Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Tuned structure and DNA binding properties of metal complexes base on a new 4-acylpyrazolone derivative

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Contents

Instrument and methods

General

All solvents and chemicals were obtained from commercial sources and without further purification. 4-benzoyl-3-methyl-1-(4-nitrophenyl)-1H-pyrazol-5(4H)-one and salicylhydrazide were prepared according to the literature.[1] All melting points were determined on a Kofler apparatus. Infrared spectra (4000~400 cm^{-1}) were recorded on a FT-170SX instrument using KBr pellets. ^{1}H-NMR spectra were recorded on a Bruker model (500 MHz) Ultra in $CDCl_3$ solution at room temperature with tetramethylsilane(TMS) as an internal standard, chemical shifts are reported as δ ppm units. The emission spectra of the sample was collected with a Hitachi F-7000 spectrophotometer and the excitation and emission slit widths were 10 nm at the room temperature. UV-Vis absorption spectra were determined by a Varian UV-Cary100 spectrophotometer. The ratio of the UV absorbance of the CT-DNA solution at 260 and 280 nm is between 1.8 and 1.9, indicating that there is no protein in the CT-DNA.[2] The concentration of CT-DNA was determined by the absorption intensity at 260 nm and the molar extinction coefficient (6600 M^{-1} cm^{-1}).[3]

DNA-binding properties

Electronic Absorption Titration. All spectrophotometric measurements were prepared in a constant temperature quartz sample cell at room temperature of 25℃ and all the experiments involving CT-DNA were performed in buffer solution (5 mM Tris–HCl/10 mM NaCl, pH = 7.2).[4] A stock solution of CT-DNA was obtained by dissolving the required amount of CT-DNA in a buffer solution, stored at 4℃ and used within 3 days. The ligand and complexes are dissolved in DMF solution to obtain a test sample. The required amount of CT-DNA was added to both the compounds and reference solution, reaching to eliminate the absorbance of CT-DNA itself. All solutions were scanned in the 190~500 nm range.[5] The possible binding modes and binding constants of the ligand and its complexes to DNA were studied by absorption spectrum titration. The binding constant is determined by the following equation:[6]

$$[DNA] / (\varepsilon_a - \varepsilon_f) = [DNA] / (\varepsilon_b - \varepsilon_f) + 1/K_b (\varepsilon_b - \varepsilon_f),$$

where ε_a corresponds to the extinction coefficient observed (A_{obsd}/[M]), ε_f corresponds to the extinction coefficient of the free compound, ε_b is the extinction coefficient of the compound fully bounded to DNA,

[DNA] is the concentration of DNA in base pairs, and K_b is the intrinsic binding constant. The ratio of slope to intercept in the plot of [DNA] / ($\varepsilon_a - \varepsilon_f$) versus [DNA] gives the values of K_b.

EB–DNA fluorescence competition experiment. It was previously reported that, ethidium bromide (EB) does not show any appreciable emission in buffer solution due to fluorescence quenching by the solvent. Upon adding the ligand or complex into a solution containing EB, it is observed that there is no change in the fluorescence spectra. However, when CT-DNA is added to EB solution, the fluorescence intensity is greatly enhanced, which is derived from the strong insertion of EB into DNA base pair. Normally, the fluorescence emitted by the binding of EB to DNA can compete with EB for DNA by adding additional molecules, resulting in fluorescence quenching.[7,8] Therefore, the degree of fluorescence quenching can determine the degree of binding of other molecules to CT-DNA, and its fluorescence quenching constant is calculated according to the Stern-Volmer equation:[9]

$$I_0 / I = 1 + K_{SV}[Q]$$

where I_0 and I are the fluorescence intensities at 596 nm in the absence and presence of the quencher, respectively, K_{SV} is the linear Stern-Volmer quenching constant, and [Q] is the concentration of the quencher.

X-ray single crystal diffraction analysis

Intensity data of **1**, **2** and **3** were recorded with a Bruker Smart Apex II CCD diffractometer with agraphite-monochromated Mo-Kα radiation (λ = 0. 71073 Å) using the w-scan mode. There was no crystal attenuation during the data collection. The diffaction data were corrected for absorption effects using the empirical multiscan method (SADABS).[10] The structures were solved by direct methods and refined on F^2 by a full-matrix least-squares procedure. SHELXL-2014 was used for both structural solutions and refinements.[11] Nonhydrogen atoms of the compounds were refined with anisotropic temperature parameters. Graphics of **1**, **2** and **3** were drawn with DIAMOND (Version 3.2).[12]

Table S1. Crystallographic data and data collection parameters for the **1**, **2** and **3**.

	1	**2**	**3**
Empirical formula	Cu2C48H34Cl2N10O	Cu2C52H48N10O14	MnC26H26N5O8
Temperature (K)，M	296(2), 1108.85	296(2), 1164.10	296(2), 1182.92
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	P21/c
a (Å)	8.5903(10)	10.7140(5)	12.1612(17)
b (Å)	11.9318(12)	11.3202(6)	12.5232(14)
c (Å)	13.5523(11)	11.9538(7)	17.883(3)
α (°)	74.564(8)	114.677(6)	90.00
β(°)	84.335(8)	91.405(4)	95.074(14)
γ (°)	71.586(10)	102.244(4)	90.00
Volume (Å3), Z	1270.3(2), 1	1277.0(1), 1	2712.9(6), 4
Absorption coefficient (mm– 1)	1.008	1.077	0.545
F(000)	564	1442	1224
Crystal size (mm)	0.37×0.25×0.24	0.21×0.18×0.14	0.21×0.18×0.13
θ Range for data collection (°)	2.96~25.99	1.53~25.02	1.20~25.00
Index ranges	-10≤ h ≤ 10	-15≤ h ≤ 15	-15≤ h ≤ 9
	-14 ≤ k ≤ 14	-18 ≤ k ≤ 15	-12 ≤ k ≤15
	-16 ≤ l ≤ 15	-21≤ l ≤ 21	-21 ≤ l ≤ 22
Reflections collected/unique	8347/5006	7432/5679	6604/6608
Rint	0.0415	0.0242	0.0346
Data/restraints/parameters	5006/0/ 317	5679/0/ 341	6608/0/ 368
Goodness-of-fit on F2	1.032	1.057	0.869
Final R indices [I >2σ(I)]	R1 = 0.0533	R1 = 0.0540	R1 = 0.0623
	wR2 = 0.1372	wR2 = 0.1343	wR2 = 0.1349
R indices (all data)	R1 = 0.0692	R1 = 0.0624	R1 = 0.1580
	wR2 = 0.1555	wR2 = 0.1652	wR2 = 0.1591
Goodness-of-fit on F2	1.032	1.057	0.869
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R indices (all data)	R1 = 0.0692	R1 = 0.0624	R1 = 0.1580
	wR2 = 0.1555	wR2 = 0.1652	wR2 = 0.1591

Table S2. Selected bond distances (Å) and angles (º) in the **1**, **2** and **3**.

[Cu(HL)Cl] (**1**)					
Cu1–O2	1.944(2)	Cu1–O3	1.904(2)	Cu1–N2	1.988(3)
Cu1–Cl1	2.216 (1)	O3–C15	1.271(4)	C15–C16	1.422(4)
O2–Cu1–O3	170.87 (1)	Cl1–Cu1–N2	173.05(8)	O2–Cu1–N2	81.03(1)
O2–Cu1–Cl1	92.87(8)	O3–Cu1–Cl1	93.64(7)	O3–Cu1–N2	92.80(1)
$[Cu_2L_2(CH_3OH)_2]\cdot CH_3OH$ (**2**)					
Cu1–O3	1.902(2)	Cu1–O4	1.922(2)	Cu1–O5	2.686(2)
Cu1–O6	1.950(2)	Cu1–N5	1.926(2)	O3–C10	1.297(3)
C9–C10	1.405(4)				
O6–Cu1–N6	176.74(1)	O4–Cu1–O3	176.62(8)	N5–O3–O6	89.98(9)
O4–N5–O3	90.63(9)	O5–O4–O6	94.68(1)	O4–O6–O3	87.71(9)
O5–Cu1–O3	87.28(8)	O5–Cu1–O6	85.44(8)	O5–Cu1–O4	95.60(8)
O5–Cu1–N5	96.88(8)				
$[Mn_2L_2(CH_3OH)_2(H_2O)_2]\cdot CH_3OH$ (**3**)					
Mn1–O2	1.912(3)	Mn1–O3	1.915(3)	Mn1–O6	2.324(4)
Mn1–O7	2.172(3)	Mn1–O7A	1.872(3)	Mn1–N2	1.990(4)
O3–C15	1.270(5)	C15–C16	1.407(6)		
O6–Mn1–O7	177.26(2)	O7A–Mn1–N2	169.90(2)	O3–Mn1–O2	168.56(2)
O6–Mn1–N2	90.66(2)	O7–Mn1–N2	91.74(1)		

Table S3. Hydrogen-bonding distances (Å) and angles (º) of **1**, **2** and **3**.

Complex	D-H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A	Symmetry code
1	C5–H5···O2	0.931(4)	2.413(2)	3.341(5)	175.19(2)	1-x, 2-y, -z
	C11–H11···O4	0.930(3)	2.711(4)	3.333(6)	125.03(3)	1+x, 1+y, -1+z
	C2–H2···N3	0.930(3)	2.543(4)	3.457(5)	167.55(3)	1-x, 2-y, 1-z
2	O6–H6a···O7	0.849(4)	1.828(4)	2.651(4)	162.82(2)	x, -1+y, z
	O7–H7···O1	0.820(7)	2.096(5)	2.877(5)	159.01(1)	1-x, -y, -1-z
	C6–H6···O1	0.930(4)	2.577(6)	3.460(3)	158.61(4)	1-x, 1-y, 1-z
3	O8–H8···N3	0.820(4)	2.011(4)	2.815(5)	166.58(3)	1.5-x, -0.5+y,0.5- z
	O6–H6B···O8	0.957(5)	1.896(8)	2.818(6)	160.82(3)	-0.5+x,1.5 -y, -0.5+z

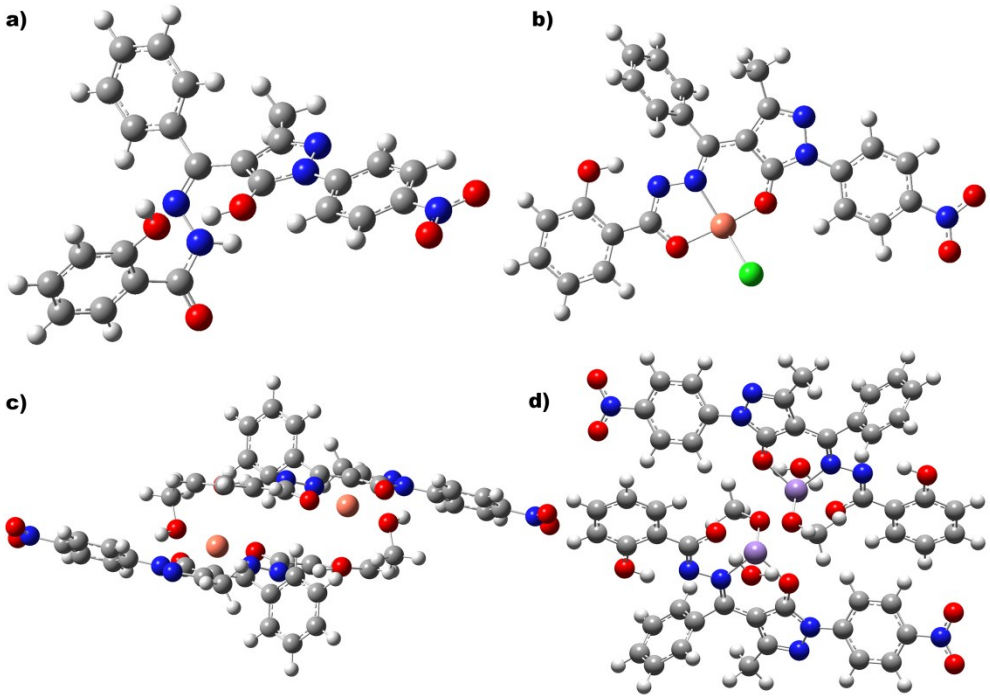

Figure S1. Optimized molecular structures of H_2L (a), **1** (b), **2** (c), and **3** (d).

The cartesian coordinate of the optimized structure of H_2L are as follows:

B3LYP/6-31G in gas phase, E = -1575.285 a.u., Charge = 0, Multiplicity = 1

N	-1.55698	3.56404	-0.00128
C	-1.1524	4.26624	1.13025
C	-0.4816	5.42498	-0.7191
C	-0.48229	5.42571	0.71577
N	-1.15116	4.26513	-1.13304
C	0.13739	6.49994	1.62879
N	0.7315	7.52768	1.11479
N	1.37446	8.63995	0.55851
H	0.91396	9.47553	0.85807
C	0.04951	6.35017	3.15897
C	-0.5907	5.24267	3.7158
C	0.61003	7.32161	3.98823
C	-0.67092	5.10707	5.10158
H	-1.03317	4.47737	3.06175
C	0.53073	7.18562	5.37446
H	1.11481	8.19446	3.54953
C	-0.10972	6.07866	5.93122
H	-1.17607	4.23448	5.54055
H	0.97313	7.95151	6.02805
H	-0.17305	5.9715	7.02384
C	2.77614	8.66754	1.00059
O	3.53063	9.61384	0.65587
C	3.32312	7.53449	1.88863

C	2.48867	6.48423	2.27219
C	4.65275	7.55815	2.30943
C	2.98364	5.45824	3.07691
H	1.44025	6.46627	1.94091
C	5.1483	6.53141	3.11359
C	4.31398	5.48162	3.49748
H	2.32581	4.6307	3.37979
H	6.19681	6.55012	3.44487
H	4.70404	4.67252	4.13192
O	5.50828	8.63442	1.91623
H	6.39186	8.48338	2.25986
C	-1.45329	3.74758	2.54871
H	-0.53375	3.57553	3.06809
H	-2.03184	4.47481	3.07912
H	-2.00335	2.83204	2.48449
O	0.0947	6.42159	-1.56735
H	-0.25664	6.32831	-2.45587
C	0.08333	3.46941	-1.19429
C	1.12121	3.8563	-2.04257
C	0.21716	2.32767	-0.40431
C	2.29236	3.10119	-2.10129
H	1.01509	4.75605	-2.66582
C	1.38899	1.57277	-0.4622
H	-0.60069	2.0227	0.26446
C	2.42648	1.95925	-1.3106
H	3.11022	3.40574	-2.77036
H	1.49439	0.67284	0.16109
N	3.661	1.16363	-1.37266
O	4.18311	1.23397	-2.62648
O	3.38075	-0.13238	-1.07034

The cartesian coordinate of the optimized structure of **1** are as follows:

B3LYP/6-31G + LANL2DZ in gas phase, E = -3674.651 a.u., Charge = 0, Multiplicity = 1

Cu	8.106	9.019	1.97
C	9.377	13.422	4.334
H	9.414	12.779	5.005
C	10.044	14.627	4.492
H	10.523	14.795	5.272
C	10.001	15.573	3.499
H	10.452	16.379	3.604
C	9.289	15.327	2.358
H	9.26	15.97	1.686
C	8.61	14.125	2.194

H	8.124	13.964	1.417
C	8.659	13.174	3.186
C	8.024	11.827	3.06
C	9.765	10.435	0.351
C	10.71	10.75	-0.738
C	11.055	12.057	-1.127
C	11.937	12.25	-2.167
H	12.145	13.117	-2.432
C	12.517	11.192	-2.82
H	13.114	11.343	-3.516
C	12.203	9.876	-2.433
H	12.605	9.152	-2.857
C	11.295	9.676	-1.42
H	11.065	8.807	-1.182
C	6.701	10.018	4.168
C	7.079	11.38	4.006
C	6.293	12.087	4.97
C	6.188	13.565	5.219
H	5.464	13.736	5.827
H	6.025	14.019	4.39
H	7.009	13.885	5.602
C	5.232	8.901	5.888
C	4.682	9.102	7.133
H	4.655	9.958	7.497
C	4.173	8.035	7.841
H	3.8	8.165	8.682
C	4.22	6.793	7.296
C	4.738	6.575	6.065
H	4.748	5.715	5.708
C	5.251	7.633	5.337
H	5.604	7.493	4.488
Cl	7.831	6.861	1.549
N	9.335	11.391	1.164
N	8.398	10.98	2.113
N	5.534	11.287	5.675
N	5.805	10.003	5.2
N	3.706	5.663	8.068
O	9.355	9.247	0.499
O	7.079	8.961	3.572
O	3.323	5.862	9.212
O	3.74	4.553	7.578
O	10.466	13.111	-0.494
H	10.074	12.842	0.176

The cartesian coordinate of the optimized structure of **2** are as follows:

B3LYP/6-31G + LANL2DZ in gas phase, E = -3772.915 a.u., Charge = 0, Multiplicity = 1

Cu	4.5101	-1.5715	2.4453
C	8.2676	-5.9551	6.4405
C	9.2031	-4.9802	6.6959
H	9.965	-5.1771	7.1915
C	8.9952	-3.7011	6.2067
H	9.6322	-3.0382	6.3468
C	7.832	-3.417	5.5065
C	6.8971	-4.4256	5.2522
H	6.1258	-4.2361	4.7674
C	7.1218	-5.6933	5.7176
H	6.5079	-6.3715	5.5495
C	8.8164	1.259	5.2209
H	9.4097	1.1045	5.96
H	9.3202	1.5801	4.4689
H	8.1596	1.9113	5.4731
C	8.1361	-0.016	4.8557
C	7.0424	-0.2464	3.9712
C	6.7045	-1.5952	4.163
C	6.3962	0.6085	3.0242
C	6.936	1.9763	2.7398
C	8.153	2.1164	2.1181
H	8.6353	1.3593	1.8746
C	8.6689	3.3769	1.8498
H	9.4916	3.4667	1.4254
C	7.9512	4.4971	2.2172
H	8.2857	5.3462	2.0362
C	6.7453	4.3551	2.8475
H	6.2682	5.1119	3.1007
C	6.2245	3.1068	3.1158
H	5.4033	3.0227	3.5446
C	3.6633	0.4516	0.9492
C	2.9087	1.2569	-0.028
C	3.4953	2.3481	-0.6928
C	2.7512	3.0636	-1.6096
H	3.1426	3.781	-2.0556
C	1.4535	2.7361	-1.8746
H	0.9707	3.2296	-2.4974
C	0.85	1.677	-1.2239
H	-0.0375	1.4627	-1.3974
C	1.5782	0.9419	-0.3167
H	1.1765	0.2223	0.1131
C	2.4154	-3.6344	1.7755

H	1.8886	-2.8531	1.5837
H	2.6998	-4.0404	0.9502
H	1.8903	-4.2665	2.2743
N	8.5083	-7.3108	6.9372
N	7.6263	-2.0974	5.0389
N	8.5008	-1.1035	5.4828
N	4.7575	1.0045	1.4361
N	5.3561	0.1567	2.3659
O	7.7422	-8.2005	6.5806
O	9.4464	-7.4972	7.6806
O	5.7596	-2.3293	3.6619
O	3.2326	-0.7202	1.2885
O	4.7857	2.7172	-0.473
H	5.1059	2.2552	0.1185
O	3.5469	-3.2651	2.5297
H	3.9658	-3.9676	2.7581
Cu	6.2039	1.5715	-2.4453
C	2.4464	5.9551	-6.4405
C	1.5109	4.9802	-6.6959
H	0.749	5.1771	-7.1915
C	1.7188	3.7011	-6.2067
H	1.0818	3.0382	-6.3468
C	2.882	3.417	-5.5065
C	3.8169	4.4256	-5.2522
H	4.5882	4.2361	-4.7674
C	3.5922	5.6933	-5.7176
H	4.2061	6.3715	-5.5495
C	1.8976	-1.259	-5.2209
H	1.3043	-1.1045	-5.96
H	1.3938	-1.5801	-4.4689
H	2.5544	-1.9113	-5.4731
C	2.5779	0.016	-4.8557
C	3.6716	0.2464	-3.9712
C	4.0095	1.5952	-4.163
C	4.3178	-0.6085	-3.0242
C	3.778	-1.9763	-2.7398
C	2.561	-2.1164	-2.1181
H	2.0787	-1.3593	-1.8746
C	2.0451	-3.3769	-1.8498
H	1.2224	-3.4667	-1.4254
C	2.7628	-4.4971	-2.2172
H	2.4283	-5.3462	-2.0362
C	3.9687	-4.3551	-2.8475
H	4.4458	-5.1119	-3.1007

C	4.4895	-3.1068	-3.1158
H	5.3107	-3.0227	-3.5446
C	7.0507	-0.4516	-0.9492
C	7.8053	-1.2569	0.028
C	7.2187	-2.3481	0.6928
C	7.9628	-3.0636	1.6096
H	7.5714	-3.781	2.0556
C	9.2605	-2.7361	1.8746
H	9.7433	-3.2296	2.4974
C	9.864	-1.677	1.2239
H	10.7515	-1.4627	1.3974
C	9.1358	-0.9419	0.3167
H	9.5375	-0.2223	-0.1131
C	8.2986	3.6344	-1.7755
H	8.8254	2.8531	-1.5837
H	8.0142	4.0404	-0.9502
H	8.8237	4.2665	-2.2743
N	2.2057	7.3108	-6.9372
N	3.0877	2.0974	-5.0389
N	2.2132	1.1035	-5.4828
N	5.9565	-1.0045	-1.4361
N	5.3579	-0.1567	-2.3659
O	2.9718	8.2005	-6.5806
O	1.2676	7.4972	-7.6806
O	4.9544	2.3293	-3.6619
O	7.4814	0.7202	-1.2885
O	5.9283	-2.7172	0.473
H	5.6081	-2.2552	-0.1185
O	7.1671	3.2651	-2.5297
H	6.7482	3.9676	-2.7581

The cartesian coordinate of the optimized structure of **3** are as follows:

B3LYP/6-31G + LANL2DZ in gas phase, E = -3740.169 a.u., Charge = 0, Multiplicity = 1

Mn	6.3087	6.9185	7.9339
C	4.1962	10.9351	5.3795
C	3.2845	11.5024	4.512
H	3.2501	12.4266	4.4194
C	2.435	10.7247	3.7924
H	1.8239	11.1154	3.2099
C	2.4829	9.366	3.9242
H	1.9151	8.83	3.4165
C	3.3626	8.7899	4.797
H	3.3727	7.8644	4.8879

C	4.2279	9.5425	5.5434
C	5.1433	8.8838	6.4929
C	7.8669	9.4148	8.4719
C	8.0333	10.89	8.2955
C	7.3805	11.7841	9.0882
H	6.8477	11.4798	9.7883
C	7.508	13.1479	8.8566
H	7.0416	13.7528	9.3857
C	8.3076	13.5975	7.8627
H	8.3928	14.5117	7.7113
C	8.9873	12.7096	7.0825
H	9.5528	13.0177	6.4109
C	8.8351	11.3408	7.2909
H	9.2811	10.7347	6.7458
C	8.72	7.2458	9.3554
C	8.7891	8.6459	9.2343
C	9.9566	9.0178	9.9468
C	10.536	10.3778	10.1606
H	11.3203	10.3089	10.7092
H	9.8891	10.9363	10.5988
H	10.7704	10.7623	9.3144
C	10.1297	5.5965	10.6005
C	10.899	5.4913	11.7299
H	11.2305	6.254	12.1467
C	11.1791	4.2378	12.2465
H	11.6971	4.1564	13.0142
C	10.7015	3.1358	11.639
C	9.9516	3.2184	10.5239
H	9.6348	2.4432	10.1196
C	9.6501	4.4544	9.9753
H	9.1361	4.5183	9.2022
C	6.1185	4.0249	7.8092
H	6.9469	4.1977	7.355
H	5.546	3.5027	7.2446
H	6.2946	3.5428	8.6215
N	6.0577	9.6227	7.07
N	6.8774	8.8237	7.8645
N	10.5607	7.9822	10.458
N	9.8044	6.8664	10.0857
N	10.9628	1.8021	12.2037
O	5.0444	11.7729	6.0315
H	5.4571	11.3534	6.6015
O	5.0285	7.604	6.6904
O	7.8442	6.4143	8.9605

O	11.6416	1.7582	13.2012
O	10.5243	0.8328	11.6497
O	5.4905	5.2459	8.1172
O	7.6252	6.4293	6.0832
H	8.0843	6.8125	6.8847
H	8.4012	5.8695	6.0814
Mn	4.2719	5.6045	9.8791
C	6.3844	1.5879	12.4335
C	7.2962	1.0206	13.301
H	7.3305	0.0964	13.3936
C	8.1456	1.7983	14.0206
H	8.7567	1.4076	14.6031
C	8.0977	3.157	13.8888
H	8.6656	3.693	14.3965
C	7.2181	3.7331	13.016
H	7.2079	4.6586	12.9251
C	6.3528	2.9805	12.2696
C	5.4374	3.6392	11.3202
C	2.7138	3.1082	9.3412
C	2.5473	1.633	9.5175
C	3.2001	0.7389	8.7248
H	3.7329	1.0432	8.0248
C	3.0726	-0.6249	8.9564
H	3.5391	-1.2298	8.4273
C	2.273	-1.0745	9.9504
H	2.1878	-1.9887	10.1018
C	1.5933	-0.1866	10.7306
H	1.0278	-0.4947	11.4021
C	1.7455	1.1822	10.5222
H	1.2995	1.7883	11.0672
C	1.8606	5.2772	8.4576
C	1.7915	3.8771	8.5788
C	0.624	3.5052	7.8662
C	0.0447	2.1452	7.6525
H	-0.7397	2.2141	7.1038
H	0.6916	1.5867	7.2143
H	-0.1897	1.7607	8.4986
C	0.4509	6.9265	7.2125
C	-0.3184	7.0317	6.0832
H	-0.6499	6.269	5.6663
C	-0.5985	8.2852	5.5666
H	-1.1165	8.3666	4.7988
C	-0.1209	9.3872	6.174
C	0.629	9.3046	7.2891

H	0.9458	10.0798	7.6934
C	0.9306	8.0686	7.8377
H	1.4445	8.0047	8.6108
C	4.4621	8.4981	10.0038
H	3.6338	8.3253	10.458
H	5.0346	9.0203	10.5685
H	4.2861	8.9802	9.1915
N	4.523	2.9003	10.743
N	3.7033	3.6993	9.9486
N	0.02	4.5408	7.355
N	0.7762	5.6566	7.7273
N	-0.3821	10.7209	5.6093
O	5.5363	0.7501	11.7815
H	5.1235	1.1696	11.2115
O	5.5522	4.919	11.1226
O	2.7364	6.1087	8.8525
O	-1.061	10.7648	4.6118
O	0.0564	11.6902	6.1633
O	5.0902	7.2771	9.6958
O	2.9554	6.0937	11.7299
H	2.4963	5.7105	10.9283
H	2.1794	6.6535	11.7317

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