Supporting Information

for

Synthesis and Biological Evaluation of a Valinomycin Analog bearing a Pentafluorophenyl Active Ester Moiety

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Table of Contents

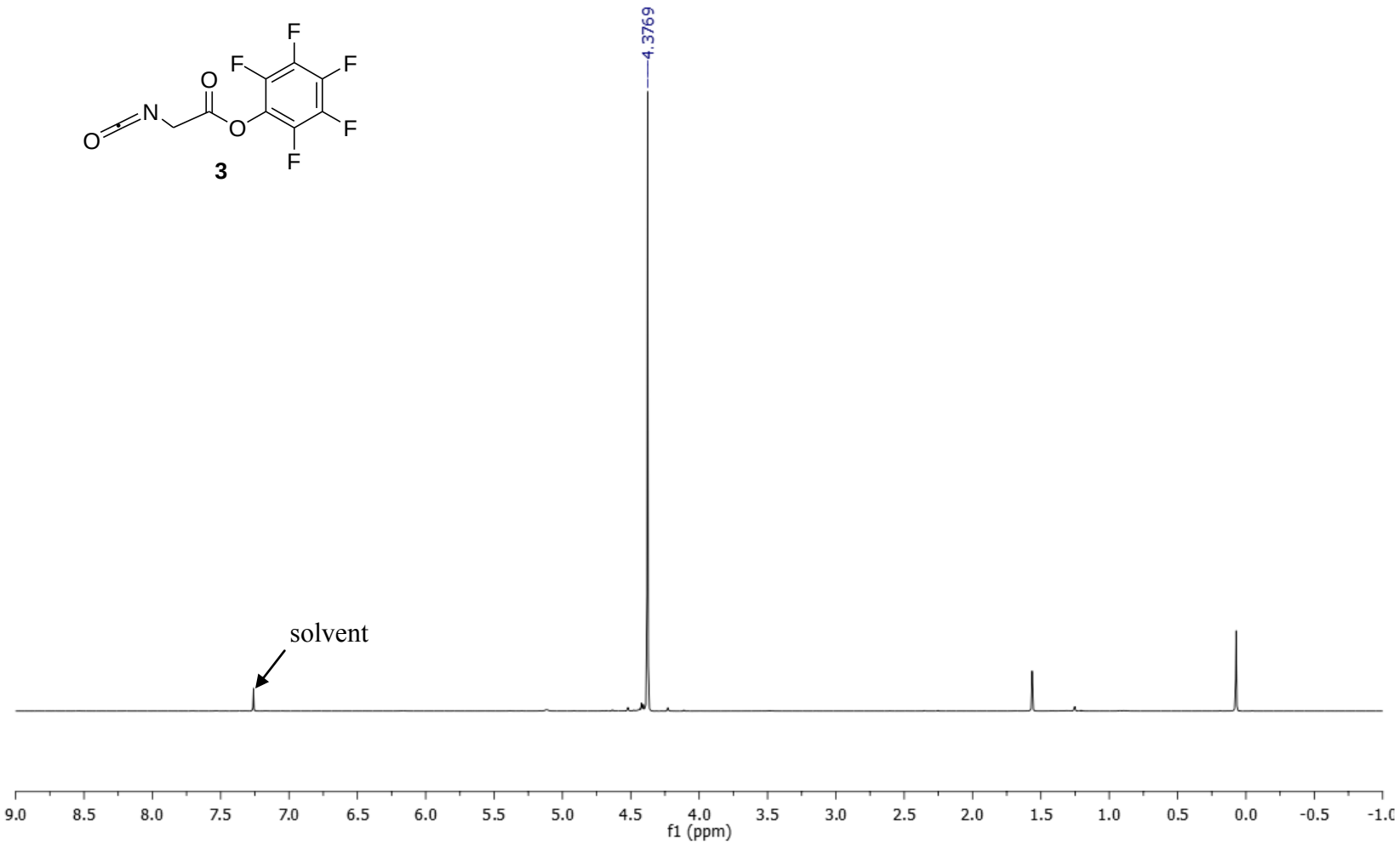


Figure *S1*. ^{1}H NMR spectrum (chloroform-*d*, 500 MHz) of pentafluorophenyl *N*-carbonyl glycinate (**3**).

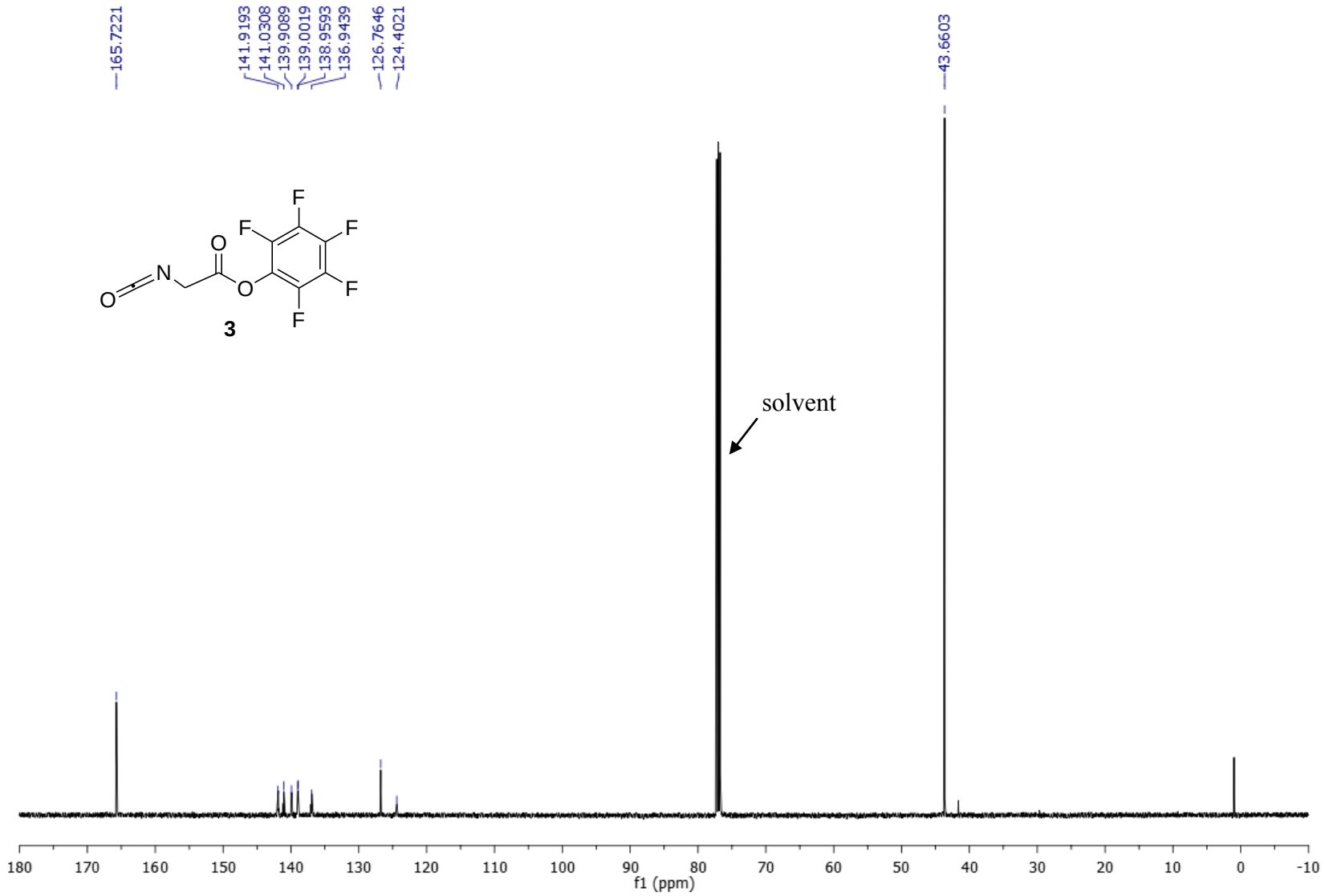


Figure *S2*. ^{13}C NMR spectrum (chloroform-*d*, 125 MHz) of pentafluorophenyl *N*-carbonyl glycinate (**3**).

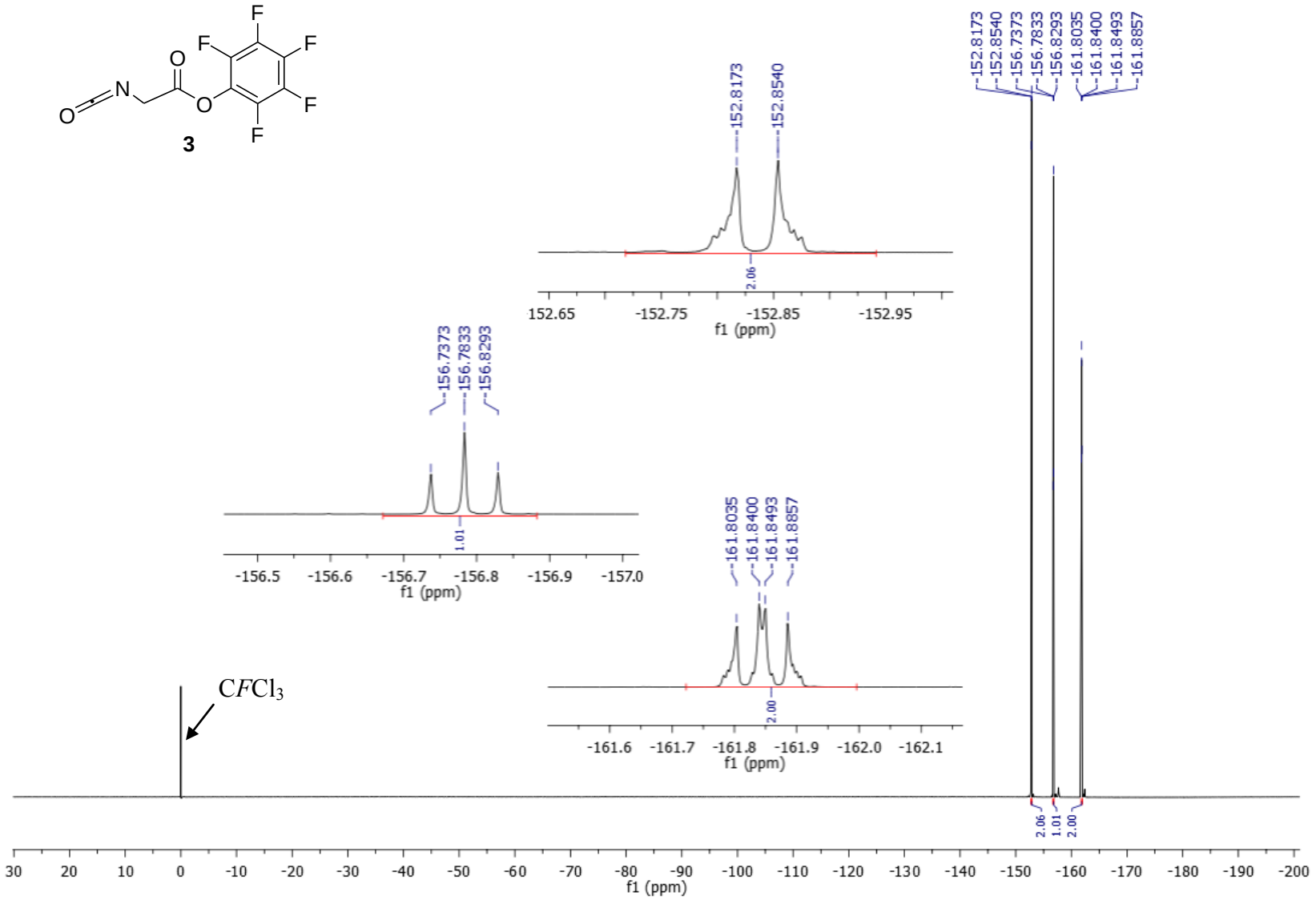


Figure *S3*. ^{19}F NMR spectrum (chloroform-*d*, 470 MHz) of pentafluorophenyl *N*-carbonyl glycinate (**3**).

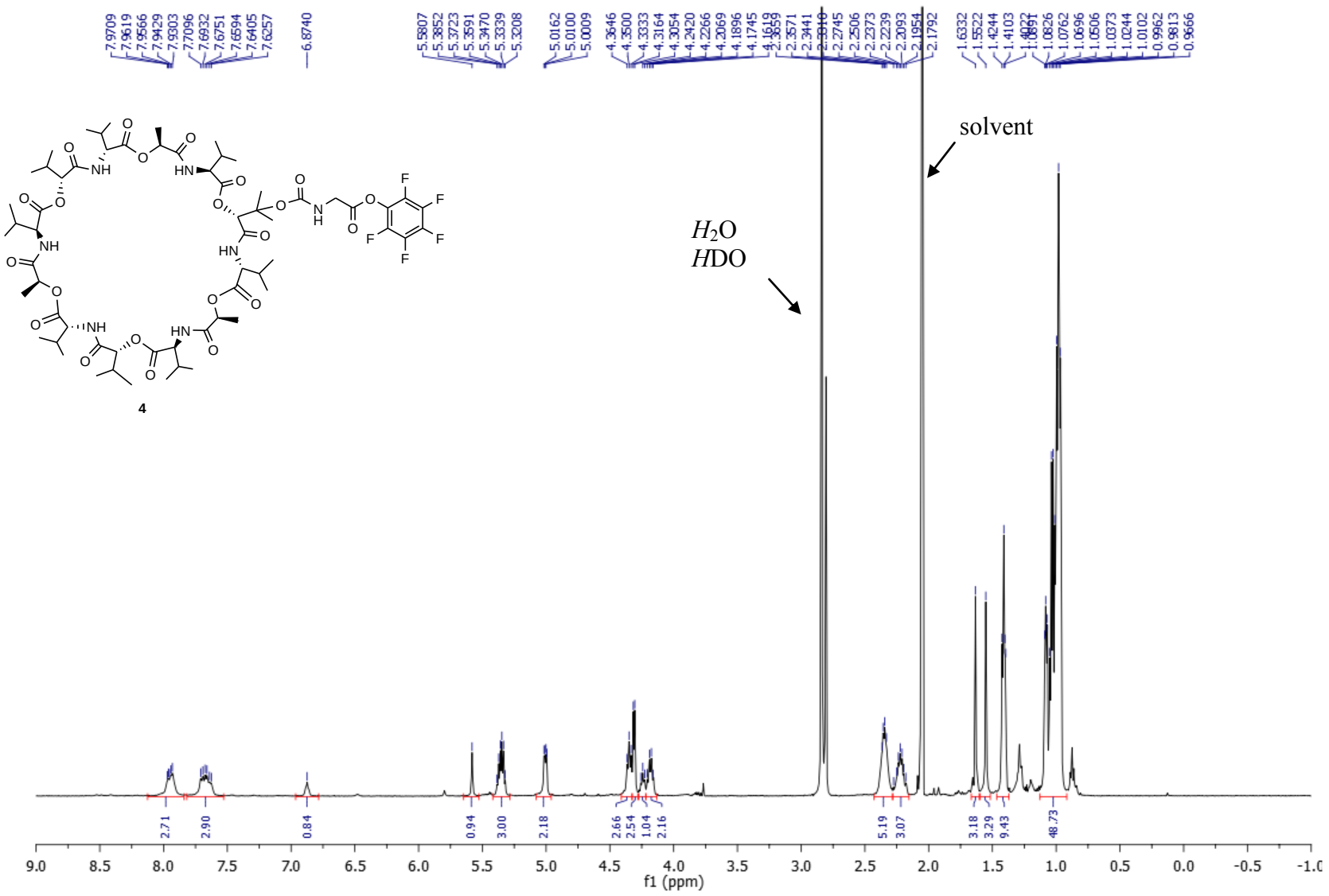


Figure *S4*. ^{1}H NMR spectrum (acetone-d_6, 500 MHz) of VLM analog **4**.

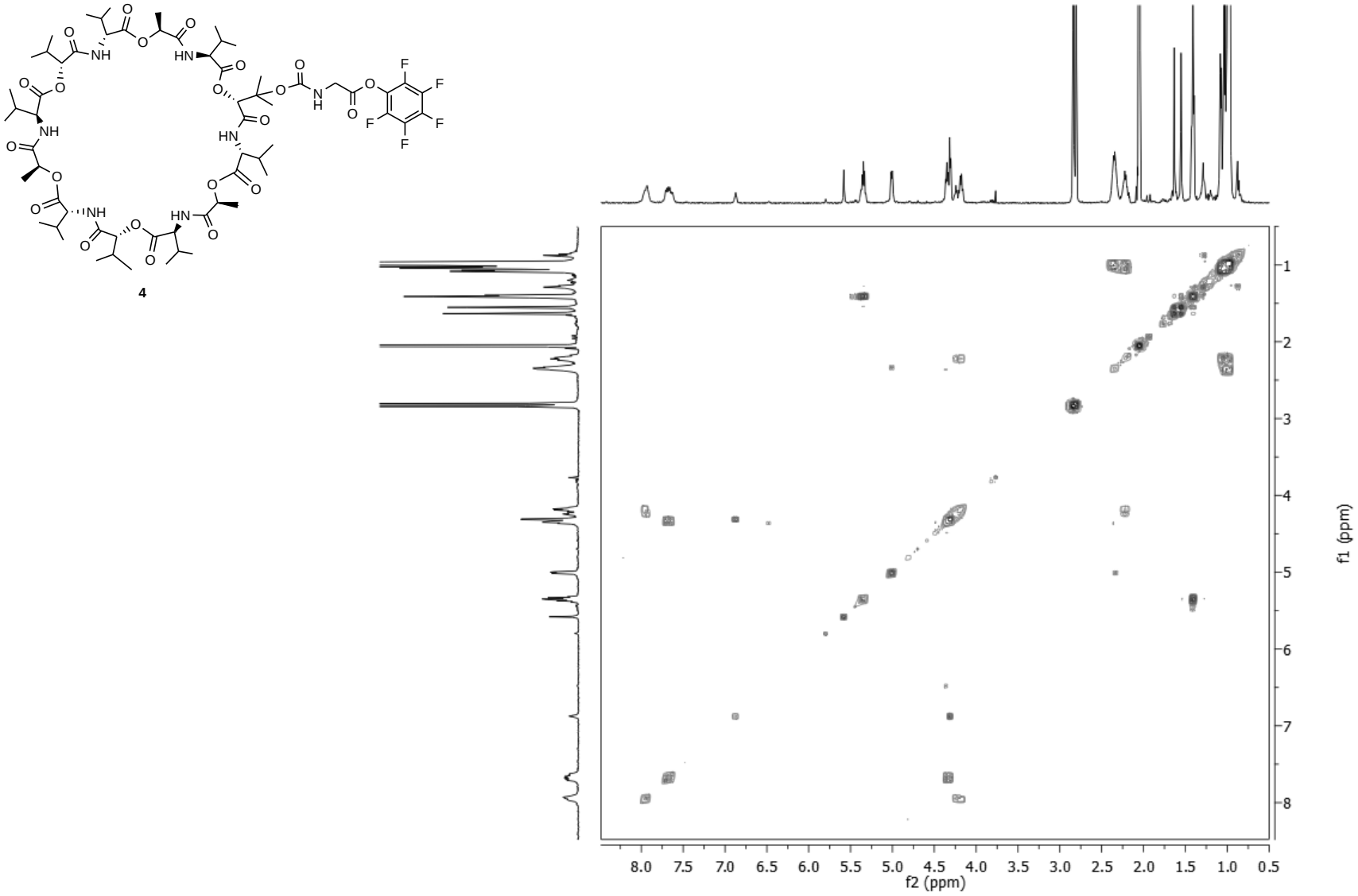


Figure *S5.* ^{1}H-^{1}H gCOSY spectrum (acetone-d_6, 500 MHz) of VLM analog **4**.

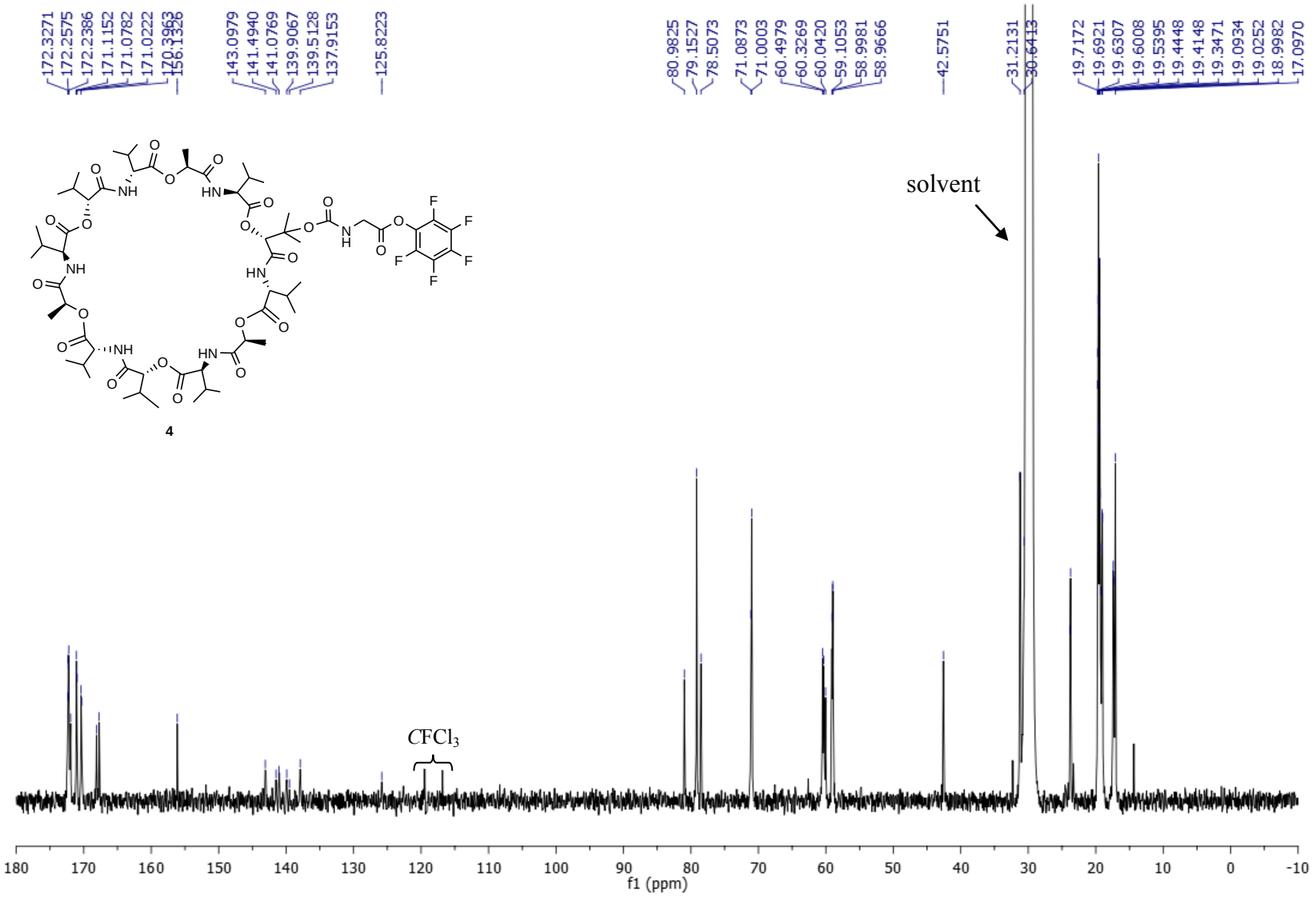


Figure *S6*. ^{13}C NMR spectrum (acetone-d_6, 125 MHz) of VLM analog (**4**).

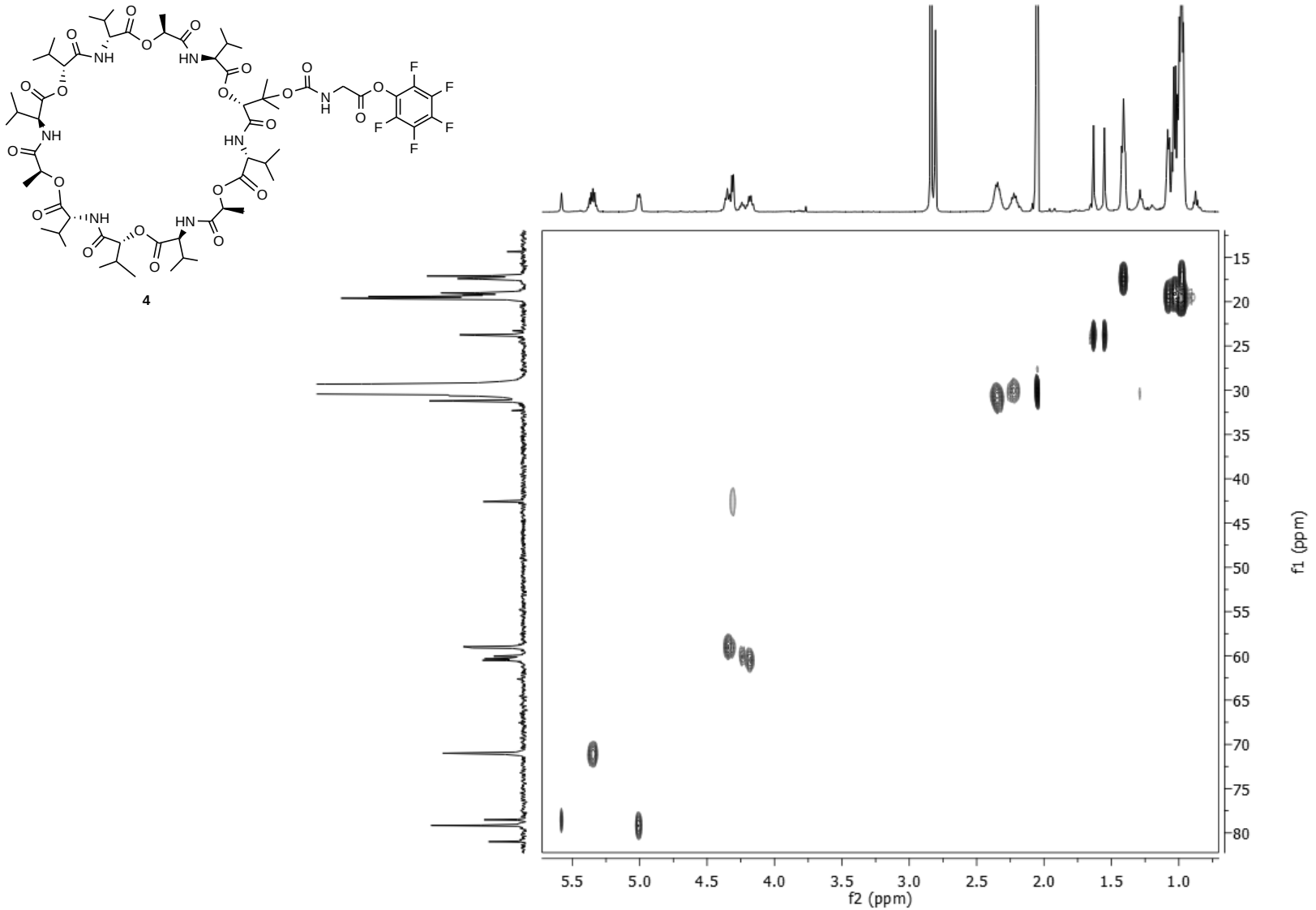


Figure *S7.* ^{1}H-^{13}C HSQCAD spectrum (acetone-d_6, 500 MHz) of VLM analog **4**.

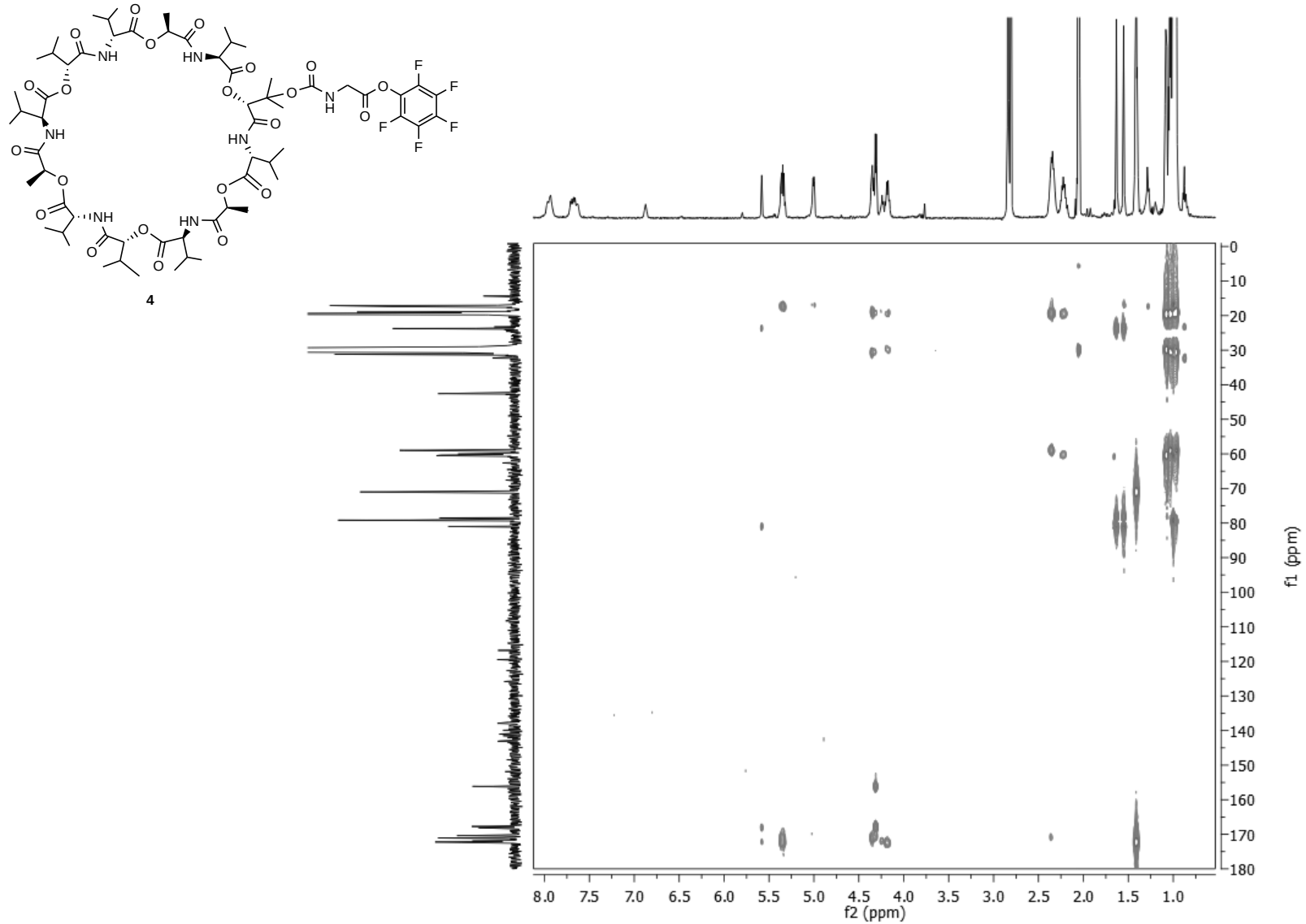


Figure *S8.* ^{1}H-^{13}C gHMBCAD spectrum (acetone-d_6, 500 MHz) of VLM analog **4**.

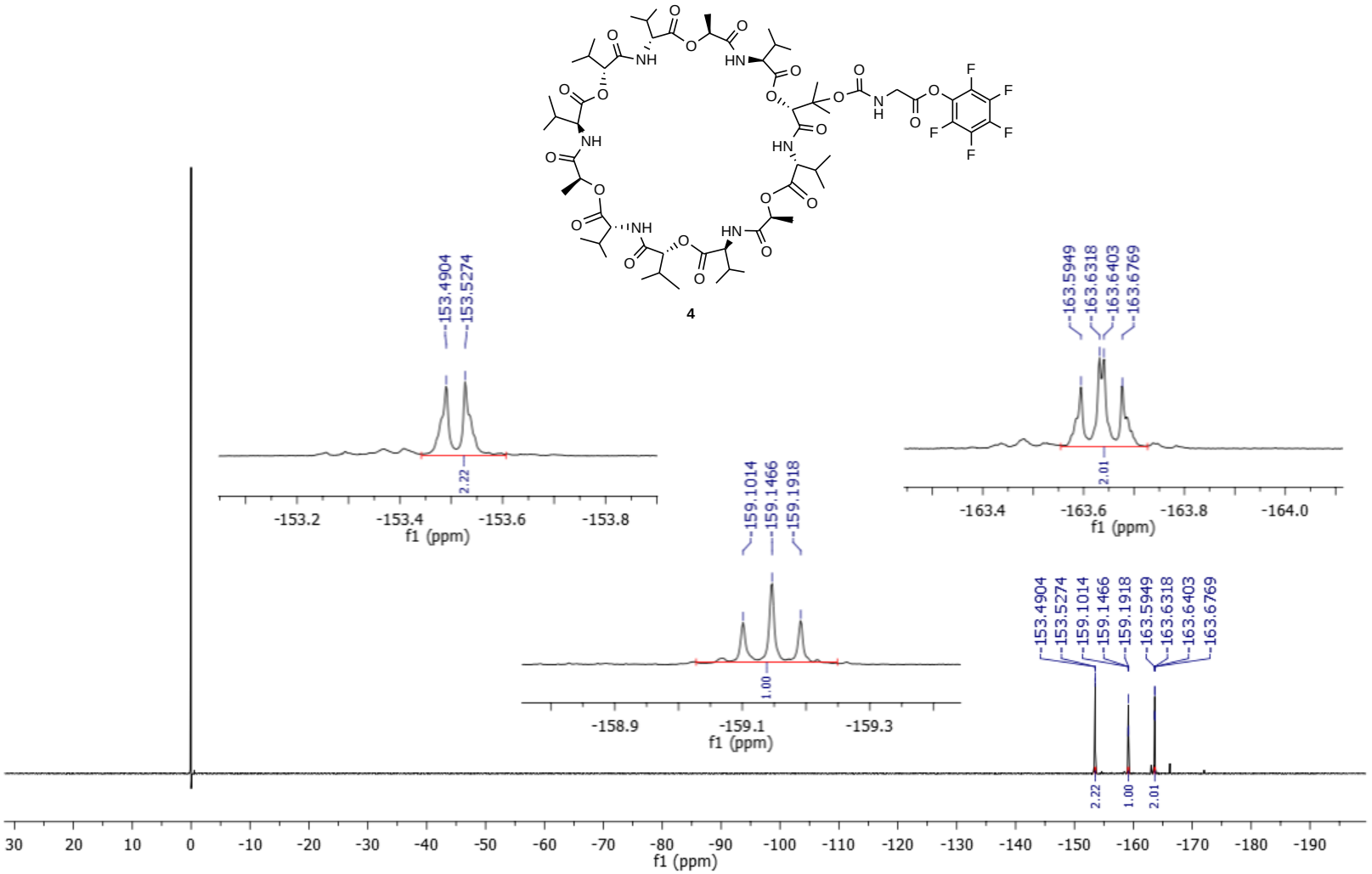
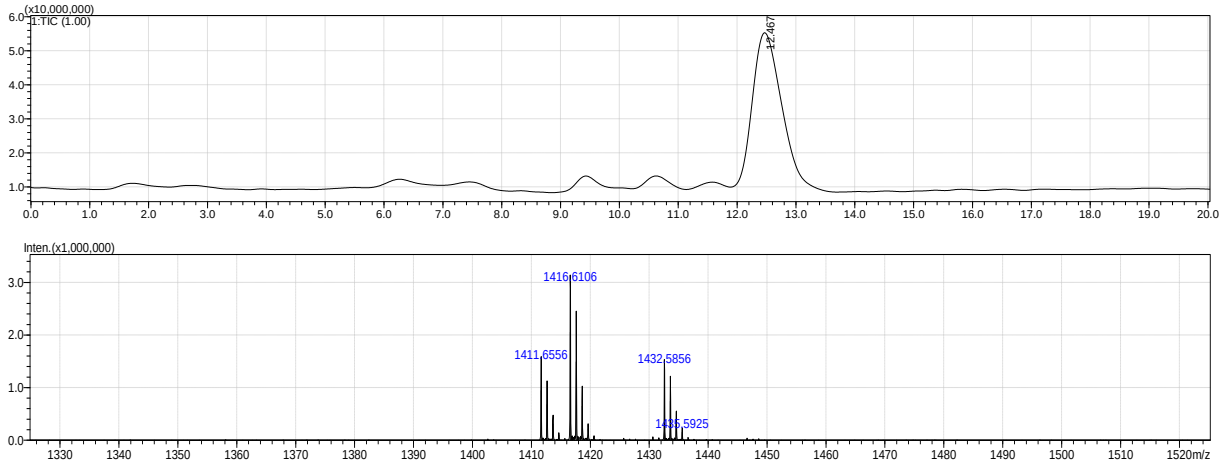


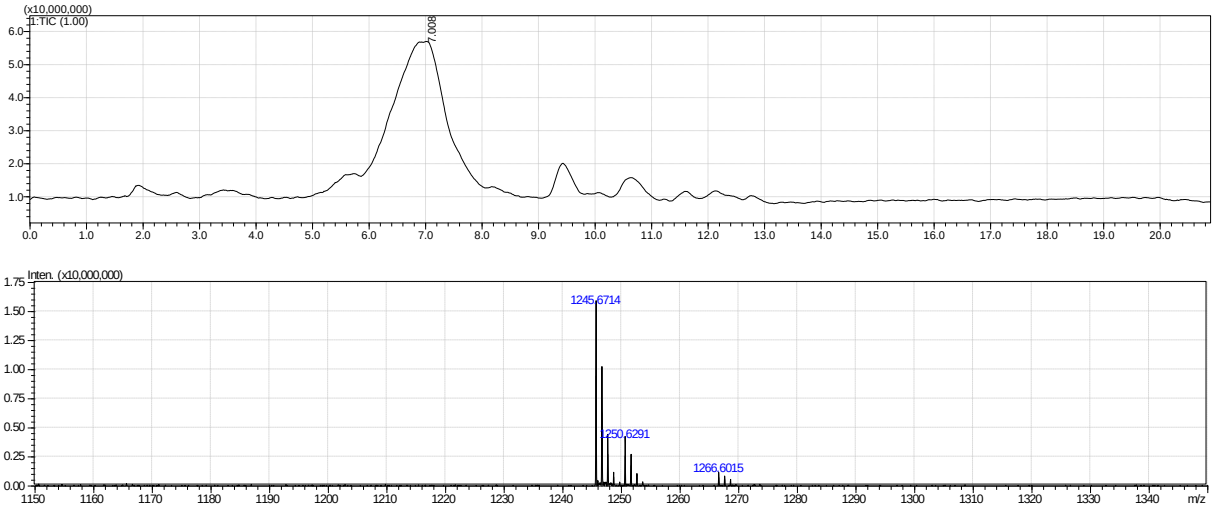
Figure *S9*. ^{19}F NMR spectrum (acetone-d_6, 470 MHz) of VLM analog **4**.

LC-HRMS data for analog 4 and reaction mixtures of analog 4 with OH- and NH_2-containing compounds, according to Scheme 3

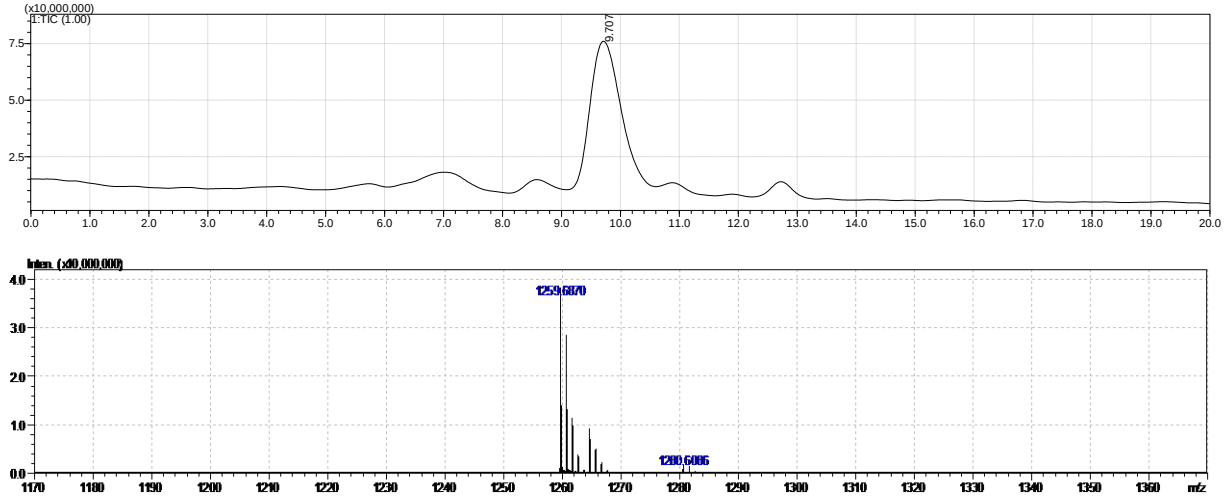
(a) Analog **4**



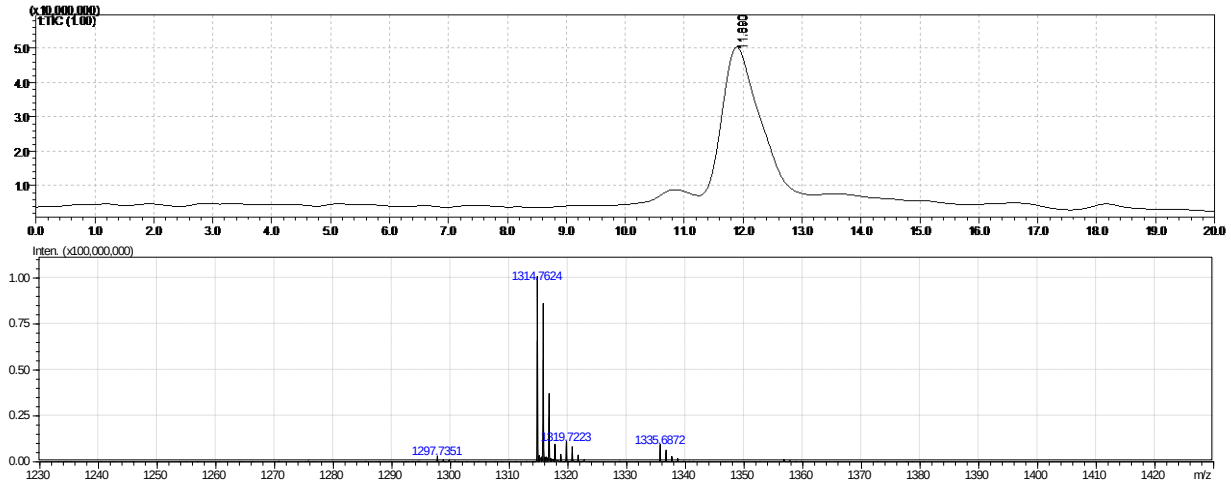
(b) ***cbx*-4**



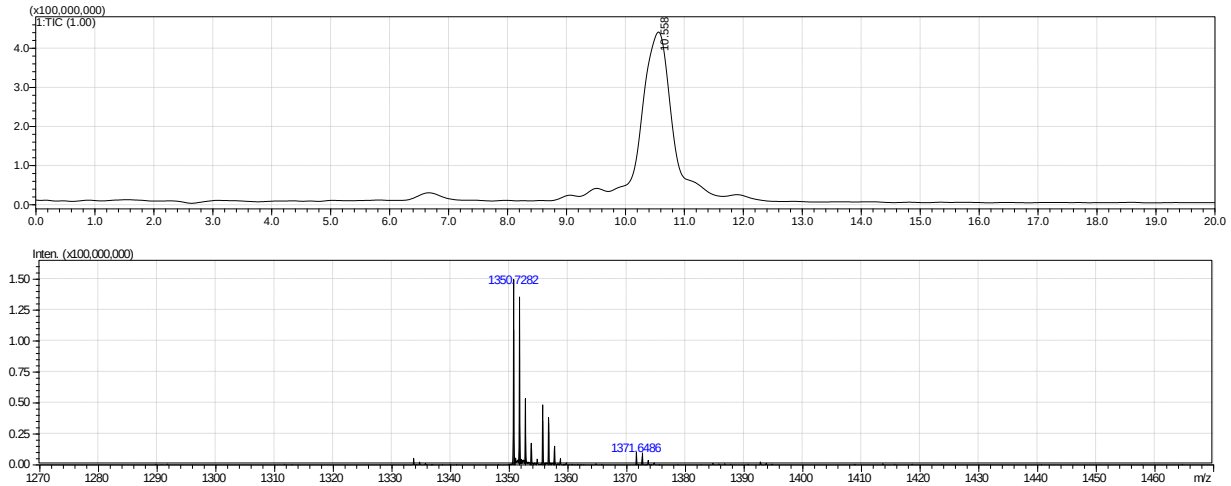
(c) ***met*-4**



(d) ***pen*-4**



(e) ***anis*-4**



(f) ***leu*-4**

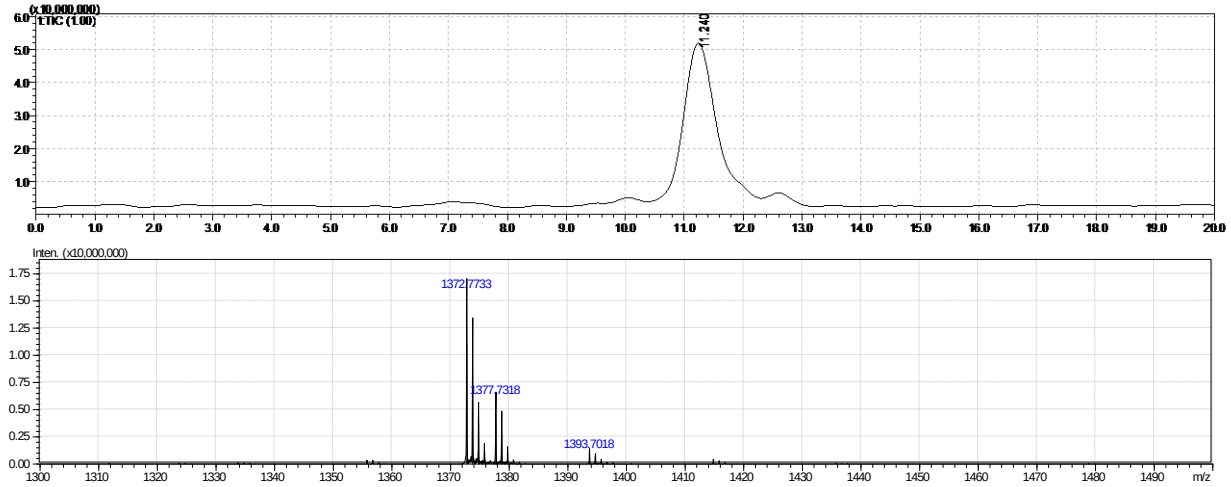


Figure *S10.* LC-HRMS (ESI-TOF) data for (a) **4**, (b) ***cbx*-4**, (c) ***met*-4**, (d) ***pen*-4**, (e) ***anis*-4**, and (f) ***leu*-4**. LC conditions: Eurospher II 100-3 C18 column (100 × 2 mm ID); water (A) – methanol (B) mobile phase, gradient elution 90-100% B in 10 min, 0.15 mL/min; high-resolution mass spectrometer settings: electrospray ion source in ion-positive mode.

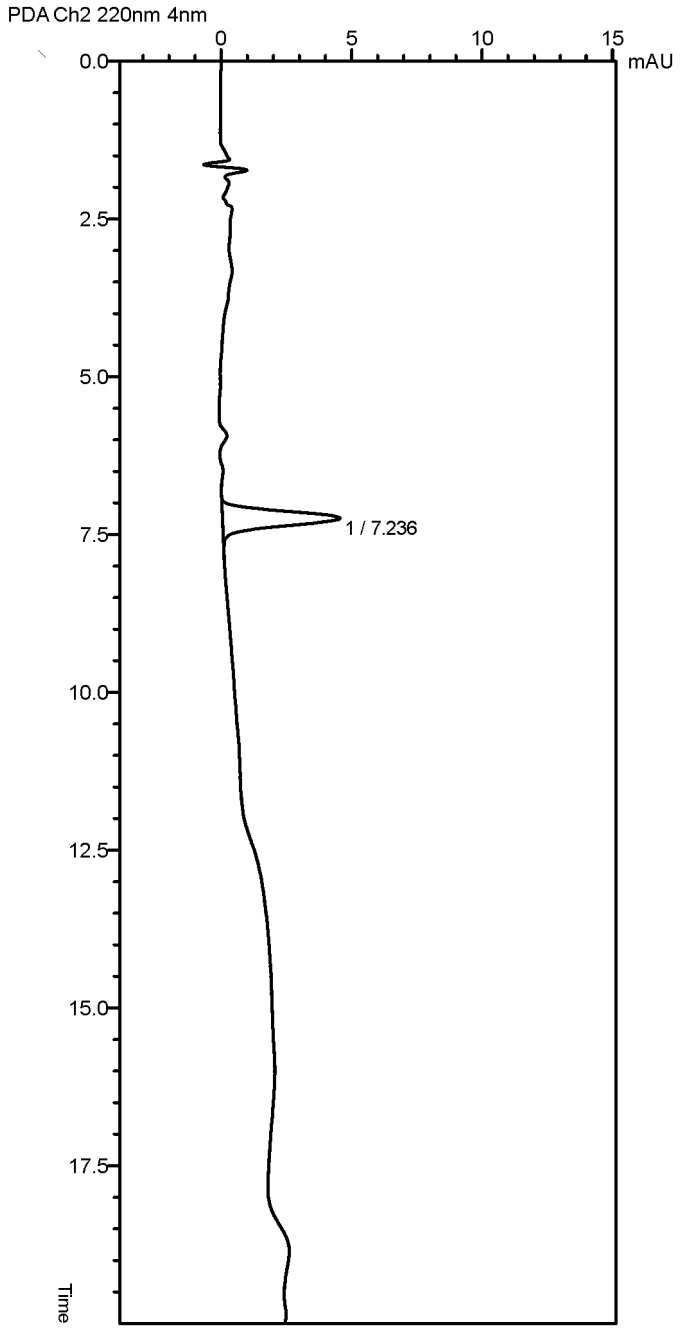


Figure *S11*. HPLC chromatogram of a purified sample of ***cbx*-4**. Conditions: Eurospher II 100-3 C18 column (100 × 2 mm ID); water (A) – methanol (B) mobile phase, gradient elution 90-100% B in 10 min, 0.15 mL/min; UV detector 220 nm.

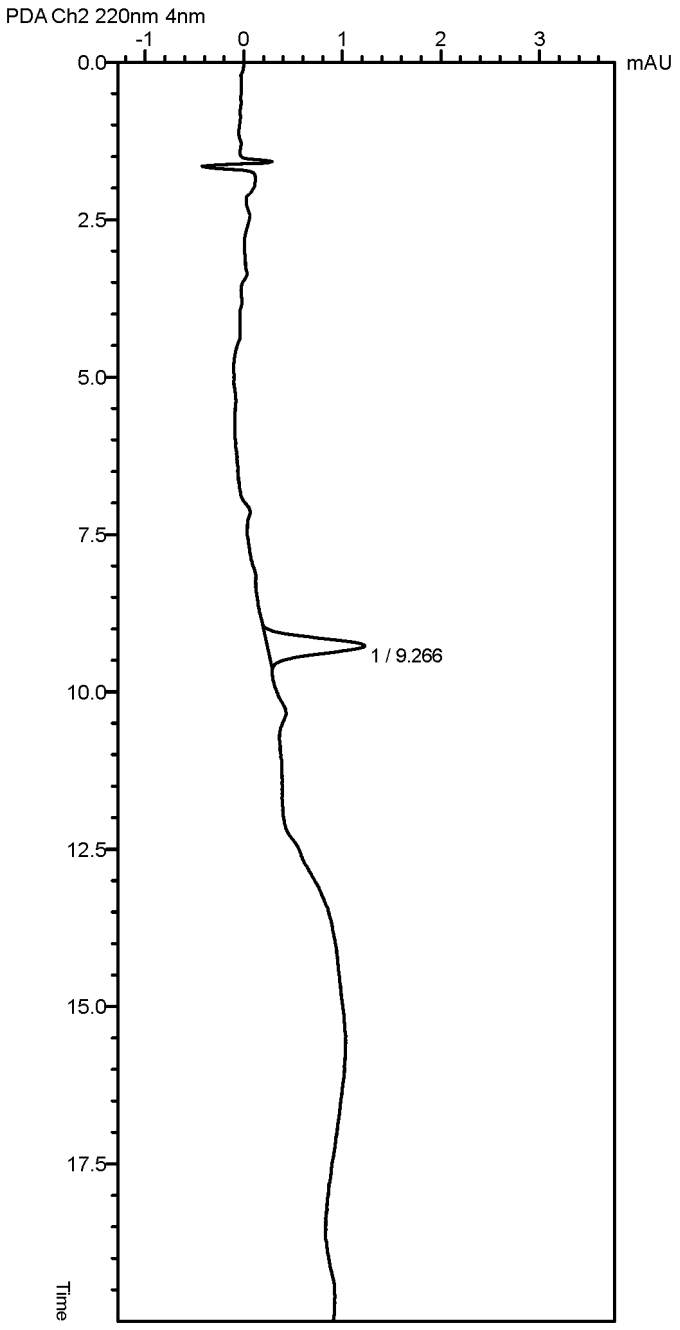


Figure *S12*. HPLC chromatogram of a purified sample of ***met*-4**. Conditions: Eurospher II 100-3 C18 column (100 × 2 mm ID); water (A) – methanol (B) mobile phase, gradient elution 90-100% B in 10 min, 0.15 mL/min; UV detector 220 nm.

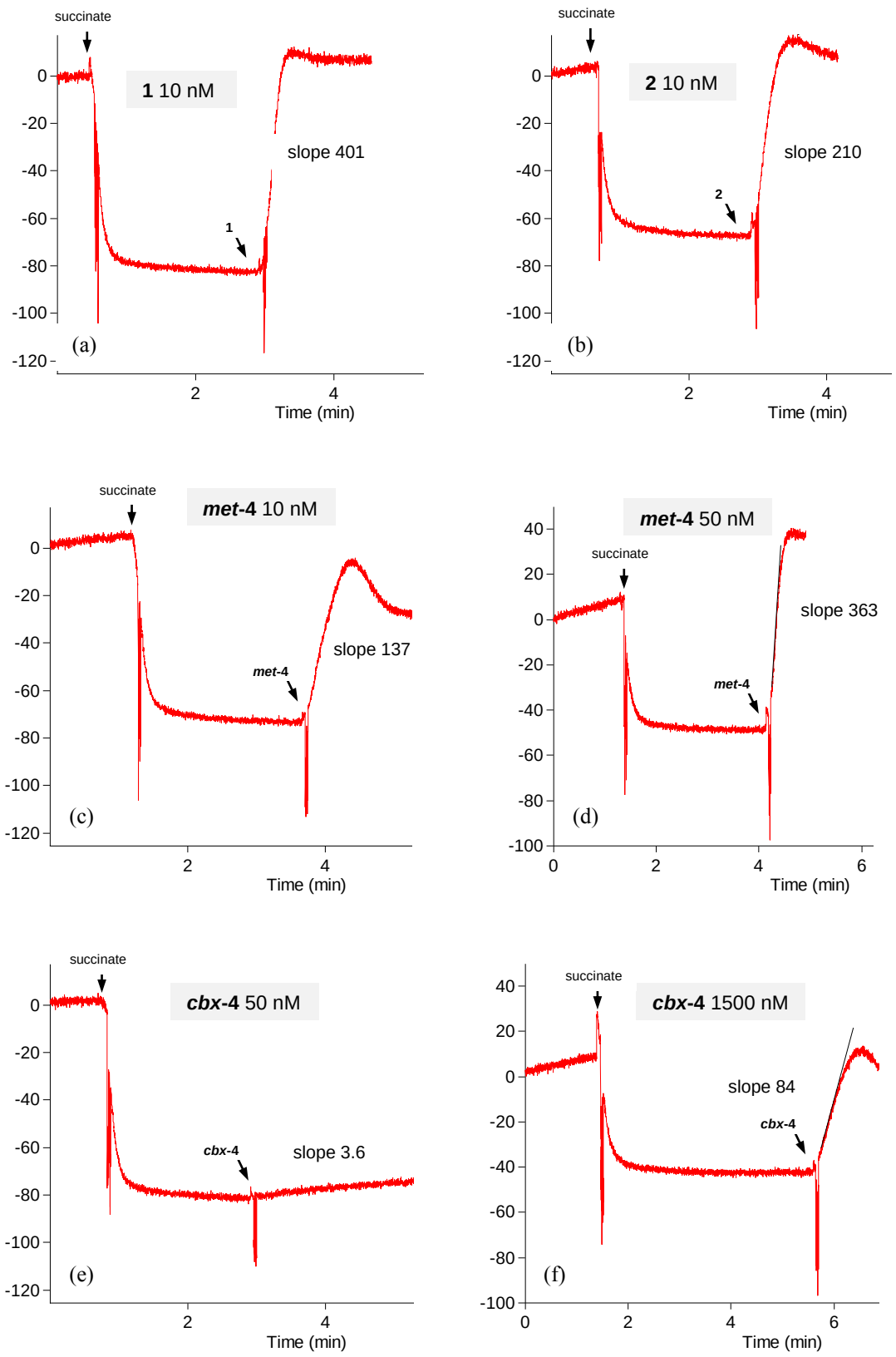


Figure *S13*. $\Delta\Psi_m$ decay induced by (a) 10 nM **1**, (b) 10 nM **2**, (c) 10 nM ***met*-4**, (d) 50 nM ***met*-4**, (e) 50 nM ***cbx*-4**, (f) 1500 nM ***cbx*-4**.