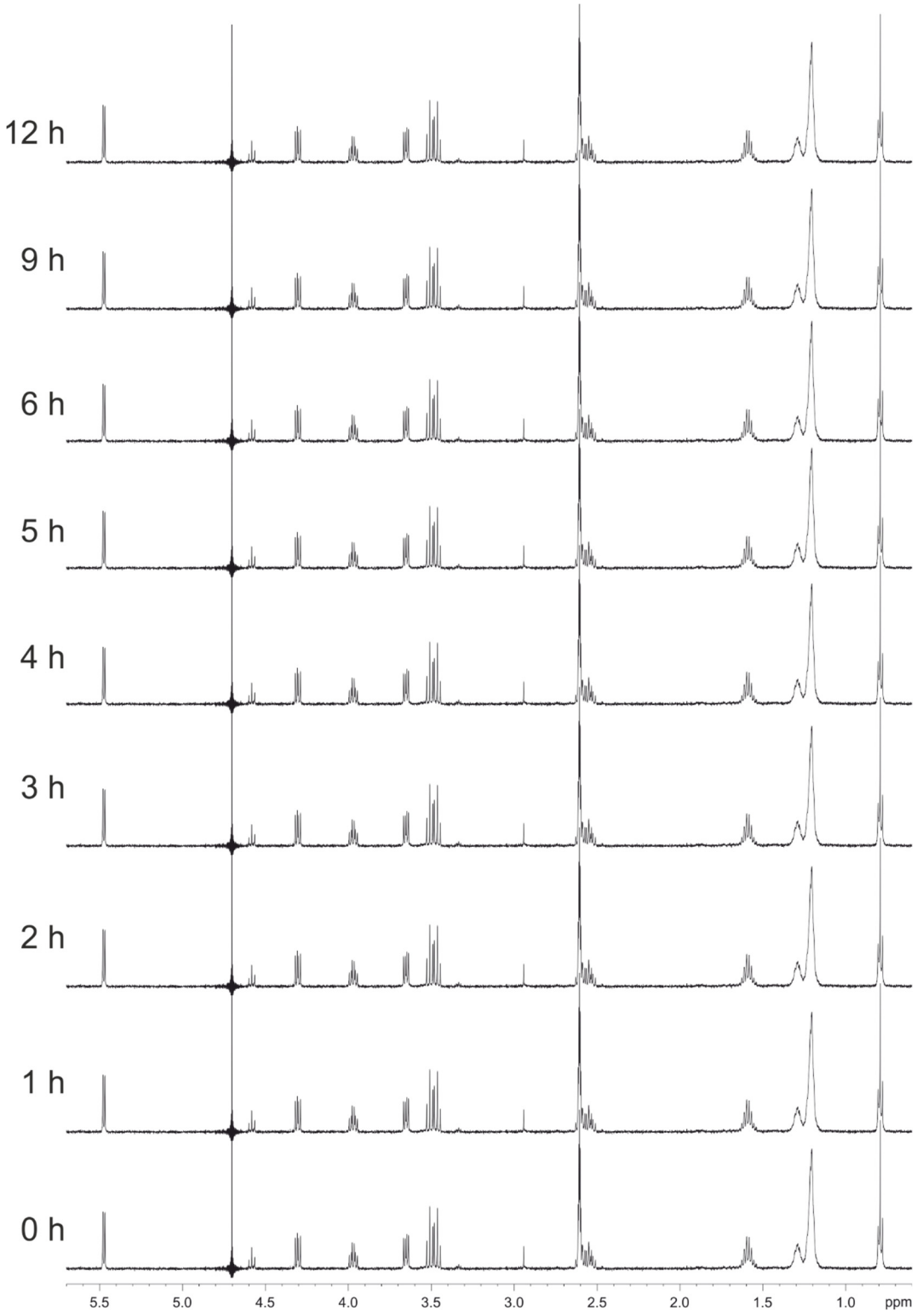

Figure S16. ^{1}H-NMR-monitored kinetic evaluation of the stability of **9** (1 mM) in 9:1 D_2O-DMSO-d_6 at pH 4.6 (10 mM formate buffer).

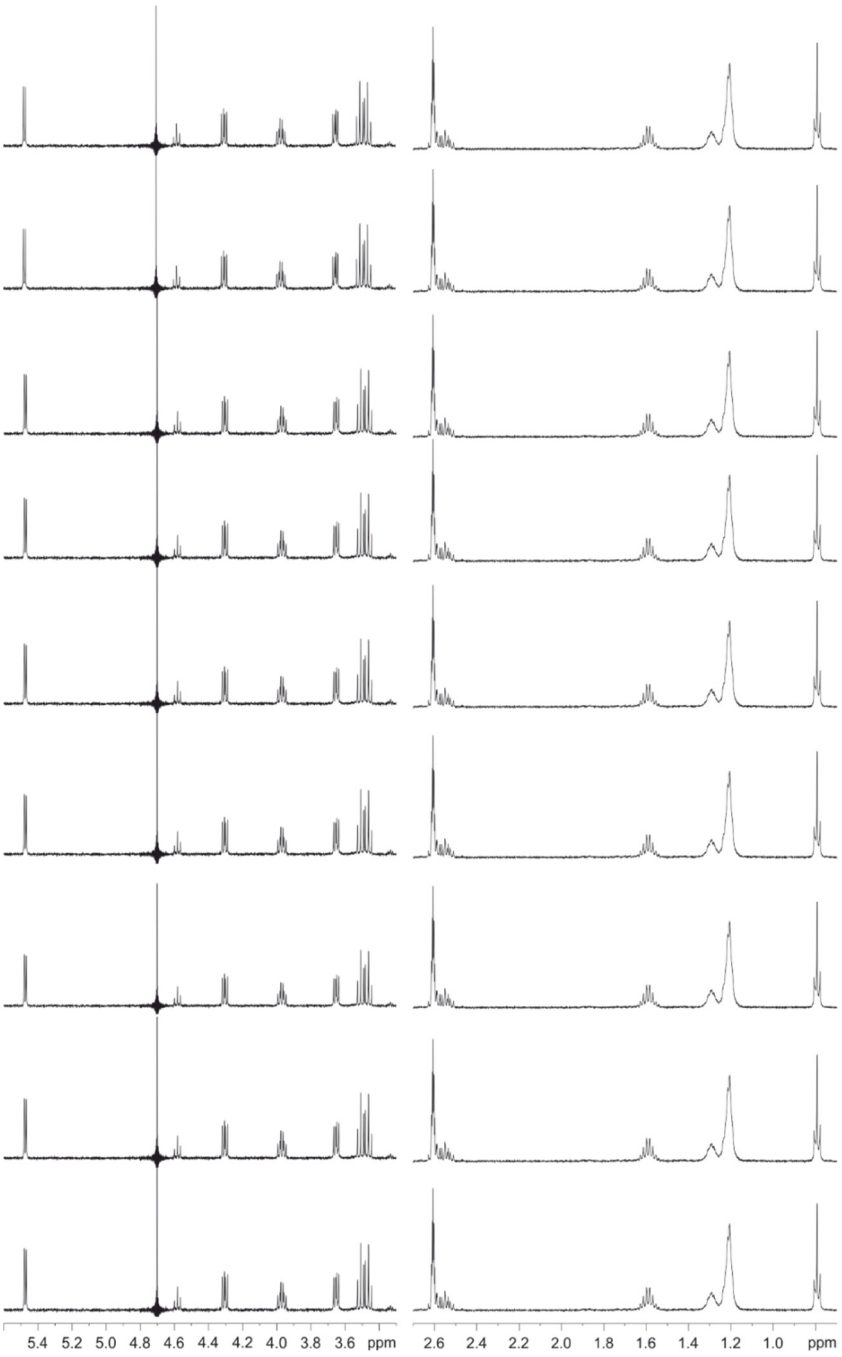

Figure S17. ^{1}H-NMR-monitored (selected regions) kinetic evaluation of the stability of **9** (1 mM) in 9:1 D_2O-DMSO-d_6 at pH 4.6 (10 mM formate buffer).

Table S1. GI_{50} values (μM) of the sp^2-IGLs (**8**-**14**) tested as antiproliferative agents by HTS.

	A549	**SW1573**	**HBL-100**	**T-47D**	**HeLa**	**WiDr**
Compound	*Lung*		*Breast*		*Cervix*	*Colon*
8 (Se–Ph)	>100	>100	>100	>100	>100	>100
9 (Se–C_8)	36(± 9.5)	>100	>100	71(± 16)	49(± 14)	64(± 11)
10 (Se–C_{12})	18(± 4.3)	28(± 3.7)	24(± 8.1)	21(± 5.3)	22(± 5.5)	22(± 8.8)
11 (NH–C_8)	>100	>100	>100	>100	>100	>100
12 (NH–C_{12})	18(± 4.4)	30(± 0.4)	23(± 7.0)	23(± 5.5)	23(± 7.7)	22(± 7.6)
13 (S–C_8)	58(± 7.1)	>100	73(± 38)	95(± 7.2)	92(± 12)	89(± 15)
14 (S–C_{12})	16(± 2.0)	18(± 1.2)	17(± 3.7)	18(± 1.9)	17(± 2.2)	18(± 0.2)