Supporting Information

Bioorg. Med. Chem. Rep. 1:1 (2018) 29-36

Analyzing of some druggable properties of hydrazono-pyridazinones

Burak Kuzu[1] and Nurettin Menges[1] *

[1] *Pharmaceutical Chemistry Section, Faculty of Pharmacy, Van Yüzüncü Yil University, 65080, Van,Türkiye*

Table of Contents	Page
Figure S1. Optimized 3D structures of some pyridazinone derivatives (Atoms are color-coded: Green:Cl; Blue: N; Red: Oxygen; Gray: Carbon; White: Hydrogen).	2
Table S1. Some distances between atoms based on theoretical calculation	2
Table S2. Bond and dihedral angles for 4	3
Figure S2. HOMOs and LUMOs of some pyridazinones	4
Table S3. NBO analyze for some bonds of compound **4[a]**	4
S4. Coordinates for Compound **1**	6
S5. Coordinates for Compound **2**	8
S6. Coordinates for Compound **3**	11

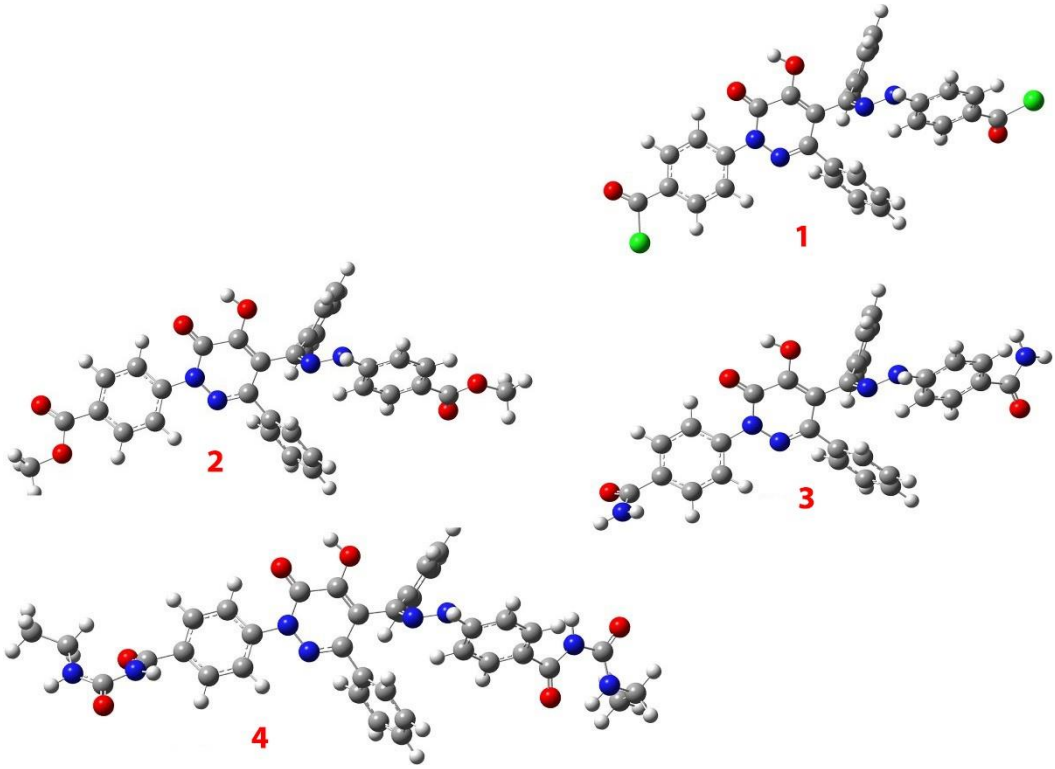
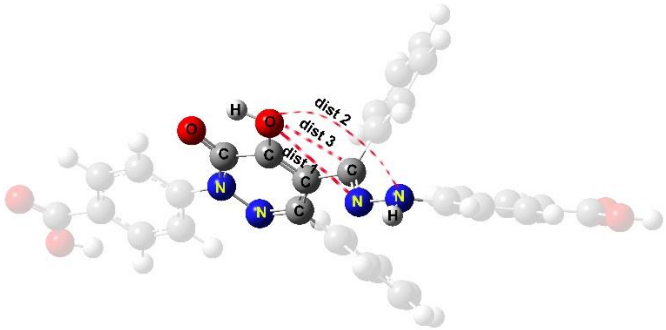


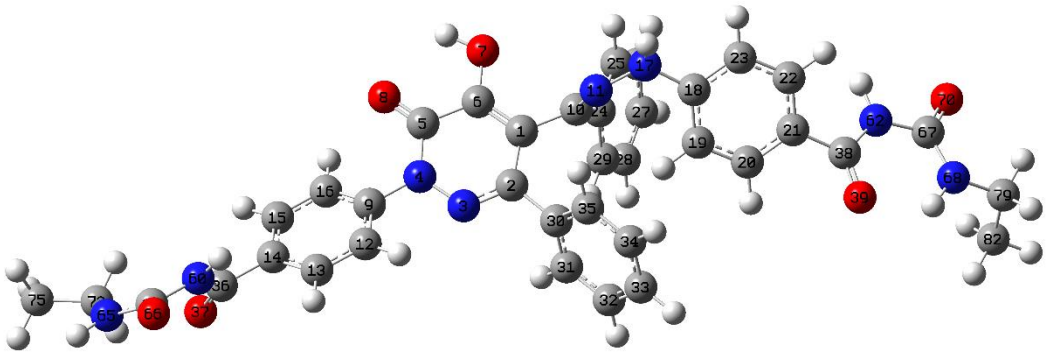
Figure S1. Optimized 3D structures of some pyridazinone derivatives (Atoms are color-coded: Green:Cl; Blue: N; Red: Oxygen; Gray: Carbon; White: Hydrogen).

Table S1. Some distances between atoms based on theoretical calculation



Compound	Distances (Aº)		
	HO……..**N**=CH (dist 1)	**HO**…….**N**HN=CPh (dist 2)	**HO**…….**C**=NNH (dist 3)
PAC-1	4.01	4.90	2.70
1	3.51	4.50	2.85
2	3.50	4.49	2.85
3	3.50	4.48	2.85
4	3.50	4.48	2.85

Table S2. Bond and dihedral angles for 4



Atoms	Bond Angles(º)	Dihedral Angles(º)
N3-N4-C9	114.27	-
C2-N3-N4	120.50	-
N4-C5-C6	114.57	-
C5-N4-N3	123.06	-
O8-C5-N4	123.78	-
C1-C2-N3	123.07	
C5-C6-C1	122.08	
C6-C1-C10-C24	-	-80.88
C6-C1-C2-N3	-	0.28
C1-C2-N3-N4	-	0.02
C2-N3-N4-C5	-	0.07
N11-N17-C18-C19	-	0.20
C30-C2-C1-C10	-	0.42
N3-C2-C30-C31	-	64.88
C16-C9-N4-N3	-	-151.51
C6-C1-C10-N11	-	97.42

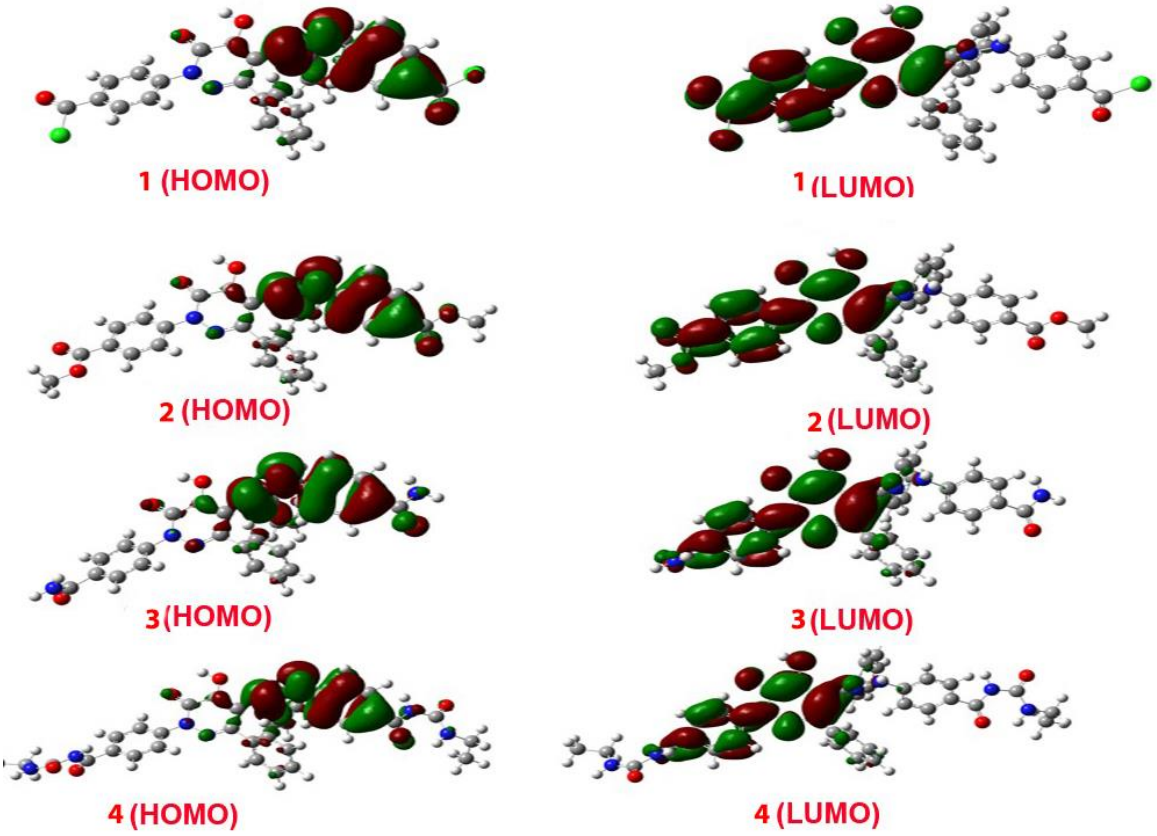


Figure S2. HOMOs and LUMOs of some pyridazinones

Table S3. NBO analyze for some bonds of compound **4**[a]

Bond	**Compound 4 (C5-O8)**
(C-O)$_{\sigma bond}$	$(0.5924sp^{2.00})C + (0.8057sp^{1.40})O$
(C-O)$_{\sigma}$ anti-bond	$(0.8043sp^{2.00})C – (0.5924sp^{1.40})O$
(C-O)$_{\pi bond}$	$(0.5429p)C + (0.8398p)O$
(C-O)$_{\pi}$ anti-bond	$(0.8398p)C – (0.5429p)O$
Bond	**Compound 4 (C6-O7)**
(C-O)$_{\sigma bond}$	$(0.5782sp^{2.84})C + (0.8159sp^{1.87})O$
(C-O)$_{\sigma}$ anti-bond	$(0.8159sp^{2.84})C – (0.5782sp^{1.87})O$
Bond	**Compound 4 (C10-N11)**
(C-N)$_{\sigma bond}$	$(0.6401sp^{2.06})C + (0.7684sp^{1.36})N$
(C-N)$_{\sigma}$ anti-bond	$(0.7684sp^{2.10})C – (0.6401sp^{1.36})N$
(C-N)$_{\pi bond}$	$(0.6605p)C + (0.7508p)N$
(C-N)$_{\pi}$ anti-bond	$(0.7508p)C – (0.6605p)N$

Bond	**Compound 4 (N11-N17)**
$(N\text{-}N)_{\sigma bond}$	$(0.6935sp^{3.06})N + (0.7204sp^{2.59})N$
$(N\text{-}N)_{\sigma\ anti\text{-}bond}$	$(0.7204sp^{3.06})N - (0.6935sp^{2.59})N$
Bond	**Compound 4 (C36-O37)**
$(C\text{-}O)_{\sigma bond}$	$(0.5872sp^{2.18})C + (0.8094sp^{1.44})O$
$(C\text{-}O)_{\sigma\ anti\text{-}bond}$	$(0.8094sp^{2.18})C - (0.5872sp^{1.44})O$
$(C\text{-}O)_{\pi bond}$	$(0.5582p)C + (0.8297p)O$
$(C\text{-}O)_{\pi\ anti\text{-}bond}$	$(0.8297p)C - (0.5582p)O$
Bond	**Compound 4 (C38-O39)**
$(C\text{-}O)_{\sigma bond}$	$(0.5864sp^{2.22})C + (0.8100sp^{1.45})O$
$(C\text{-}O)_{\sigma\ anti\text{-}bond}$	$(0.8100sp^{2.22})C - (0.5864sp^{1.45})O$
$(C\text{-}O)_{\pi bond}$	$(0.5482p)C + (0.8363p)O$
$(C\text{-}O)_{\pi\ anti\text{-}bond}$	$(0.8363p)C - (0.5482p)O$

a: for atom numbering see figure of Table S2

S4. Coordinates for Compound **1**

Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	0.371525	1.083348	-0.519218
2	6	0	0.996458	-0.209599	-0.265570
3	7	0	2.305357	-0.371104	-0.164755
4	7	0	3.152310	0.697772	-0.296316
5	6	0	2.693880	2.020608	-0.543221
6	6	0	1.208068	2.153380	-0.658664
7	8	0	0.728558	3.394960	-0.902543
8	8	0	3.430165	2.985557	-0.652029
9	6	0	4.565416	0.356533	-0.186574
10	6	0	-1.105578	1.234165	-0.610634
11	7	0	-1.610592	0.948053	-1.778459
12	6	0	4.996311	-0.945527	-0.501729
13	6	0	6.347085	-1.271074	-0.388120
14	6	0	7.272974	-0.302911	0.031111
15	6	0	6.833535	1.000875	0.331764
16	6	0	5.485737	1.334556	0.231932
17	7	0	-2.955630	1.117989	-2.072700
18	6	0	-4.005325	0.404435	-1.432882
19	6	0	-3.810119	-0.459369	-0.334012
20	6	0	-4.907229	-1.052001	0.273806
21	6	0	-6.217183	-0.816342	-0.200938
22	6	0	-6.402938	0.027401	-1.312224
23	6	0	-5.313157	0.626965	-1.930450
24	6	0	-1.774227	1.721860	0.623070
25	6	0	-2.564488	2.879855	0.560967
26	6	0	-3.184766	3.359391	1.717801
27	6	0	-3.021860	2.686295	2.932700
28	6	0	-2.232079	1.532842	2.993908
29	6	0	-1.603588	1.051187	1.843279
30	6	0	0.177502	-1.437388	-0.095217
31	6	0	0.160128	-2.097938	1.142618
32	6	0	-0.622295	-3.244722	1.301571
33	6	0	-1.374393	-3.736683	0.229583
34	6	0	-1.339407	-3.085970	-1.008244
35	6	0	-0.561414	-1.937707	-1.177272
36	6	0	8.713587	-0.576892	0.163576
37	8	0	9.618155	0.200946	0.189304
38	6	0	-7.307265	-1.483471	0.507826
39	8	0	-7.244888	-2.243335	1.428437
40	1	0	1.488552	4.066007	-0.971956
41	1	0	4.279686	-1.706830	-0.825384
42	1	0	6.667928	-2.286962	-0.639829
43	1	0	7.559881	1.757855	0.646989
44	1	0	5.161684	2.355975	0.462504
45	1	0	-3.053237	1.211384	-3.100560
46	1	0	-2.807805	-0.678952	0.035394

47	1	0	-4.762799	-1.719062	1.131047
48	1	0	-7.404730	0.223626	-1.707423
49	1	0	-5.472539	1.283712	-2.784257
50	1	0	-2.692106	3.403533	-0.387705
51	1	0	-3.798391	4.258457	1.670557
52	1	0	-3.510431	3.059781	3.832235
53	1	0	-2.106119	1.009715	3.940990
54	1	0	-0.987134	0.154211	1.894262
55	1	0	0.763916	-1.726400	1.970642
56	1	0	-0.640334	-3.760099	2.261632
57	1	0	-1.983252	-4.631692	0.357128
58	1	0	-1.917432	-3.476481	-1.845716
59	1	0	-0.527290	-1.432984	-2.145111
60	17	0	9.082418	-2.321848	0.333293
61	17	0	-8.941443	-1.073176	-0.123790

S5. Coordinates for Compound **2**

Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	0.365399	1.053846	-0.544545
2	6	0	0.985673	-0.234830	-0.261458
3	7	0	2.292790	-0.394323	-0.130162
4	7	0	3.140047	0.672964	-0.256877
5	6	0	2.687284	1.991836	-0.528806
6	6	0	1.205126	2.122376	-0.677893
7	8	0	0.731659	3.362303	-0.946337
8	8	0	3.426175	2.956158	-0.631919
9	6	0	4.553319	0.337047	-0.112794
10	6	0	-1.109311	1.202117	-0.669813
11	7	0	-1.590504	0.902815	-1.844150
12	6	0	5.000353	-0.953371	-0.453334
13	6	0	6.350497	-1.266699	-0.310820
14	6	0	7.252301	-0.301557	0.163957
15	6	0	6.797936	0.984351	0.498191
16	6	0	5.448834	1.309507	0.364348
17	7	0	-2.923699	1.075282	-2.175953
18	6	0	-4.000961	0.409618	-1.509732
19	6	0	-3.826444	-0.461815	-0.417788
20	6	0	-4.941400	-1.015381	0.204381
21	6	0	-6.235205	-0.723507	-0.261790
22	6	0	-6.405244	0.132429	-1.364674

23	6	0	-5.300767	0.693536	-1.993527
24	6	0	-1.802720	1.705307	0.544075
25	6	0	-2.581022	2.869532	0.453271
26	6	0	-3.223602	3.365138	1.590918
27	6	0	-3.095173	2.701714	2.815303
28	6	0	-2.318079	1.541682	2.904976
29	6	0	-1.667444	1.043887	1.773512
30	6	0	0.163902	-1.460975	-0.092702
31	6	0	0.122380	-2.106724	1.152358
32	6	0	-0.665382	-3.249921	1.310873
33	6	0	-1.399264	-3.753075	0.231528
34	6	0	-1.339768	-3.117687	-1.013291
35	6	0	-0.555957	-1.973334	-1.181928
36	6	0	8.693735	-0.598148	0.327360
37	8	0	9.568201	0.128927	0.741079
38	6	0	-7.382394	-1.336337	0.430575
39	8	0	-7.377787	-2.093860	1.376209
40	1	0	1.494584	4.030094	-1.006255
41	1	0	4.299095	-1.708721	-0.817459
42	1	0	6.714558	-2.266008	-0.570373
43	1	0	7.510244	1.731030	0.865874
44	1	0	5.106775	2.319192	0.614272
45	1	0	-2.998906	1.066350	-3.210337
46	1	0	-2.829773	-0.719815	-0.058762
47	1	0	-4.818334	-1.689019	1.058949
48	1	0	-7.416149	0.352721	-1.721972
49	1	0	-5.439581	1.363846	-2.839474
50	1	0	-2.682496	3.383794	-0.503717
51	1	0	-3.827954	4.268556	1.521112

52	1	0	-3.601189	3.087318	3.699426
53	1	0	-2.219978	1.025192	3.858659
54	1	0	-1.061792	0.141202	1.846160
55	1	0	0.711116	-1.725454	1.986689
56	1	0	-0.703166	-3.752577	2.276797
57	1	0	-2.014268	-4.643493	0.359299
58	1	0	-1.904514	-3.515981	-1.855845
59	1	0	-0.503602	-1.479473	-2.154473
60	8	0	-8.573255	-0.935345	-0.150411
61	6	0	-9.787268	-1.467165	0.442797
62	1	0	-9.872542	-1.115024	1.475625
63	1	0	-10.568845	-1.050332	-0.200135
64	1	0	-9.766306	-2.561206	0.409461
65	8	0	8.967711	-1.892667	-0.070503
66	6	0	10.352804	-2.318173	0.037840
67	1	0	10.669600	-2.271563	1.084603
68	1	0	10.314543	-3.346528	-0.335722
69	1	0	10.983996	-1.676757	-0.585582

S6. Coordinates for Compound **3**

Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-0.386061	-0.887487	-0.573877
2	6	0	-0.995694	0.399653	-0.263117
3	7	0	-2.301011	0.564199	-0.115464
4	7	0	-3.153787	-0.496092	-0.252633
5	6	0	-2.712859	-1.811494	-0.554370
6	6	0	-1.233769	-1.948594	-0.718457
7	8	0	-0.770216	-3.187290	-1.011639
8	8	0	-3.461326	-2.767670	-0.671153
9	6	0	-4.564103	-0.159876	-0.079874
10	6	0	1.086432	-1.041907	-0.712894
11	7	0	1.562624	-0.728506	-1.885267
12	6	0	-5.018846	1.128661	-0.415612
13	6	0	-6.368523	1.438695	-0.252201
14	6	0	-7.258944	0.473075	0.235546
15	6	0	-6.795964	-0.803312	0.581098
16	6	0	-5.448329	-1.129099	0.422203
17	7	0	2.887535	-0.906797	-2.235647
18	6	0	3.982527	-0.305054	-1.522861
19	6	0	3.820599	0.580168	-0.443024
20	6	0	4.945655	1.078497	0.211734
21	6	0	6.232359	0.702080	-0.200617
22	6	0	6.391520	-0.158588	-1.296857
23	6	0	5.277487	-0.662695	-1.961262
24	6	0	1.783843	-1.569219	0.488643

25	6	0	2.526585	-2.755043	0.380305
26	6	0	3.167731	-3.277543	1.506559
27	6	0	3.073586	-2.619368	2.737015
28	6	0	2.333540	-1.436931	2.843611
29	6	0	1.684398	-0.911932	1.723407
30	6	0	-0.165556	1.618315	-0.082088
31	6	0	-0.112912	2.246017	1.171797
32	6	0	0.684170	3.380970	1.342583
33	6	0	1.416802	3.893833	0.266981
34	6	0	1.345684	3.277181	-0.986638
35	6	0	0.551968	2.141597	-1.167695
36	6	0	-8.707709	0.788845	0.440536
37	8	0	-9.314699	0.604384	1.480435
38	6	0	7.402433	1.280126	0.521592
39	8	0	7.506641	2.452584	0.841951
40	1	0	-1.538385	-3.848038	-1.076745
41	1	0	-4.323596	1.885372	-0.787498
42	1	0	-6.724152	2.441211	-0.496323
43	1	0	-7.491384	-1.544166	0.985268
44	1	0	-5.098228	-2.134315	0.677544
45	1	0	2.960653	-0.793281	-3.264766
46	1	0	2.827983	0.897241	-0.120202
47	1	0	4.828721	1.777613	1.044688
48	1	0	7.391499	-0.428063	-1.640834
49	1	0	5.405356	-1.338490	-2.804878
50	1	0	2.599709	-3.264804	-0.581744
51	1	0	3.741426	-4.199357	1.423909
52	1	0	3.575355	-3.027804	3.612926
53	1	0	2.260931	-0.924992	3.801949

54	1	0	1.106429	0.007759	1.809207
55	1	0	-0.700561	1.857201	2.003503
56	1	0	0.730020	3.869856	2.315187
57	1	0	2.040370	4.777050	0.404319
58	1	0	1.909630	3.683511	-1.826024
59	1	0	0.490073	1.662842	-2.147096
60	7	0	-9.367884	1.332552	-0.663244
61	1	0	-8.947722	1.408631	-1.571023
62	7	0	8.433083	0.388905	0.835759
63	1	0	8.350312	-0.604135	0.723058
64	1	0	9.225772	0.716627	1.366420
65	1	0	-10.355616	1.529201	-0.605110

Coordinates for 4

Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	0.324514	1.280037	-0.585373
2	6	0	0.883926	-0.058094	-0.438369
3	7	0	2.172951	-0.284397	-0.240771
4	7	0	3.057023	0.757086	-0.163978
5	6	0	2.665178	2.116671	-0.285855
6	6	0	1.202669	2.323772	-0.515973
7	8	0	0.785703	3.605486	-0.645366
8	8	0	3.440024	3.055269	-0.207537
9	6	0	4.445293	0.352263	0.031925
10	6	0	-1.132264	1.500514	-0.788191
11	7	0	-1.537199	1.378415	-2.021560

12	6	0	4.882533	-0.894918	-0.452831
13	6	0	6.211395	-1.271777	-0.265373
14	6	0	7.098968	-0.411851	0.395795
15	6	0	6.656083	0.823411	0.884922
16	6	0	5.328551	1.213846	0.703962
17	7	0	-2.836245	1.645765	-2.417088
18	6	0	-3.979689	0.953328	-1.901910
19	6	0	-3.907848	-0.068498	-0.937307
20	6	0	-5.081223	-0.641529	-0.453255
21	6	0	-6.330941	-0.206423	-0.921685
22	6	0	-6.399614	0.791010	-1.907871
23	6	0	-5.236374	1.368713	-2.403046
24	6	0	-1.895944	1.864071	0.433380
25	6	0	-2.626336	3.062285	0.451116
26	6	0	-3.333047	3.427243	1.600060
27	6	0	-3.315810	2.600219	2.727695
28	6	0	-2.586318	1.406462	2.709354
29	6	0	-1.872380	1.037945	1.566580
30	6	0	0.016629	-1.262951	-0.494952
31	6	0	-0.133515	-2.068242	0.644284
32	6	0	-0.963192	-3.191370	0.590942
33	6	0	-1.631354	-3.516110	-0.594317
34	6	0	-1.463582	-2.721812	-1.733533
35	6	0	-0.636730	-1.596306	-1.690446
36	6	0	8.521762	-0.817692	0.633410
37	8	0	9.016477	-0.946016	1.733711
38	6	0	-7.552676	-0.862725	-0.384868
39	8	0	-7.676218	-2.068592	-0.240325
40	1	0	1.569809	4.245767	-0.563875

41	1	0	4.188737	-1.569895	-0.961831
42	1	0	6.552567	-2.243700	-0.629099
43	1	0	7.347089	1.482526	1.415802
44	1	0	4.993923	2.188509	1.074694
45	1	0	-2.840208	1.748346	-3.449552
46	1	0	-2.945127	-0.431833	-0.574756
47	1	0	-5.031748	-1.442999	0.289367
48	1	0	-7.368045	1.110117	-2.299306
49	1	0	-5.296231	2.148263	-3.160873
50	1	0	-2.639598	3.705205	-0.430535
51	1	0	-3.899113	4.357787	1.615111
52	1	0	-3.870209	2.885690	3.620899
53	1	0	-2.573019	0.763717	3.588329
54	1	0	-1.302831	0.109195	1.555531
55	1	0	0.404683	-1.826084	1.560745
56	1	0	-1.083844	-3.818557	1.473673
57	1	0	-2.278890	-4.391883	-0.632237
58	1	0	-1.976628	-2.981917	-2.659270
59	1	0	-0.498704	-0.979439	-2.580932
60	7	0	9.250673	-1.018024	-0.559270
61	1	0	8.734300	-0.980246	-1.454208
62	7	0	-8.593233	0.016606	-0.010374
63	1	0	-8.444689	1.034068	-0.069217
64	6	0	10.587217	-1.553736	-0.737198
65	7	0	11.622808	-1.254982	0.122952
66	8	0	10.768453	-2.240000	-1.735982
67	6	0	-9.897241	-0.341280	0.518895
68	7	0	-10.240005	-1.683239	0.535201
69	1	0	-9.528948	-2.408857	0.353151

70	8	0	-10.624826	0.582242	0.849429
71	1	0	12.510496	-1.727974	-0.065712
72	6	0	11.589774	-0.336562	1.290804
73	1	0	11.145379	-0.871292	2.168610
74	1	0	10.919559	0.524627	1.070160
75	6	0	12.999634	0.149694	1.606500
76	1	0	13.457071	0.674442	0.757937
77	1	0	12.981354	0.853081	2.449853
78	1	0	13.670208	-0.670544	1.891044
79	6	0	-11.479927	-2.108066	1.234683
80	1	0	-11.962812	-2.890623	0.605592
81	1	0	-12.187728	-1.245061	1.289669
82	6	0	-11.185385	-2.643500	2.632999
83	1	0	-10.489016	-3.490134	2.615111
84	1	0	-10.743487	-1.870948	3.276099
85	1	0	-12.105020	-2.985350	3.123078
