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Supplementary Material for

Contemplating Thiadiazole Inspired Cyclic Peptide Mimics: A Computational Investigation

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Contents:

Table 1. Crystal data and structure refinement for 446xs1.

Identification code	446xs1	
Empirical formula	C_{20} H_{36} N_4 O_4 S	
Formula weight	428.59	
Temperature	293(2) K	
Wavelength	1.54180 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.1529(3) Å	α= 90°.
	b = 10.1893(2) Å	β= 93.620(2)°.
	c = 11.1550(3) Å	γ = 90°.
Volume	1265.13(5) $Å^3$	
Z	2	
Density (calculated)	1.125 Mg/m^3	
Absorption coefficient	1.375 mm^{-1}	
F(000)	464	
Crystal size	0.5 x 0.4 x 0.4 mm^3	
Theta range for data collection	3.97 to 62.49°.	
Index ranges	-11<=h<=12, -11<=k<=11, -12<=l<=12	
Reflections collected	18336	
Independent reflections	3989 [R(int) = 0.0247]	
Completeness to theta = 62.49°	99.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3989 / 1 / 262	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0331, wR2 = 0.0928	
R indices (all data)	R1 = 0.0353, wR2 = 0.0945	
Absolute structure parameter	0.009(16)	
Largest diff. peak and hole	0.121 and -0.179 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 446xs1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5147(2)	1543(2)	3630(2)	51(1)
C(2)	6792(2)	2160(2)	4628(2)	51(1)
C(3)	4043(2)	1586(2)	2781(2)	51(1)
C(4)	3137(2)	2572(2)	3199(2)	58(1)
C(5)	2648(2)	2233(3)	4402(2)	76(1)
C(6)	2123(2)	2784(3)	2236(2)	80(1)
C(7)	4077(2)	-581(2)	1869(2)	65(1)
C(8)	3859(3)	-2783(3)	1040(3)	89(1)
C(9)	5101(4)	-3216(4)	1445(6)	160(2)
C(10)	2977(4)	-3863(3)	1275(4)	123(1)
C(11)	3743(4)	-2370(4)	-258(3)	127(1)
C(12)	7798(2)	3115(2)	4918(2)	53(1)
C(13)	8393(2)	3520(2)	3767(2)	64(1)
C(14)	8825(2)	2345(3)	3082(2)	88(1)
C(15)	9396(2)	4517(3)	4029(2)	79(1)
C(16)	9127(2)	3241(2)	6753(2)	55(1)
C(17)	10700(2)	2954(3)	8382(2)	75(1)
C(18)	11282(3)	1720(3)	8878(3)	110(1)
C(19)	11600(3)	3762(4)	7780(4)	132(1)
C(20)	10064(4)	3694(6)	9322(3)	168(2)
N(1)	5887(1)	2526(1)	3804(1)	50(1)
N(2)	6783(2)	970(2)	5076(2)	74(1)
N(3)	3553(1)	272(2)	2613(1)	56(1)
N(4)	8632(1)	2549(2)	5824(1)	60(1)
O(1)	3470(1)	-1711(2)	1802(1)	75(1)
O(2)	4980(2)	-333(2)	1379(2)	92(1)
O(3)	9823(1)	2443(1)	7460(1)	71(1)
O(4)	8974(1)	4403(2)	6914(1)	68(1)
S(1)	5588(1)	206(1)	4467(1)	81(1)

Table 3. Bond lengths [Å] and angles [°] for 446xs1.

C(1)-N(1)	1.304(2)
C(1)-C(3)	1.505(3)
C(1)-S(1)	1.7062(18)
C(2)-N(2)	1.311(3)
C(2)-N(1)	1.373(2)
C(2)-C(12)	1.505(3)
C(3)-N(3)	1.455(2)
C(3)-C(4)	1.519(3)
C(4)-C(5)	1.520(3)
C(4)-C(6)	1.526(3)
C(7)-O(2)	1.203(3)
C(7)-O(1)	1.335(2)
C(7)-N(3)	1.359(3)
C(8)-O(1)	1.466(3)
C(8)-C(9)	1.497(5)
C(8)-C(11)	1.505(5)
C(8)-C(10)	1.511(4)
C(12)-N(4)	1.449(2)
C(12)-C(13)	1.539(3)
C(13)-C(14)	1.516(3)
C(13)-C(15)	1.525(3)
C(16)-O(4)	1.211(2)
C(16)-N(4)	1.344(2)
C(16)-O(3)	1.345(2)
C(17)-O(3)	1.469(2)
C(17)-C(19)	1.491(5)
C(17)-C(18)	1.504(4)
C(17)-C(20)	1.505(4)
N(2)-S(1)	1.6514(19)

N(1)-C(1)-C(3)	123.75(15)
N(1)-C(1)-S(1)	111.92(13)
C(3)-C(1)-S(1)	124.33(12)
N(2)-C(2)-N(1)	118.89(16)
N(2)-C(2)-C(12)	122.65(16)
N(1)-C(2)-C(12)	118.34(15)

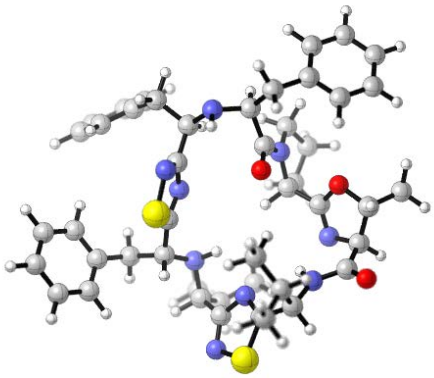
N(3)-C(3)-C(1)	109.85(15)
N(3)-C(3)-C(4)	113.36(14)
C(1)-C(3)-C(4)	111.10(14)
C(3)-C(4)-C(5)	113.80(17)
C(3)-C(4)-C(6)	110.83(16)
C(5)-C(4)-C(6)	111.22(17)
O(2)-C(7)-O(1)	126.30(19)
O(2)-C(7)-N(3)	123.21(19)
O(1)-C(7)-N(3)	110.47(16)
O(1)-C(8)-C(9)	110.3(3)
O(1)-C(8)-C(11)	109.8(2)
C(9)-C(8)-C(11)	113.2(3)
O(1)-C(8)-C(10)	102.8(2)
C(9)-C(8)-C(10)	109.5(3)
C(11)-C(8)-C(10)	110.7(3)
N(4)-C(12)-C(2)	109.24(15)
N(4)-C(12)-C(13)	113.34(15)
C(2)-C(12)-C(13)	110.45(14)
C(14)-C(13)-C(15)	111.72(18)
C(14)-C(13)-C(12)	112.13(18)
C(15)-C(13)-C(12)	111.67(17)
O(4)-C(16)-N(4)	124.88(17)
O(4)-C(16)-O(3)	125.88(17)
N(4)-C(16)-O(3)	109.24(16)
O(3)-C(17)-C(19)	108.6(2)
O(3)-C(17)-C(18)	102.4(2)
C(19)-C(17)-C(18)	109.9(3)
O(3)-C(17)-C(20)	110.1(2)
C(19)-C(17)-C(20)	113.4(3)
C(18)-C(17)-C(20)	112.0(3)
C(1)-N(1)-C(2)	108.82(14)
C(2)-N(2)-S(1)	107.73(14)
C(7)-N(3)-C(3)	119.67(15)
C(16)-N(4)-C(12)	122.95(16)
C(7)-O(1)-C(8)	120.44(16)
C(16)-O(3)-C(17)	122.03(16)
N(2)-S(1)-C(1)	92.64(9)

Symmetry transformations used to generate equivalent atoms:

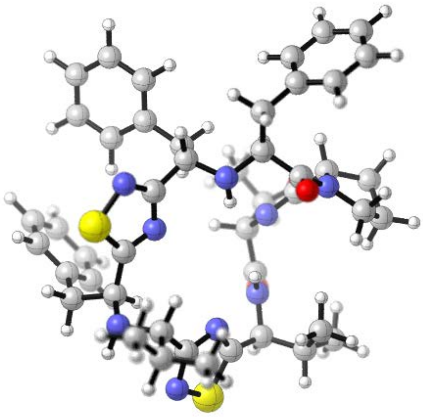
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 446xs1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(1)	47(1)	55(1)	1(1)	1(1)	-7(1)
C(2)	48(1)	48(1)	58(1)	2(1)	-6(1)	-1(1)
C(3)	53(1)	48(1)	51(1)	0(1)	-2(1)	-11(1)
C(4)	55(1)	50(1)	68(1)	-3(1)	-6(1)	-8(1)
C(5)	78(1)	76(1)	77(1)	-13(1)	14(1)	-2(1)
C(6)	64(1)	79(2)	95(2)	1(1)	-21(1)	1(1)
C(7)	69(1)	56(1)	71(1)	-9(1)	11(1)	-15(1)
C(8)	95(2)	64(1)	111(2)	-32(1)	25(1)	-11(1)
C(9)	109(3)	96(3)	272(6)	-59(3)	-16(3)	13(2)
C(10)	142(3)	70(2)	162(3)	-44(2)	41(2)	-36(2)
C(11)	172(3)	116(3)	96(2)	-42(2)	39(2)	-14(2)
C(12)	48(1)	48(1)	62(1)	-2(1)	-9(1)	3(1)
C(13)	51(1)	67(1)	72(1)	3(1)	-4(1)	-4(1)
C(14)	83(2)	97(2)	85(1)	-19(1)	14(1)	-9(1)
C(15)	64(1)	77(1)	97(2)	1(1)	8(1)	-14(1)
C(16)	48(1)	55(1)	62(1)	-6(1)	-6(1)	5(1)
C(17)	71(1)	80(1)	69(1)	-13(1)	-24(1)	6(1)
C(18)	123(2)	100(2)	99(2)	12(2)	-52(2)	12(2)
C(19)	84(2)	123(3)	182(3)	38(3)	-54(2)	-26(2)
C(20)	151(3)	246(6)	99(2)	-86(3)	-41(2)	72(4)
N(1)	47(1)	45(1)	58(1)	1(1)	-5(1)	-4(1)
N(2)	74(1)	58(1)	85(1)	16(1)	-26(1)	-9(1)
N(3)	56(1)	53(1)	59(1)	-9(1)	8(1)	-15(1)
N(4)	59(1)	49(1)	69(1)	-6(1)	-18(1)	6(1)
O(1)	82(1)	59(1)	86(1)	-24(1)	24(1)	-21(1)
O(2)	85(1)	76(1)	122(1)	-23(1)	45(1)	-21(1)
O(3)	77(1)	61(1)	71(1)	-4(1)	-29(1)	5(1)
O(4)	61(1)	59(1)	82(1)	-15(1)	-13(1)	9(1)
S(1)	83(1)	55(1)	103(1)	25(1)	-27(1)	-19(1)

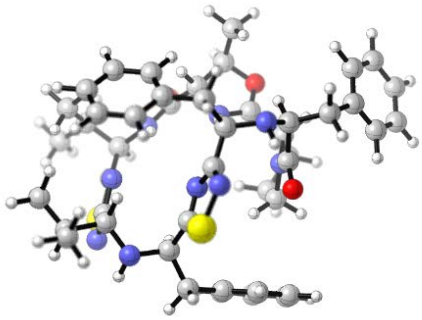
Peptide 9



Peptide 10



Peptide 11



Peptide 12

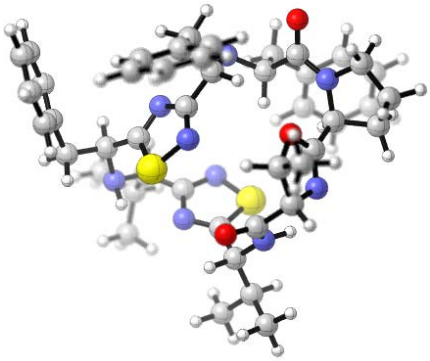
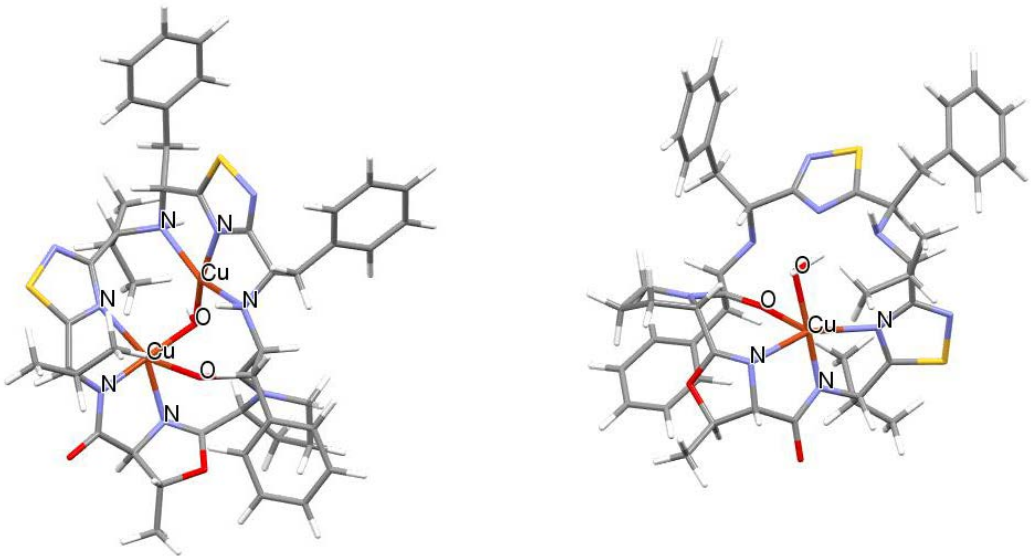


Figure S1. The minimum energy conformers for peptides 9-12 determined using a forcefield-based approach involving the MacroModel 10.6 Macrocycle Conformational Sampling algorithm in conjunction with the MMFFs force field.



(a)

(b)

Figure S2. Labelled calculated structures of (a) $[Cu_2(\mu\text{-}OH)(\mathbf{9}\text{-}H)]^{2+}$ and (b) $[Cu(\mathbf{9}\text{-}H)(H_2O)]^{+}$

The Cartesian coordinates for the Single Point calculations of the optimized geometries are listed below, together with the following energies (in Hartree):

M06 solution-phase electronic energy (E),

Ligand 9-H
No imaginary frequencies
E = -3298.640634 H

N	1.793545	1.275529	-0.004047
C	1.441816	2.337689	-0.808121
N	2.274461	2.726470	-1.746311
S	3.637758	1.744069	-1.671398
C	2.976794	0.825689	-0.337886
C	-3.076541	0.372480	1.985313
C	-4.027982	0.993937	3.039807
C	-4.943367	1.920971	2.227903
C	-4.009190	2.484690	1.155054
N	-3.106363	1.347478	0.874995
C	-4.861119	-2.549555	0.612919
O	-4.600408	-1.114190	0.790545
C	-3.490786	-1.012543	1.559358
N	-2.893747	-2.085022	1.918893
C	-3.619843	-3.198119	1.296870
S	2.157780	-5.155519	-0.255401
C	0.818559	-4.051293	-0.108060
N	1.136871	-3.018665	0.631099
C	2.436909	-3.131253	1.072412
N	3.142691	-4.179270	0.701027
C	-0.546227	-4.265096	-0.719559
N	-1.518091	-3.549456	0.100342
C	-2.767403	-4.001612	0.309788
O	-3.243096	-5.007011	-0.239274
C	-2.307396	1.165512	-0.196310
O	-1.613033	0.136597	-0.303425
C	-2.210937	2.250391	-1.293361
N	-0.811389	2.429554	-1.700017
C	0.079483	2.976993	-0.644889
C	3.644918	-0.357522	0.326445
N	2.886311	-0.709380	1.534873
C	3.053558	-2.090606	1.997214
C	-6.191359	-2.900896	1.249287
C	-3.011021	1.836112	-2.556591
C	-4.514529	1.777661	-2.393453
C	0.116699	4.519219	-0.739585
C	0.854449	5.187221	0.402202
C	5.128435	-0.067694	0.690322
C	6.089690	-0.032157	-0.480685
C	2.557072	-2.255339	3.466862
C	1.114225	-1.781438	3.694624
C	3.519539	-1.552524	4.434747

C	-0.643823	-3.877562	-2.232197
C	0.106861	-4.872028	-3.125900
C	-0.220620	-2.433511	-2.516929
C	6.259712	-1.157098	-1.306308
C	7.164823	-1.135672	-2.367720
C	7.924689	0.010497	-2.621501
C	7.773921	1.131220	-1.803329
C	6.862953	1.108256	-0.743416
C	0.252397	5.312050	1.664343
C	0.928978	5.912371	2.727709
C	2.224911	6.403827	2.546582
C	2.834508	6.290454	1.295233
C	2.154153	5.686530	0.234420
C	-5.167743	0.565322	-2.131507
C	-6.555777	0.517295	-1.975942
C	-7.314551	1.684934	-2.083561
C	-6.676511	2.899589	-2.351676
C	-5.289531	2.942934	-2.506379
H	-2.057506	0.277943	2.368445
H	-3.429383	1.573501	3.750316
H	-4.571677	0.229958	3.601910
H	-5.393622	2.710768	2.835696
H	-5.747360	1.347178	1.754579
H	-3.434062	3.337227	1.538734
H	-4.538372	2.793859	0.253484
H	-4.883756	-2.729768	-0.464271
H	-3.938100	-3.917719	2.060275
H	-0.796091	-5.329108	-0.650059
H	-2.587583	3.206658	-0.921999
H	-0.468972	1.505574	-1.963534
H	-0.267320	2.696347	0.359467
H	3.631730	-1.174174	-0.416186
H	1.900015	-0.517897	1.370108
H	4.122853	-2.318916	2.008658
H	-6.395453	-3.966599	1.094172
H	-6.172976	-2.703218	2.327227
H	-7.004594	-2.323738	0.796558
H	-2.633562	0.860260	-2.886232
H	-2.750477	2.563596	-3.332662
H	-0.923658	4.865656	-0.755234
H	0.563814	4.796419	-1.699334
H	5.444589	-0.860833	1.377101
H	5.174010	0.871354	1.252045
H	2.598577	-3.332968	3.677940
H	0.817033	-1.979606	4.731475
H	1.018133	-0.701327	3.528143
H	0.399126	-2.289707	3.040209
H	4.541644	-1.938276	4.333542
H	3.546075	-0.472495	4.252139
H	3.203294	-1.711168	5.472807
H	-1.714438	-3.977948	-2.451605

H	-0.180180	-5.908673	-2.909731
H	-0.125129	-4.674664	-4.178895
H	1.194612	-4.787193	-3.014565
H	0.853847	-2.288639	-2.348307
H	-0.425748	-2.185866	-3.565238
H	-0.761875	-1.714888	-1.893271
H	5.686196	-2.060317	-1.109488
H	7.281198	-2.016308	-2.994571
H	8.630670	0.026381	-3.447931
H	8.363481	2.025828	-1.987796
H	6.753004	1.984365	-0.108453
H	-0.760056	4.941672	1.812628
H	0.442413	6.001582	3.696035
H	2.752044	6.874971	3.372367
H	3.840262	6.674270	1.141732
H	2.635777	5.604119	-0.736879
H	-4.583002	-0.347933	-2.054235
H	-7.044017	-0.433696	-1.777635
H	-8.394665	1.648666	-1.966376
H	-7.259374	3.812545	-2.446488
H	-4.800508	3.890375	-2.724073

$[Cu_2(9\text{-}H)(\mu\text{-}OH)]^{2+}$

No imaginary frequencies

E = -4606.850189 H

N	-2.389530	0.676937	-0.142203
C	-2.479417	1.964059	0.320754
N	-3.640528	2.346555	0.764920
S	-4.729830	1.083531	0.585162
C	-3.533984	0.043725	-0.078578
C	3.294448	0.547744	-2.341636
C	4.201177	1.291334	-3.340373
C	4.339020	2.696423	-2.763184
C	2.982923	2.937668	-2.125489
N	2.689785	1.622649	-1.532084
C	5.576762	-1.161115	-0.050378
O	5.101936	-0.039292	-0.863740
C	4.019675	-0.454315	-1.505585
N	3.678820	-1.692355	-1.394596
C	4.649375	-2.312593	-0.490478
S	-0.581837	-4.705037	2.186885
C	0.565026	-3.689454	1.413599
N	0.055357	-3.130678	0.332460
C	-1.244445	-3.549971	0.157310
N	-1.749437	-4.370381	1.045955
C	1.964310	-3.448124	1.871564
N	2.668542	-2.856701	0.753561
C	3.995221	-2.970197	0.707672
O	4.718639	-3.529243	1.549790
C	2.080543	1.367514	-0.364931

O	2.152066	0.266971	0.203144
C	1.240842	2.445599	0.304673
N	-0.107995	1.868396	0.460510
C	-1.232736	2.798597	0.247499
C	-3.623542	-1.387693	-0.493201
N	-2.369281	-1.778763	-1.196705
C	-2.119901	-3.237399	-1.028314
C	7.036976	-1.393339	-0.305546
C	1.906711	2.802955	1.644870
C	3.305362	3.314163	1.434745
C	-1.268888	4.026607	1.163496
C	-2.230176	5.099330	0.720786
C	-4.881223	-1.685732	-1.320551
C	-6.153244	-1.380497	-0.577209
C	-1.709670	-4.014386	-2.296940
C	-0.439998	-3.571282	-3.003407
C	-2.862543	-4.072575	-3.292121
C	2.016261	-2.573714	3.156037
C	1.665293	-3.372441	4.401414
C	1.170710	-1.312593	3.054120
C	-6.429970	-2.004469	0.644747
C	-7.588122	-1.696888	1.349124
C	-8.491385	-0.767495	0.837187
C	-8.234252	-0.153558	-0.384520
C	-7.070502	-0.457147	-1.085591
C	-2.025446	5.760249	-0.493516
C	-2.883075	6.775270	-0.905449
C	-3.955895	7.151169	-0.101039
C	-4.162369	6.506431	1.115470
C	-3.305638	5.487654	1.520827
C	4.394821	2.439229	1.436215
C	5.675758	2.899461	1.144756
C	5.883163	4.244825	0.850780
C	4.804952	5.127477	0.856000
C	3.525371	4.663288	1.145384
H	2.490762	-0.000360	-2.844853
H	3.696181	1.325508	-4.313270
H	5.162392	0.784806	-3.481238
H	4.583223	3.446767	-3.522283
H	5.115280	2.723848	-1.984597
H	2.220981	3.193262	-2.876857
H	3.005615	3.717079	-1.358025
H	5.393681	-0.869866	0.994345
H	5.219919	-3.086947	-1.025786
H	2.420952	-4.420229	2.126719
H	1.154347	3.337928	-0.329906
H	-1.145236	3.142725	-0.797408
H	-3.651942	-1.972862	0.441117
H	-3.080588	-3.695838	-0.747056
H	7.368315	-2.246434	0.300874
H	7.209280	-1.631480	-1.363482

H	7.637166	-0.518172	-0.031419
H	1.918178	1.896190	2.267701
H	1.296367	3.550147	2.167288
H	-0.259661	4.461404	1.164218
H	-1.483589	3.706654	2.193738
H	-4.854887	-2.747772	-1.602657
H	-4.832509	-1.101111	-2.251576
H	-1.545223	-5.037727	-1.921006
H	-0.176904	-4.309686	-3.771732
H	-0.602143	-2.622345	-3.538390
H	0.422275	-3.482031	-2.328844
H	-3.780866	-4.462167	-2.833188
H	-3.085929	-3.085341	-3.724028
H	-2.597568	-4.732997	-4.127753
H	3.075420	-2.283522	3.229587
H	2.246108	-4.302694	4.467726
H	1.875411	-2.779595	5.301280
H	0.596176	-3.631248	4.443480
H	0.093671	-1.545835	3.046504
H	1.351972	-0.668185	3.925020
H	1.404879	-0.729376	2.153715
H	-5.732733	-2.742766	1.044589
H	-7.788918	-2.187337	2.300268
H	-9.397563	-0.525849	1.390226
H	-8.938396	0.569565	-0.792781
H	-6.860482	0.033515	-2.036943
H	-1.172383	5.484310	-1.117136
H	-2.707610	7.280930	-1.854081
H	-4.626190	7.948154	-0.419463
H	-4.996005	6.797079	1.753410
H	-3.472945	4.980101	2.471442
H	4.231953	1.385847	1.671218
H	6.515202	2.204471	1.151339
H	6.884726	4.607111	0.624181
H	4.962004	6.182312	0.635181
H	2.678486	5.352807	1.143487
Cu	-0.814574	-0.212167	-0.812622
H	-0.181359	1.444414	1.390811
H	-2.491648	-1.575732	-2.195247
Cu	1.676247	-1.963063	-0.622684
O	0.637134	-0.856586	-1.809369
H	0.292504	-1.412821	-2.524622

[Cu(9-H)(H_2O)]$^+$
No imaginary frequencies
E = -3990.010606 H

N	1.873492	1.243058	-0.180328
C	1.641372	2.413740	-0.859073
N	2.627245	2.995635	-1.491584

S	3.999678	2.070088	-1.266102
C	3.129241	0.914370	-0.290254
C	-2.823893	1.135608	1.760372
C	-3.703492	2.030085	2.643887
C	-4.630050	2.736644	1.660070
C	-3.739268	2.985167	0.453688
N	-2.853948	1.808798	0.455453
C	-4.868345	-1.852415	1.196007
O	-4.595553	-0.416808	1.282320
C	-3.331855	-0.267649	1.653311
N	-2.653491	-1.333089	1.904788
C	-3.528089	-2.473701	1.625292
S	1.675398	-4.813060	-1.046140
C	0.430200	-3.787208	-0.462361
N	0.912895	-2.882886	0.368087
C	2.269064	-3.066750	0.533275
N	2.841972	-4.025054	-0.151089
C	-1.026002	-3.897779	-0.773455
N	-1.709260	-3.039468	0.171451
C	-2.943969	-3.369584	0.551408
O	-3.622847	-4.313380	0.115769
C	-2.076596	1.344215	-0.541014
O	-1.465049	0.274522	-0.434002
C	-1.899841	2.188853	-1.797314
N	-0.461919	2.303928	-2.007633
C	0.239147	2.955223	-0.896635
C	3.739389	-0.331572	0.286286
N	2.936144	-0.861883	1.401622
C	3.125460	-2.313607	1.517235
C	-6.037670	-2.190991	2.073136
C	-2.552842	1.479628	-2.987663
C	-4.034759	1.331810	-2.785457
C	0.167453	4.482445	-0.911345
C	0.658418	5.090514	0.373371
C	5.214203	-0.149456	0.681404
C	6.170407	-0.031860	-0.475310
C	2.964005	-2.874231	2.945396
C	1.649479	-2.539693	3.633856
C	4.143549	-2.468231	3.820620
C	-1.368505	-3.565961	-2.247924
C	-0.977726	-4.693959	-3.190139
C	-0.783630	-2.238775	-2.703561
C	6.215053	-1.025054	-1.460030
C	7.102278	-0.928849	-2.525517
C	7.965439	0.160952	-2.621127
C	7.939330	1.147957	-1.641242
C	7.047958	1.050060	-0.575990
C	-0.044429	4.866901	1.562309
C	0.402428	5.399346	2.766538
C	1.564398	6.167878	2.800826
C	2.271456	6.397754	1.624529

C	1.821719	5.859844	0.421137
C	-4.559127	0.232403	-2.098703
C	-5.921099	0.155970	-1.819378
C	-6.778013	1.174867	-2.227903
C	-6.267806	2.267838	-2.923992
C	-4.905632	2.343808	-3.197719
H	-1.789494	1.078045	2.119403
H	-3.056441	2.757749	3.150820
H	-4.234848	1.459201	3.413747
H	-5.046408	3.665955	2.062366
H	-5.464728	2.081872	1.376426
H	-3.146369	3.906616	0.569784
H	-4.303254	3.045556	-0.483936
H	-5.089264	-2.057687	0.139828
H	-3.652729	-3.084812	2.532282
H	-1.331281	-4.945314	-0.600713
H	-2.390574	3.169674	-1.660645
H	-0.223568	2.601518	0.037657
H	3.680023	-1.078346	-0.524165
H	4.155249	-2.588898	1.225519
H	-6.233467	-3.268864	2.001862
H	-5.819164	-1.945041	3.120941
H	-6.938800	-1.652003	1.757193
H	-2.068878	0.499939	-3.109497
H	-2.342097	2.068964	-3.891777
H	-0.886023	4.759651	-1.073692
H	0.738638	4.868392	-1.767811
H	5.499345	-1.022046	1.288595
H	5.297430	0.727685	1.341269
H	3.012575	-3.967827	2.814214
H	1.543380	-3.147606	4.541860
H	1.631432	-1.488191	3.954811
H	0.773104	-2.733982	2.998478
H	5.101340	-2.766989	3.373774
H	4.174377	-1.383047	3.999781
H	4.065807	-2.951150	4.803658
H	-2.467443	-3.491480	-2.247941
H	-1.359376	-5.665871	-2.847760
H	-1.384391	-4.506694	-4.192604
H	0.113564	-4.775451	-3.310185
H	0.313135	-2.291825	-2.790868
H	-1.172531	-1.976006	-3.696704
H	-1.026722	-1.416723	-2.016713
H	5.555802	-1.892530	-1.385131
H	7.123529	-1.710457	-3.283622
H	8.659364	0.236903	-3.456848
H	8.614655	1.999997	-1.704200
H	7.026884	1.826131	0.190531
H	-0.958766	4.267193	1.537691
H	-0.159880	5.217524	3.681738
H	1.915444	6.587643	3.742398

H	3.179884	6.998649	1.641746
H	2.379804	6.038983	-0.498785
H	-3.887931	-0.569158	-1.775169
H	-6.319357	-0.707827	-1.286651
H	-7.843306	1.112875	-2.010673
H	-6.932947	3.064581	-3.254319
H	-4.503079	3.203761	-3.735857
H	-0.287130	2.824408	-2.868881
H	3.270157	-0.419017	2.261647
Cu	-0.732355	-1.659775	1.093733
O	0.244170	-0.153238	1.999307
H	0.251656	-0.350983	2.950878
H	1.190200	-0.264001	1.694301

$[Cu_2(9\text{-}H)(\mu\text{-}OH)]^{2+}$ - metal ion and μ-OH deleted
No imaginary frequencies
E = -3298.613445

N	2.298707	0.621526	0.252011
C	2.331902	1.902077	-0.236014
N	3.473959	2.324916	-0.692823
S	4.616771	1.113100	-0.493850
C	3.468853	0.036443	0.195286
C	-3.366199	0.293387	2.479794
C	-4.299991	1.016980	3.468224
C	-4.499779	2.403468	2.864766
C	-3.157627	2.689759	2.216290
N	-2.810980	1.377128	1.646927
C	-5.582306	-1.555142	0.232398
O	-5.152636	-0.398567	1.021831
C	-4.051240	-0.754652	1.666521
N	-3.658353	-1.978993	1.577792
C	-4.605030	-2.657375	0.690264
S	0.713178	-4.876662	-1.964773
C	-0.472983	-3.895957	-1.205858
N	0.016519	-3.295136	-0.138032
C	1.333673	-3.655280	0.039135
N	1.869785	-4.470561	-0.835892
C	-1.883007	-3.723298	-1.661897
N	-2.607546	-3.140780	-0.552231
C	-3.927999	-3.309696	-0.498032
O	-4.630134	-3.915239	-1.325891
C	-2.195852	1.125529	0.482093
O	-2.222576	0.012125	-0.064373
C	-1.405412	2.225161	-0.211990
N	-0.033811	1.702940	-0.362939
C	1.051077	2.684099	-0.173060
C	3.620909	-1.381545	0.636935
N	2.387138	-1.811883	1.353619
C	2.199509	-3.282804	1.214463

C	-7.030322	-1.844277	0.498738
C	-2.090997	2.527786	-1.555720
C	-3.509353	2.983024	-1.348992
C	1.031377	3.894525	-1.112661
C	1.947755	5.015553	-0.695111
C	4.893284	-1.609706	1.464037
C	6.148305	-1.265131	0.709090
C	1.827591	-4.051771	2.499683
C	0.542886	-3.649440	3.203367
C	2.985668	-4.041535	3.490455
C	-1.977058	-2.876983	-2.962700
C	-1.597105	-3.684082	-4.194091
C	-1.185639	-1.579299	-2.888961
C	6.446727	-1.900364	-0.501912
C	7.588031	-1.557529	-1.217416
C	8.452802	-0.580800	-0.727635
C	8.174389	0.045243	0.483220
C	7.027308	-0.293908	1.195373
C	1.719663	5.690610	0.507199
C	2.534807	6.748994	0.895564
C	3.587567	7.154503	0.079121
C	3.816709	6.495640	-1.125708
C	3.002639	5.433666	-1.507436
C	-4.560535	2.062682	-1.328609
C	-5.858807	2.473580	-1.040131
C	-6.122234	3.814353	-0.771119
C	-5.082647	4.741808	-0.798297
C	-3.785557	4.326936	-1.084613
H	-2.537974	-0.210162	2.989728
H	-3.793211	1.091485	4.437941
H	-5.238199	0.472863	3.623252
H	-4.772847	3.157343	3.610419
H	-5.279458	2.382738	2.089402
H	-2.404420	2.992062	2.959074
H	-3.216440	3.452456	1.434098
H	-5.415777	-1.276710	-0.818575
H	-5.140011	-3.444767	1.242999
H	-2.298771	-4.718720	-1.896203
H	-1.354616	3.132510	0.404907
H	0.952965	3.044401	0.865433
H	3.670668	-1.983001	-0.286081
H	3.177787	-3.705338	0.937640
H	-7.327298	-2.722297	-0.089627
H	-7.188293	-2.068952	1.561837
H	-7.668301	-1.000913	0.210609
H	-2.066181	1.609442	-2.160939
H	-1.515045	3.289991	-2.095228
H	0.004540	4.285898	-1.117074
H	1.255599	3.564052	-2.137540
H	4.913312	-2.666229	1.766636
H	4.823245	-1.009727	2.383869

H	1.705473	-5.088283	2.144265
H	0.314416	-4.383321	3.986952
H	0.666471	-2.684268	3.719245
H	-0.324973	-3.610057	2.531201
H	3.918016	-4.400555	3.034859
H	3.168424	-3.037500	3.902264
H	2.752263	-4.696295	4.339846
H	-3.047894	-2.633590	-3.036917
H	-2.138001	-4.639307	-4.239824
H	-1.835719	-3.118293	-5.104213
H	-0.518105	-3.897951	-4.236121
H	-0.099616	-1.766334	-2.881839
H	-1.397507	-0.960216	-3.771243
H	-1.441025	-0.989212	-1.998868
H	5.780069	-2.675274	-0.884253
H	7.805931	-2.057362	-2.159878
H	9.345752	-0.311603	-1.289405
H	8.848630	0.805447	0.874238
H	6.800187	0.205756	2.138073
H	0.881505	5.390790	1.139949
H	2.341566	7.265049	1.835097
H	4.224499	7.985303	0.379054
H	4.634773	6.809050	-1.772968
H	3.187811	4.915337	-2.448874
H	-4.353816	1.012820	-1.544061
H	-6.667885	1.743517	-1.029463
H	-7.137464	4.138043	-0.546897
H	-5.283667	5.793090	-0.597078
H	-2.968830	5.051761	-1.099899
H	0.054023	1.264479	-1.285244
H	2.504541	-1.584490	2.347503

$[Cu(9\text{-}H)(H_2O)]^+$ - metal ion and H_2O removed
No imaginary frequencies
E = -3298.634384 H

N	1.816765	1.156188	-0.100868
C	1.565080	2.305074	-0.809229
N	2.540023	2.884348	-1.460800
S	3.926660	1.985086	-1.216586
C	3.076776	0.842980	-0.207167
C	-2.871429	1.031754	1.860916
C	-3.760781	1.936352	2.724139
C	-4.701155	2.603193	1.725817
C	-3.818512	2.832738	0.509734
N	-2.916089	1.669801	0.538870
C	-4.874024	-1.999472	1.383610
O	-4.621937	-0.558286	1.431022
C	-3.359218	-0.381067	1.792859
N	-2.664431	-1.429546	2.069544

C	-3.523277	-2.589705	1.823677
S	1.704072	-4.922890	-0.806250
C	0.446147	-3.900192	-0.244643
N	0.918603	-2.967381	0.559776
C	2.277899	-3.127114	0.724275
N	2.862256	-4.094705	0.063047
C	-1.009406	-4.040055	-0.546851
N	-1.701688	-3.167142	0.377900
C	-2.930046	-3.505011	0.771390
O	-3.596641	-4.469724	0.363471
C	-2.135672	1.190436	-0.448150
O	-1.508163	0.132930	-0.315503
C	-1.975865	2.004139	-1.726938
N	-0.540558	2.134498	-1.946011
C	0.154966	2.824961	-0.855366
C	3.707175	-0.378338	0.399486
N	2.915839	-0.890665	1.531612
C	3.126783	-2.335941	1.684609
C	-6.035071	-2.331750	2.274052
C	-2.622766	1.254378	-2.895575
C	-4.101619	1.090442	-2.683581
C	0.060894	4.350070	-0.909959
C	0.547607	4.998852	0.356319
C	5.180598	-0.164483	0.783717
C	6.130759	-0.063549	-0.379534
C	2.978749	-2.861000	3.127673
C	1.662000	-2.527545	3.812389
C	4.155424	-2.414985	3.987144
C	-1.362109	-3.752230	-2.028136
C	-0.958322	-4.898886	-2.941924
C	-0.798361	-2.429162	-2.520889
C	6.186319	-1.081602	-1.337956
C	7.068154	-1.000655	-2.409178
C	7.914935	0.098662	-2.536905
C	7.877975	1.110679	-1.583223
C	6.992025	1.027967	-0.512180
C	-0.147555	4.796484	1.553555
C	0.295865	5.366928	2.741549
C	1.446593	6.152884	2.750922
C	2.145919	6.361903	1.566140
C	1.699703	5.785982	0.379141
C	-4.607351	0.002023	-1.966027
C	-5.967030	-0.086782	-1.679302
C	-6.840229	0.908446	-2.111026
C	-6.348605	1.989976	-2.837681
C	-4.988689	2.078472	-3.118806
H	-1.834994	0.998693	2.217162
H	-3.122592	2.686440	3.209137
H	-4.280925	1.378302	3.510888
H	-5.129586	3.536643	2.105206
H	-5.527204	1.929124	1.462870

H	-3.238727	3.765439	0.599150
H	-4.386733	2.860194	-0.426878
H	-5.095773	-2.235711	0.334095
H	-3.635659	-3.178437	2.746925
H	-1.298707	-5.086988	-0.345373
H	-2.480379	2.980994	-1.614141
H	-0.299121	2.489335	0.089765
H	3.655772	-1.147008	-0.390792
H	4.159416	-2.603847	1.396091
H	-6.215351	-3.413854	2.231943
H	-5.816357	-2.055116	3.314129
H	-6.945131	-1.814417	1.947669
H	-2.124984	0.278946	-2.993551
H	-2.423965	1.822665	-3.815729
H	-0.997102	4.607570	-1.075295
H	0.623251	4.721548	-1.778582
H	5.480678	-1.016530	1.412498
H	5.253403	0.730874	1.419942
H	3.042832	-3.956858	3.025103
H	1.568113	-3.112792	4.736489
H	1.629751	-1.468322	4.105636
H	0.786241	-2.751221	3.185880
H	5.115842	-2.711485	3.544449
H	4.171040	-1.325126	4.137568
H	4.088340	-2.872899	4.982854
H	-2.462003	-3.693738	-2.025684
H	-1.324471	-5.866870	-2.572557
H	-1.371332	-4.744033	-3.947315
H	0.133597	-4.967660	-3.064189
H	0.298732	-2.468567	-2.611196
H	-1.194682	-2.198350	-3.519021
H	-1.050934	-1.592906	-1.854928
H	5.540099	-1.956285	-1.237603
H	7.098061	-1.801589	-3.146533
H	8.604616	0.162619	-3.377126
H	8.540542	1.970478	-1.671300
H	6.962399	1.823587	0.233737
H	-1.053114	4.183123	1.548409
H	-0.260383	5.201145	3.663476
H	1.794893	6.602373	3.679700
H	3.045514	6.976173	1.563882
H	2.251743	5.948890	-0.547416
H	-3.923328	-0.780901	-1.624231
H	-6.350672	-0.941928	-1.122430
H	-7.903709	0.836745	-1.887946
H	-7.026523	2.767990	-3.186171
H	-4.600721	2.929689	-3.681002
H	-0.376539	2.634574	-2.821353
H	3.246486	-0.420483	2.378339

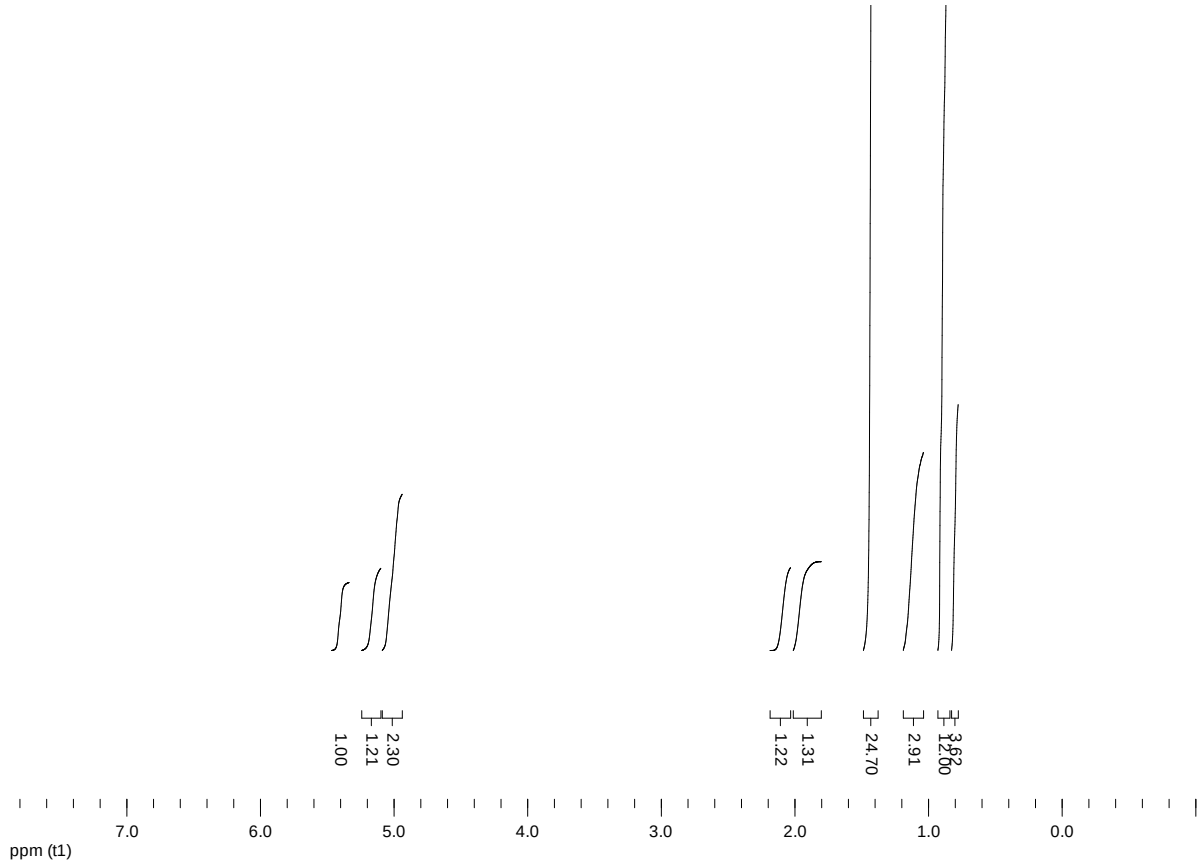


Figure S2. ^{1}H NMR spectra of compound **7**

Figure S3. ^{13}C NMR spectra of compound **7**

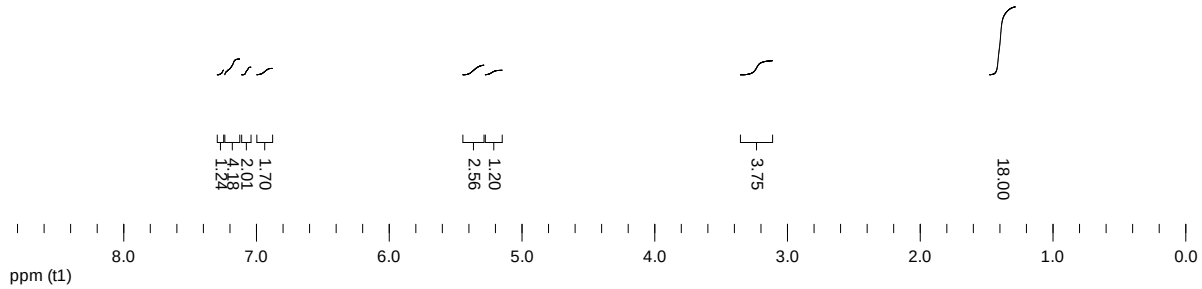


Figure S4. ^{1}H NMR spectra of compound **8**

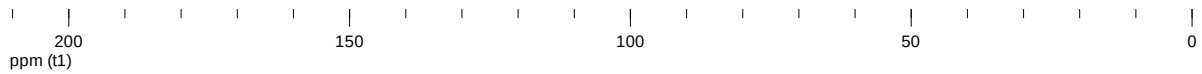


Figure S5. ^{13}C NMR spectra of compound **8**