Supporting Information:

Molecular Structures and Intermolecular Hydrogen Bonding of Silylated 2-Aminopyrimidines

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Table S1: Details of chemicals used and purification methods applied

substance	*Source*	*purification*
Anisole	VWR (AnalaR Normapuran)	Distillation from Na/benzophenone
Diethyl ether	VWR (AnalaR Normapuran)	MBRAUN MB-SPS-800
Tetrahydrofuran	VWR (AnalaR Normapuran)	MBRAUN MB-SPS-800
Tetrahydrofuran-d8	Deutero, 99.5 %	none
n-Pentane	VWR TECHNICAL	standing several days over activated molecular sieve (type 3 Å, purchased from Sigma-Aldrich)
Triethylamine	AppliChem (pure)	Distillation from Na/benzophenon
Deuterated Chloroform	Deutero	Distillation from CaH_2
Chloroform (stabilized with amylenes)	Fisher Scientific	standing serveral days over activated molecular sieve (type 3 Å, purchased from Sigma-Aldrich) and activated alumina (purchased from Supelco)
Chlorotrimethylsilane	Sigma-Aldrich	Distillation over 20 cm filled column
Dichlorodimethylsilane	Sigma-Aldrich	Distillation over 20 cm filled column
Trichloromethylsilane	Sigma-Aldrich	Distillation over 20 cm filled column
Tetrachlorsilane	Sigma-Aldrich	Distillation over 20 cm filled column
2-Aminopyrimidine	Sigma-Aldrich (97 %)	none
CO_2 (gaseous)	Linde, purity '5.3'	Passed through a column with molecular sieves 3 Å prior to use

2 NMR spectra

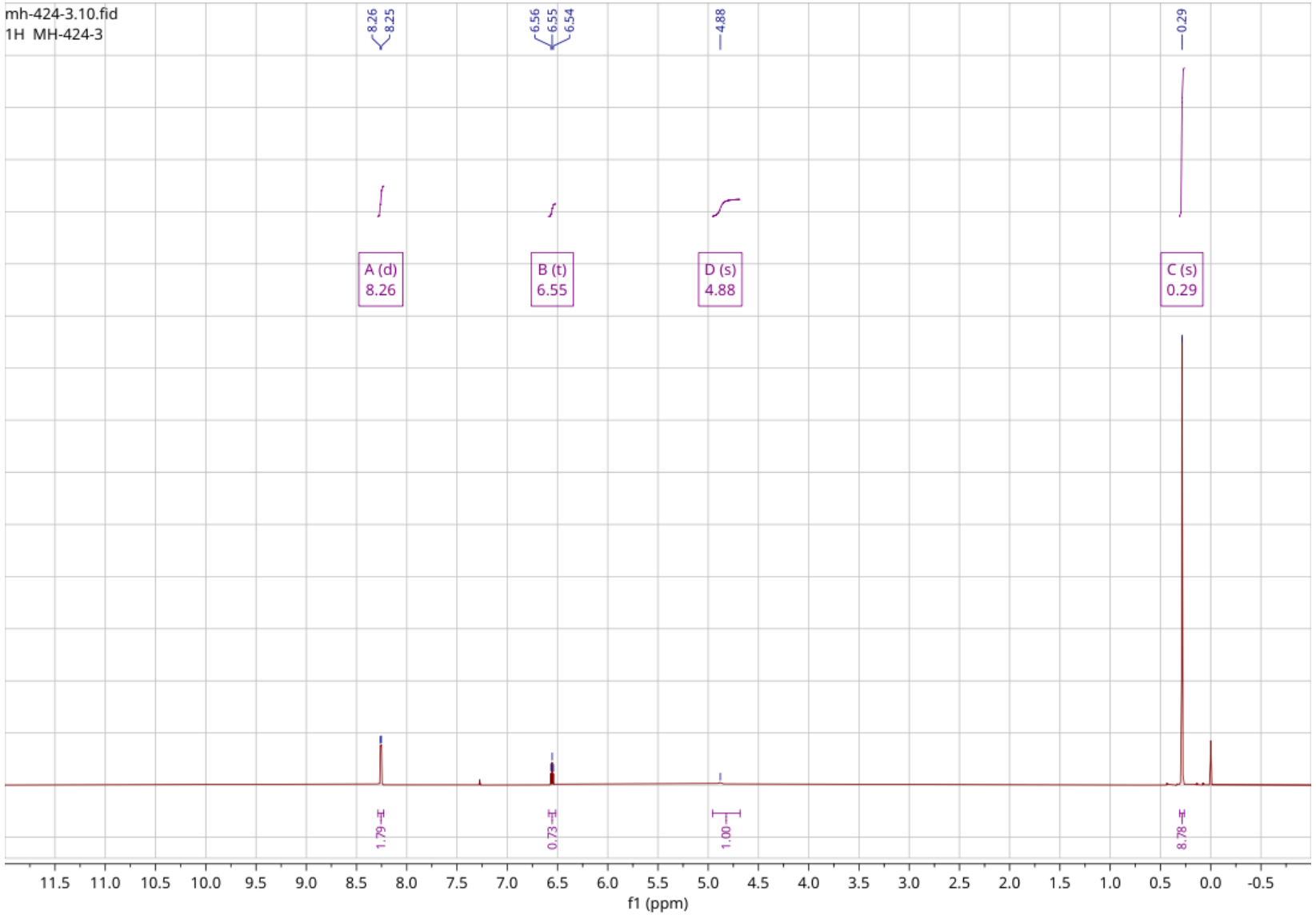

Figure S1: ^{1}H NMR spectrum of **1** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

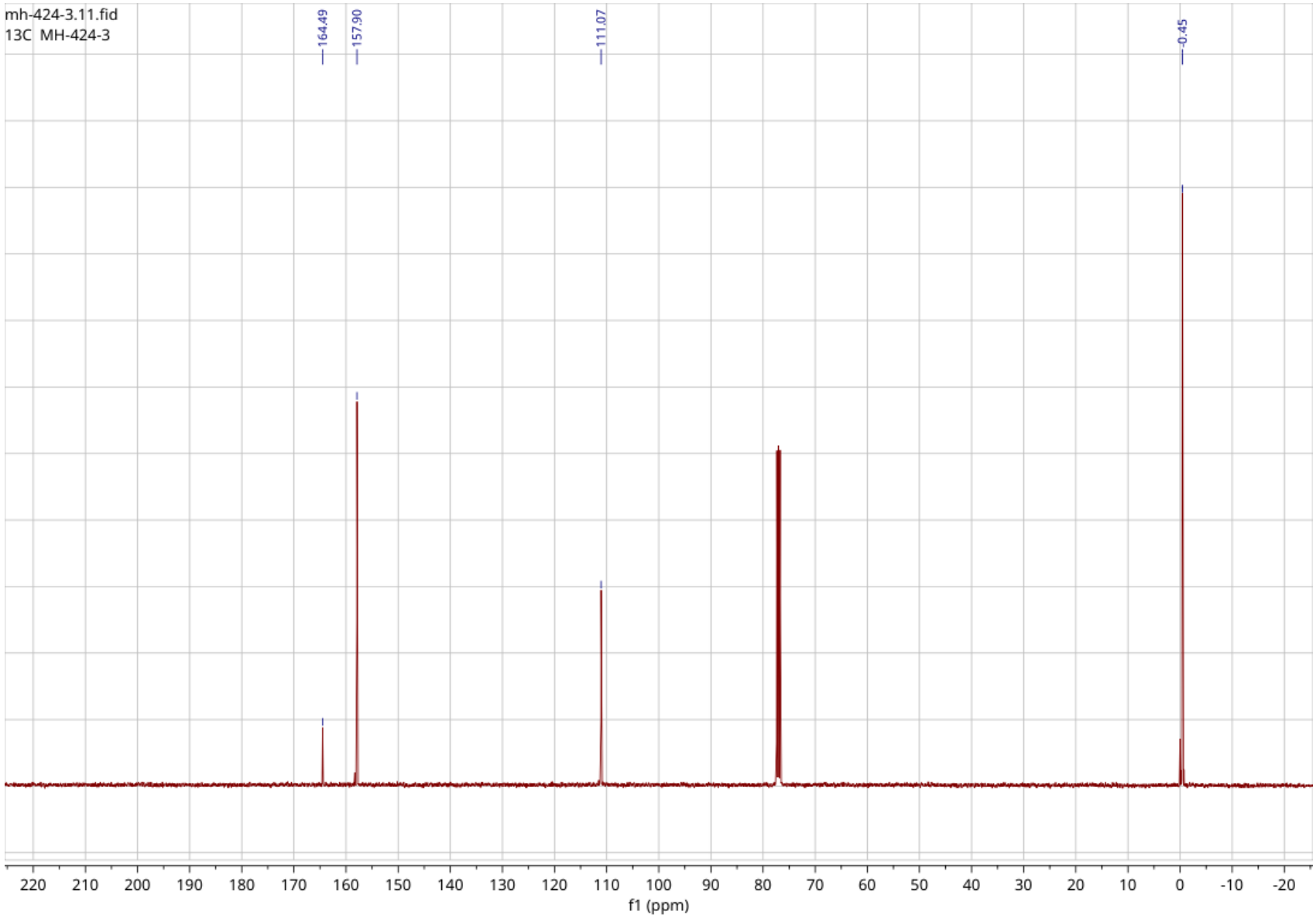

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

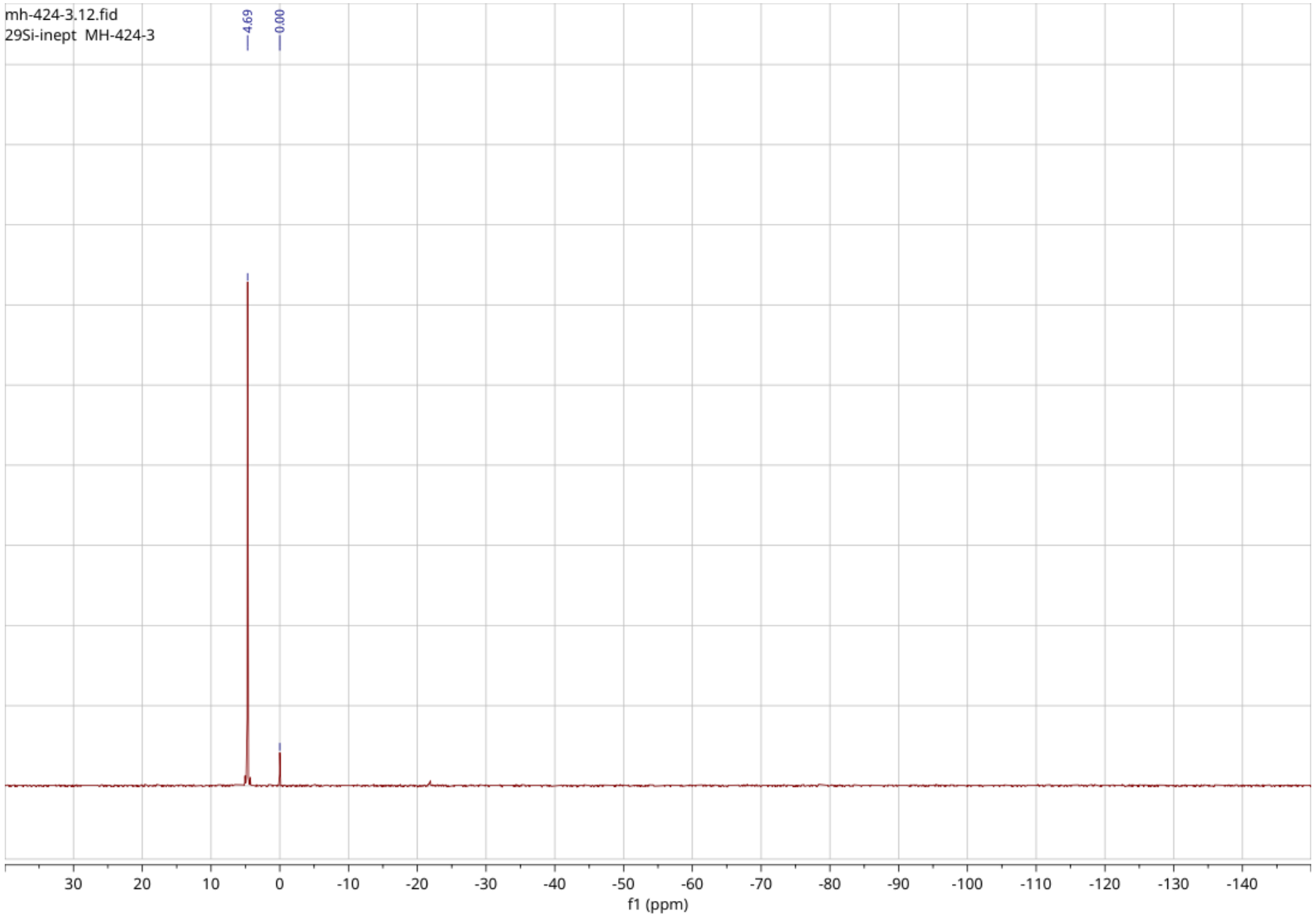

Figure S3: $^{29}Si\{^{1}H\}$ INEPT NMR spectrum of **1** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

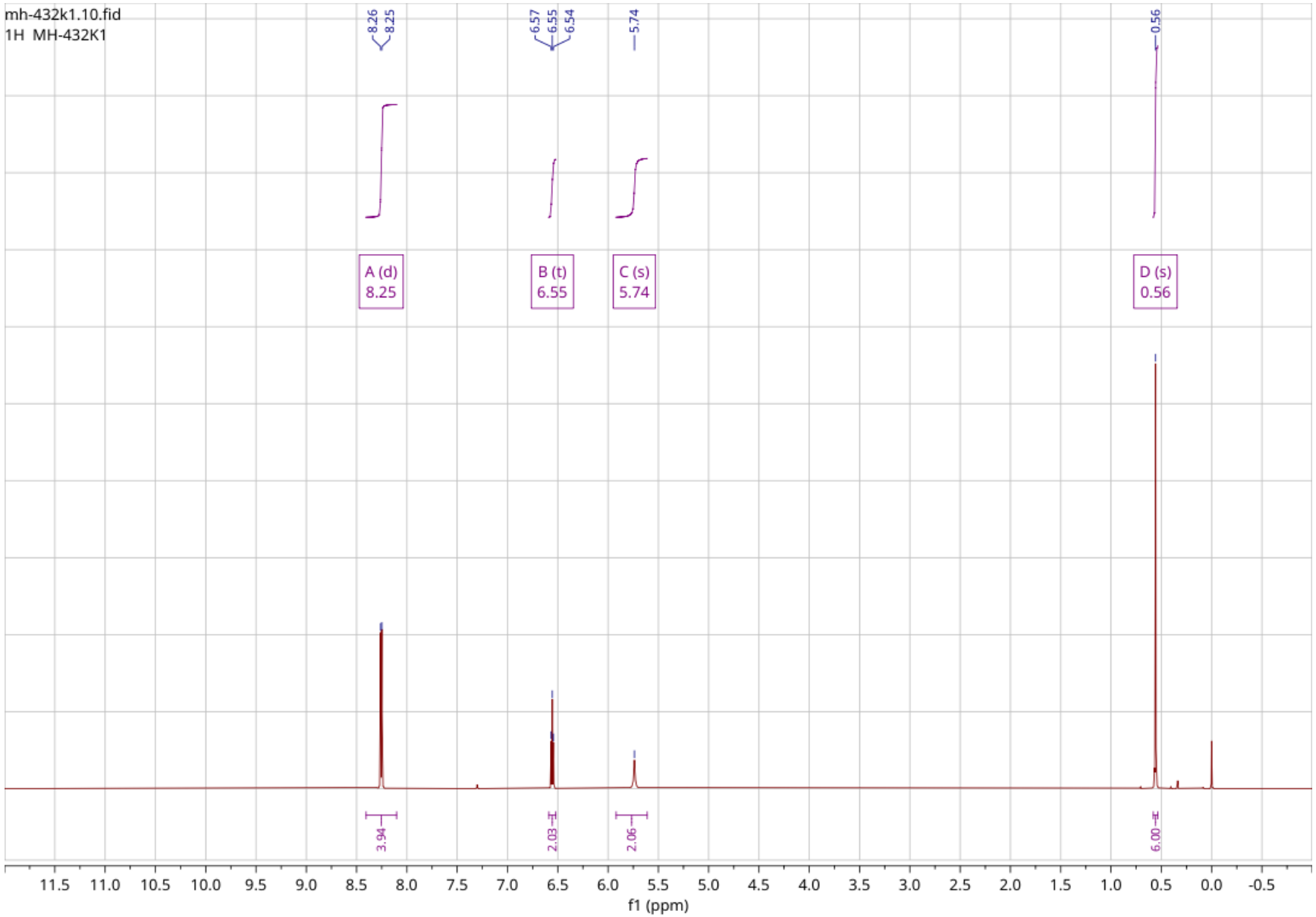

Figure S4: ^{1}H NMR spectrum of **2** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

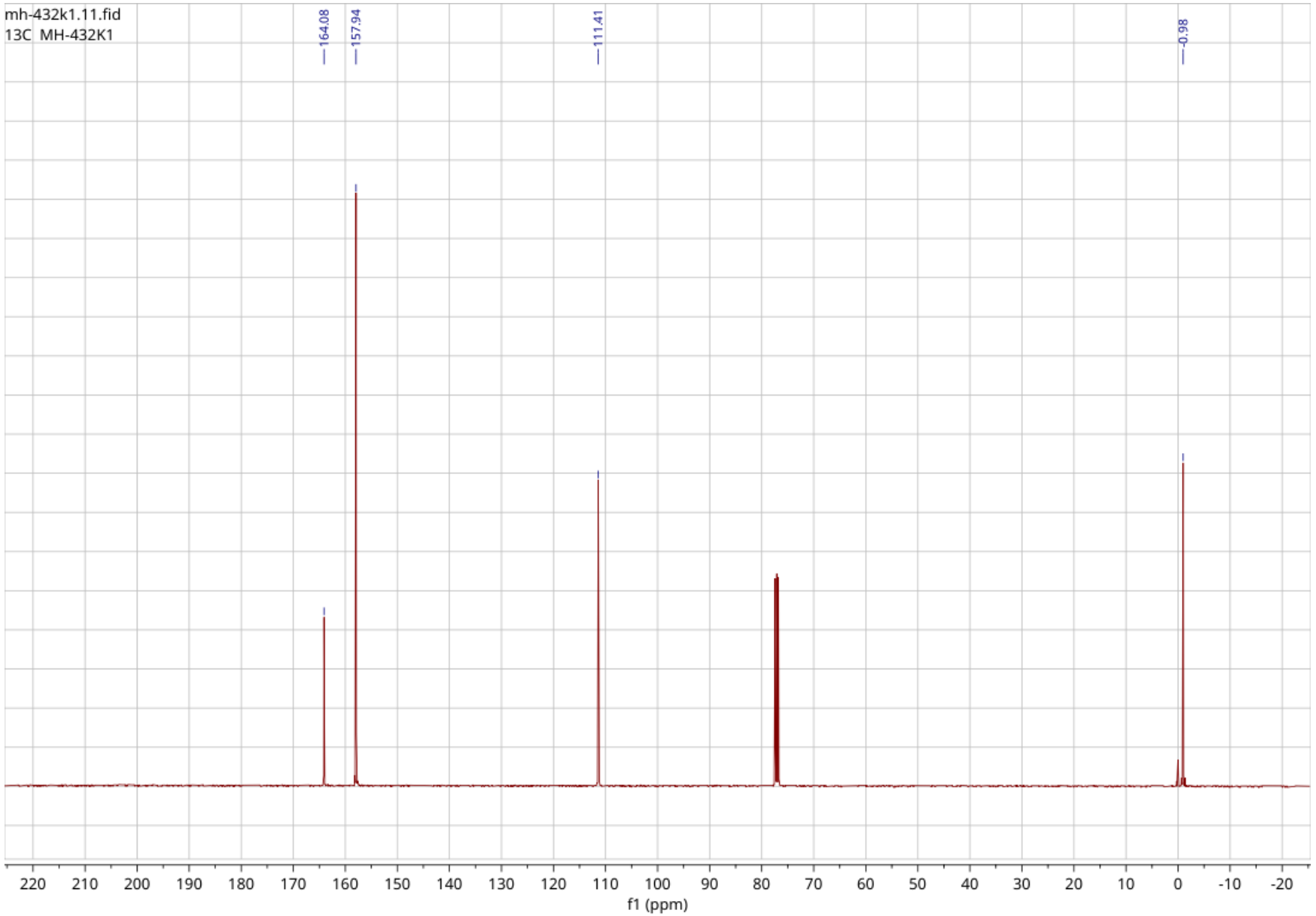

Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **2** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

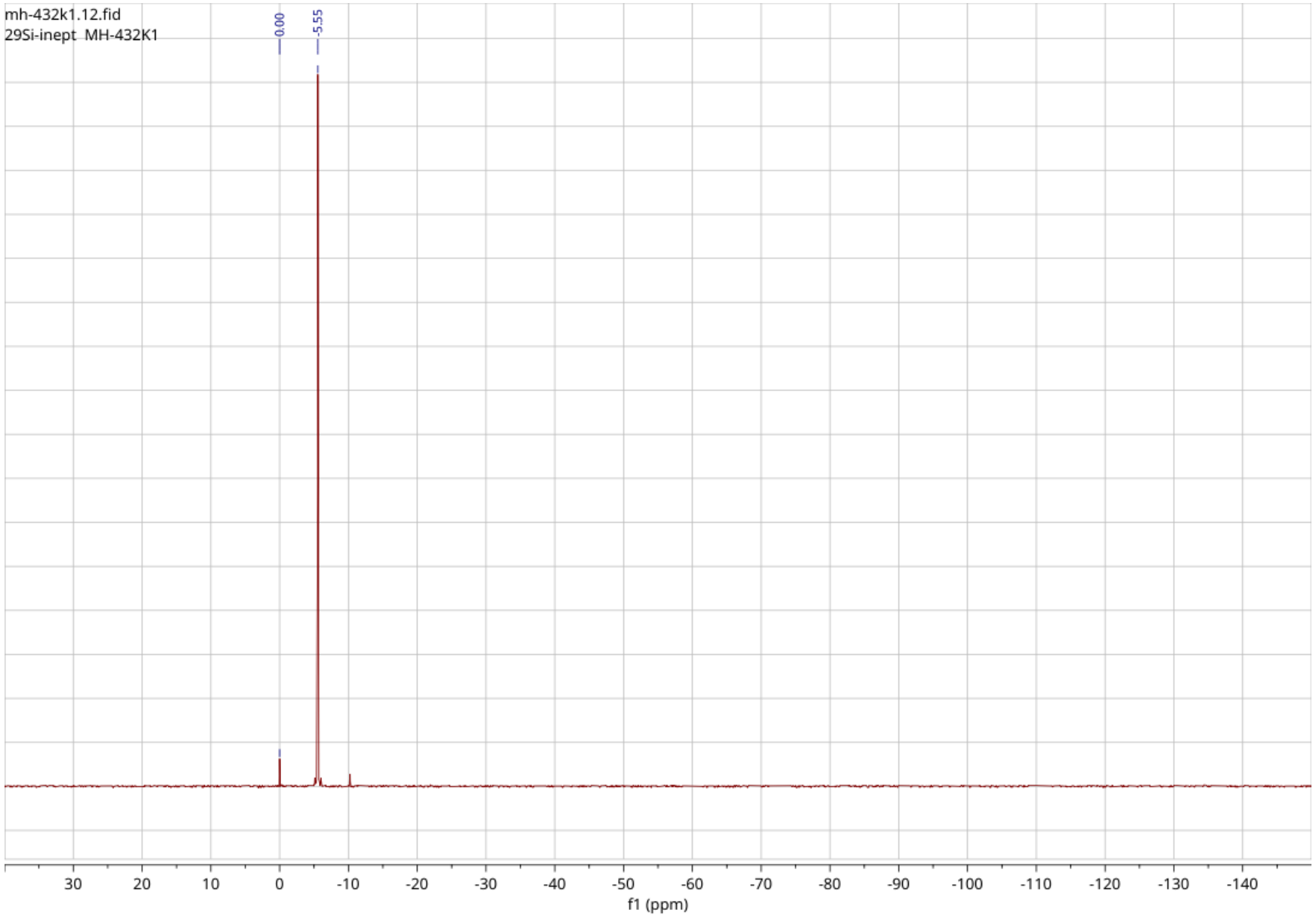

Figure S6: $^{29}Si\{^{1}H\}$ INEPT NMR spectrum of **2** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

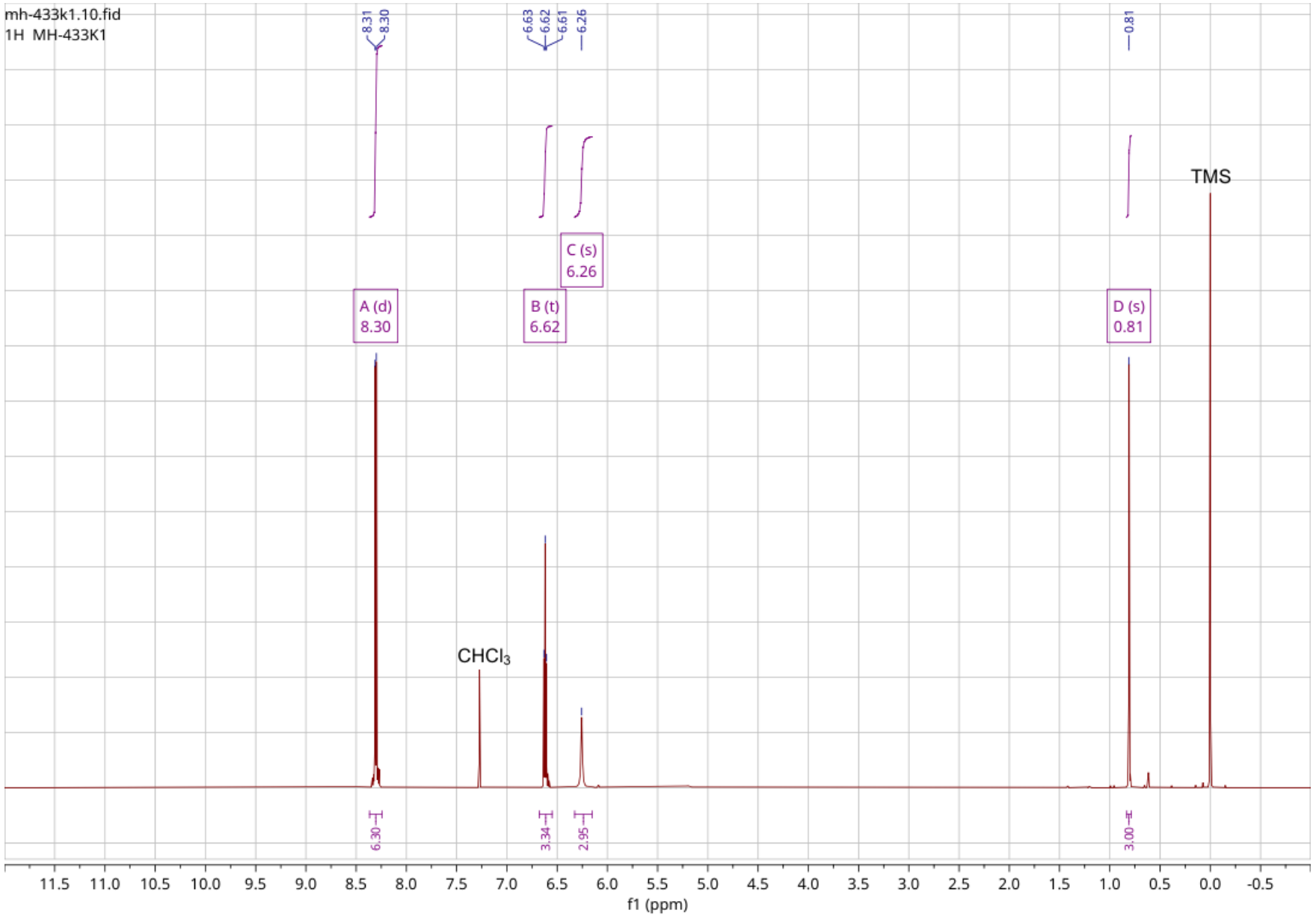

Figure S7: ^{1}H NMR spectrum of **3** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

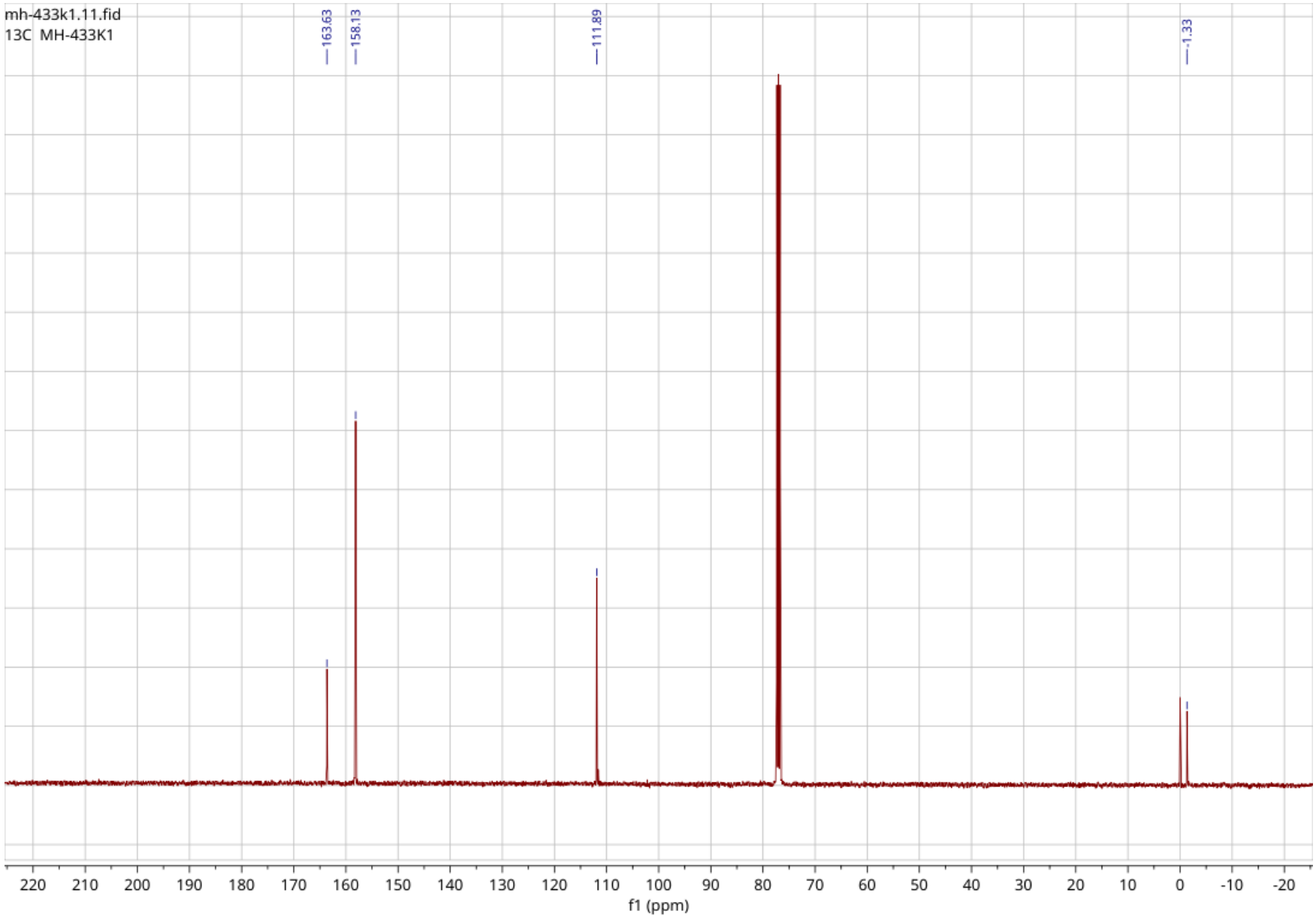

Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of **3** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

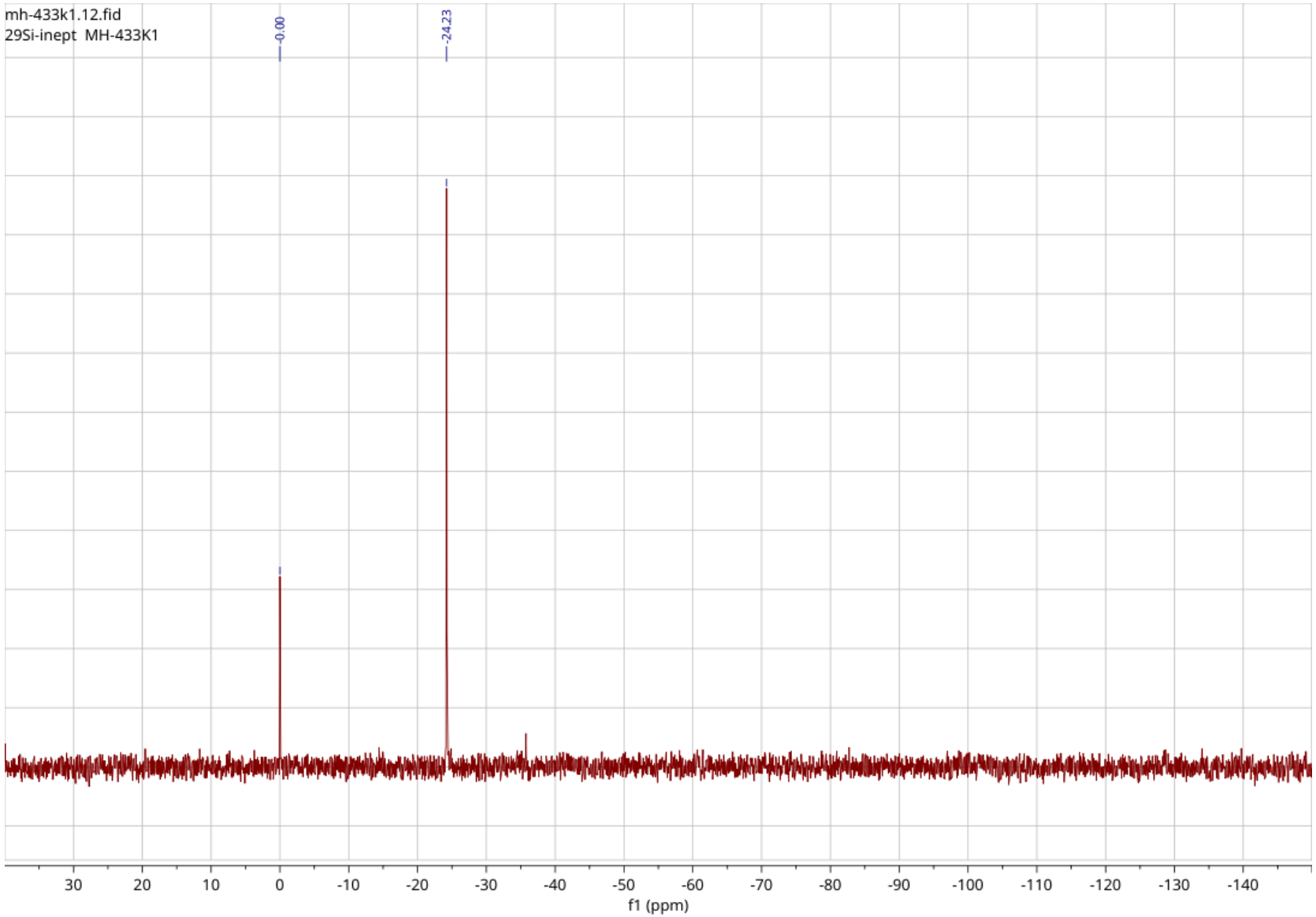

Figure S9: $^{29}Si\{^{1}H\}$ INEPT NMR spectrum of **3** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

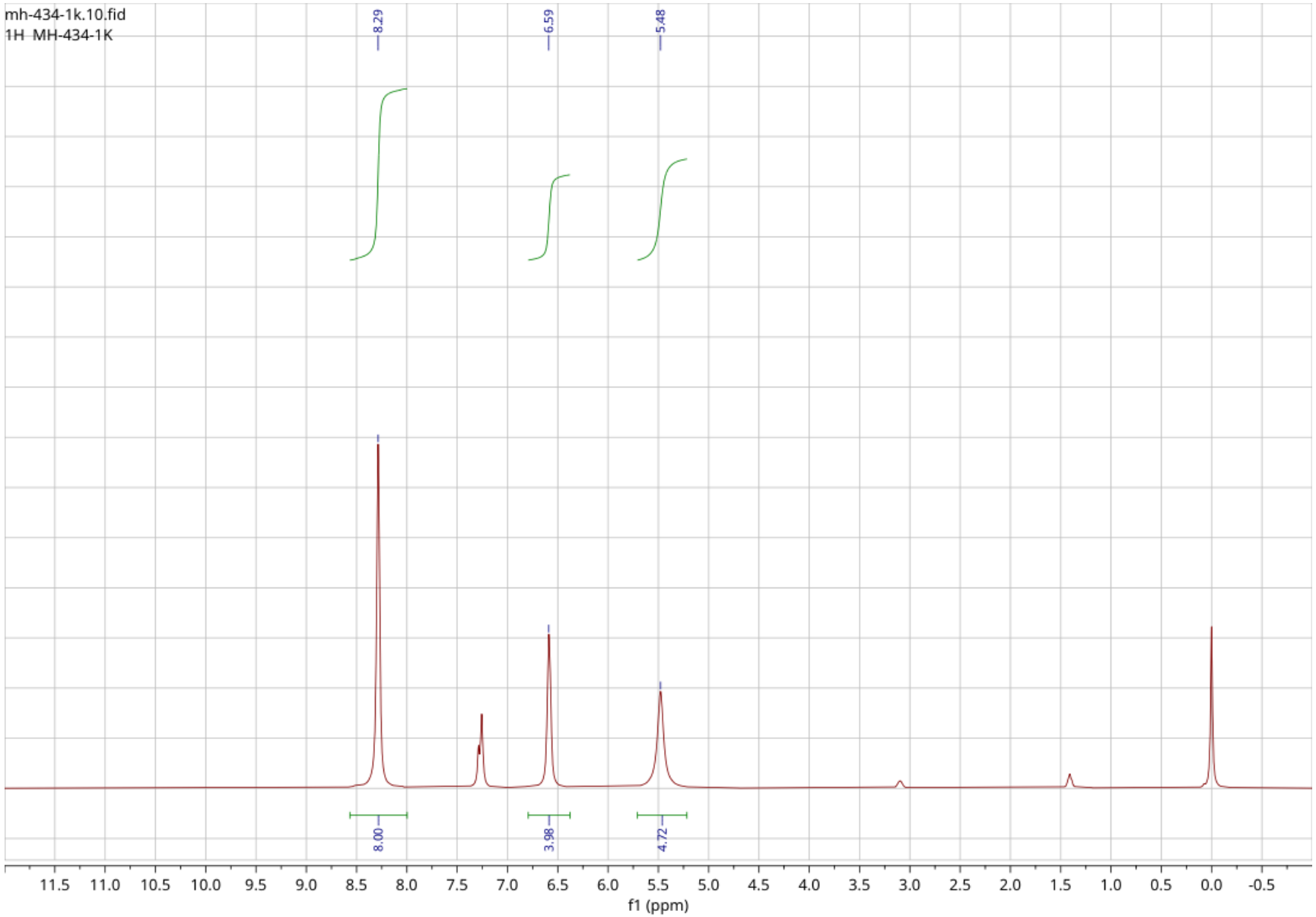

Figure S10: ^{1}H NMR spectrum of **4** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

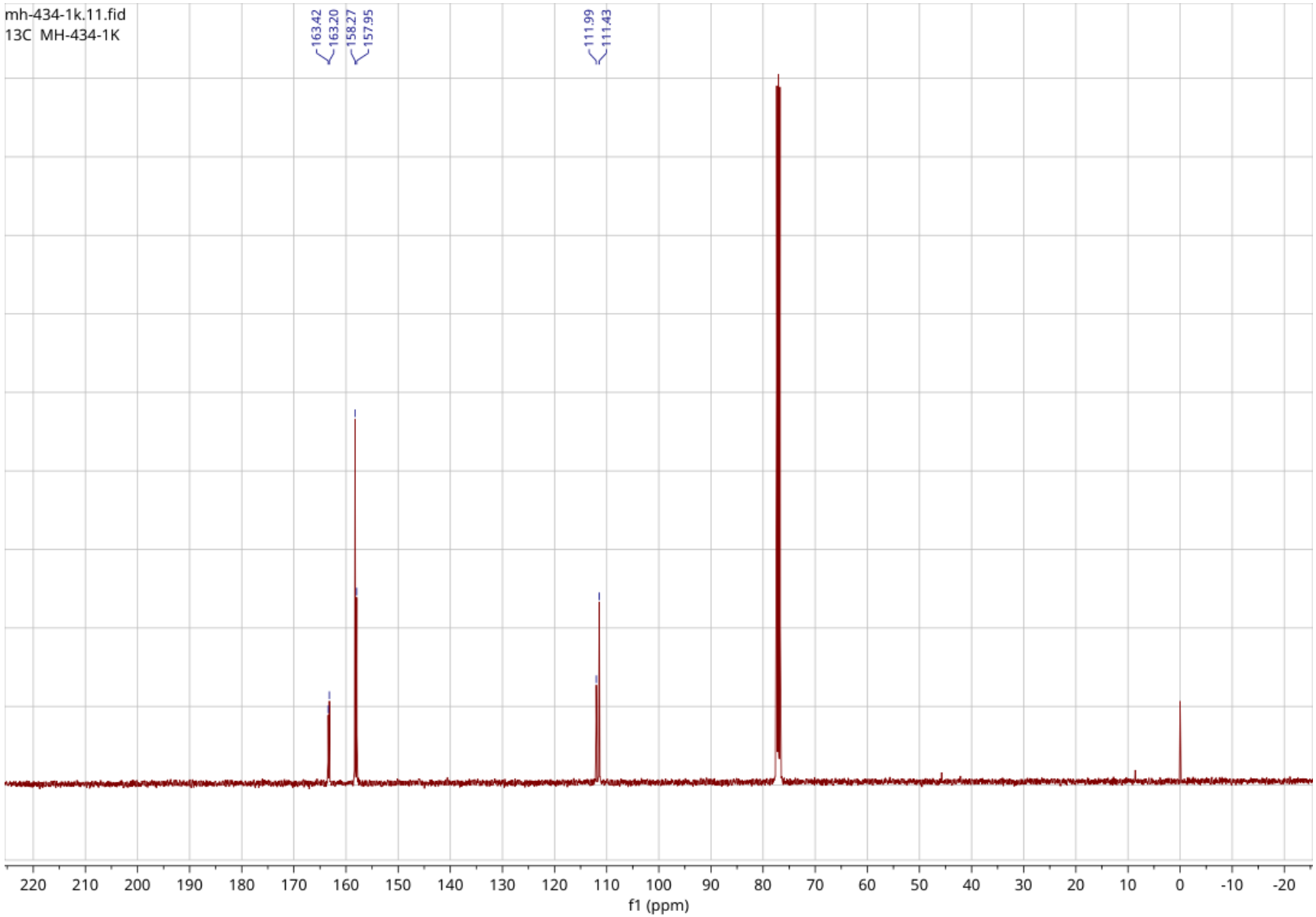

Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of **4** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

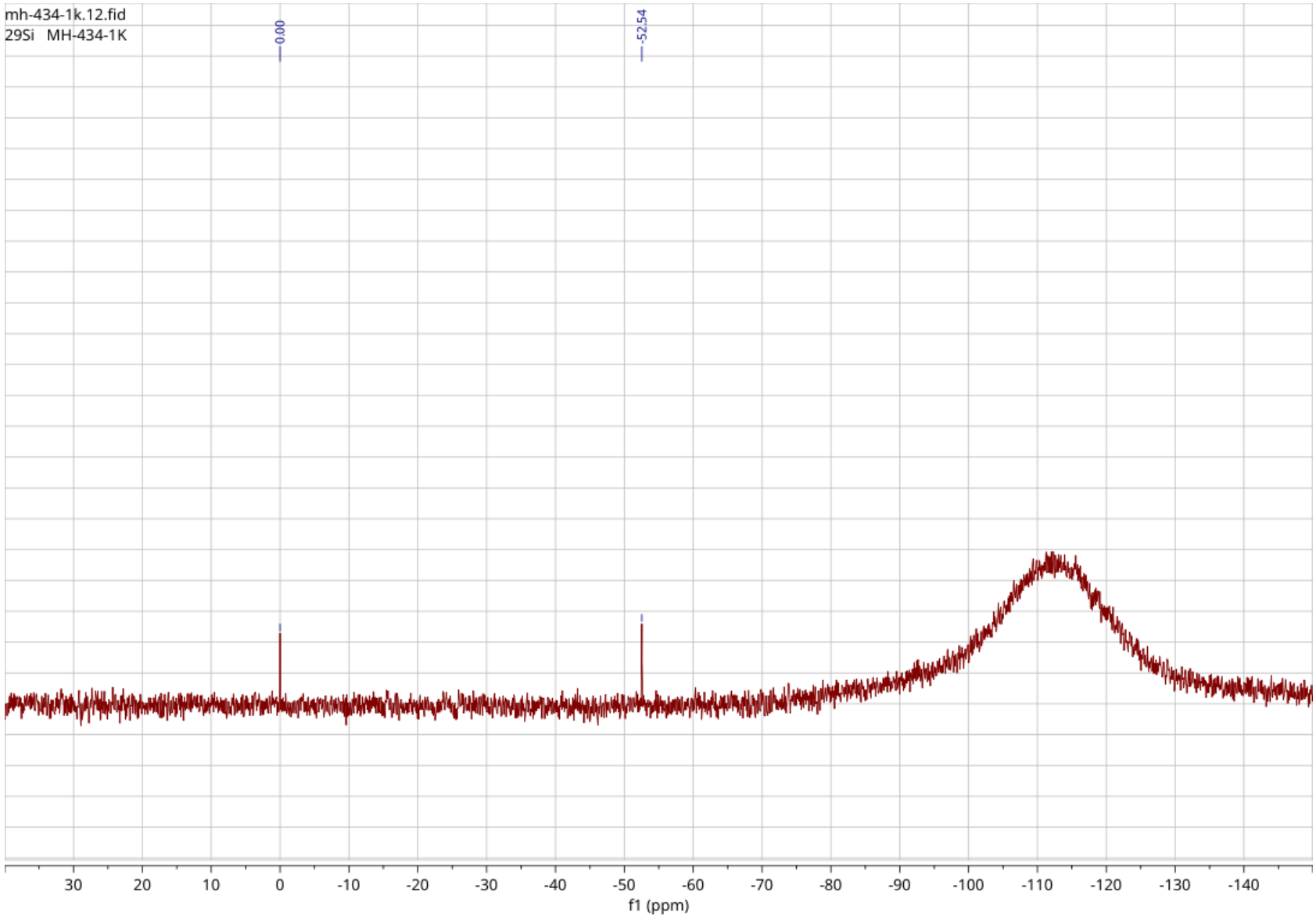

Figure S12: $^{29}Si\{^{1}H\}$ NMR spectrum of **4** (in $CDCl_3$, with $SiMe_4$ as internal shift reference).

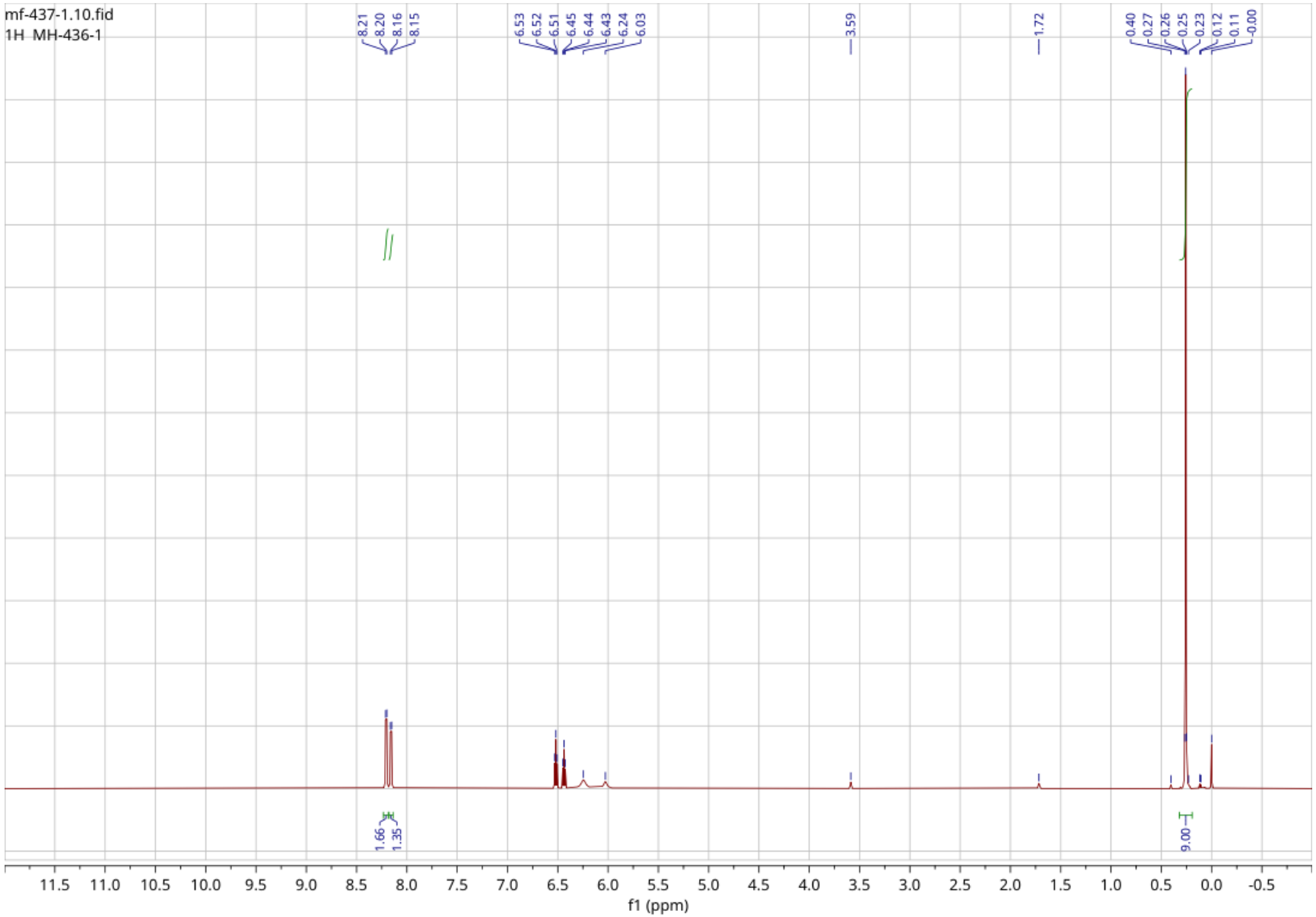

Figure S13: ^{1}H NMR spectrum of **1** (containing 2-aminopyrimidine) in a solution with CO_2 (in THF-d_8, with $SiMe_4$ as internal shift reference).

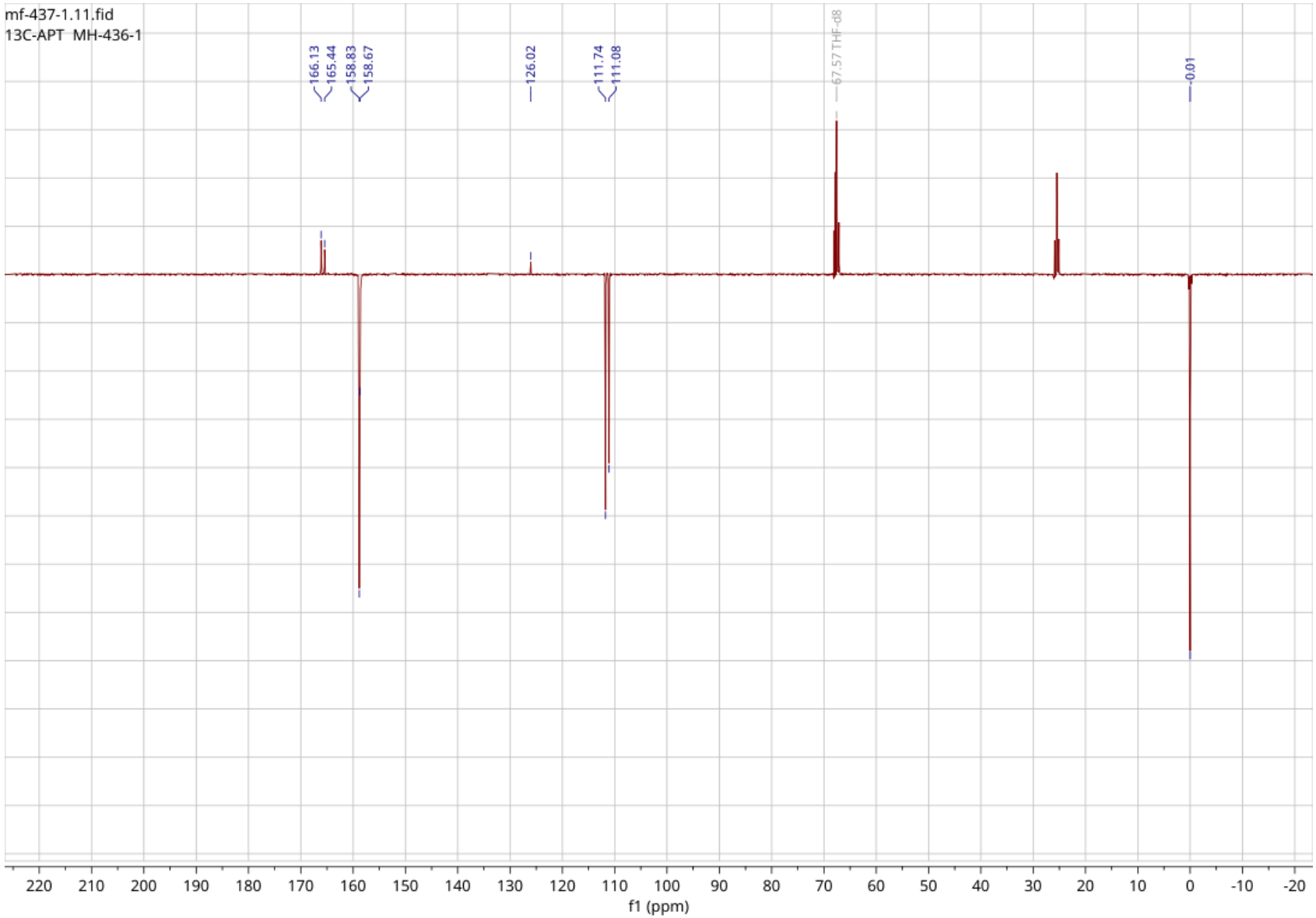

Figure S14: $^{13}C\{^{1}H\}$ APT NMR spectrum of **1** (containing 2-aminopyrimidine) in a solution with CO_2 (in THF-d_8, with $SiMe_4$ as internal shift reference). The relaxation delay was set to 10 seconds to detect signals of carbonyl moieties.

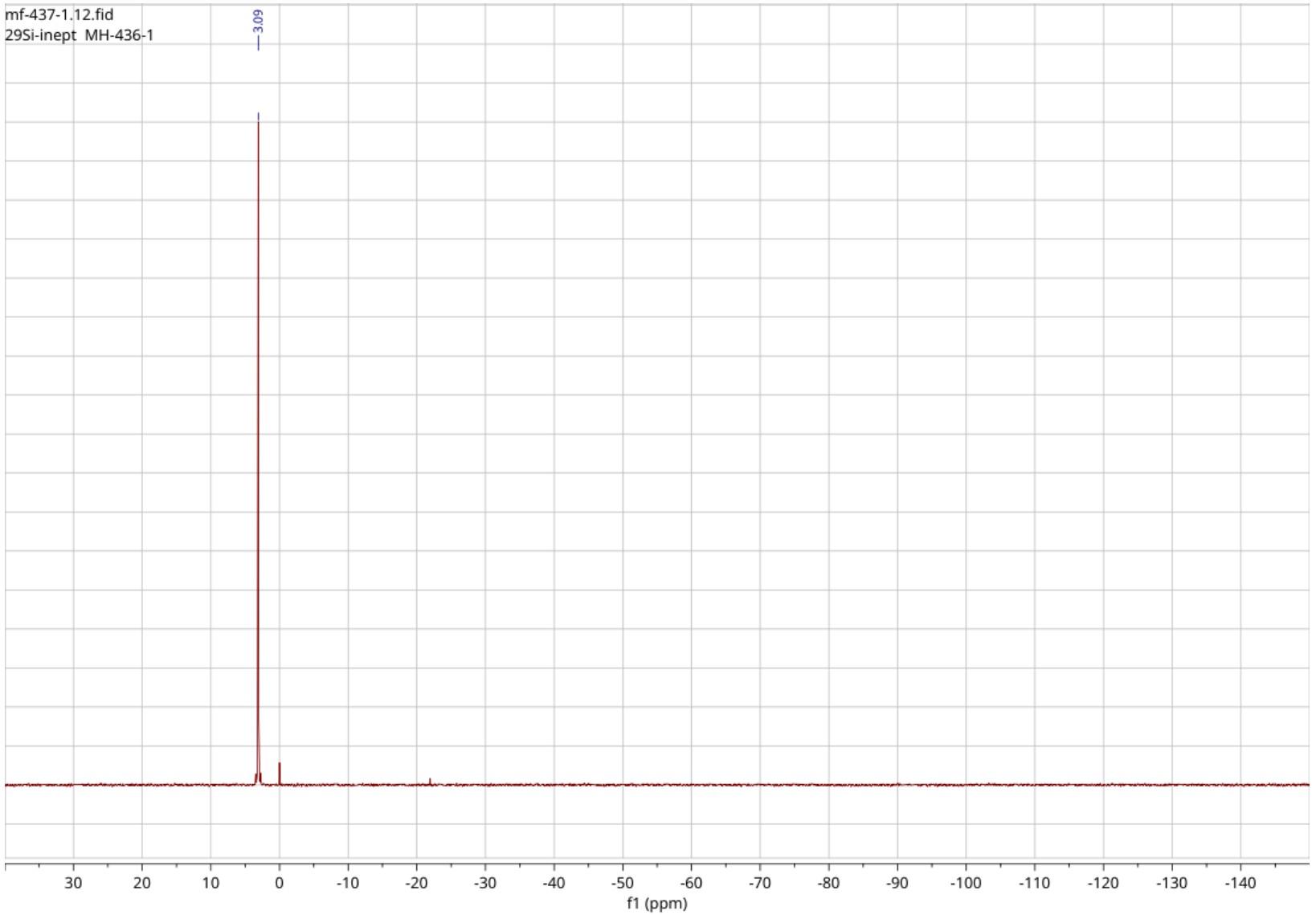

Figure S15: $^{29}Si\{^{1}H\}$ INEPT NMR spectrum of **1** (containing 2-aminopyrimidine) in a solution with CO_2 (in THF-d_8, with $SiMe_4$ as internal shift reference).

Table S2: Representative parameters used in NMR data acquisition

Spectrum	**^{1}H**	**^{13}C{^{1}H}**	**^{13}C{^{1}H} APT**	**^{29}Si{^{1}H}**	**^{29}Si{^{1}H} INEPT**
Pulse Sequence	zg30	zgpg30	jmod	zgig30	ineptrd-Si
Number of Scans	8	400	208	800	56
Receiver Gain	109.0	204.7	204.7	204.7	204.7
Relaxation Delay [s]	1.0	10.0	10.0	30.0	5.0
Pulse Width	13.80	8.70	8.79	9.30	9.30
Acquisition Time [s]	4.0894	1.9038	1.9999	1.9999	1.9999
Frequency [MHz]	400.13	100.62	100.62	79.49	79.49
Spectral Width [Hz]	8012.8	25252.5	25252.5	32051.3	23809.5
Lowest Frequency [Hz]	–1540.3	–2565.5	–2573.0	–23949.6	–19837.4
Acquired Size	32768	48075	50503	64100	47617
Spectral Size	65536	131072	131072	131072	131072

3 Raman spectra

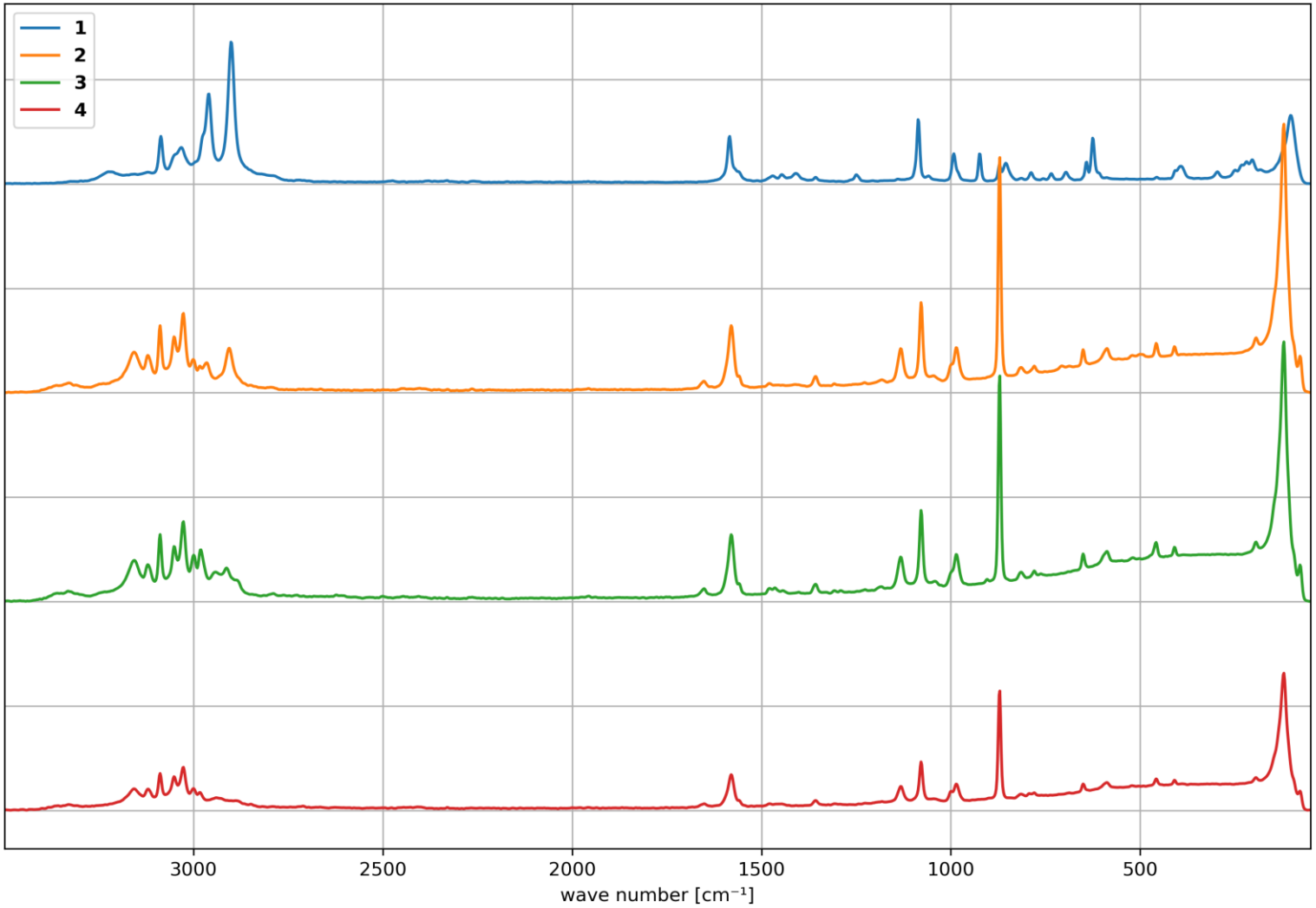

Figure S16: Raman spectra of compounds **1 – 4**.