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Electronic Supplementary Information

N-Hydroxy-Phe-Phe, a New Dipeptide and Cytotoxic Macrocyclic Trichothecenes from a Lethal Toxic Mushroom *Podostroma cornu-damae*

Bum Soo Lee,[a,†] Su Myung Jung,[b,†] Rhim Ryoo,[c] Sang Un Choi,[d] Seongpil An,[e,*] and Ki Hyun Kim [a,*]

[a.] *School of Pharmacy, Sungkyunkwan University, Suwon 440-746, Republic of Korea. E-mail: khkim83@skku.edu; Fax: +82-31-290-7730; Tel: +82-31-290-7700*

[b.] *Department of Biological Sciences, Sungkyunkwan University, Suwon 16419, Republic of Korea.*

[c.] *Special Forest Products Division, Forest Bioresources Department, National Institute of Forest Science, Suwon 16631, Republic of Korea*

[d.] *Korea Research Institute of Chemical Technology, Deajeon 34114, Republic of Korea*

[e.] *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea. E-mail: esan@skku.edu*

Electronic Supplementary Information Contents:

Figure S1. The HR-ESIMS data of compound **1**

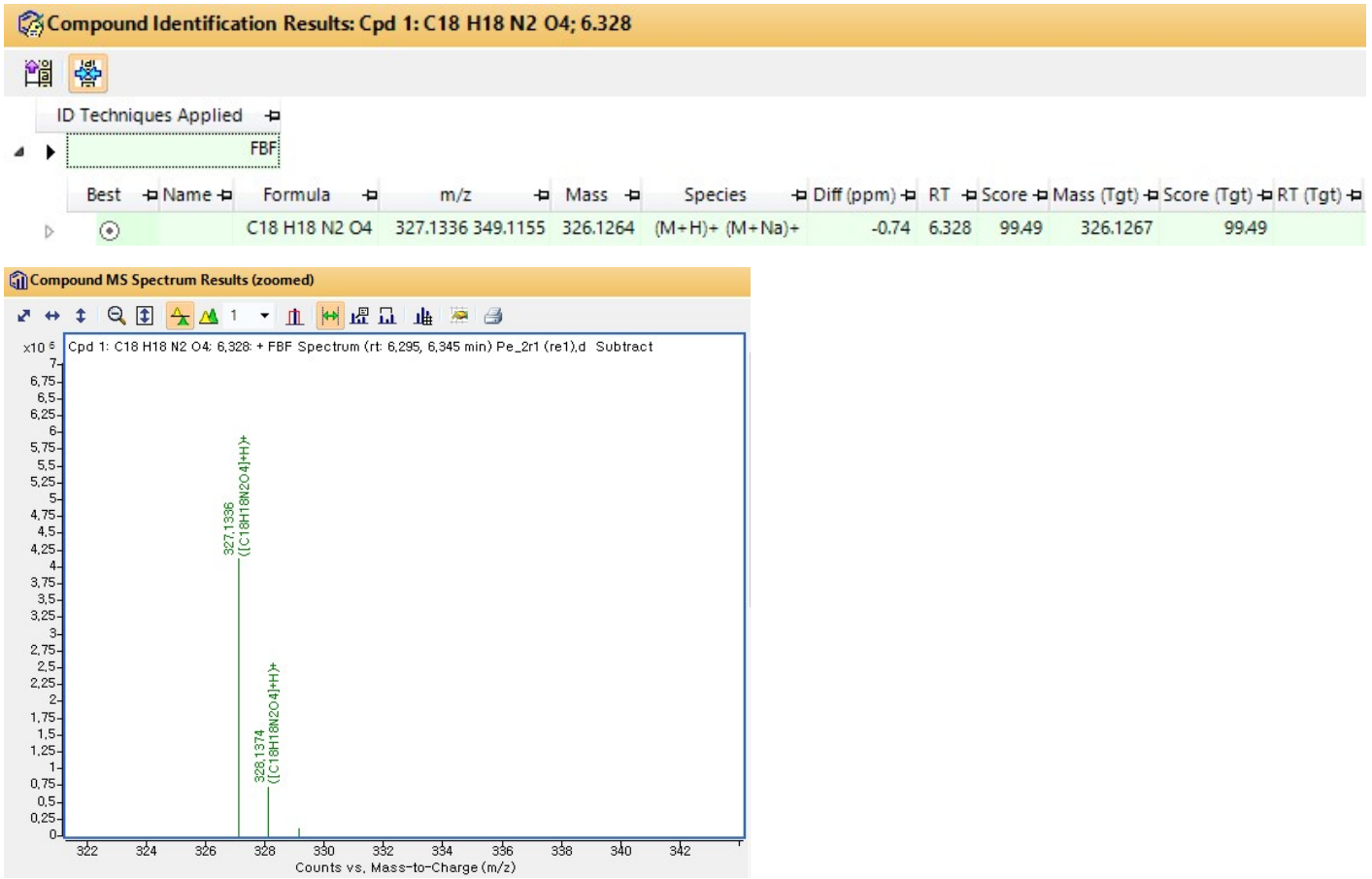

Figure S2. The UV spectrum of compound **1**

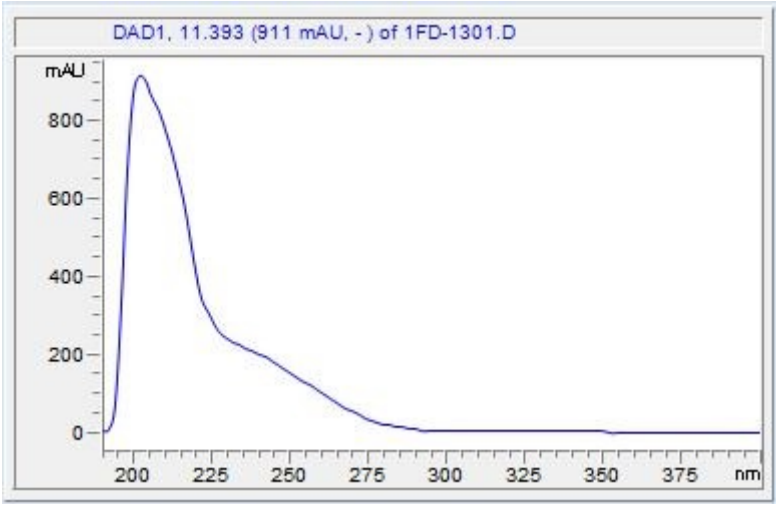

Figure S3. The IR spectrum of compound **1**

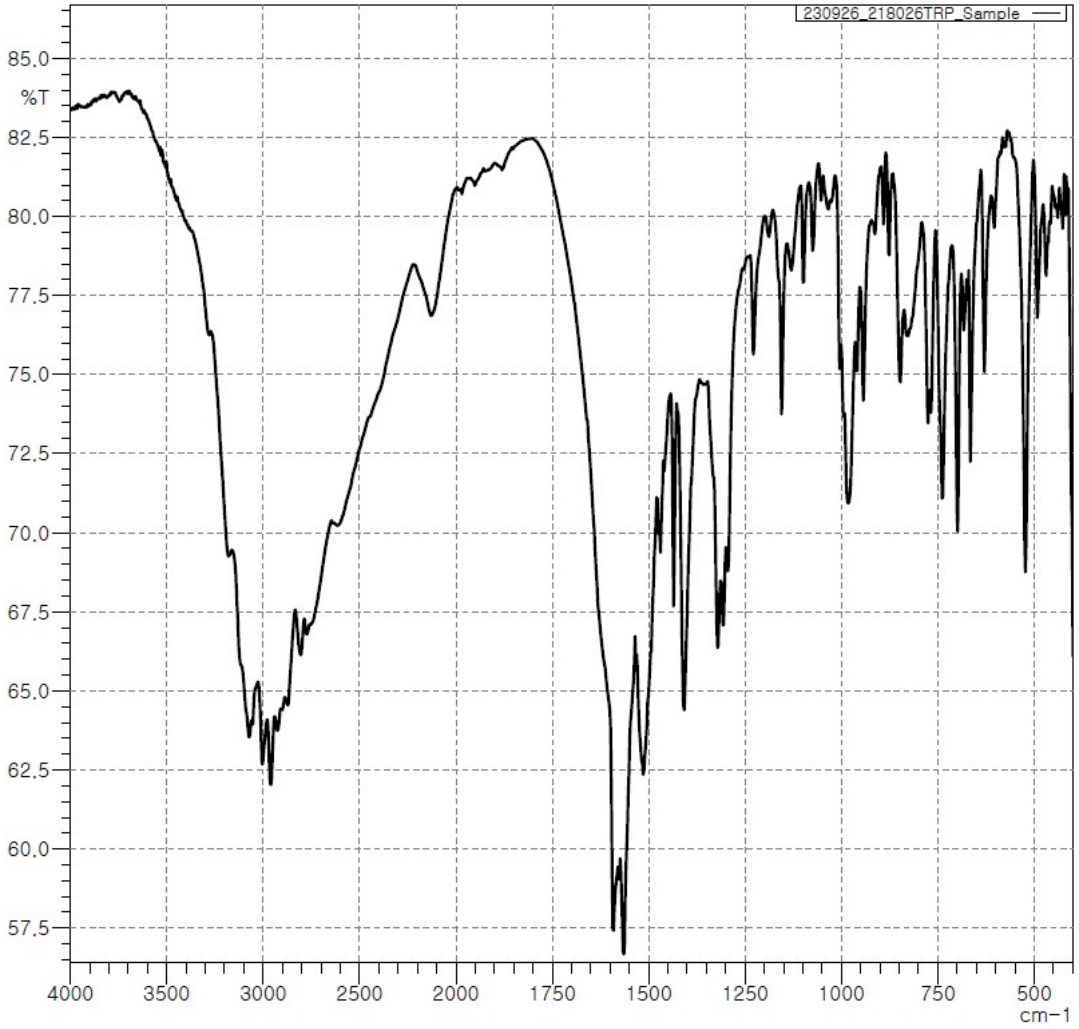

Figure S4. The ^{1}H NMR spectrum of compound **1** (CD_3OD, 850 MHz)

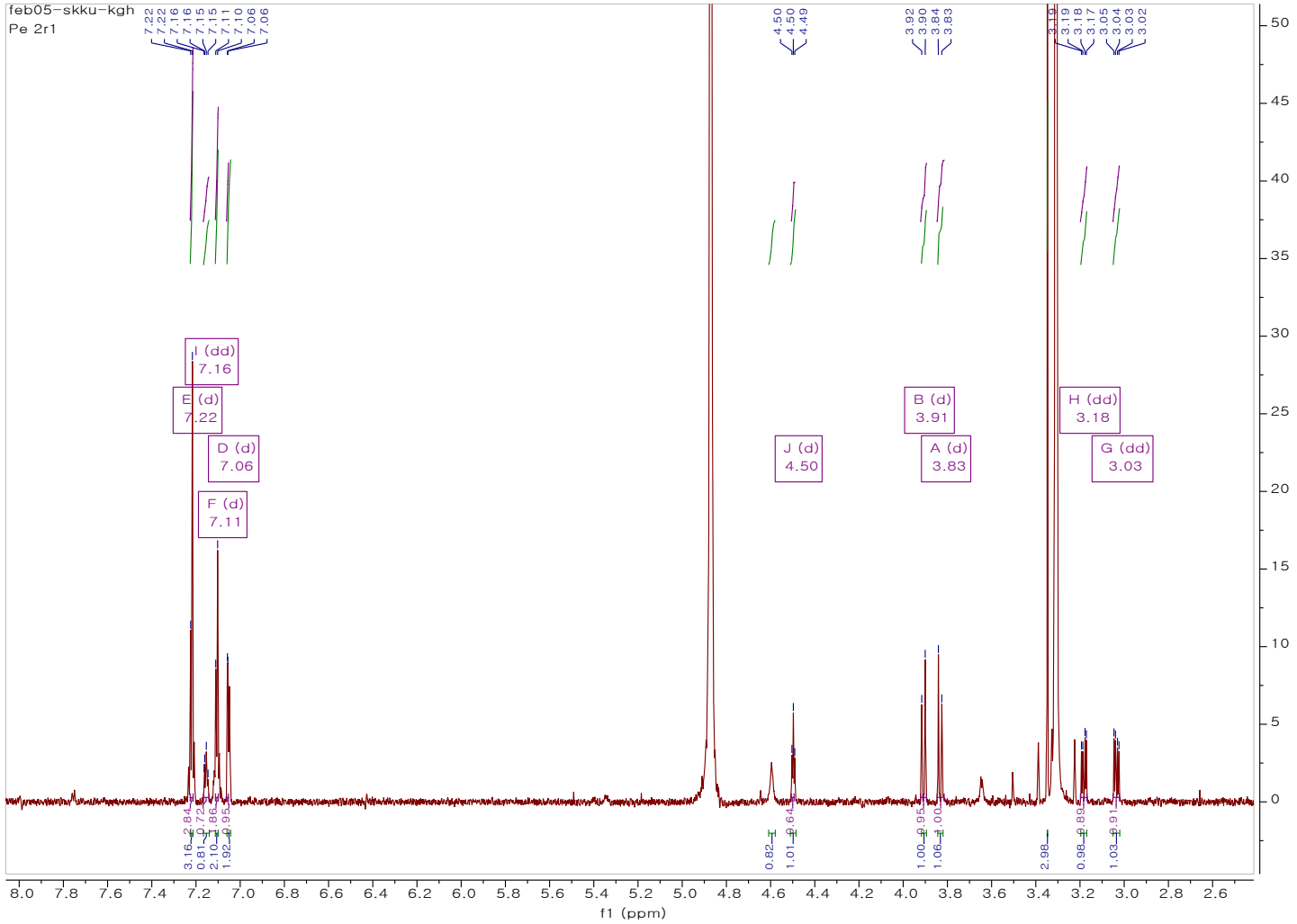

Figure S5. The ^{1}H-^{1}H COSY spectrum of compound **1**

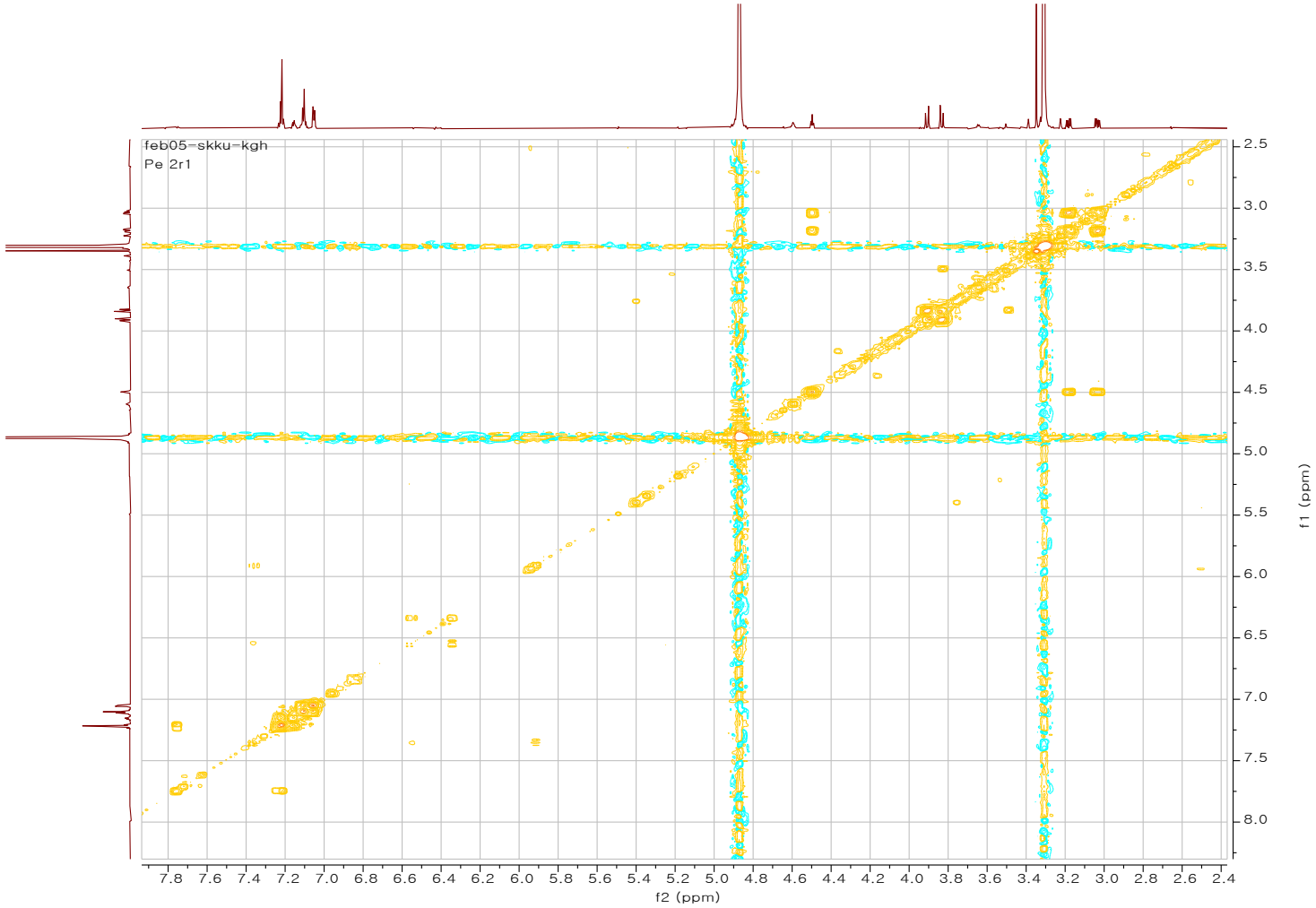

Figure S6. The HSQC spectrum of compound **1**

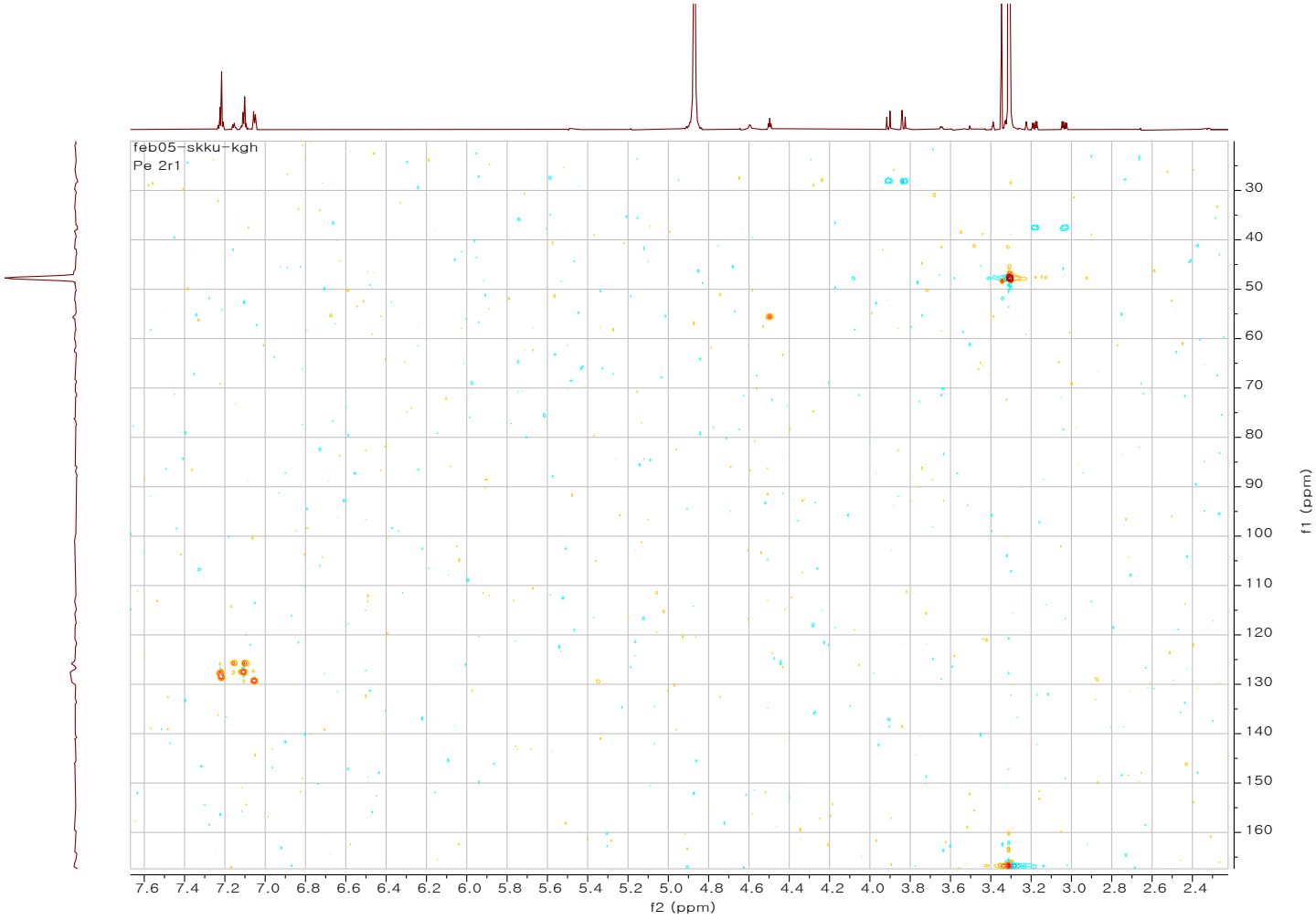

Figure S7. The HMBC spectrum of compound **1**

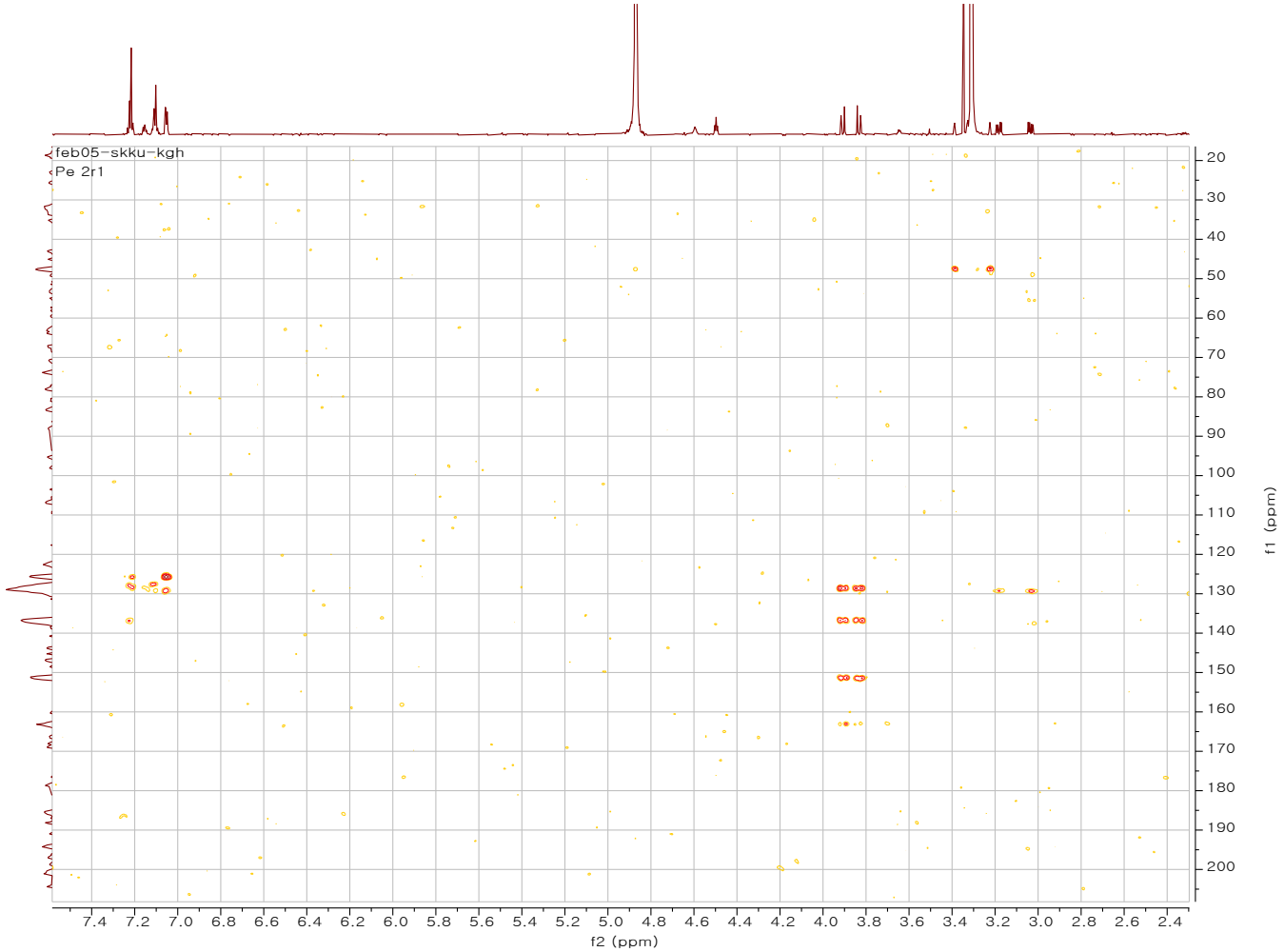

Figure S8. The ROESY spectrum of compound **1**

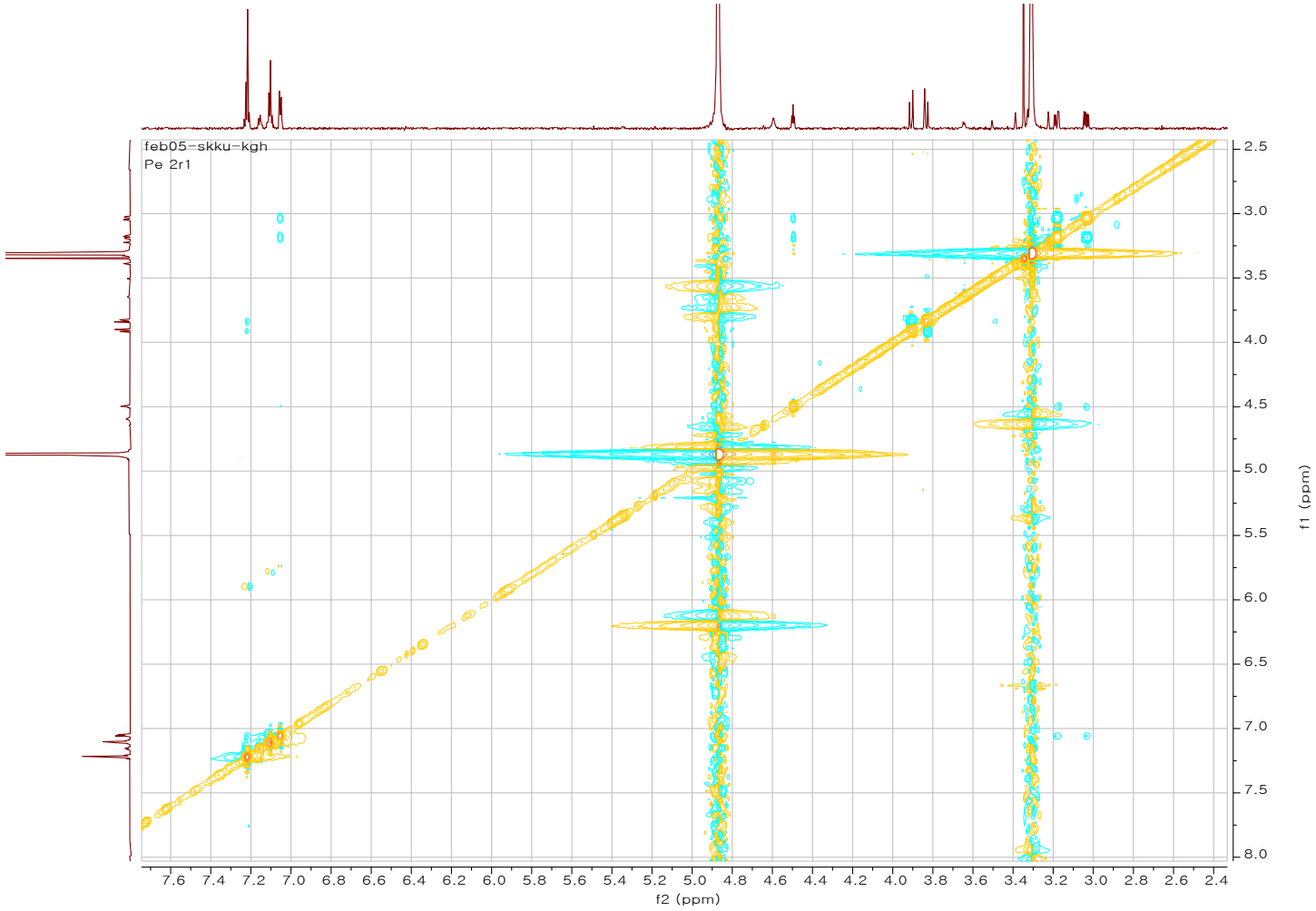

Table S1. Gibbs free energies and Boltzmann distribution of conformers **1a.**

Conformers	B3LYP/6-31+G(d,p) Gibbs free energy (298.15 K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann distribution (%)
1a-1	-1106.508070741	0.00	**21.86%**
1a-2	-1106.508168102	-0.06	**24.23%**
1a-3	-1106.508173240	-0.06	**24.36%**
1a-4	-1106.508354830	-0.18	**29.53%**

Coordinates of the conformers

1a_1

Coordinates (Angstroms) X	Y	Z	atom	charge
3.700283	-3.11009	-3.77491	o	8
3.056131	-2.97777	-1.54203	c	6
5.287313	1.013557	-0.90457	c	6
6.866691	2.201776	1.186039	c	6
6.507286	1.13228	3.479059	o	8
8.302729	3.950727	0.845048	o	8
3.762664	3.088898	-2.33381	c	6
1.757883	4.376034	-0.75309	c	6
2.324361	6.561164	0.639381	c	6
0.487908	7.722386	2.135216	c	6
-1.94912	6.718208	2.26224	c	6
-2.53869	4.550007	0.878687	c	6
-0.70014	3.392264	-0.61763	c	6
1.41856	-5.00991	-0.37205	c	6

0.389778	-7.0302	-2.10316	c	6
-2.1364	-6.26095	-3.25625	c	6
-4.41585	-7.03747	-2.1561	c	6
-6.72612	-6.31921	-3.20848	c	6
-6.78638	-4.80439	-5.368	c	6
-4.52185	-4.01216	-6.46846	c	6
-2.21076	-4.73314	-5.42022	c	6
-0.52108	-6.71562	2.965086	o	8
6.625409	0.217225	-2.27264	h	1
3.127919	-1.08249	1.818247	h	1
7.576736	2.059587	4.650964	h	1
5.131624	4.469416	-3.03707	h	1
2.912636	2.152732	-3.96895	h	1
4.215721	7.355893	0.538175	h	1
0.958876	9.418817	3.19304	h	1
-3.38219	7.627531	3.418116	h	1
-4.43373	3.761997	0.954175	h	1
-1.18107	1.719045	-1.70832	h	1
0.177092	-8.77963	-1.02747	h	1

1.780617	-7.32139	-3.60092	h	1
-4.37076	-8.20007	-0.4644	h	1
-8.47942	-6.94659	-2.34166	h	1
-8.58437	-4.24818	-6.18942	h	1
-4.55205	-2.83697	-8.15278	h	1
-0.4458	-4.1098	-6.26382	h	1
-0.59591	-6.31492	4.746829	h	1

1a_2

Coordinates (Angstroms) X	Y	Z	atom	charge
0.398932	-1.10424	-5.29874	o	8
-0.02442	-1.00508	-3.01539	c	6
2.781567	2.625586	-2.33129	c	6
5.489057	2.147564	-1.42004	c	6
5.815035	-0.14752	-0.36535	o	8
7.193206	3.660119	-1.6679	o	8
1.964865	5.375752	-1.72909	c	6
1.556325	5.889387	1.058626	c	6
3.55927	6.689413	2.603718	c	6

3.184445	7.123221	5.178011	c	6
0.801486	6.764734	6.254878	c	6
-1.20662	5.973136	4.738409	c	6
-0.82942	5.541719	2.162284	c	6
-1.78175	-2.89436	-1.78188	c	6
-2.9548	-4.8979	-3.44068	c	6
-1.36553	-7.29847	-3.56056	c	6
0.686501	-7.46252	-5.22869	c	6
2.138353	-9.66109	-5.3472	c	6
1.564017	-11.7203	-3.79881	c	6
-0.4697	-11.5654	-2.12496	c	6
-1.92202	-9.36591	-2.00412	c	6
-3.72836	-4.4333	1.630839	o	8
2.850567	2.403279	-4.3908	h	1
0.579141	0.634664	0.413695	h	1
7.597163	-0.25511	0.072135	h	1
3.427253	6.626033	-2.48195	h	1
0.219623	5.737888	-2.7786	h	1
5.41547	6.97132	1.773195	h	1

4.75457	7.753035	6.342406	h	1
0.509329	7.112434	8.257406	h	1
-3.07189	5.70432	5.554936	h	1
-2.40597	4.945302	0.986873	h	1
-3.13953	-4.09528	-5.33373	h	1
-4.83562	-5.33499	-2.7075	h	1
1.137442	-5.85133	-6.41845	h	1
3.717655	-9.7676	-6.65604	h	1
2.691255	-13.434	-3.89774	h	1
-0.93113	-13.1589	-0.91386	h	1
-3.49619	-9.24147	-0.692	h	1
-3.77565	-3.9701	3.398484	h	1

1a_3

Coordinates (Angstroms) X	Y	Z	atom	charge
4.48488	-3.57853	-1.45495	o	8
2.535557	-2.31272	-1.50532	c	6
4.654473	1.592183	-0.16709	c	6
4.629991	2.22691	2.660226	c	6

2.802085	1.016052	3.956083	o	8
6.136652	3.640595	3.652562	o	8
5.144019	4.005418	-1.75562	c	6
2.956876	5.853837	-1.77287	c	6
2.732193	7.717157	0.102466	c	6
0.689681	9.385502	0.105427	c	6
-1.16447	9.222968	-1.76595	c	6
-0.95976	7.382915	-3.64463	c	6
1.085405	5.715173	-3.6456	c	6
0.03682	-3.52364	-2.19195	c	6
0.023553	-6.32245	-2.74557	c	6
-0.48069	-7.90281	-0.39008	c	6
1.492339	-8.4798	1.281364	c	6
1.035181	-9.927	3.438356	c	6
-1.39728	-10.8116	3.956256	c	6
-3.37258	-10.2362	2.304556	c	6
-2.91718	-8.78656	0.147654	c	6
-4.12504	-3.26874	-2.8433	o	8
6.258295	0.30556	-0.42232	h	1

0.736005	1.048832	-0.99193	h	1
3.014653	1.509629	5.714005	h	1
6.839211	4.905343	-0.99088	h	1
5.567683	3.392899	-3.68542	h	1
4.170849	7.852358	1.561271	h	1
0.552313	10.82261	1.566222	h	1
-2.74914	10.5287	-1.7672	h	1
-2.38314	7.251073	-5.11929	h	1
1.244807	4.298186	-5.12556	h	1
1.876164	-6.80387	-3.51976	h	1
-1.42216	-6.70097	-4.17056	h	1
3.378466	-7.77532	0.880449	h	1
2.583409	-10.3676	4.714349	h	1
-1.75012	-11.9436	5.633019	h	1
-5.27084	-10.9188	2.69147	h	1
-4.45803	-8.32746	-1.12928	h	1
-5.35047	-1.91352	-2.7897	h	1

1a_4

Coordinates (Angstroms)			atom	charge
X	Y	Z		

3.76777	-6.65523	-3.44741	o	8
2.538131	-2.59039	-1.57462	c	6
4.258517	1.715849	-1.47492	c	6
6.615621	2.131472	0.158959	c	6
6.974698	0.313886	1.907066	o	8
8.05756	3.891103	-0.1229	o	8
2.867231	4.253167	-1.93705	c	6
1.557669	5.30324	0.384012	c	6
2.854342	6.869255	2.088682	c	6
1.655131	7.792944	4.248337	c	6
-0.86178	7.169855	4.742984	c	6
-2.17451	5.620765	3.059211	c	6
-0.97263	4.698225	0.898021	c	6
0.808977	-4.4709	-0.28843	c	6
0.535788	-7.04891	-1.47911	c	6
-1.59899	-7.13695	-3.41169	c	6
-4.01863	-7.95446	-2.71424	c	6
-5.96996	-8.03543	-4.48796	c	6
-5.52786	-7.2908	-6.98042	c	6

-3.12391	-6.46084	-7.6863	c	6
-1.17181	-6.38029	-5.91425	c	6
-1.86021	-5.49946	2.815711	o	8
4.97758	1.020991	-3.28989	h	1
1.598487	0.045557	1.068528	h	1
8.544925	0.740786	2.762266	h	1
4.269202	5.598031	-2.64095	h	1
1.486241	3.929692	-3.44182	h	1
4.811045	7.361128	1.709174	h	1
2.686284	9.010261	5.541601	h	1
-1.7954	7.897475	6.420731	h	1
-4.13865	5.139415	3.417419	h	1
-2.01277	3.510409	-0.41767	h	1
0.191971	-8.42979	0.017037	h	1
2.32794	-7.48892	-2.40467	h	1
-4.36674	-8.52184	-0.77198	h	1
-7.83469	-8.68506	-3.92239	h	1
-7.04475	-7.35943	-8.36295	h	1
-2.76403	-5.8786	-9.62291	h	1

0.695682	-5.71853	-6.45204	h	1
-2.48565	-4.64196	4.303936	h	1

Table S2. Gibbs free energies and Boltzmann distribution of conformers **1b.**

Conformers	B3LYP/6-31+G(d,p) Gibbs free energy (298.15 K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann distribution (%)
1b-1	-1106.480430267	0.00	**67.40%**
1b-2	-1106.479143266	0.81	**17.24%**
1b-3	-1106.478717568	1.07	**10.98%**
1b-4	-1106.477843396	1.62	**4.35%**

1b_1

Coordinates (Angstroms) X	Y	Z	atom	charge
-2.94924	-1.4227	-1.35821	c	6
-1.92824	-3.33237	0.517559	c	6
-2.77849	-2.83072	3.221306	c	6
-5.35695	-2.86216	3.838164	c	6
-6.14352	-2.49929	6.327332	c	6
-4.36437	-2.10031	8.2379	c	6
-1.79761	-2.05448	7.638263	c	6
-1.01181	-2.4119	5.143184	c	6
-1.16745	0.712151	-2.06351	c	6
-0.32638	4.804342	-3.36606	o	8
-4.36809	4.306306	-1.46943	c	6
-6.08829	5.09309	-3.68309	c	6
-6.06642	3.37141	-5.57585	o	8
-7.39441	6.963892	-3.72031	o	8
-3.85289	6.605823	0.263729	c	6
-2.5029	5.985254	2.706316	c	6
-3.87126	5.666551	4.951704	c	6

-2.63803	5.162328	7.227519	c	6
-0.00792	4.970228	7.290314	c	6
1.375853	5.271601	5.063863	c	6
0.138192	5.774542	2.790164	c	6
1.073132	0.284205	-2.59447	o	8
-5.4002	2.860254	-0.40521	h	1
-5.50415	-0.37374	-3.68216	h	1
0.133991	-3.33988	0.405681	h	1
-2.61778	-5.18691	-0.08686	h	1
-6.73729	-3.1837	2.351092	h	1
-8.14671	-2.54252	6.77929	h	1
-4.97669	-1.83097	10.1793	h	1
-0.40003	-1.74093	9.109553	h	1
0.991265	-2.37657	4.687834	h	1
1.147834	3.674373	-3.54904	h	1
-7.24647	3.974706	-6.84943	h	1
-2.78135	7.995552	-0.82507	h	1
-5.69506	7.453547	0.656665	h	1
-5.91961	5.838856	4.921736	h	1

-3.73113	4.927625	8.949251	h	1
0.957114	4.593296	9.063142	h	1
3.424208	5.127797	5.096982	h	1
1.216142	6.018183	1.060793	h	1

1b_2

Coordinates (Angstroms) X	Y	Z	atom	charge
-6.13376	-1.02636	-1.09676	c	6
-6.06624	-3.57646	0.207937	c	6
-4.10163	-3.66725	2.30323	c	6
-1.60104	-4.38727	1.801738	c	6
0.199732	-4.42105	3.731396	c	6
-0.47495	-3.74116	6.190117	c	6
-2.96217	-3.02274	6.70879	c	6
-4.75804	-2.97707	4.775568	c	6
-3.81722	-0.44861	-2.68209	c	6
-0.74065	2.246734	-4.24549	o	8
-2.94935	3.872051	-0.69332	c	6
-3.79299	6.335057	-1.98658	c	6

-6.18234	6.108455	-2.87862	o	8
-2.54644	8.229621	-2.22417	o	8
-0.45547	4.188429	0.789767	c	6
-0.80375	5.653604	3.229375	c	6
-1.66931	4.416137	5.408815	c	6
-2.01229	5.738694	7.664297	c	6
-1.48685	8.322519	7.77739	c	6
-0.61946	9.570579	5.62087	c	6
-0.28325	8.247057	3.363373	c	6
-2.9149	-2.03996	-4.14726	o	8
-4.45825	3.2973	0.592967	h	1
-7.86098	2.021242	-1.96743	h	1
-5.63759	-5.01025	-1.22153	h	1
-7.95862	-3.927	0.955323	h	1
-1.07211	-4.92166	-0.10931	h	1
2.127517	-4.99279	3.314307	h	1
0.923007	-3.78003	7.69309	h	1
-3.5084	-2.50814	8.6205	h	1
-6.69216	-2.41693	5.185885	h	1

-0.6453	0.550145	-5.01231	h	1
-6.59353	7.688163	-3.72236	h	1
0.236766	2.283852	1.210786	h	1
0.931097	5.104918	-0.43202	h	1
-2.05717	2.398004	5.346745	h	1
-2.67684	4.747932	9.336076	h	1
-1.74519	9.353417	9.534508	h	1
-0.2009	11.57978	5.692826	h	1
0.365942	9.226741	1.68203	h	1

1b_3

Coordinates (Angstroms) X	Y	Z	atom	charge
-0.48181	-0.83578	1.644525	c	6
-1.22488	-3.5935	1.485312	c	6
-4.08181	-3.91468	1.40394	c	6
-5.33514	-4.46902	-0.85889	c	6
-7.96034	-4.73879	-0.90835	c	6
-9.36449	-4.45218	1.305565	c	6
-8.13172	-3.88453	3.57176	c	6

-5.50966	-3.61291	3.617849	c	6
-0.58347	0.611788	-0.8301	c	6
-1.27651	4.277792	-3.12337	o	8
-3.628	3.94567	0.652186	c	6
-6.06871	3.20573	-0.74099	c	6
-8.11212	4.33672	0.294998	o	8
-6.19346	1.735805	-2.48107	o	8
-3.43829	6.81035	1.228159	c	6
-1.1724	7.471775	2.844335	c	6
1.223162	7.797944	1.754265	c	6
3.313731	8.375616	3.255805	c	6
3.042826	8.635439	5.868995	c	6
0.668773	8.314161	6.973183	c	6
-1.42048	7.736332	5.468501	c	6
0.308971	-0.26144	-2.7952	o	8
-3.63965	2.90944	2.442571	h	1
0.74855	1.992307	3.502927	h	1
-0.43525	-4.53479	3.146459	h	1
-0.37029	-4.40439	-0.21382	h	1

-4.25054	-4.67883	-2.5898	h	1
-8.90402	-5.17111	-2.67973	h	1
-11.4057	-4.67417	1.269594	h	1
-9.21149	-3.66402	5.30505	h	1
-4.54984	-3.17193	5.380859	h	1
-0.79425	2.861885	-4.23002	h	1
-9.57282	3.695022	-0.61779	h	1
-3.3684	7.823384	-0.57225	h	1
-5.18467	7.363904	2.180372	h	1
1.437196	7.590445	-0.2777	h	1
5.155282	8.627117	2.38262	h	1
4.670298	9.088784	7.035521	h	1
0.438848	8.51976	9.003289	h	1
-3.2681	7.501345	6.339919	h	1

1b_4

Coordinates (Angstroms) X	Y	Z	atom	charge
-7.12342	-0.14463	0.969127	c	6
-6.5987	-2.96371	1.056203	c	6

-4.19426	-3.55061	2.518684	c	6
-4.20544	-3.49563	5.168743	c	6
-2.00781	-4.00377	6.536516	c	6
0.241944	-4.5641	5.27044	c	6
0.275474	-4.61165	2.631666	c	6
-1.92684	-4.10412	1.265688	c	6
-5.33024	1.30156	-0.77342	c	6
-5.64246	5.004762	1.87512	o	8
-3.03866	5.240293	-1.8703	c	6
-3.59035	4.9886	-4.70325	c	6
-6.08497	5.081533	-5.20959	o	8
-1.97291	4.910331	-6.31565	o	8
-0.24499	4.621545	-1.27356	c	6
0.389109	5.062843	1.481024	c	6
0.171227	3.100016	3.255776	c	6
0.648198	3.536423	5.819045	c	6
1.367689	5.936794	6.644271	c	6
1.61688	7.896608	4.892128	c	6
1.127188	7.461649	2.337939	c	6

-4.39817	0.257992	-2.63156	o	8
-3.43337	7.215346	-1.38569	h	1
-9.0549	2.698339	1.995605	h	1
-6.43318	-3.67381	-0.87722	h	1
-8.23217	-3.84582	1.96115	h	1
-5.95345	-3.05703	6.15605	h	1
-2.0547	-3.97649	8.589844	h	1
1.951763	-4.96999	6.332476	h	1
2.015507	-5.04836	1.632099	h	1
-1.89442	-4.12295	-0.78692	h	1
-4.3007	4.711459	3.10804	h	1
-6.23963	4.926874	-7.03348	h	1
0.098383	2.655292	-1.80683	h	1
0.929593	5.796522	-2.50243	h	1
-0.32887	1.209208	2.627402	h	1
0.474309	1.985308	7.152143	h	1
1.747035	6.27573	8.633215	h	1
2.194355	9.76594	5.515463	h	1