Electronic Supplementary Information

For

Peptoid-based siderophore mimics as dinuclear Fe^{3+} chelators

Assunta D'Amato, ‡[a] Pritam Ghosh, ‡[b] Chiara Costabile,[a] Giorgio Della Sala,[a] Irene Izzo,[a] Galia Maayan[b*] and Francesco De Riccardis[a*]

[a] *Department of Chemistry and Biology "A. Zambelli", University of Salerno, Via Giovanni Paolo II, 132, Fisciano (SA), 84084, Italy*

[b] *Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa 32000, Israel*

‡ Equal contribution.

Corresponding authors: Francesco De Riccardis, dericca@unisa.it;

Galia Maayan, gm92@technion.ac.il

1.0 List of abbreviations

ACN: acetonitrile

Ar: aryl

Bn: benzyl

DCM: dichloromethane

DMSO: dimethyl sulfoxide

DIC: *N,N′*-diisopropylcarbodiimide

DIPEA: *N,N*-diisopropylethylamine

DMF: *N*,*N*-dimethylformamide

ESI: electrospray ionisation

ES-MS: electrospray mass spectrometry

HATU: *O*-(7-azabenzotriazol-1-yl)-*N*,*N*,*N'*,*N'*-tetramethyluronium hexafluorophosphate

HFIP: 1,1,1,3,3,3-hexafluoroisopropanol

MALDI-FTICR: matrix assisted laser desorption ionization-Fourier transform ion cyclotron resonance

Ph: phenyl

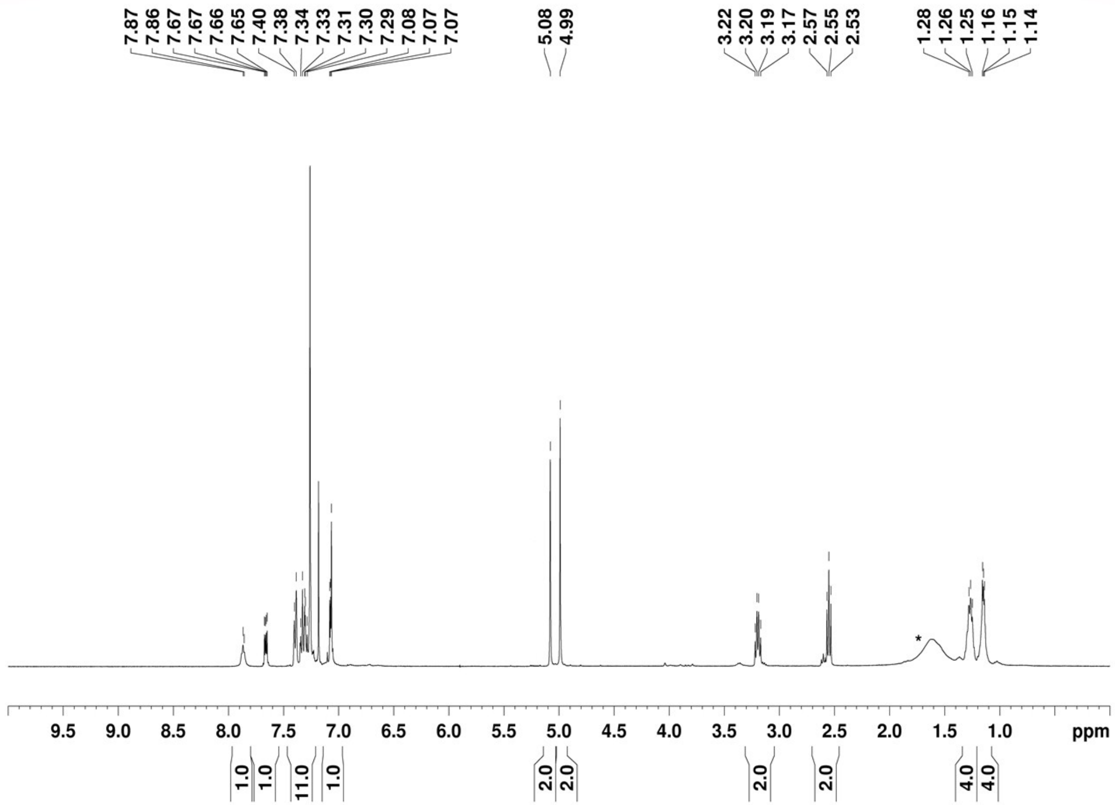
RP-HPLC: reversed-phase high-performance liquid chromatography

TFA: trifluoroacetic acid

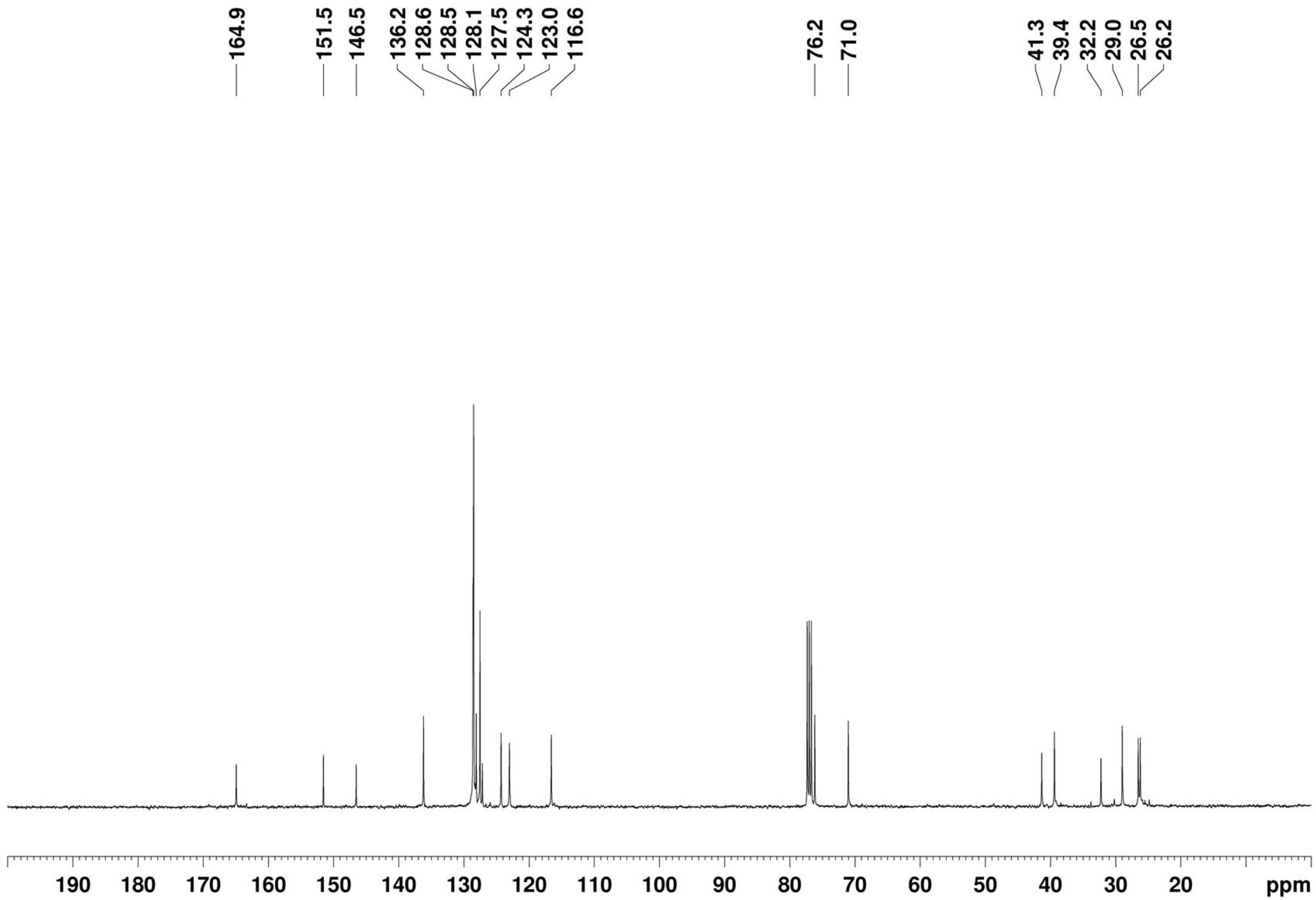
TLC: thin layer chromatography

2.0 ¹H, ¹³C-NMR spectra

2.1 ¹H-, ¹³C-NMR spectra of 8c

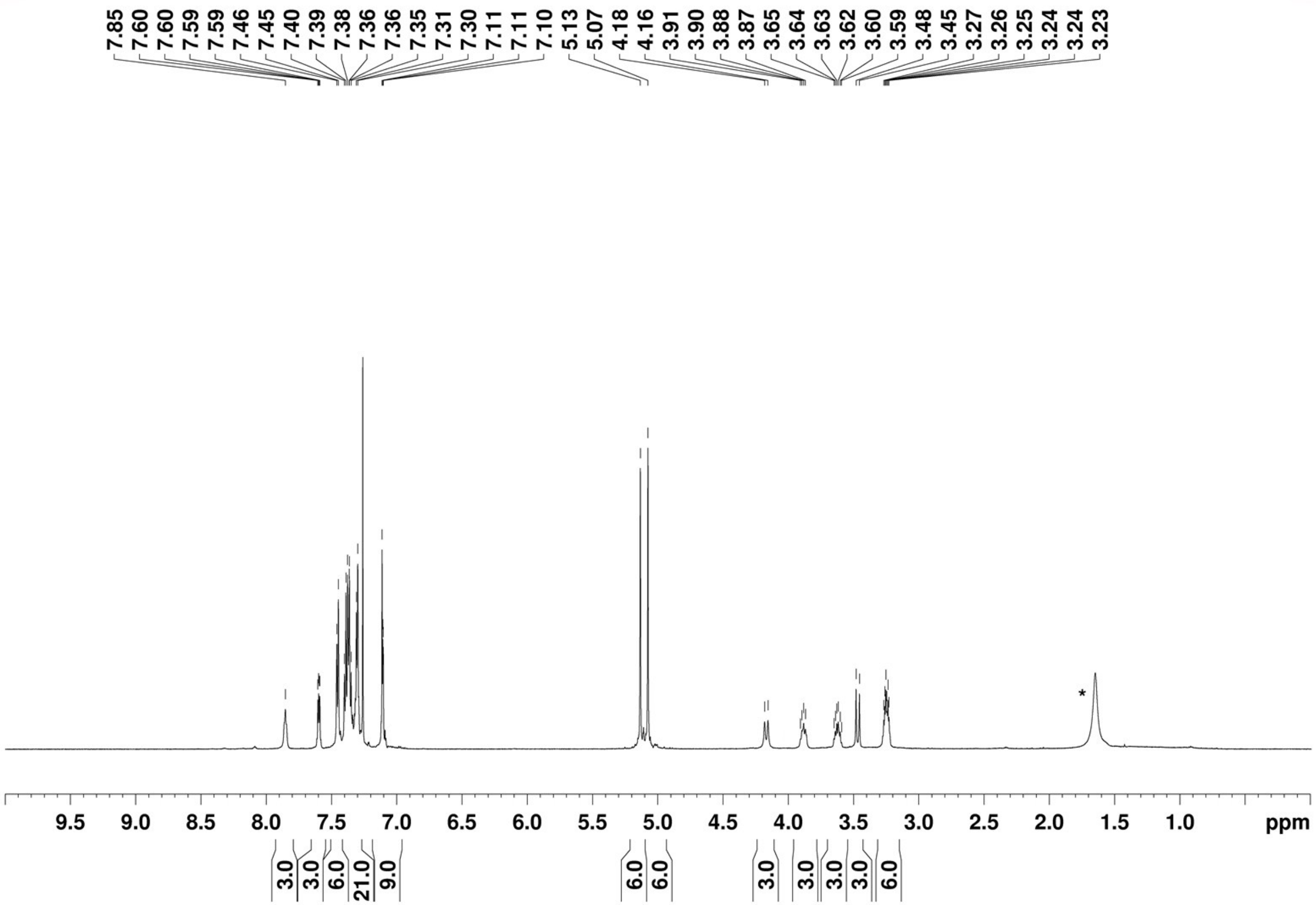


8c: ¹H NMR (400 MHz, $CDCl_3$). Water impurity marked with a black asterisk.

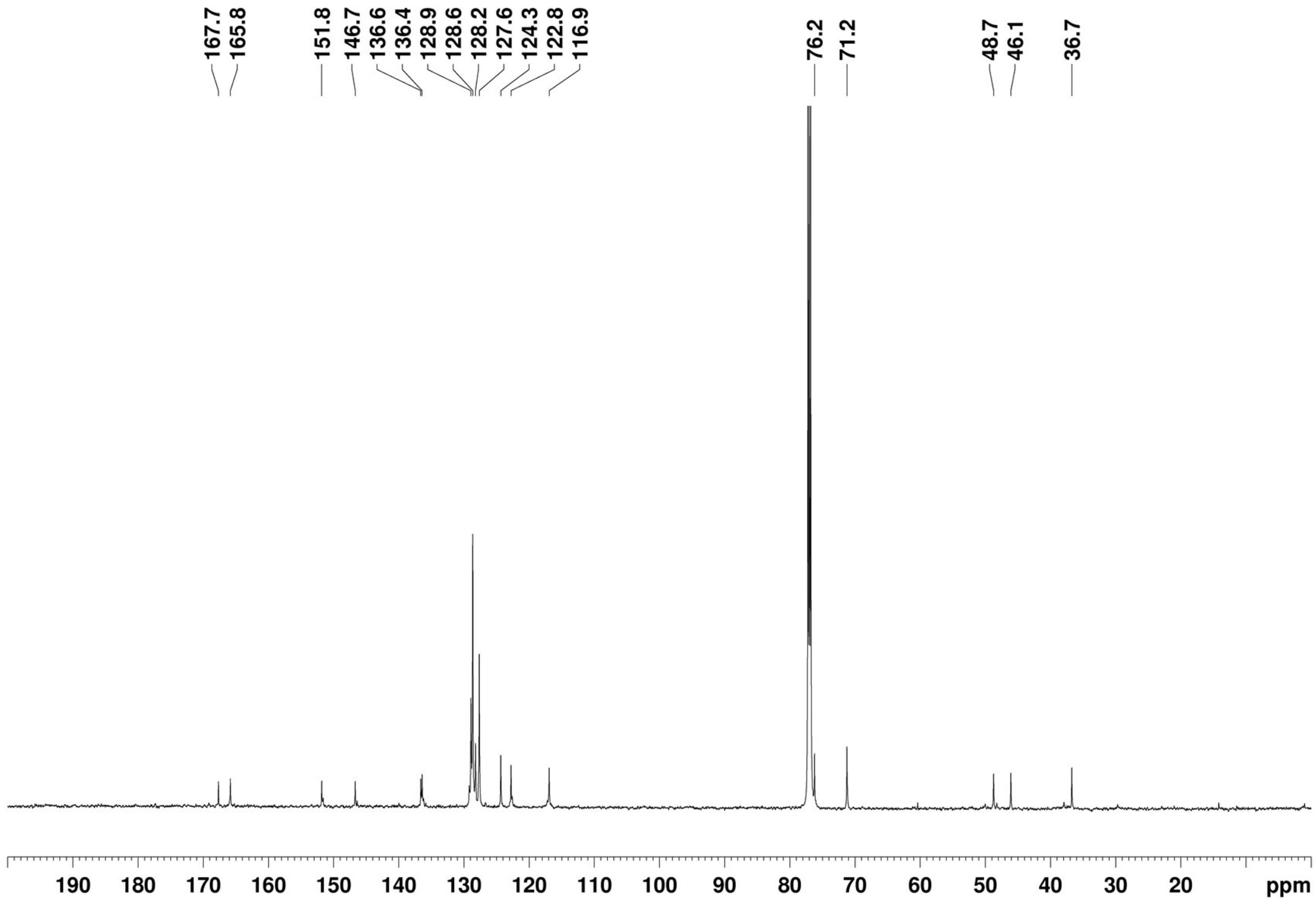


8c: ^{13}C NMR (100 MHz, $CDCl_3$)

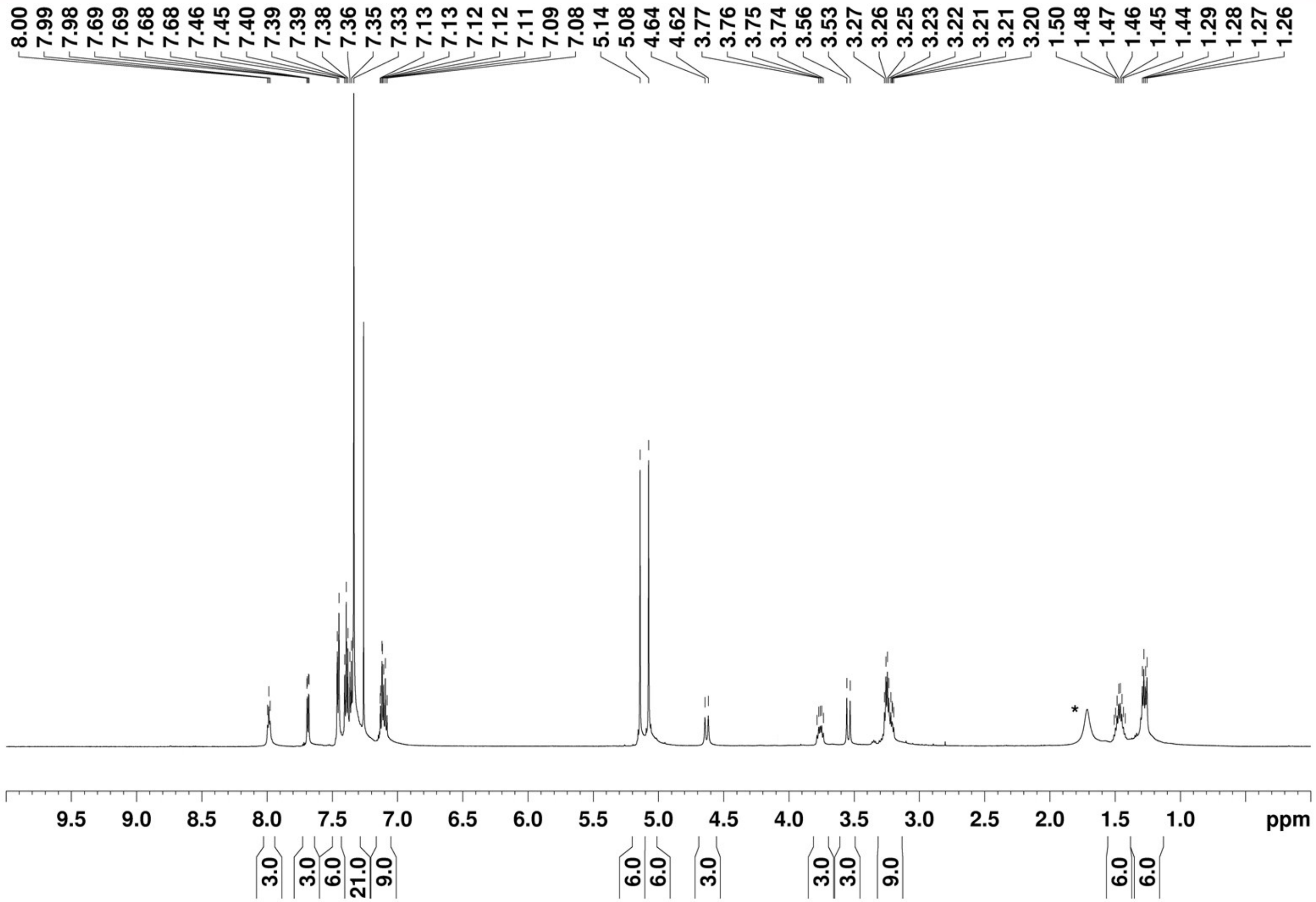
2.2 ¹H-, ¹³C-NMR spectra of cyclic peptoids 10a, 10b, 10c, 3a, 3b, 3c



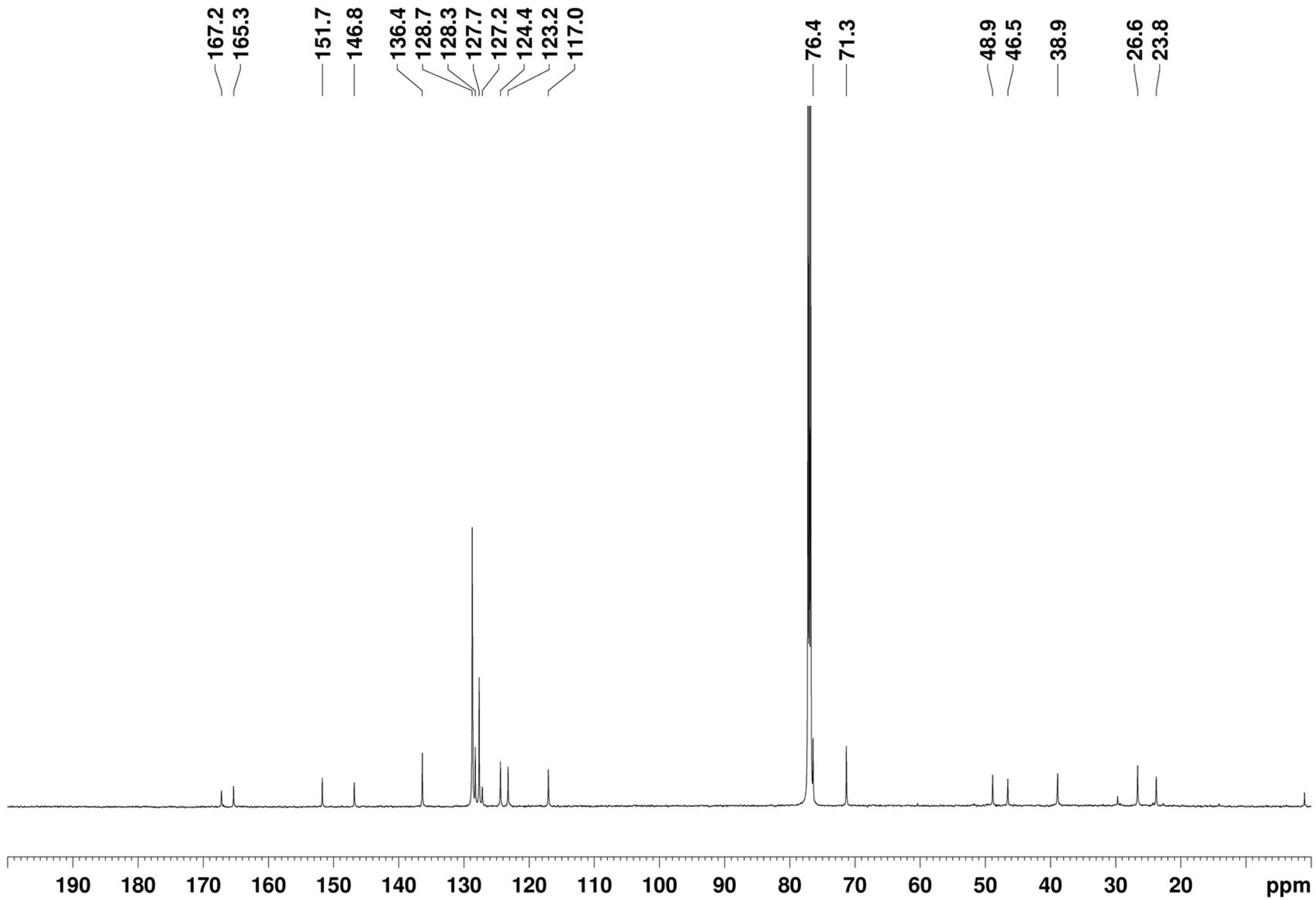
10a: ^{1}H NMR (600 MHz, $CDCl_3$). Water impurity marked with a black asterisk.



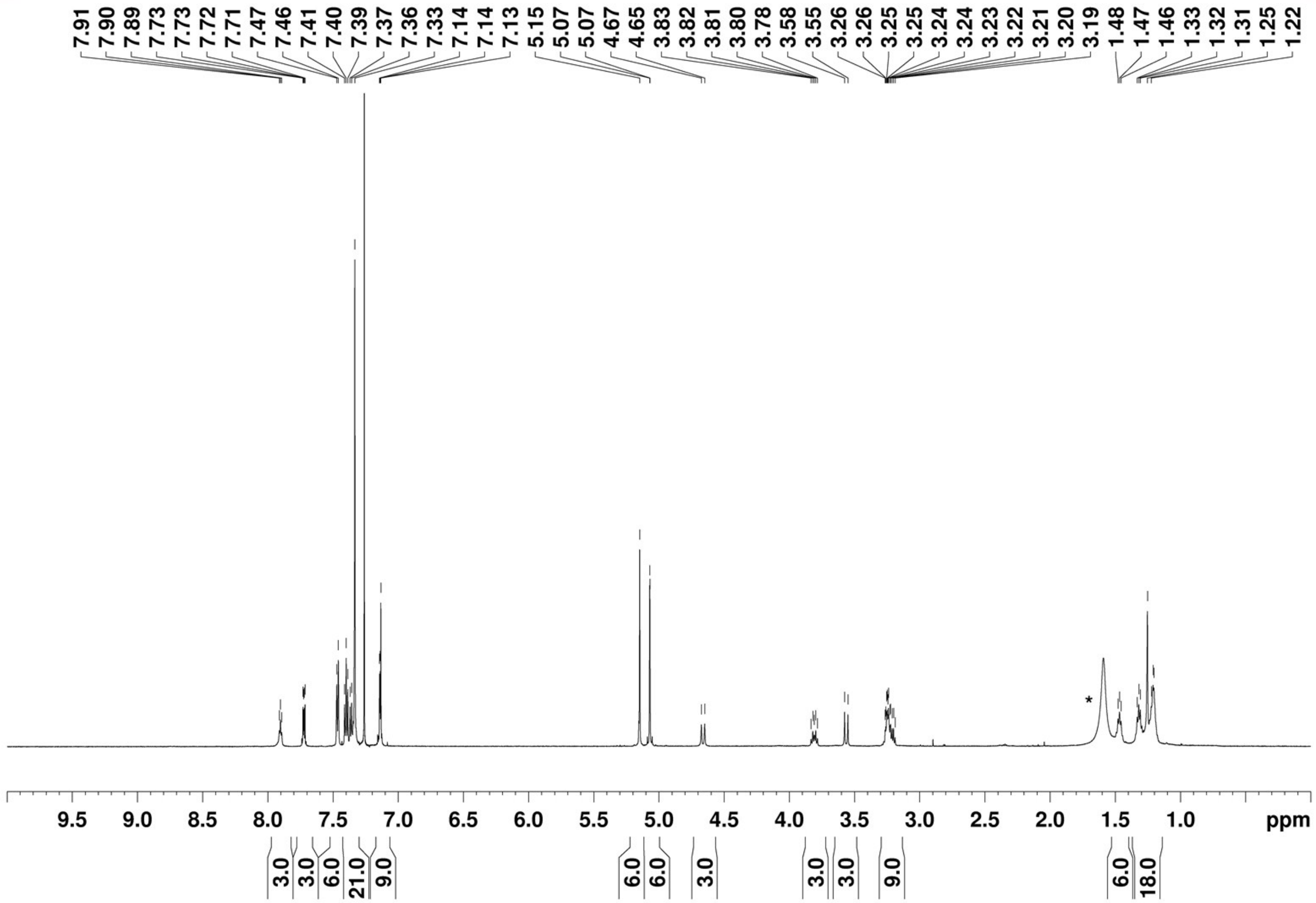
10a: ^{13}C NMR (150 MHz, $CDCl_3$)



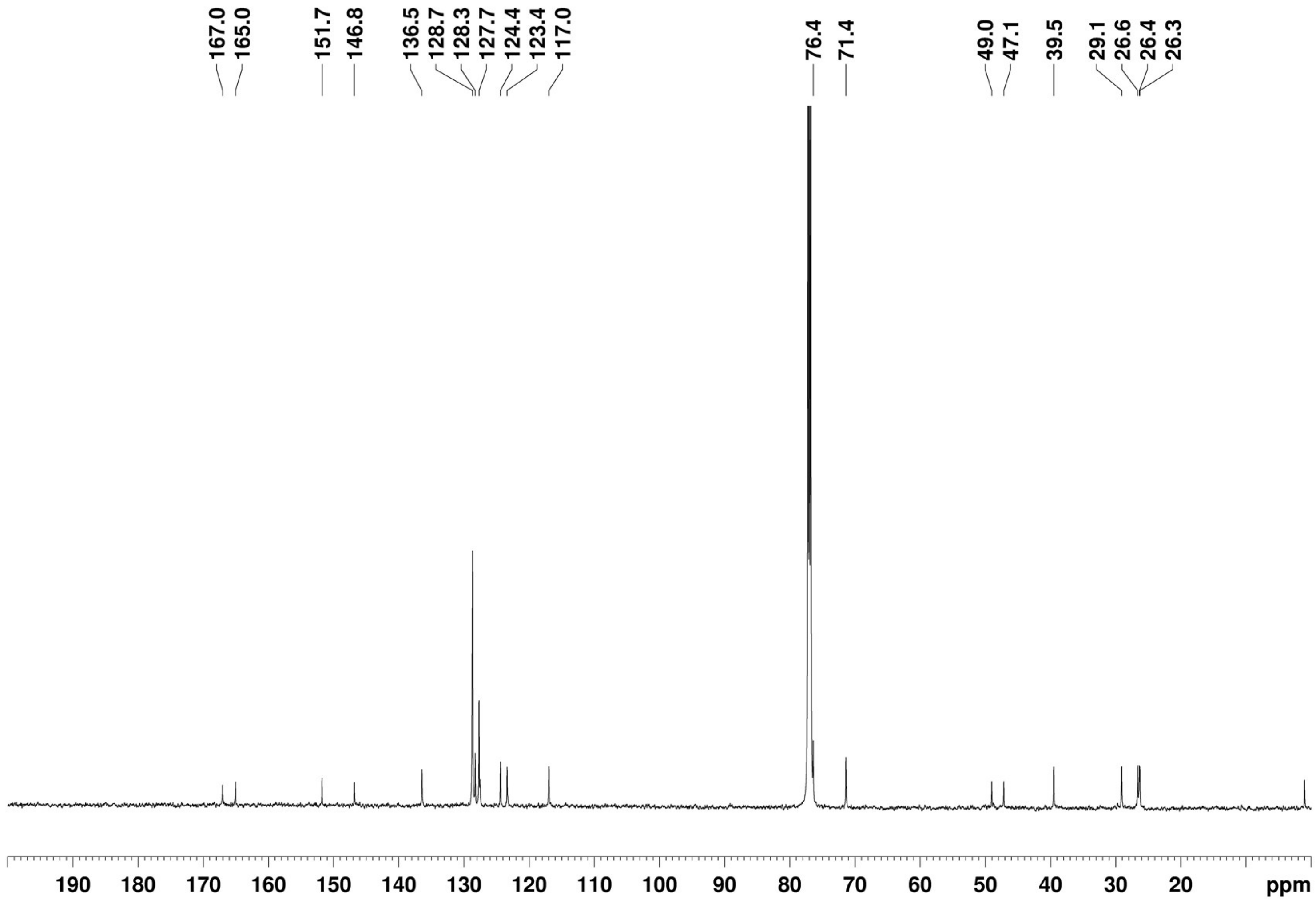
10b: ^{1}H NMR (600 MHz, $CDCl_3$). Water impurity marked with a black asterisk.



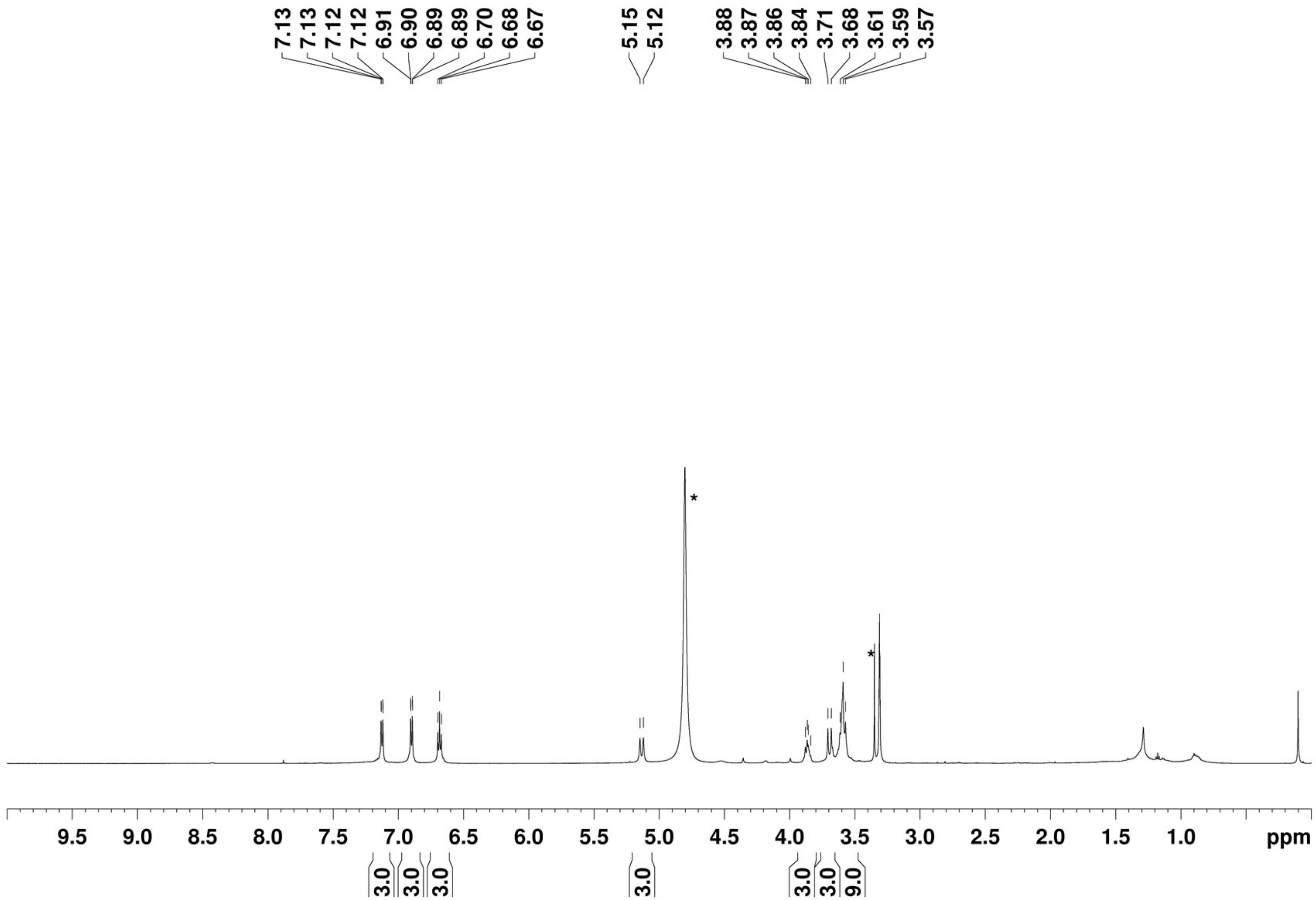
10b: ^{13}C NMR (150 MHz, $CDCl_3$)



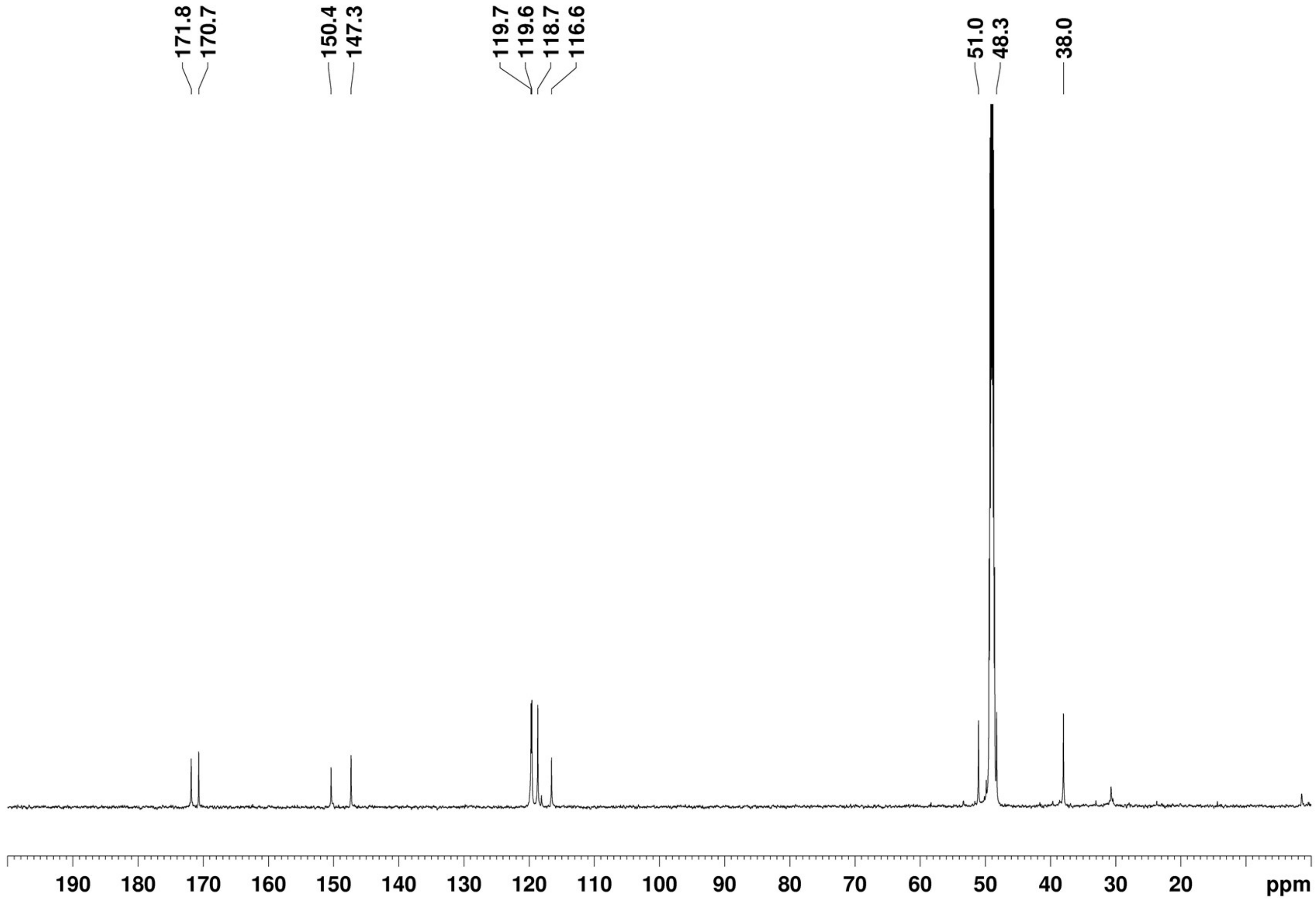
10c: ^{1}H NMR (600 MHz, $CDCl_3$). Water impurity marked with a black asterisk.



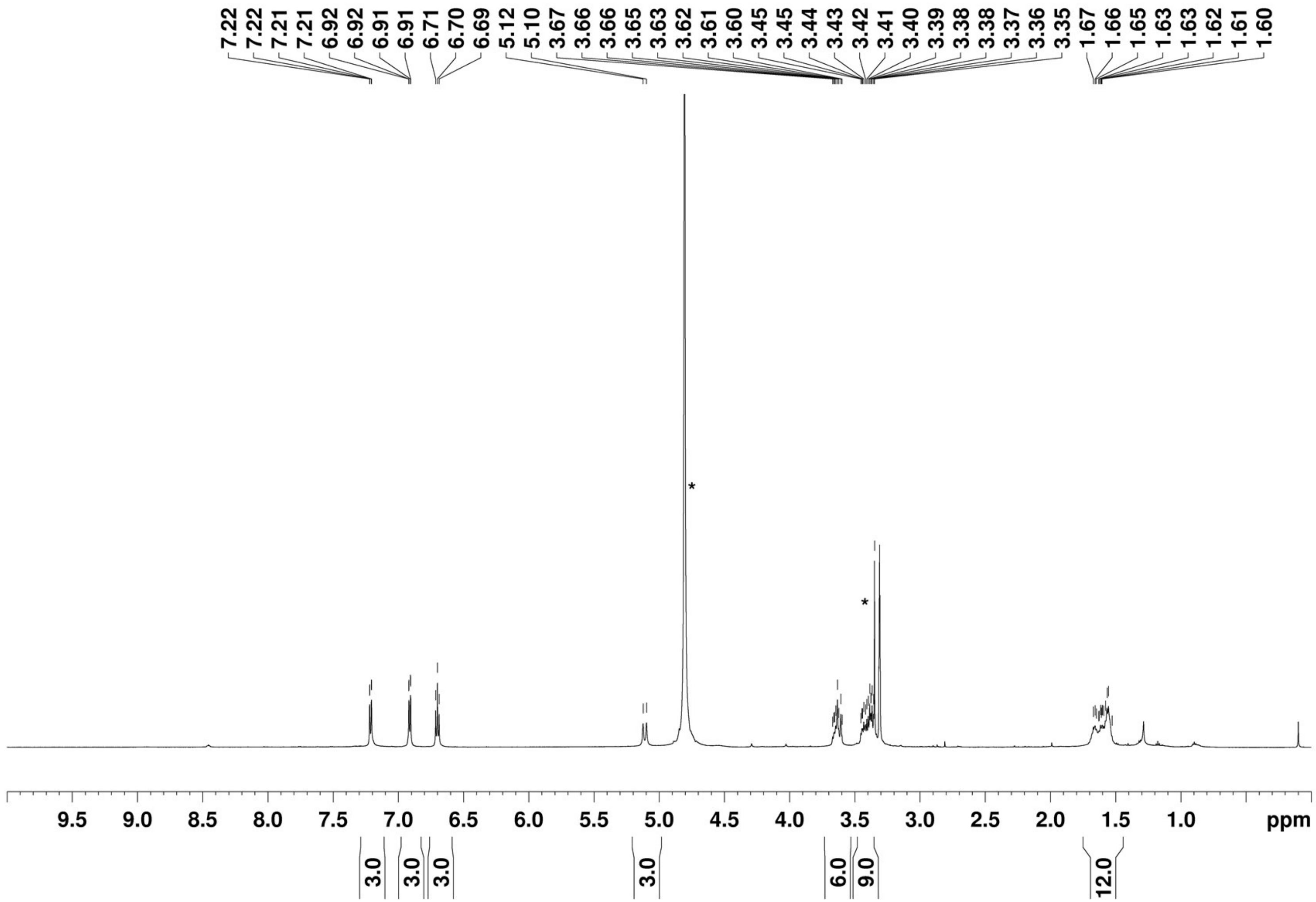
10c: ^{13}C NMR (150 MHz, $CDCl_3$)



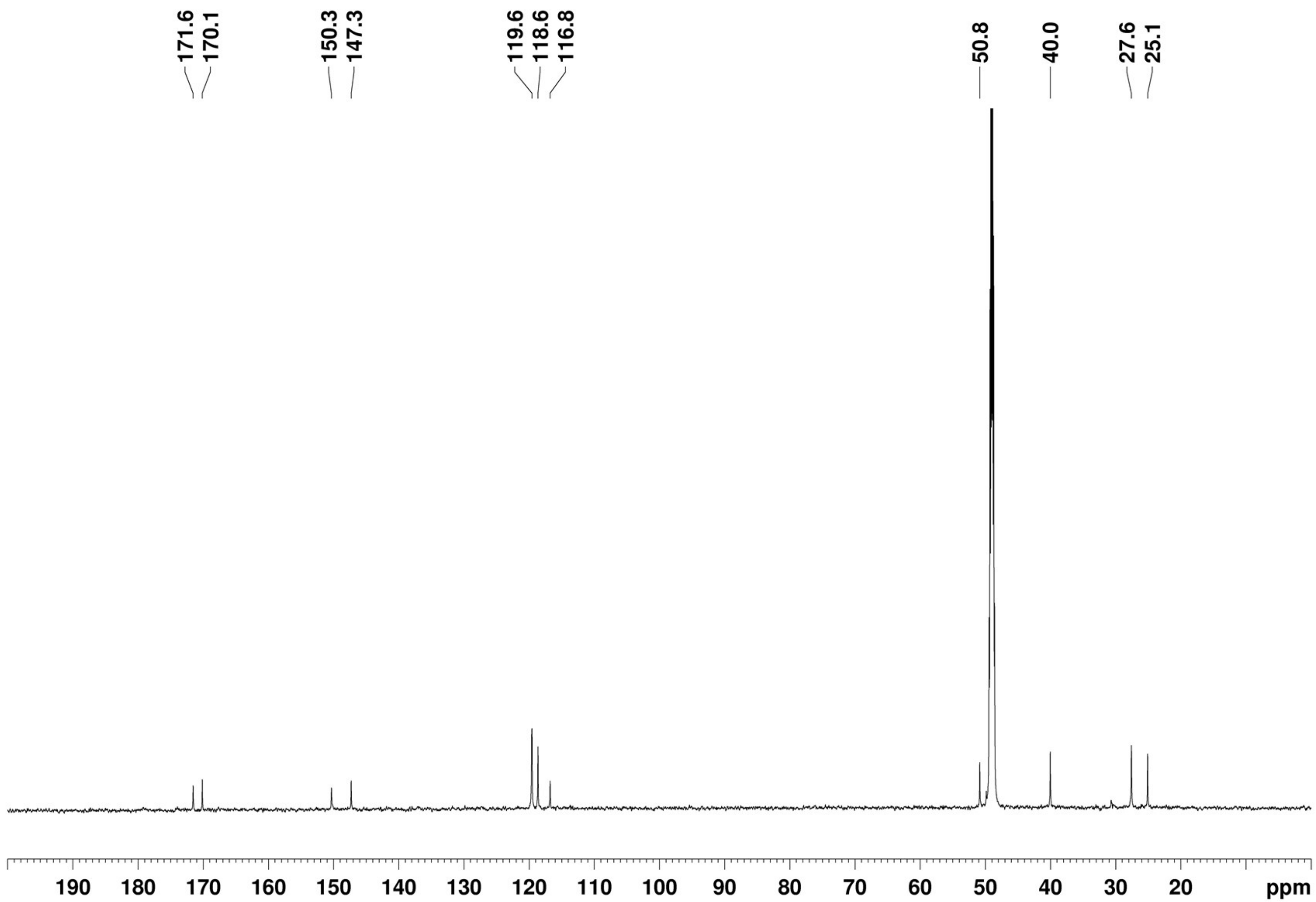
3a: [1]H NMR (600 MHz, CD_3OD). Water impurity and residual solvent marked with a black asterisk.



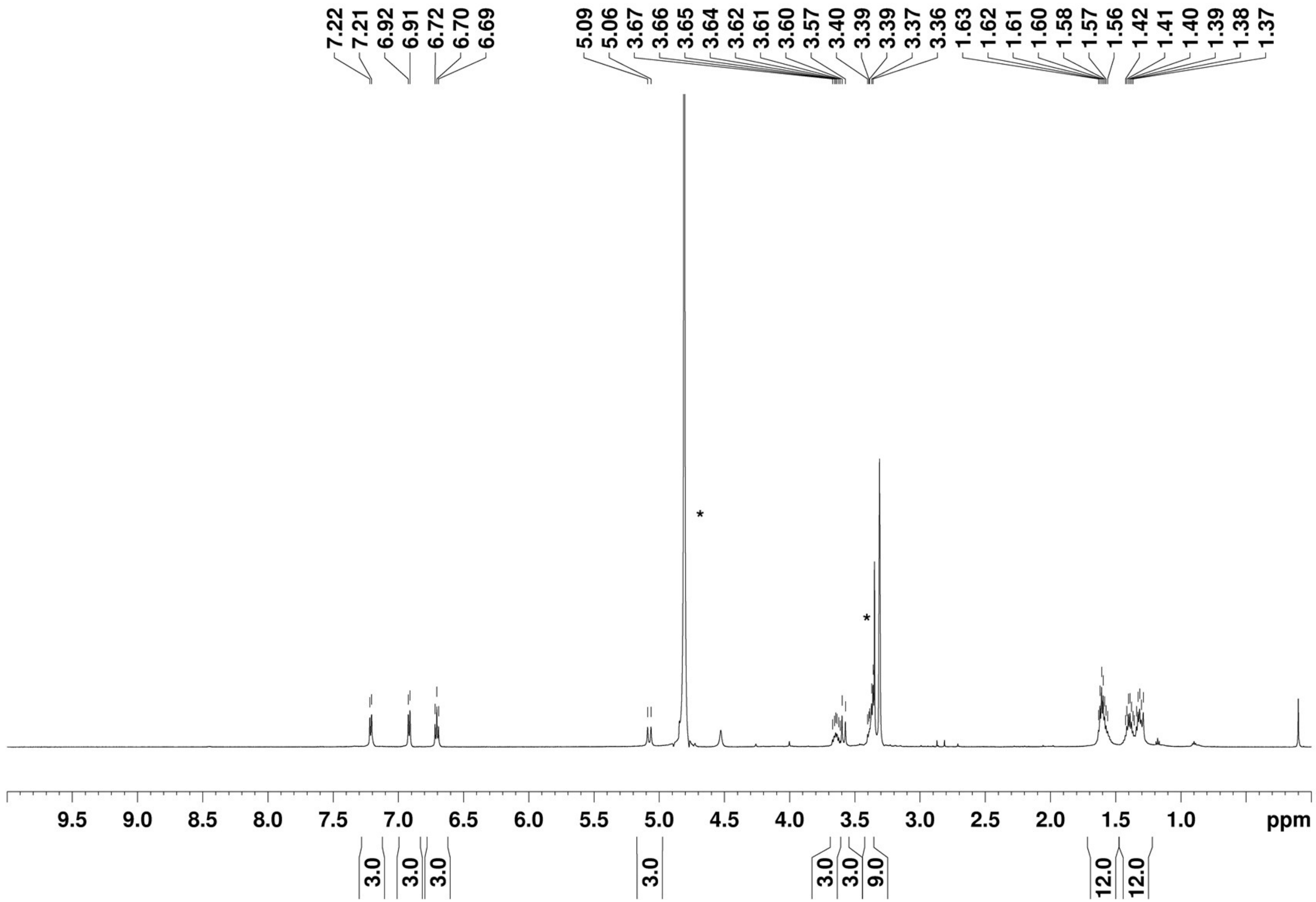
3a: ^{13}C NMR (150 MHz, CD_3OD)



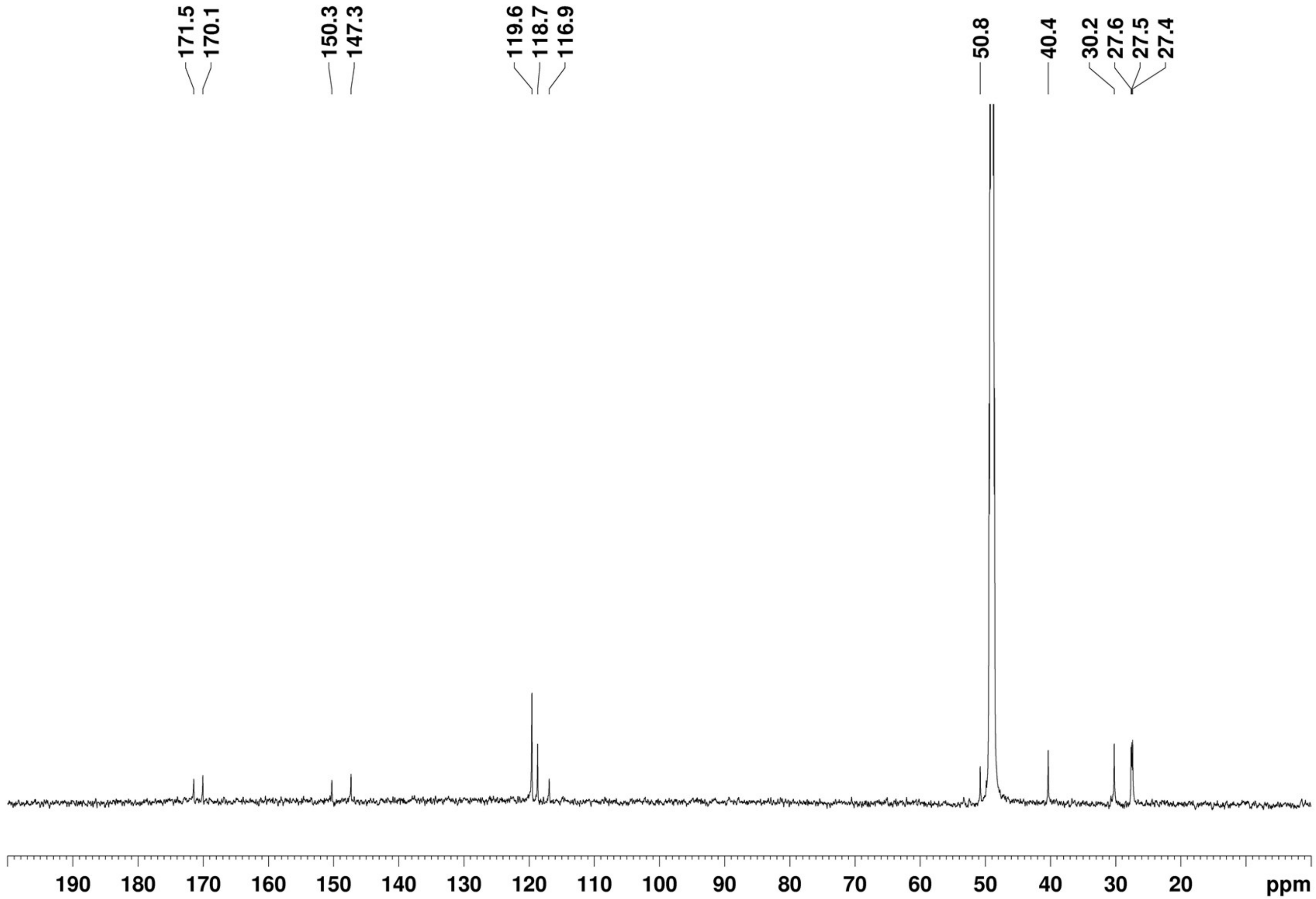
3b: ^{1}H NMR (600 MHz, CD_3OD). Water impurity and residual solvent marked with a black asterisk.



3b: ^{13}C NMR (150 MHz, CD_3OD)



3c: [1]H NMR (600 MHz, CD_3OD). Water impurity and residual solvent marked with a black asterisk.



3c: ^{13}C NMR (150 MHz, CD_3OD)

3.0 HPLC chromatograms

3.1 HPLC chromatograms of linear peptoids 9a, 9b, 9c as crude mixtures (Figure S1-S3)

Conditions: 5 → 100% A in 30 min (A, 0.1% TFA in acetonitrile, B, 0.1% TFA in water); flow: 1 mL min^{-1}, 220 nm.

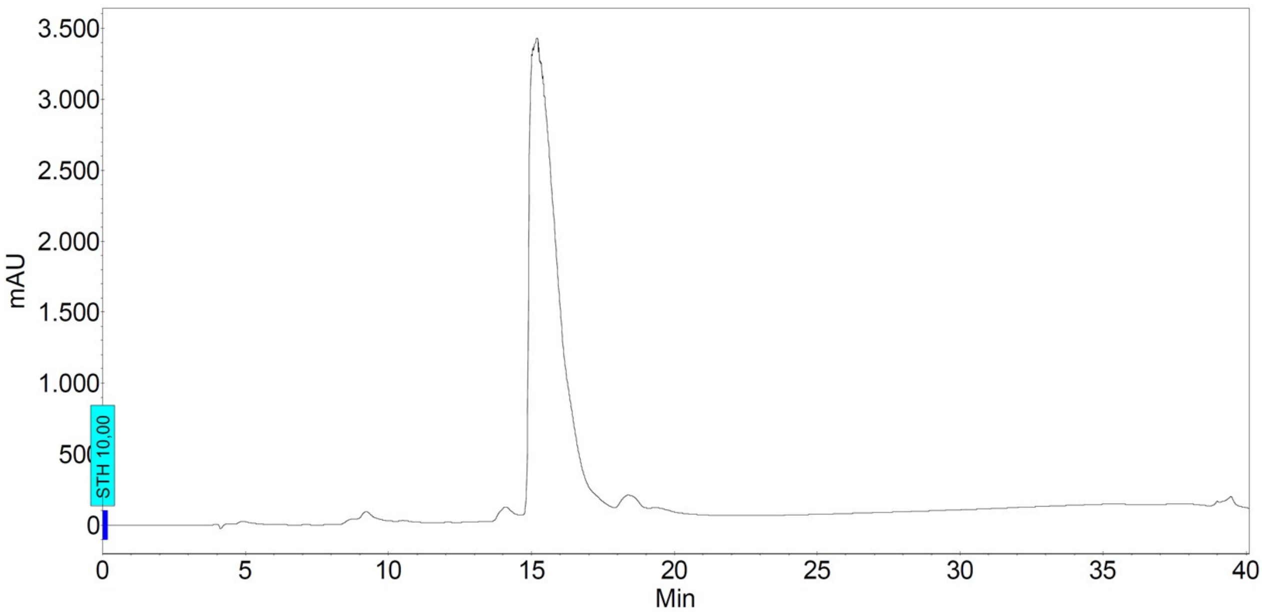


Figure S1. HPLC analysis of **9a**

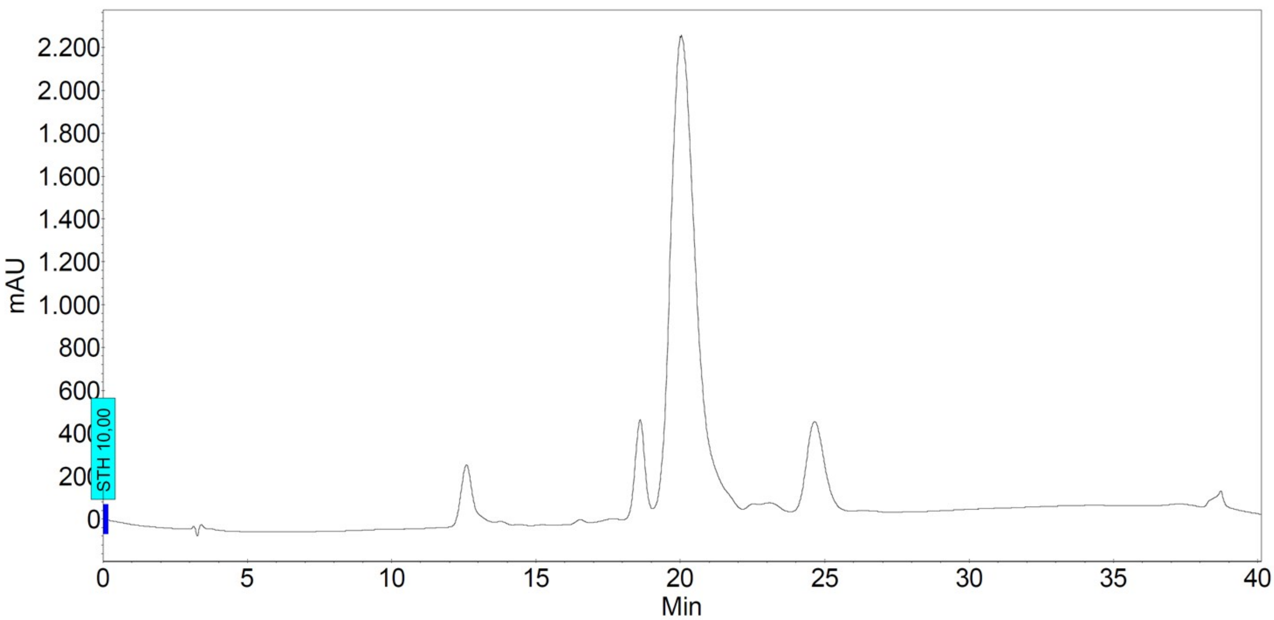


Figure S2. HPLC analysis of **9b**

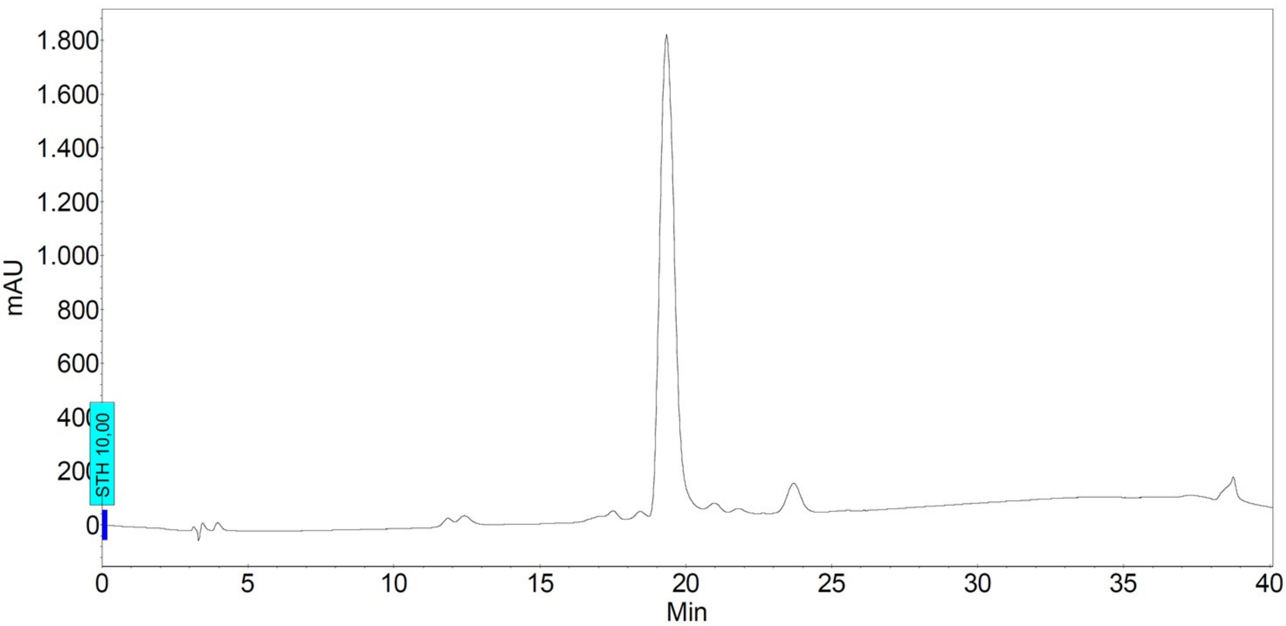


Figure S3. HPLC analysis of **9c**

3.2 HPLC chromatograms of cyclic peptoids 10a, 10b, 10c (Figure S4-S6)

Conditions: 5 → 100% A in 30 min (A, 0.1% TFA in acetonitrile, B, 0.1% TFA in water); flow: 1 mL min^{-1}, 220 nm.

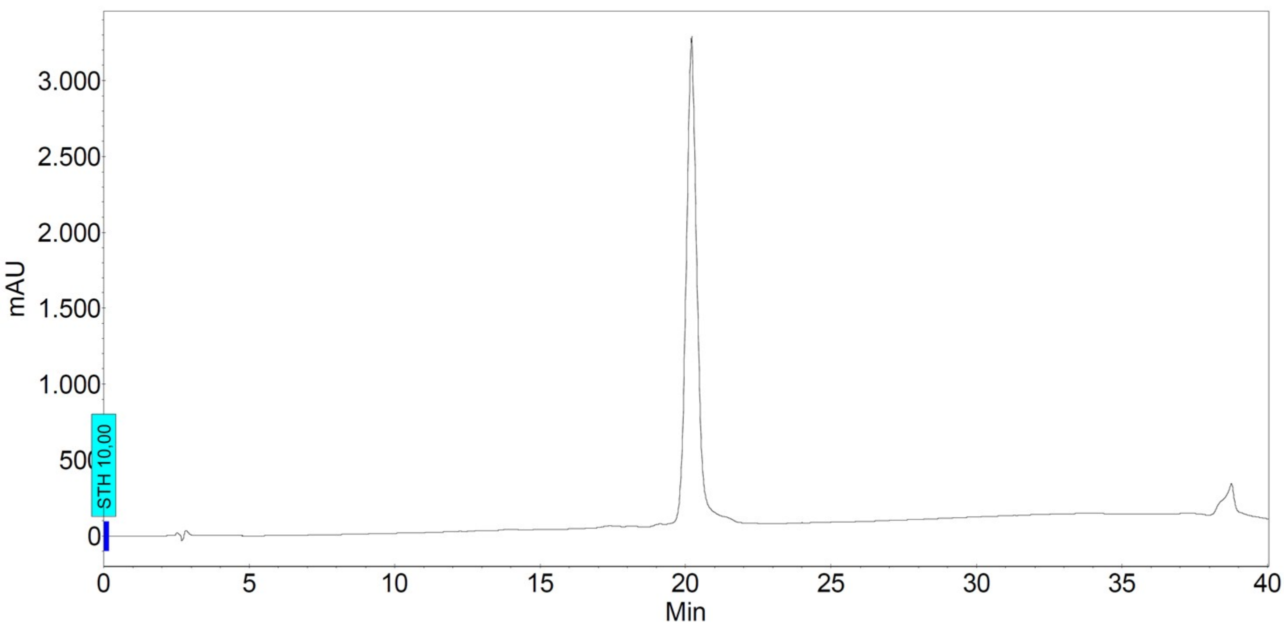


Figure S4. HPLC analysis of **10a**

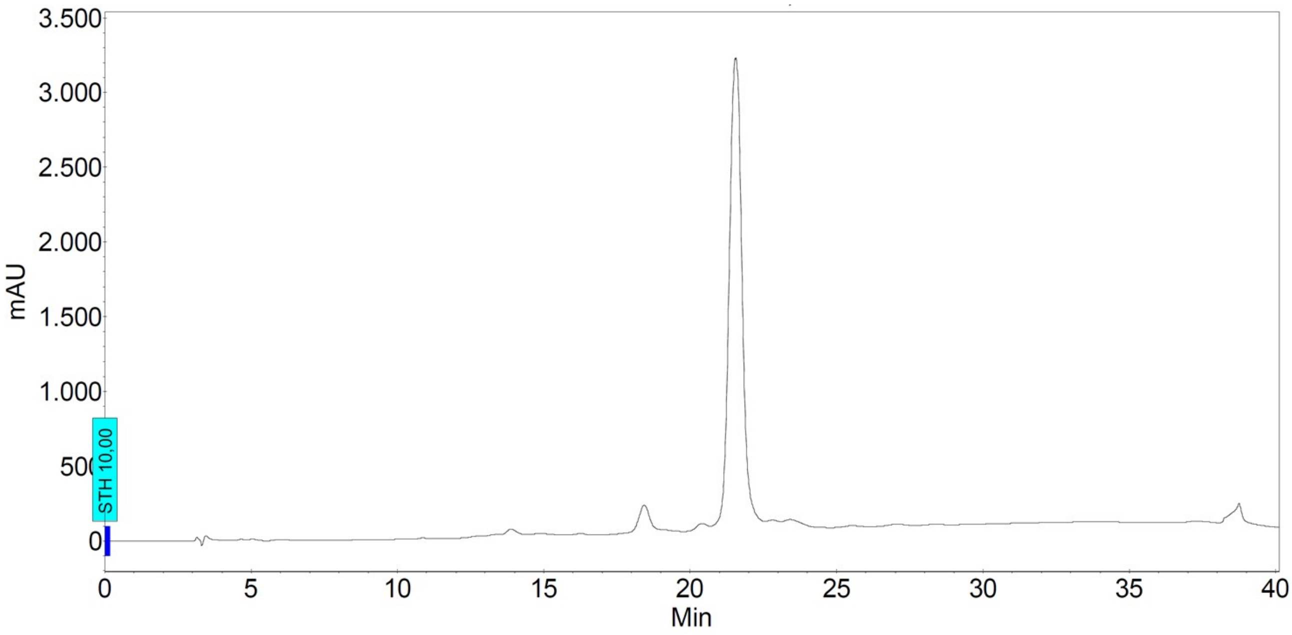


Figure S5. HPLC analysis of **10b**

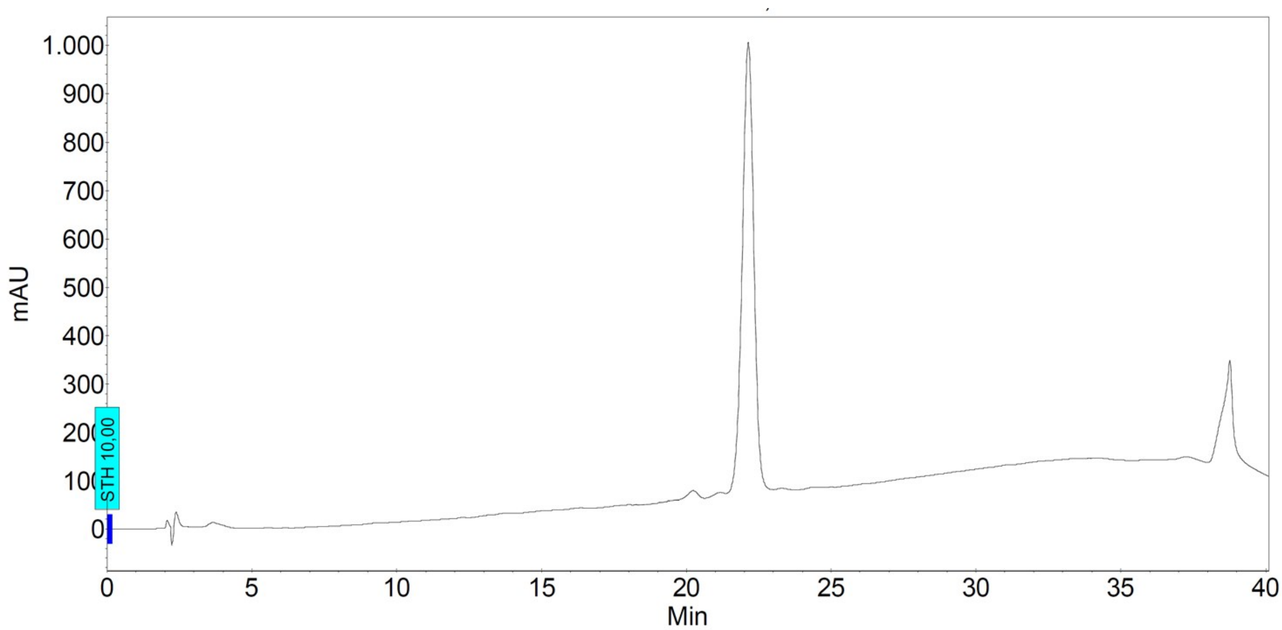


Figure S6. HPLC analysis of **10c**

3.3 HPLC chromatograms of cyclic peptoids 3a, 3b, 3c (Figure S7-S9)

Conditions: 5 → 100% A in 30 min (A, 0.1% TFA in acetonitrile, B, 0.1% TFA in water); flow: 1 mL min^{-1}, 220 nm.

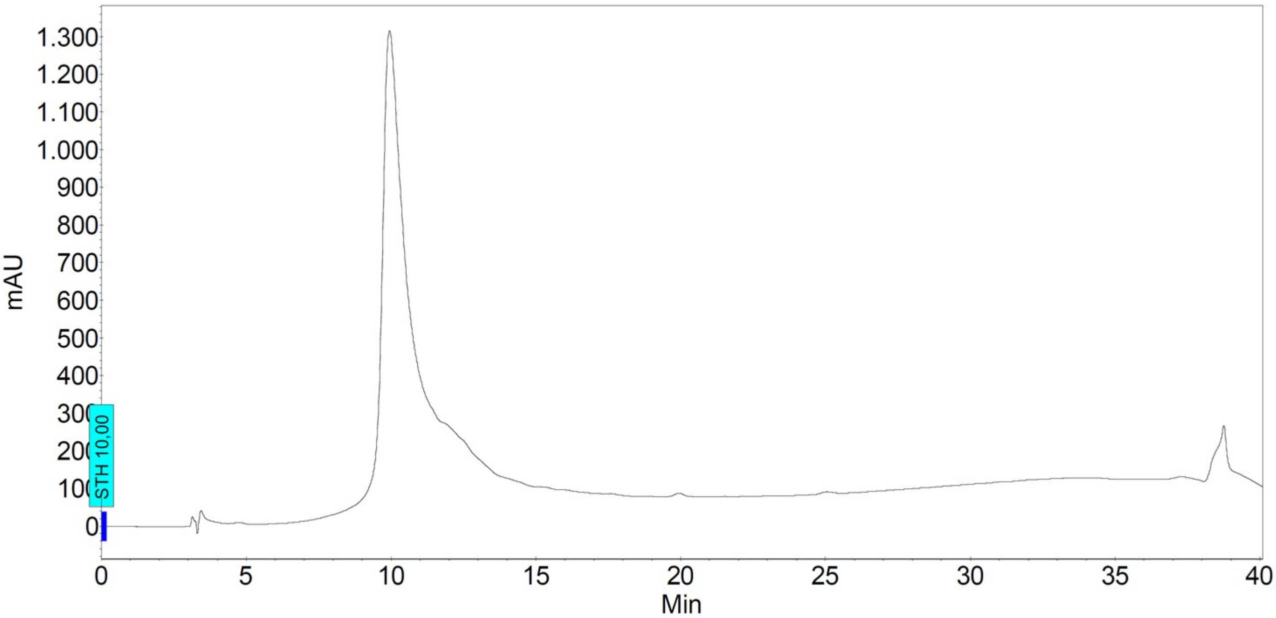


Figure S7. HPLC analysis of **3a**

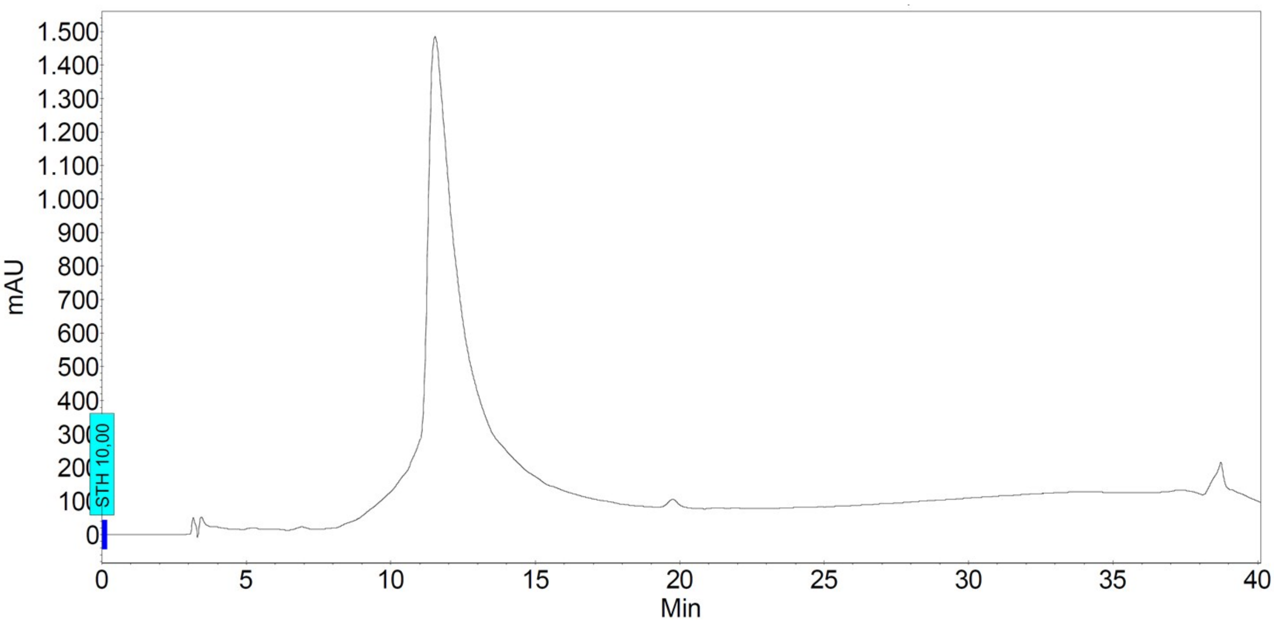


Figure S8. HPLC analysis of **3b**

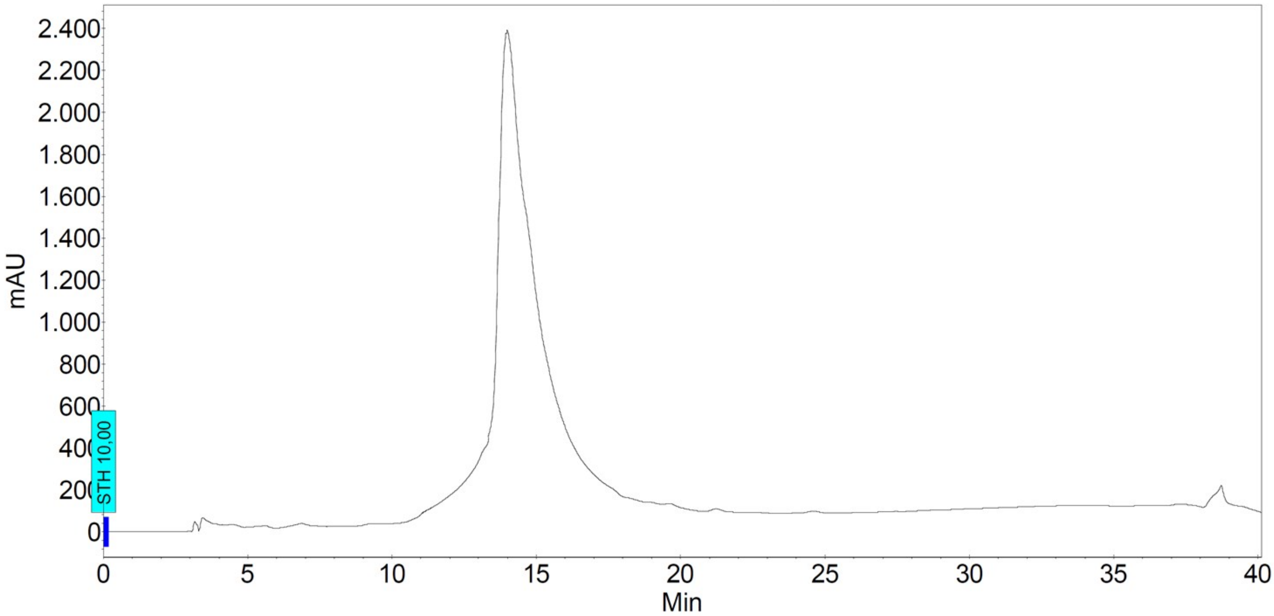


Figure S9. HPLC analysis of **3c**

4.0 UV-Vis titration of 3a-c with metal ions in MeOH (Figure S10-S15)

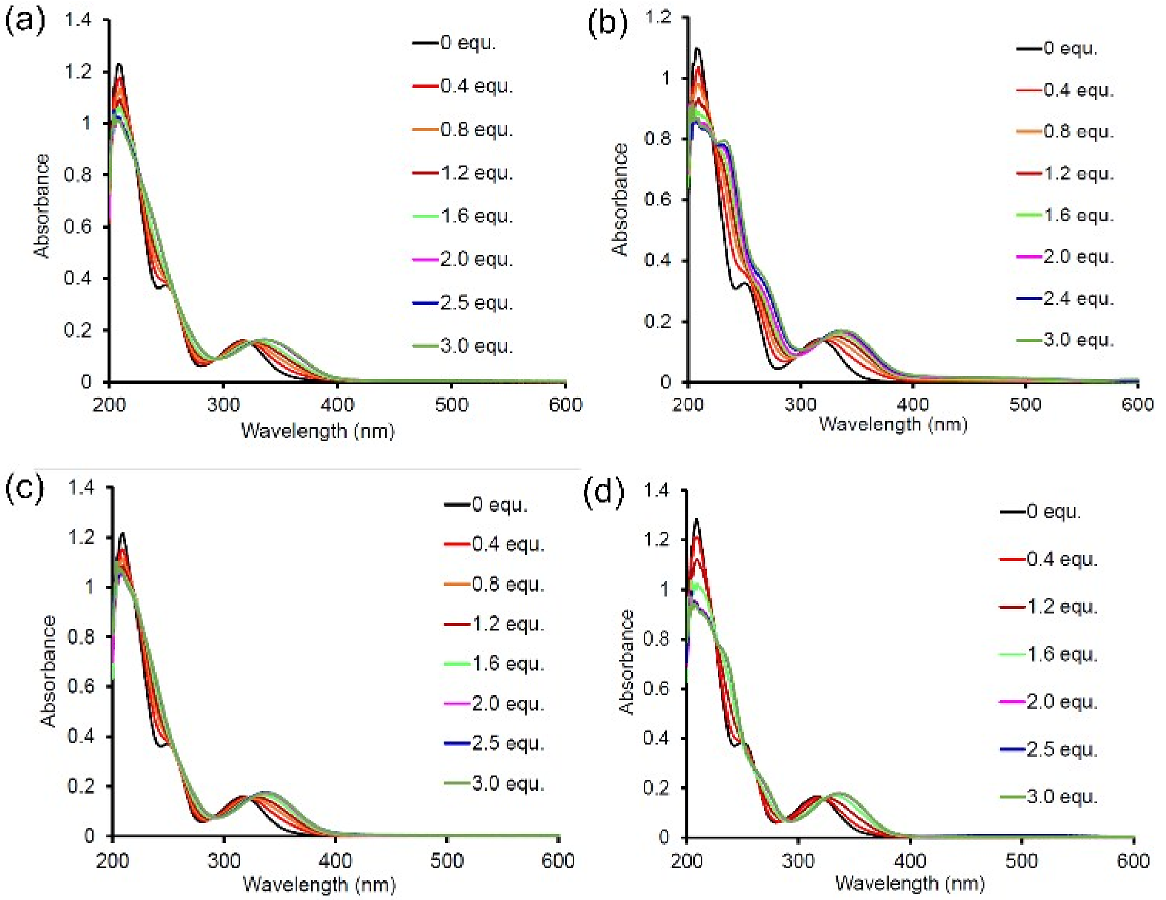


Figure S10. UV-Vis of **3a** with (a) Co^{2+}, (b) Cu^{2+}, (c) Ni^{2+} and (d) Zn^{2+} in methanol, concentration: 17 µM with three equivalents of metal ions.

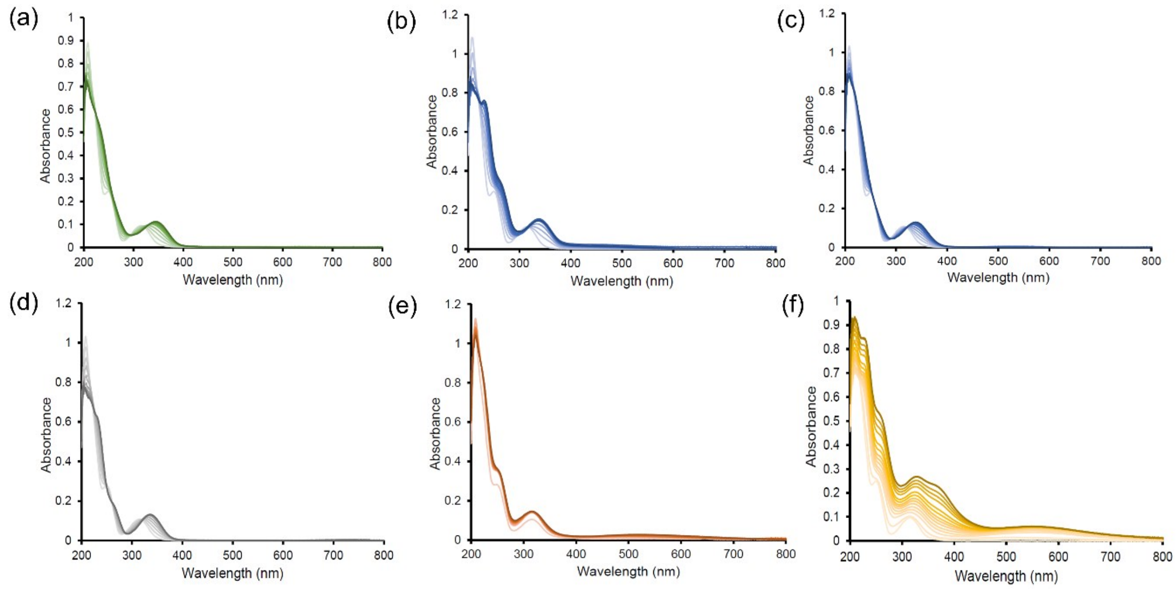


Figure S11. UV-Vis of **3b** with (a) Co^{2+}, (b) Cu^{2+}, (c) Ni^{2+}, (d) Zn^{2+}, (e) Fe^{2+} and (f) Fe^{3+} in methanol, concentration: 17 µM with three equivalents of metal ions.

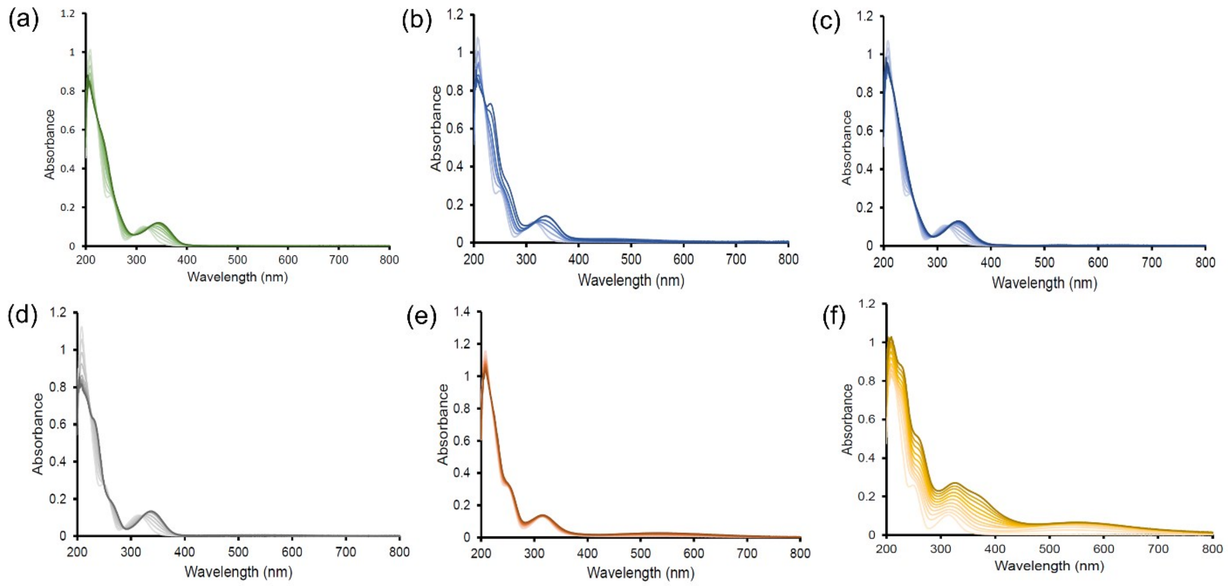


Figure S12. UV-Vis of **3c** with (a) Co^{2+}, (b) Cu^{2+}, (c) Ni^{2+}, (d) Zn^{2+}, (e) Fe^{2+} and (f) Fe^{3+} in methanol, concentration: 17 µM with three equivalents of metal ions.

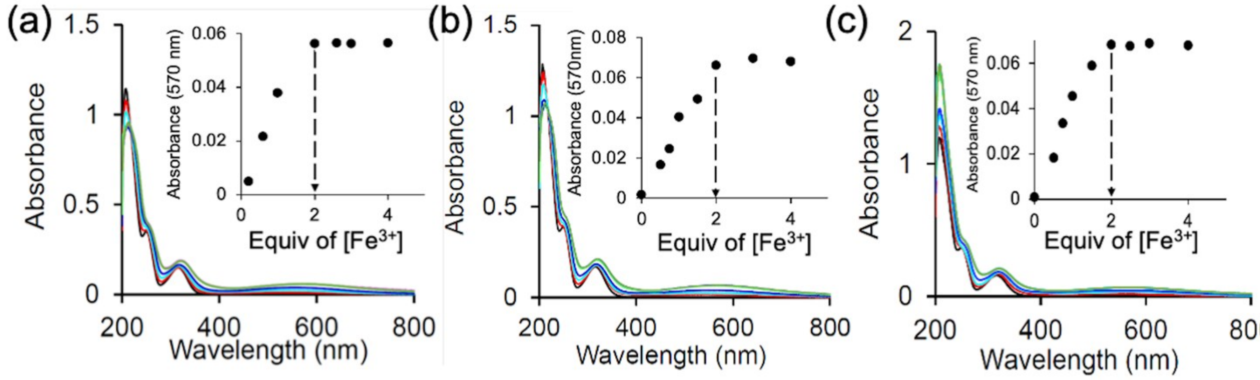


Figure S13. UV-Vis of **3a** with varying counterion of Fe^{3+} (a) Cl^-, (b) ClO_4^- and (c) NO_3^- in methanol, concentration: 17 µM with four equivalents of metal ions.

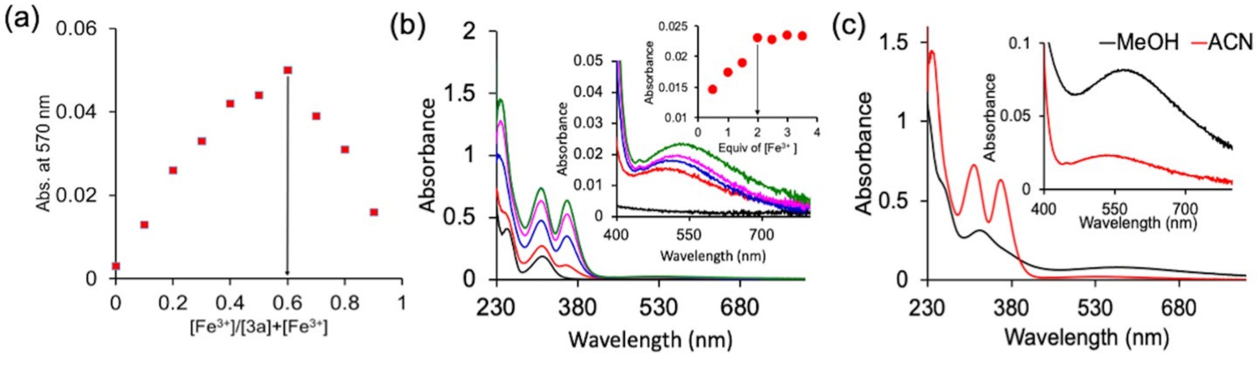


Figure S14. (a) Job's plot analysis of **3a**-Fe^{3+} measured in methanol (17 µM); UV-Vis of (b) titration of **3a** (8 µM) with aliquots addition of 0.5 equivalents Fe^{3+} in acetonitrile [1st inset: expanded view of 400-800 nm range; 2nd inset: metal to peptoid ratio for **3a** with Fe^{3+}], (c) overlapping of the UV-Vis spectra of **3a**-Fe^{3+} complex as obtained from the titration in acetonitrile (8 µM) and methanol (17 µM).

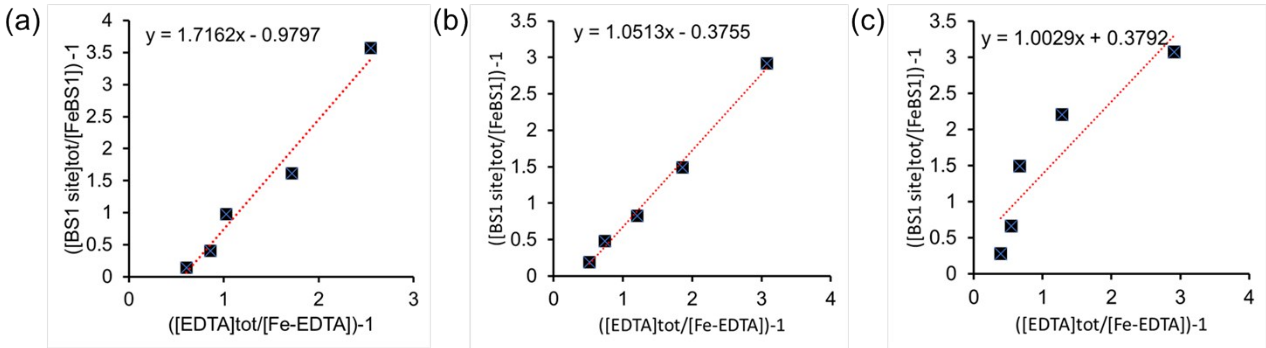


Figure S15. Dissociation constant calculation for the ferric ion complex for (a) **3a**, (b) **3b** and (c) **3c**, method: competition with EDTA.

The experiment has been executed in pH 7, using EDTA as competitor agent. $FeCl_3$. $6H_2O$ is used in the experiment. In pH 7, to correct the formation constant for EDTA's acid–base properties we need to calculate the fraction, $\alpha_{(EDTA)}$.[1]

$K_{A(FeEDTA)}\alpha_{(EDTA)}$ [K_D: Dissociation constant of Fe-Host complex, K_A: Association constant of Fe-EDTA ($5x10^{25}M^{-1}$) and $\alpha_{(EDTA)}$ is the pH correction factor].

Slope= $K_{D(Fe\text{-}\mathbf{peptoid})}$ $K_{A(FeEDTA)}$ $\alpha_{(EDTA)}$, for **3a**: 6.86 x 10^{-19}M, for **3b**: 4.21 x 10^{-19}M and for **3c**: 4.01 x 10^{-19}M.

[1] Harvey D., *Modern Analytical Chemistry, ISBN 0–07–237547–7*, McGraw-Hill.

5.0 ESI-MS spectra of Fe(III) complexes (Figure S16-S18) Advion expression CMS mass spectrometer

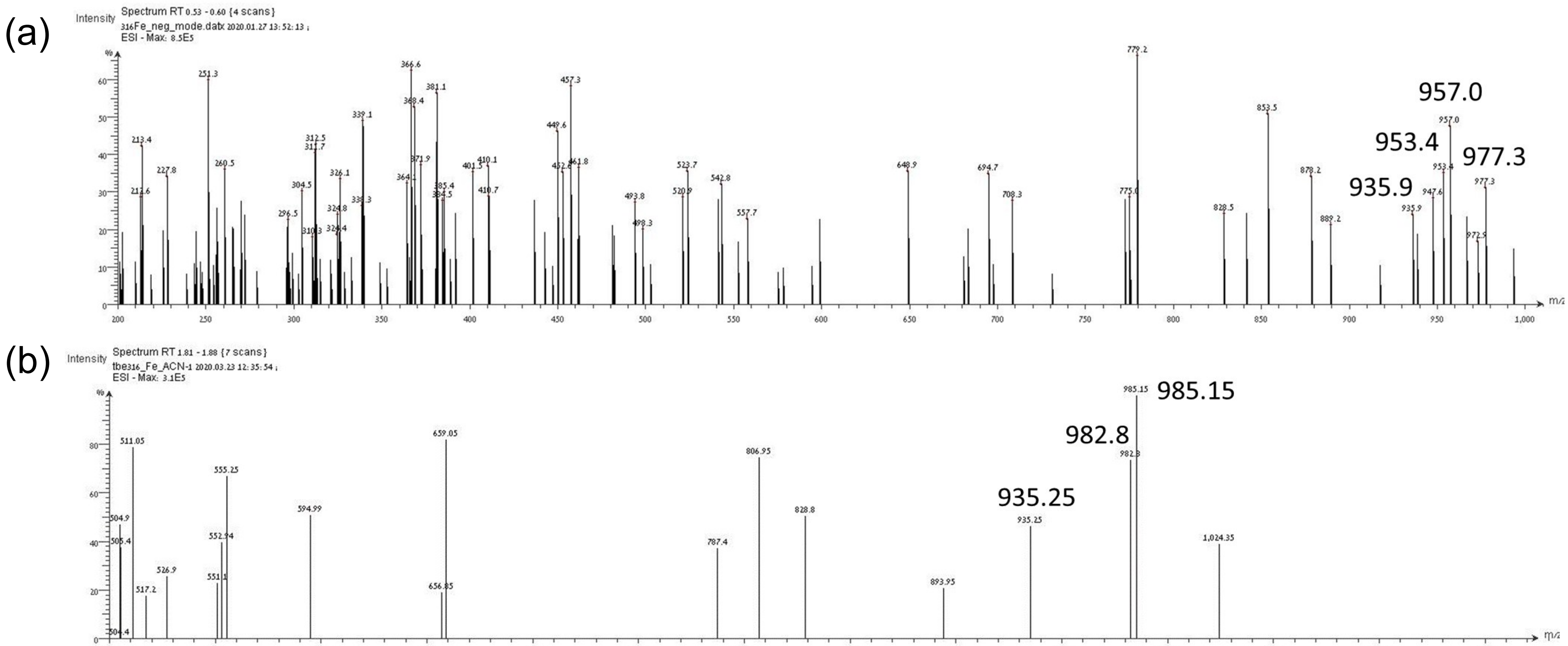


Figure S16. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3a** complex. (a) In methanol: The calculated mass for $[Fe_2($**3a**$)+2H_2O+4CH_3OH-H]^-$ exact mass: 977.18, $[Fe_2($**3a**$)+5H_2O+CH_3OH+Na^+-2H]^-$ exact mass: 957.12, $[Fe_2($**3a**$)+3H_2O+2CH_3OH+Na^+-2H]^-$ exact mass: 953.12, $[Fe_2($**3a**$)+5H_2O+CH_3OH-H]^-$ exact mass: 935.13. (b) In acetonitrile: Calculated mass for $[Fe_2($**3a**$)+4H_2O+2CH_3CN-H]^- \cdot H_2O$ exact mass: 985.16, $[Fe_2($**3a**$)+5H_2O+CH_3CN+K^+-2H]^-$ exact mass: 982.53, $[Fe_2($**3a**$)+5H_2O+CH_3OH-H]^-$ exact mass: 935.13 (as the methanolic stock solution of **3a** was used during titration, coordination of methanol is plausible).

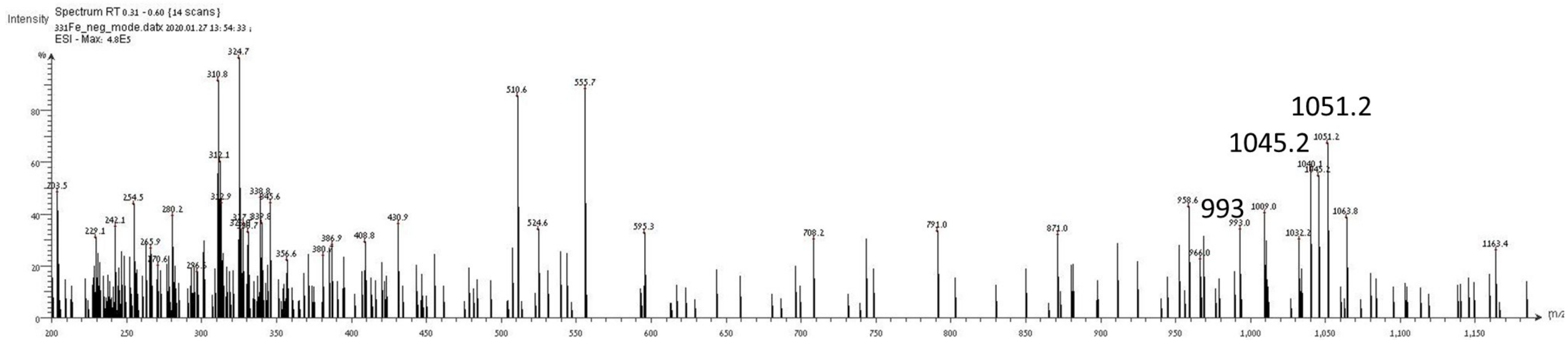


Figure S17. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3b** complex in methanol. The calculated mass for [Fe_2(**3b**)+$5H_2O$+CH_3OH-H]$^{-}$·CH_3OH, exact mass: 1051.25, [Fe_2(**3b**)+$6H_2O$+Na^{+}-2H]$^{-}$·H_2O, exact mass: 1045.20, [Fe_2(**3b**)+$3CH_3OH$-H]$^{-}$ exact mass: 993.23.

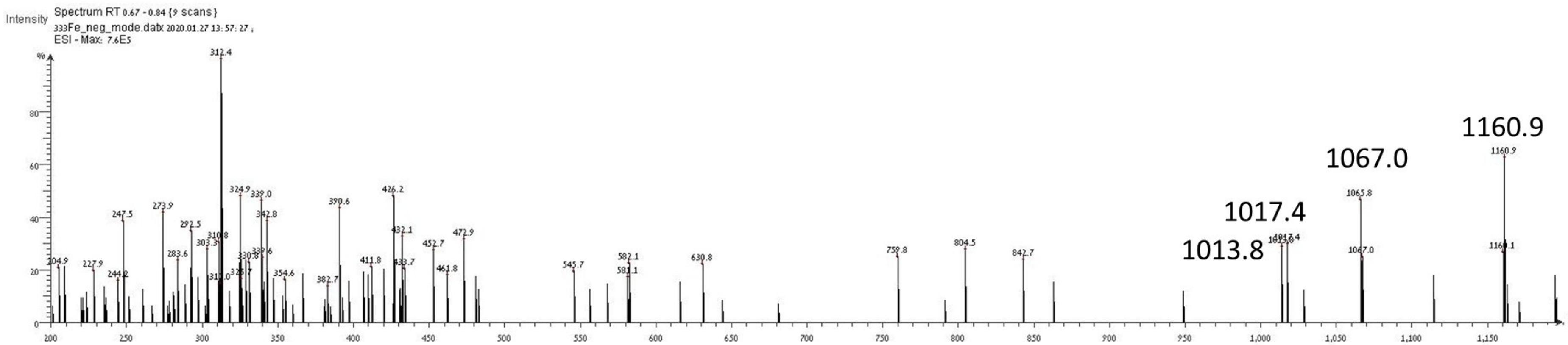


Figure S18. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3c** complex in methanol. The calculated mass for [Fe_2(**3c**)+$6H_2O$-H]$^{-}$·$4H_2O$ exact mass: 1161.35, [Fe_2(**3c**)+$3H_2O$+CH_3OH-H]$^{-}$, exact mass: 1067.30, [Fe_2(**3c**)+$2H_2O$-H]$^{-}$, exact mass: 1017.26, [Fe_2(**3c**)+CH_3OH-H]$^{-}$, exact mass: 1013.27.

6.0 ESI-MS spectra of Fe(III) complexes (Figure S19-S24) with Bruker Maxis impact instrument plus isotopic analysis

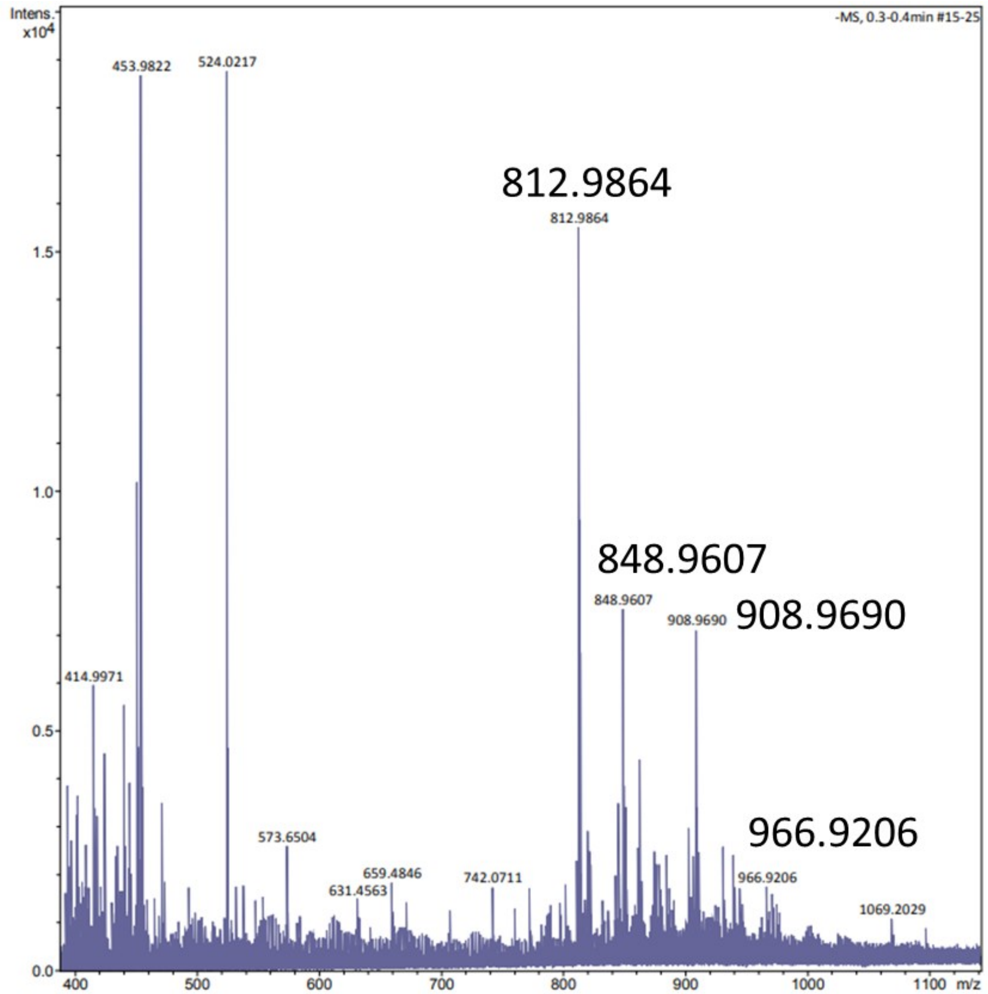


Figure S19. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3a** complex in methanol. The calculated mass for [Fe_2(**3a**)+$4H_2O$+$2CH_3OH$-H]$^{-}\cdot H_2O$ exact mass: 967.16, [Fe_2(**3a**)+$3CH_3OH$-H]$^-$ exact mass: 909.13, [Fe_2(**3a**)+$2H_2O$-H]$^-$ exact mass: 849.08, [Fe_2(**3a**)-H]$^-$ exact mass: 813.05.

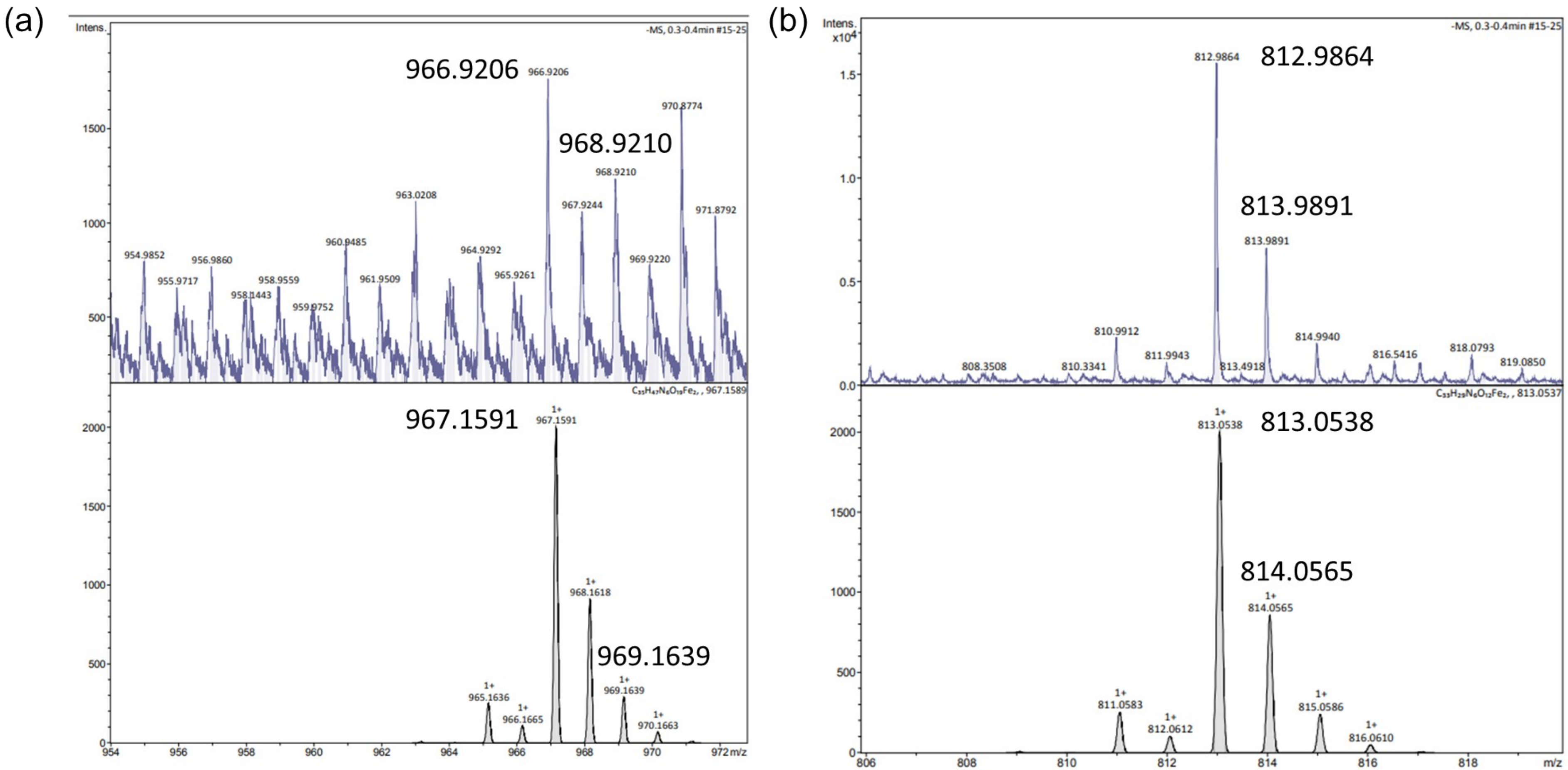


Figure S20. Experimental isotopic analysis by ESI-MS(-ve mode) of Fe^{3+}-**3a** complex (top) and calculated ESI-MS spectrum (bottom). The calculated mass for (a) [Fe_2(**3a**)+4H_2O+2CH_3OH-H]$^-$·H_2O exact mass: 967.16; (b) [Fe_2(**3a**)-H]$^-$ exact mass: 813.05.

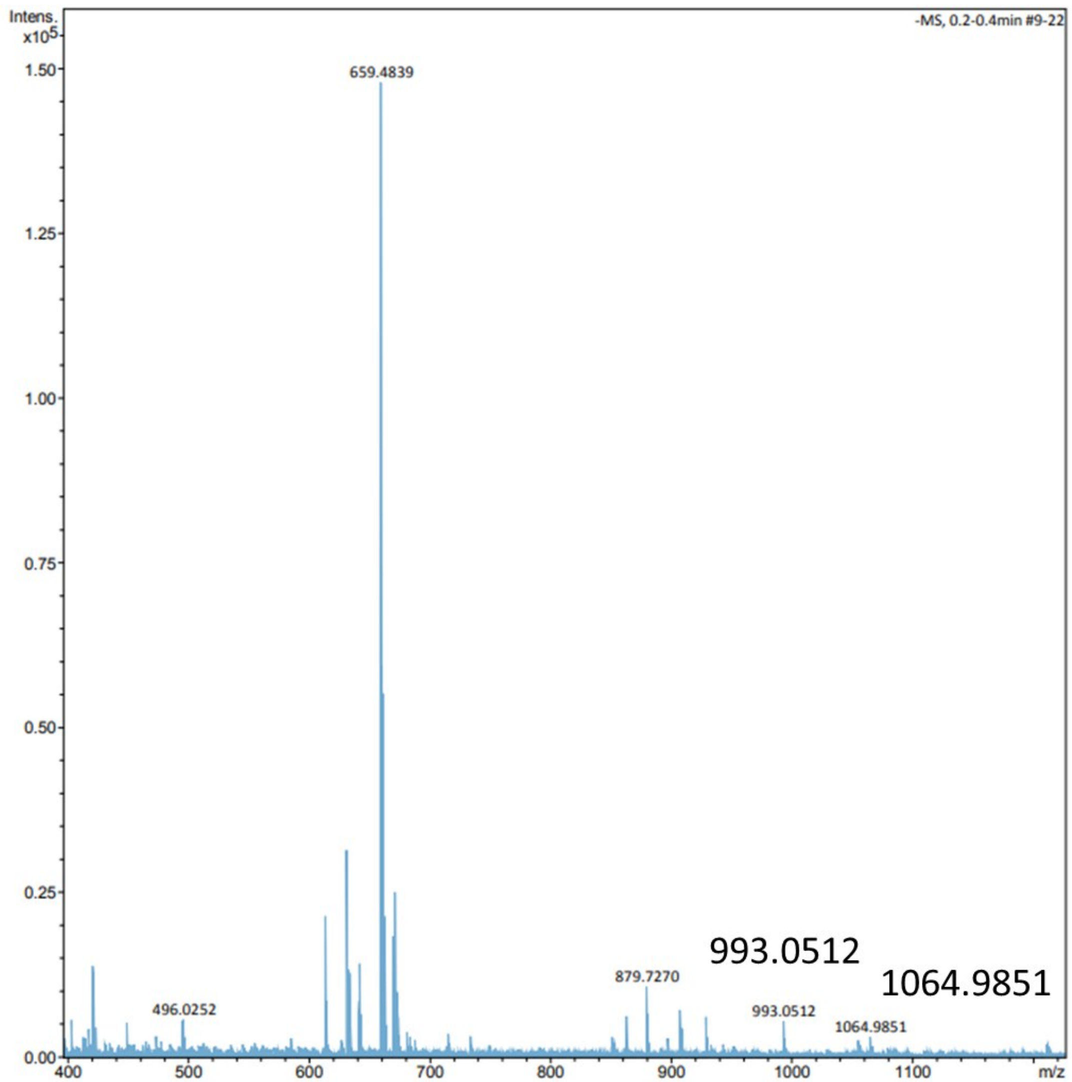


Figure S21. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3b** complex in methanol. The calculated mass for $[Fe_2(\mathbf{3b})+6H_2O+Na^{+}+K^{+}-3H]^{-}$, exact mass: 1065.15, $[Fe_2(\mathbf{3b})+3CH_3OH-H]^{-}$ exact mass: 993.23.

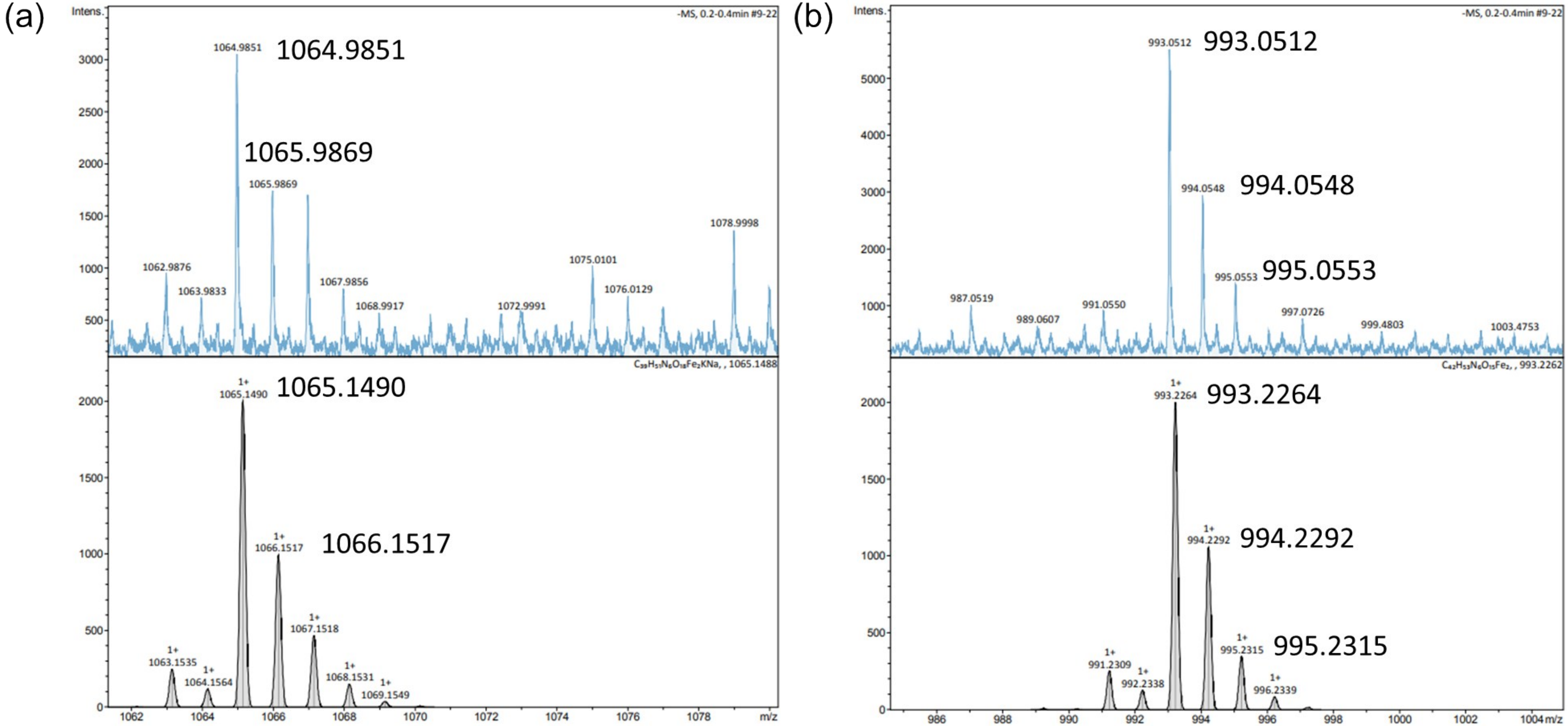


Figure S22. Experimental isotopic analysis by ESI-MS(-ve mode) of Fe^{3+}-**3b** complex (top) and calculated ESI-MS spectrum (bottom). The calculated mass for (a) $[Fe_2($**3b**$)+6H_2O+Na^++K^+-3H]^-$, exact mass: 1065.15; (b) $[Fe_2($**3b**$)+3CH_3OH-H]^-$ exact mass: 993.23.

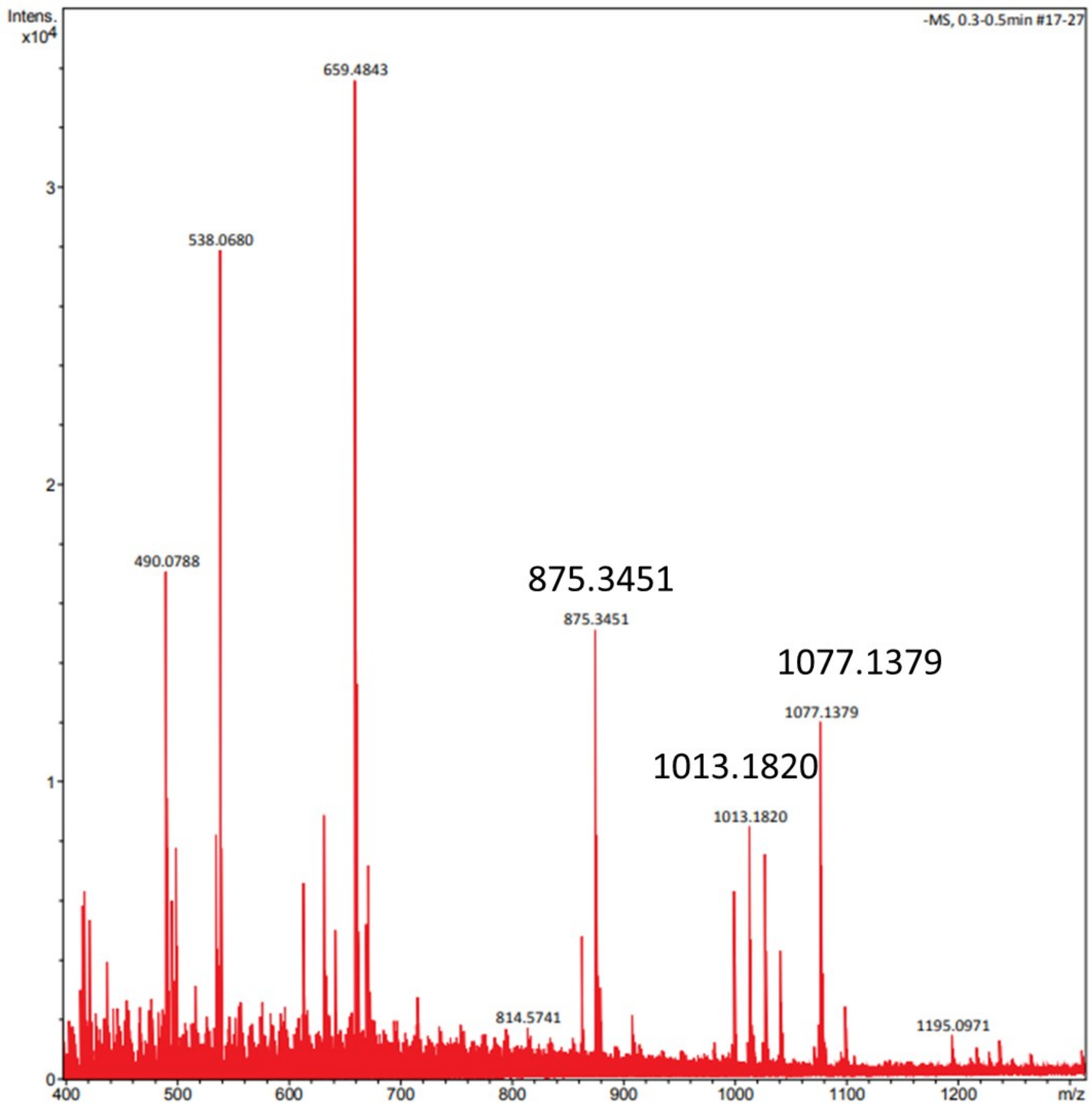


Figure S23. ESI-MS spectrum (-ve mode) of Fe^{3+}-**3c** complex in methanol. The calculated mass for $[Fe_2($**3c**$)+5CH_3OH+H_2O-H]^{-}\cdot 2H_2O$, exact mass: 1195.40, $[Fe_2($**3c**$)+3CH_3OH-H]^{-}$, exact mass: 1077.32, $[Fe_2($**3c**$)+CH_3OH-H]^{-}$, exact mass: 1013.27 and [**3c**-H]$^{-}$, exact mass: 875.42.

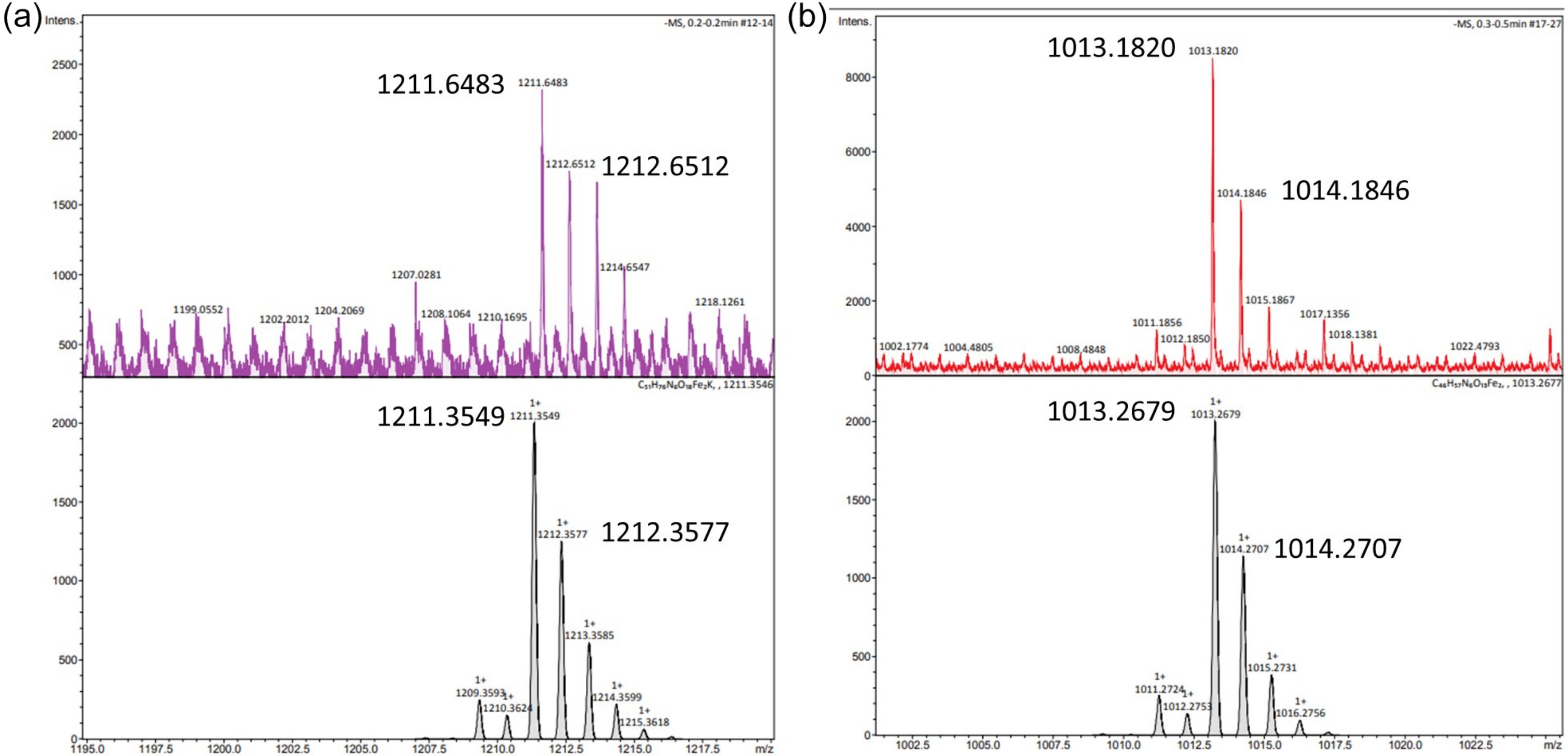


Figure S24. Experimental isotopic analysis by ESI-MS(-ve mode) of Fe^{3+}-**3c** complex (top) and calculated ESI-MS spectrum (bottom). The calculated mass for (a) [Fe_2(**3c**)+6CH_3OH+K^+-2H]$^-$ (not evidenced, but present, in the spectrum of Figure S23), exact mass: 1211.36; (b) [Fe_2(**3c**)+CH_3OH-H]$^-$, exact mass: 1013.27.

7.0 Computational details relative to calculations on iron complexes

The DFT calculations were performed with the Gaussian09 set of programs,[2] using the B3LYP functional.[3] The electronic configuration of the molecular systems was described with 6-311G* basis set for H, C, N, O.[4] For Fe we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential (standard SDD keywords in Gaussian09).[5] The geometry optimizations were performed without symmetry constraints.

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[2] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; N. Kudin, K.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

[3] (a) Becke, Axel D "Density-functional thermochemistry. III. The role of exact exchange". *J. Chem. Phys.* **1993** 98 (7): 5648–5652. (b) K. Kim; K. D. Jordan "Comparison of Density Functional and MP2 Calculations on the Water Monomer and Dimer". *J. Phys. Chem.* **1994**, 98 (40), 10089–10094. (c) P.J. Stephens; F. J. Devlin; C. F. Chabalowski; M. J. Frisch (1994). "Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields". *J. Phys. Chem.* **1994**, 98 (45): 11623–11627.

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7.1 Cartesian coordinates and energies

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Δ-Fe-**3a'**$^{3-}$ E(gas)=-2631.51859310 A.U.

C	-3.915469	-0.540660	-2.001369
C	-4.566479	-1.453544	-0.941789
N	-3.730103	0.790278	-1.724032
C	-4.584689	1.513815	-0.776273
C	-3.935072	1.978053	0.543822
N	-3.732505	1.070295	1.552526
C	-4.577313	-0.118719	1.708937
C	-3.915763	-1.488753	1.453622
N	-3.715265	-1.908974	0.163010
O	-3.632509	3.157537	0.653166
O	-3.603682	-2.168286	2.420815
O	-3.597735	-1.037220	-3.072504
C	-3.123078	1.591091	2.804888
C	-3.124033	1.617810	-2.800313
C	-3.096587	-3.248953	-0.015112
H	-4.865511	-2.335462	-1.508430
H	-5.486546	-1.018441	-0.550678
H	-5.502352	0.953223	-0.594556
H	-4.888404	2.444376	-1.255688
H	-4.881373	-0.168602	2.754599
H	-5.495337	-0.005740	1.131507
C	-1.690365	2.142280	2.700526
H	-3.780067	2.386475	3.185340
H	-3.108834	0.778445	3.527859
H	-3.746886	-3.981734	0.484125
H	-3.083854	-3.466431	-1.080864
C	-1.660833	-3.424970	0.509939
H	-3.122967	2.651244	-2.460549
C	-1.685350	1.267852	-3.217890
H	-3.775728	1.539977	-3.682556
N	-0.655093	1.811948	-2.370940
H	-1.563368	0.188293	-3.280330
H	-1.571546	1.677349	-4.229331
N	-0.649396	1.147909	2.747904
H	-1.579179	2.731784	1.792629
H	-1.579078	2.820424	3.555674
N	-0.625549	-2.964989	-0.379661
H	-1.548678	-2.931174	1.473149
H	-1.542455	-4.503586	0.670692
H	-0.008963	1.037768	1.955193
C	-0.142076	0.739073	3.958361
H	0.009499	-2.216708	-0.083720
C	-0.112839	-3.811012	-1.334334
H	-0.010761	1.183959	-1.879628
C	-0.155862	3.069089	-2.616955
O	-0.786565	3.868865	-3.330842
C	1.158693	3.377249	-2.003324
O	-0.769453	0.955832	5.010279
C	1.177443	0.063110	3.914504
O	-0.732703	-4.837415	-1.664850
C	1.202634	-3.428100	-1.902447
C	1.966139	-2.347512	-1.392104
C	3.264521	-2.039177	-1.965019
C	3.738576	-2.839300	-3.003967

C	2.971766	-3.920295	-3.497358
C	1.733502	-4.209951	-2.961172
O	1.598127	-1.572389	-0.408777
O	3.896057	-1.010786	-1.450369
H	4.712883	-2.603742	-3.429820
H	3.366821	-4.526784	-4.313619
H	1.133036	-5.038397	-3.324110
C	1.936137	2.395501	-1.337597
C	3.233826	2.745590	-0.787558
C	3.692885	4.052350	-0.948039
C	2.911688	5.019745	-1.621628
C	1.674300	4.692685	-2.137818
O	1.581838	1.150533	-1.169421
O	3.879688	1.785800	-0.168691
H	4.666501	4.309055	-0.533054
H	3.294883	6.035550	-1.728845
H	1.062693	5.420867	-2.661549
C	1.949382	-0.023265	2.727941
C	3.252433	-0.664051	2.752715
C	3.720963	-1.169030	3.965072
C	2.944816	-1.069502	5.143086
C	1.702795	-0.468181	5.121002
O	1.585516	0.444872	1.565266
O	3.893475	-0.719589	1.609299
H	4.698520	-1.648940	3.977714
H	3.335622	-1.477218	6.076479
H	1.094584	-0.378645	6.015776
Fe	2.897909	0.014369	-0.004851

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Λ-Fe-**3a'**$^{3-}$ E(gas)=-2631.52381267 A.U.

C	-3.811624	1.760680	-1.038017
C	-4.550148	0.530931	-1.623443
N	-3.769852	1.938898	0.321311
C	-4.547225	1.145117	1.273915
C	-3.809443	0.022080	2.045037
N	-3.770026	-1.244159	1.519446
C	-4.549488	-1.671049	0.356769
C	-3.813359	-1.778902	-1.002056
N	-3.772648	-0.690625	-1.835934
O	-3.332083	0.304619	3.133039
O	-3.338056	-2.863246	-1.301669
O	-3.335908	2.561615	-1.827735
C	-3.178624	-2.328351	2.339047
C	-3.177949	3.190992	0.849405
C	-3.181930	-0.858918	-3.184844
H	-4.861928	0.879811	-2.608562
H	-5.463795	0.304403	-1.075001
H	-5.462175	0.784909	0.804800
H	-4.856739	1.824210	2.069138
H	-4.860707	-2.698664	0.547761
H	-5.463476	-1.083007	0.280422
C	-1.890662	-2.981095	1.796857
H	-2.970033	-1.920579	3.323160
H	-3.955598	-3.099717	2.442172
H	-2.974656	-1.915293	-3.323936
H	-3.958814	-0.561589	-3.904140
C	-1.893082	-0.064489	-3.479139
H	-3.954118	3.665655	1.467148

C	-1.888716	3.048191	1.683941
H	-2.971095	3.839495	0.003877
N	-0.686395	2.980853	0.898017
H	-1.849340	3.940984	2.320767
H	-1.943421	2.175075	2.335062
N	-0.687398	-2.268354	2.131319
H	-1.852295	-3.979322	2.251039
H	-1.946166	-3.107723	0.715123
N	-0.690516	-0.711892	-3.029001
H	-1.854628	0.041312	-4.570704
H	-1.947526	0.935629	-3.047826
H	-0.099089	-1.819698	1.422607
C	-0.122460	-2.418865	3.372034
H	-0.101193	-0.322319	-2.286983
C	-0.126587	-1.711629	-3.779908
H	-0.098400	2.142591	0.863504
C	-0.121095	4.130452	0.407957
O	-0.726400	5.214678	0.498529
C	1.218881	3.988853	-0.207526
O	-0.728428	-3.038736	4.265747
C	1.217909	-1.815931	3.557229
O	-0.733395	-2.175440	-4.763175
C	1.213607	-2.174458	-3.350949
C	1.921646	-1.579366	-2.276345
C	3.231812	-2.087022	-1.907672
C	3.771116	-3.141842	-2.643511
C	3.057733	-3.717453	-3.719468
C	1.807542	-3.247461	-4.065521
O	1.491043	-0.576973	-1.557520
O	3.814069	-1.504746	-0.888085
H	4.754716	-3.513535	-2.360003
H	3.502245	-4.544500	-4.275212
H	1.241338	-3.676939	-4.886093
C	1.925309	2.759772	-0.229972
C	3.235039	2.692659	-0.854643
C	3.775762	3.856773	-1.400033
C	3.064095	5.077361	-1.359872
C	1.814234	5.143603	-0.779286
O	1.493457	1.636452	0.278588
O	3.815581	1.517738	-0.860901
H	4.759104	3.795874	-1.864077
H	3.509698	5.971703	-1.798099
H	1.249362	6.069768	-0.740366
C	1.924660	-1.182319	2.504031
C	3.234973	-0.609073	2.758017
C	3.775697	-0.719200	4.038819
C	3.063552	-1.363561	5.075905
C	1.813235	-1.898510	4.843107
O	1.492642	-1.060643	1.277017
O	3.815994	-0.016816	1.743490
H	4.759431	-0.287726	4.217987
H	3.509169	-1.431522	6.069513
H	1.247994	-2.394783	5.625788
Fe	2.780592	-0.000899	-0.001260

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[Fe_2(**3a**)(H2O)$_4$](CH_3OH)(H_2O) E(gas)=-3253.54446918 A.U.

C	-1.025536	3.107078	-0.980350
C	-2.110936	4.188978	-1.121545

N	0.079173	3.361843	-0.232849
C	0.126318	4.348353	0.852915
C	-0.381707	3.746825	2.184868
N	-1.740249	3.582772	2.366377
C	-2.742651	4.428515	1.710075
C	-3.732849	3.769949	0.715029
N	-3.417177	3.774393	-0.622349
O	0.447314	3.355360	2.985532
O	-4.802467	3.358586	1.133084
O	-1.163087	2.070701	-1.636836
C	-2.174170	2.914427	3.609967
C	1.228212	2.442154	-0.347352
C	-4.498522	3.605702	-1.614585
H	-2.204318	4.332695	-2.198580
H	-1.815835	5.156761	-0.719039
H	-0.374192	5.268886	0.564347
H	1.170676	4.595962	1.030385
H	-3.399454	4.819518	2.489803
H	-2.260894	5.293468	1.260124
C	-3.060226	1.679240	3.417814
H	-1.280994	2.635501	4.160024
H	-2.727492	3.644103	4.213315
H	-5.422702	3.463438	-1.061442
H	-4.576010	4.552735	-2.164675
C	-4.320060	2.470708	-2.632059
H	2.138748	3.043112	-0.309885
C	1.297237	1.327793	0.721830
H	1.168995	1.988937	-1.334308
N	2.027134	0.174840	0.233549
H	1.776371	1.696300	1.625477
H	0.290856	1.006272	0.991188
N	-2.363558	0.511906	2.888473
H	-3.456116	1.430499	4.407652
H	-3.905886	1.897821	2.766969
N	-4.737839	1.158738	-2.179008
H	-4.934377	2.719555	-3.499115
H	-3.279849	2.403024	-2.956016
H	-2.682586	0.088145	2.027584
C	-1.619645	-0.264701	3.730223
H	-4.084589	0.533530	-1.727042
C	-5.982471	0.687536	-2.473755
H	1.497094	-0.510888	-0.288058
C	3.376919	0.075356	0.310653
O	4.055267	1.004608	0.786327
C	3.991121	-1.208631	-0.118272
O	-1.307629	0.112430	4.852686
C	-1.250634	-1.649207	3.256370
O	-6.842079	1.385189	-3.000511
C	-6.243232	-0.769144	-2.185249
C	-5.296134	-1.666053	-1.615196
C	-5.621028	-3.093799	-1.511845
C	-6.899836	-3.548187	-1.910373
C	-7.805148	-2.646315	-2.423268
C	-7.474298	-1.277965	-2.566096
O	-4.132921	-1.322291	-1.165872
O	-4.699919	-3.870183	-1.045955
H	-7.128105	-4.603302	-1.809084
H	-8.787240	-2.984198	-2.736614

H	-8.186287	-0.583758	-2.996657
C	5.256088	-1.146819	-0.723247
C	6.122201	-2.287301	-0.652613
C	5.585044	-3.511982	-0.260958
C	4.255212	-3.597770	0.177571
C	3.474442	-2.455096	0.290750
O	5.764275	-0.033554	-1.240335
O	7.421267	-2.063487	-0.899873
H	6.230473	-4.385466	-0.251169
H	3.855537	-4.557324	0.490306
H	2.498391	-2.508425	0.762638
C	-1.658634	-2.232233	2.030562
C	-1.455480	-3.668950	1.814068
C	-0.718522	-4.423033	2.762941
C	-0.258353	-3.804672	3.901363
C	-0.543547	-2.442806	4.152572
O	-2.260426	-1.594800	1.061239
O	-1.987730	-4.182273	0.763451
H	-0.551752	-5.475708	2.564827
H	0.307198	-4.367858	4.635741
H	-0.233306	-1.980256	5.081982
Fe	-3.062706	-2.894770	-0.372027
O	-1.695608	-2.773747	-2.000095
H	-2.114952	-2.663766	-2.859733
H	-1.124244	-1.980957	-1.829193
O	-0.579466	-0.593679	-1.003198
H	-0.743982	0.307863	-1.341120
H	-1.114793	-0.698738	-0.196800
Fe	7.704043	-0.086207	-0.642572
O	9.685569	-0.993465	-0.247351
H	10.364895	-0.926853	-0.927212
H	9.251171	-1.865684	-0.333600
O	8.331579	1.647332	-1.672214
H	7.510179	1.947912	-2.168823
H	8.680496	2.390948	-1.170609
O	6.814684	0.877500	1.057518
H	6.984779	0.644960	1.975003
H	5.827228	0.925239	0.920776
O	5.996229	2.061875	-2.767210
C	5.817535	1.731385	-4.141954
H	4.755013	1.731813	-4.405258
H	6.321934	2.494845	-4.735603
H	6.240701	0.750424	-4.383165
H	5.613014	1.338040	-2.213344