

## Supporting Information

### Structural characterization and QSAR modeling of 1,2,4-triazole derivatives as $\alpha$ -glucosidase inhibitors

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**Table S1.** Measured and calculated geometric parameters (distances in angstroms and angles in degrees) of 1,2,4-triazole at different levels of theory with 6-311++G(d,p) basis set.

Parameter	1H-1,2,4-Triazole								
	Exp <sup>Ref 20</sup>	HF	HF <sup>a</sup>	MP2	MP2 <sup>a</sup>	B3LYP	B3LYP <sup>a</sup>	B3LYP <sup>b</sup>	B3LYP <sup>a,b</sup>
N1N2	1.381	1.339	3.04	1.347	2.46	1.356	1.81	1.358	1.67
N2C3	1.328	1.292	2.71	1.389	-4.59	1.321	0.53	1.325	0.23
C3N4	1.354	1.356	-0.15	1.362	-0.59	1.364	-0.74	1.365	-0.81
N4C5	1.280	1.296	-1.25	1.329	-3.83	1.318	-2.97	1.321	-3.20
C5N1	1.375	1.330	3.27	1.356	1.38	1.350	1.82	1.351	1.75
N1H6	0.998	0.992	0.60	1.010	-1.20	1.008	-1.00	1.010	-1.20
C3H7	1.078	1.070	0.74	1.080	-0.19	1.079	-0.09	1.081	-0.28
C5H8	1.078	1.071	0.65	1.080	-0.19	1.079	-0.09	1.081	-0.28
N1N2C3	102.7	102.6	0.10	101.6	1.07	102.0	0.68	101.6	1.07
N2C3N4	113.0	114.7	-1.50	115.3	-2.04	115.1	-1.86	115.6	-2.30
C3N4C5	106.8	102.7	3.84	102.6	3.93	102.9	3.65	102.5	4.03
N4C5N1	109.0	110.2	-1.10	109.6	-0.55	109.8	-0.73	109.9	-0.83
C5N1N2	108.5	109.7	-1.11	110.9	-2.21	110.3	-1.66	110.4	-1.75
C5N1H6	124.0	129.5	-4.44	129.3	-4.27	129.7	-4.60	129.8	-4.68
N4C3H7	118.5	123.1	-3.88	123.5	-4.22	123.2	-3.97	123.0	-3.80
N4C5H8	120.5	126.4	-4.90	126.9	-5.31	126.6	-5.06	126.6	-5.06
<b>RMSE</b>	---	<b>2.61</b>	---	<b>2.79</b>	---	<b>2.69</b>	---	<b>2.76</b>	---

<sup>a</sup> Percentage deviation to the experimental values, <sup>b</sup> b3lyp/6-31G(d).

**Table S1. (continued).**

Parameter	1H-1,2,4-Triazole						
	Exp <sup>Ref 20</sup>	M062X	M062X <sup>a</sup>	PBE	PBE <sup>a</sup>	wB97X-D	wB97X-D <sup>a</sup>
N1N2	1.381	1.345	2.61	1.359	1.59	1.347	2.46
N2C3	1.328	1.316	0.90	1.334	-0.45	1.316	0.90
C3N4	1.354	1.360	-0.44	1.368	-1.03	1.359	-0.37
N4C5	1.280	1.313	-2.58	1.328	-3.75	1.314	-2.66
C5N1	1.375	1.345	2.18	1.358	1.24	1.344	2.25
N1H6	0.998	1.008	-1.00	1.016	-1.80	1.006	-0.80
C3H7	1.078	1.078	0	1.087	-0.83	1.079	-0.09
C5H8	1.078	1.079	-0.09	1.087	-0.83	1.079	-0.09
N1N2C3	102.7	102.2	0.49	101.6	1.07	102.1	0.58
N2C3N4	113.0	115.0	-1.77	115.5	-2.21	115.1	-1.86
C3N4C5	106.8	102.7	3.84	102.6	3.93	102.7	3.84
N4C5N1	109.0	109.8	-0.73	109.8	-0.73	109.9	-0.83
C5N1N2	108.5	110.3	-1.66	110.6	-1.94	110.3	-1.66
C5N1H6	124.0	129.6	-4.51	129.7	-4.60	129.5	-4.44
N4C3H7	118.5	123.3	-4.05	123.2	-3.97	123.2	-3.97
N4C5H8	120.5	126.7	-5.15	126.7	-5.15	126.6	-5.06
<b>RMSE</b>	---	<b>2.71</b>	---	<b>2.77</b>	---	<b>2.68</b>	---

<sup>a</sup> Percentage deviation to the experimental values.

**Table S2.** Vibrational anharmonic frequencies ( $\omega_i$ , in  $\text{cm}^{-1}$ ) and IR intensities ( $I$ ,  $\text{km}\cdot\text{mol}^{-1}$ ) for the intermonomer modes of Triazole.

Triazole	E(harm)	E(anharm)	I(harm)	I(anharm)
1(1)	3651.186	3491.641	83.67336522	66.72535495
2(1)	3257.644	3123.478	1.56825484	1.33076375
3(1)	3251.412	3127.014	1.50646222	4.40657135
4(1)	1549.867	1516.545	26.91523871	18.81451114
5(1)	1461.345	1419.574	22.59667061	20.92620383
6(1)	1386.497	1352.772	12.12631708	9.26731105
7(1)	1317.57	1283.942	21.76718097	19.88554548
8(1)	1274.682	1250.259	0.55555647	0.97769202
9(1)	1179.49	1152.651	14.37514305	17.13347353
10(1)	1137.716	1108.053	17.64308814	13.58315574
11(1)	1077.598	1044.571	41.58957083	38.95235694
12(1)	990.852	976.192	16.41651127	17.71533564
13(1)	962.419	949.174	5.49745449	4.38477947
14(1)	896.755	889.887	12.50193596	6.54686684
15(1)	842.593	860.238	19.02601397	24.03588605
16(1)	695.907	685.647	45.83334822	42.19468258
17(1)	676.879	663.364	3.7336616	1.82364638
18(1)	552.343	559.733	77.44287832	80.37530966

**Table S3.** Vibrational anharmonic frequencies ( $\omega_i$ , in  $\text{cm}^{-1}$ ) and IR intensities ( $I$ ,  $\text{km}\cdot\text{mol}^{-1}$ ) for the intermonomer modes of Triazolone.

Triazolone	E(harm)	E(anharm)	I(harm)	I(anharm)
1(1)	3683.949	3496.506	93.12790776	71.31022108
2(1)	3674.701	3492.136	101.00420844	92.55413968
3(1)	3259.561	3166.343	0.32157497	0.54067708
4(1)	1819.952	1777.969	782.12544339	633.36579315
5(1)	1609.299	1574.676	39.90169477	31.09959868
6(1)	1417.277	1375.317	32.77325077	34.23187645
7(1)	1388.62	1349.966	3.93891726	6.05356713
8(1)	1322.68	1299.142	16.32553273	13.79243232
9(1)	1214.014	1186.166	34.21406484	29.94823344
10(1)	1115.328	1090.111	2.23297066	2.29754143
11(1)	1055.031	1022.981	25.33410167	19.08997371
12(1)	999.799	993.728	24.88099437	24.21043119
13(1)	928.014	912.252	28.60761003	37.36177748
14(1)	828.67	832.297	21.12038066	17.69877553
15(1)	748.193	737.696	8.52070266	9.19248177
16(1)	743.134	735.435	6.57326732	6.60678857
17(1)	661.524	646.638	8.26225245	10.33399102
18(1)	508.367	483.975	224.49612848	201.28263541
19(1)	481.724	478.433	8.33478612	7.00889224
20(1)	436.936	422.561	4.48032683	15.04093022
21(1)	222.849	230.636	8.29480458	6.73151917

**Table S4.** Second-order perturbation analysis of the interaction between electron donor and electron acceptor orbitals within the triazole and triazolone molecules,  $E_2$  (in kcal.mol<sup>-1</sup>) is the hyperconjugative interaction energy deduced from the second-order perturbation energies,  $F_{i,j}$  is the Fock matrix element,  $F_{i,j} = \langle \Phi_i | \hat{F} | \Phi_j \rangle$ .  $\Delta E_{ij}$  ( $= E_j - E_i$ ) is the energy difference between donor and acceptor orbitals. These calculations are done using B3LYP/6-31G(d). Numbering of atoms is given in Figure 1 of the ms .

Donor (i) → Acceptor (j)	1H-1,2,4-triazole		
	$E_2$	$\Delta E_{ij}$	$F_{i,j}$
BD (2) N2 - C3 → BD*(2) C5 - N4	10.87	0.31	0.056
BD (2) C5 - N4 → BD*(2) N2 - C3	30.51	0.31	0.091
LP (1) N1 → BD*(2) N2 - C3	26.05	0.29	0.079
LP (1) N1 → BD*(2) C5 - N4	52.13	0.28	0.110
1H-1,2,4-triazolone			
LP (1) N1 → BD*(2) N2 - C3	26.93	0.27	0.077
LP (1) N1 → BD*(1) C5 - O6	59.57	0.28	0.119
LP (1) N4 → BD*(2) N2 - C3	46.53	0.27	0.102
LP (1) N4 → BD*(1) C5 - O6	51.22	0.29	0.111
LP (1) O6 → RV*(1) C5	15.95	1.41	0.134
LP (2) O6 → BD*(1) N1 - C5	27.91	0.66	0.124
LP (2) O6 → BD*(1) N4 - C5	29.92	0.63	0.125

BD is the 2-center bond. BD\* is the 2-center antibond. LP is the 1-center valence lone pair

**Table S5.** The Cartesian coordinates (X, Y, Z) in Angstrom) of TzO derivatives: The first column corresponds to the number of the atom in the structure (CN: Center Number) and the second one to its atomic number (AN: Atomic Number).

N	CN	AN	X	Y	Z
1	7	-0.545124	3.557776	0.075244	
2	7	0.518616	3.032032	-0.621268	
3	6	0.273621	1.759214	-0.692426	
4	7	-0.925955	1.435493	-0.067553	
5	6	-1.495539	2.63152	0.429441	
6	8	-2.549956	2.780497	1.011114	
7	6	-1.561588	0.160683	0.032446	
8	6	-2.80211	-0.035464	-0.576502	
9	6	-3.441863	-1.266158	-0.473236	
10	6	-2.818054	-2.281127	0.236383	
11	6	-1.589803	-2.109309	0.854574	
12	6	-0.964333	-0.869235	0.759182	
13	9	-3.433792	-3.482343	0.332407	
14	6	1.171465	0.783361	-1.383454	
15	6	2.167167	0.077277	-0.474239	
16	6	2.493928	-1.260639	-0.681576	
17	6	3.414293	-1.94823	0.093803	
18	6	4.05251	-1.270737	1.129772	
19	6	3.760305	0.072032	1.365228	
20	6	2.828898	0.734394	0.568789	
21	9	1.882531	-1.932667	-1.693429	
22	1	-0.614733	4.549721	0.22853	
23	1	-3.2684	0.777169	-1.118594	
24	1	-4.406003	-1.442673	-0.932695	
25	1	-1.144159	-2.92623	1.407474	
26	1	-0.015701	-0.701795	1.253098	
27	1	0.567877	0.041337	-1.90869	
28	1	1.718543	1.347453	-2.144465	
29	1	3.6179	-2.989748	-0.122078	
30	1	4.775939	-1.791195	1.74625	
31	1	4.25787	0.604664	2.166986	
32	1	2.605729	1.779819	0.750383	

  

N	CN	AN	X	Y	Z
1	7	1.48156	-3.328056	-0.333194	
2	7	0.383793	-3.005657	-1.097314	
3	6	0.237929	-1.724555	-0.942436	
4	7	1.207525	-1.197539	-0.098377	
5	6	2.043261	-2.258044	0.321754	
6	8	3.003289	-2.218587	1.062867	
7	6	1.39311	0.164602	0.29421	
8	6	1.67872	1.130687	-0.668841	
9	6	1.765705	2.806468	1.046098	
10	6	1.312393	0.508066	1.64239	
11	6	1.85349	2.469948	-0.307887	
12	6	1.505543	1.835064	2.010996	
13	6	2.116434	3.519473	-1.360077	
14	6	-0.882242	-0.949257	-1.55999	
15	6	-1.922435	-0.474333	-0.557432	
16	6	-2.404272	0.831101	-0.576613	
17	6	-3.369561	1.298362	0.302053	
18	6	-3.888823	0.422228	1.250764	
19	6	-3.436944	-0.896276	1.300436	
20	6	-2.465438	-1.33351	0.404587	
21	9	-1.914336	1.698503	-1.503922	
22	1	1.817094	-4.275587	-0.293994	
23	1	1.777765	0.83376	-1.707397	
24	1	1.910771	3.837984	1.349844	
25	1	1.114276	-0.255502	2.383241	
26	1	1.452909	2.113578	3.057256	
27	1	1.177651	3.874388	-1.798657	
28	1	2.631897	4.384661	-0.938121	
29	1	2.728799	3.123708	-2.17392	
30	1	-0.494156	-0.093701	-2.113021	
31	1	-1.348961	-1.618472	-2.287904	
32	1	-3.696909	2.328267	0.232492	
33	1	-4.643931	0.769799	1.946022	
34	1	-3.84078	-1.58267	2.03525	
35	1	-2.11509	-2.359406	0.443408	

N	CN	AN	X	Y	Z
	1	7	-1.747726	-3.643616	0.641944
	2	7	-2.459946	-2.919341	-0.288318
	3	6	-1.655888	-1.96555	-0.648374
	4	7	-0.437293	-2.047287	0.012181
	5	6	-0.480862	-3.164026	0.876225
	6	8	0.383865	-3.579668	1.619923
	7	6	-2.031334	-0.885432	-1.613117
	8	6	-2.370225	0.441548	-0.946509
	9	6	-1.668669	1.605372	-1.26748
	10	6	-1.991467	2.827714	-0.678954
	11	6	-3.027761	2.863567	0.237878
	12	6	-3.747599	1.730076	0.584943
	13	6	-3.410512	0.519486	-0.013755
	14	9	-3.350928	4.046486	0.817639
	15	6	0.710669	-1.210396	-0.150453
	16	6	1.010979	-0.25107	0.817575
	17	6	2.128201	0.560802	0.68567
	18	6	2.963205	0.422056	-0.446746
	19	6	2.662777	-0.550163	-1.402171
3	20	6	1.543011	-1.369002	-1.250763
	21	8	4.01886	1.277161	-0.521943
	22	6	4.877553	1.204358	-1.65465
	23	8	2.343813	1.536726	1.620346
	24	6	3.504586	1.381242	2.450366
	25	1	-2.14843	-4.46208	1.06783
	26	1	-1.222493	-0.734072	-2.332015
	27	1	-2.896254	-1.256417	-2.168989
	28	1	-0.85362	1.562752	-1.98172
	29	1	-1.449627	3.734253	-0.917661
	30	1	-4.552112	1.802793	1.306216
	31	1	-3.9619	-0.376943	0.248651
	32	1	0.375678	-0.121022	1.684354
	33	1	3.296462	-0.681092	-2.268665
	34	1	1.328367	-2.134914	-1.986417
	35	1	5.625103	1.982016	-1.5089
	36	1	5.373563	0.230164	-1.717647
	37	1	4.328696	1.397964	-2.582105
	38	1	3.484806	2.216987	3.148557
	39	1	3.451571	0.439278	3.005949
	40	1	4.421003	1.416418	1.858445

N	CN	AN	X	Y	Z
	1	7	-0.13867	-2.863028	0.648484
	2	7	0.787228	-1.848167	0.568208
	3	6	0.096273	-0.793002	0.269577
	4	7	-1.258431	-1.087073	0.144737
	5	6	-1.426707	-2.472429	0.375974
	6	8	-2.448616	-3.126607	0.340891
	7	6	-2.328585	-0.200343	-0.185201
	8	6	-2.645522	0.856713	0.668118
	9	6	-4.420246	1.512232	-0.809041
	10	6	-3.067708	-0.4181	-1.346418
	11	6	-3.687851	1.735959	0.361677
	12	6	-4.117724	0.44351	-1.649646
	13	6	-4.007134	2.899166	1.269603
	14	6	0.667524	0.579107	0.051552
	15	6	2.178203	0.601502	-0.038968
	16	6	2.959968	0.805259	1.100364
	17	6	4.351084	0.82165	1.026494
4	18	6	4.947726	0.630954	-0.208799
	19	6	4.20853	0.4286	-1.363157
	20	6	2.819378	0.415519	-1.266555
	21	9	6.301727	0.647872	-0.292674
	22	1	0.155316	-3.805813	0.84021
	23	1	-2.085805	0.982326	1.588598
	24	1	-5.242307	2.175048	-1.058443
	25	1	-2.832228	-1.258948	-1.986062
	26	1	-4.704956	0.278073	-2.545597
	27	1	-3.729325	2.685928	2.304212
	28	1	-3.463089	3.798559	0.961121
	29	1	-5.07258	3.138439	1.247568
	30	1	0.228044	0.990768	-0.863011
	31	1	0.335367	1.237727	0.860724
	32	1	2.480943	0.949025	2.062863
	33	1	4.965569	0.978557	1.90411
	34	1	4.714667	0.287007	-2.30987
	35	1	2.229623	0.255418	-2.162931

N	CN	AN	X	Y	Z
	1	7	2.889553	-2.298106	-0.394716
	2	7	1.715618	-2.490391	-1.090054
	3	6	1.028268	-1.408284	-0.891872
	4	7	1.719362	-0.51192	-0.080689
	5	6	2.964324	-1.09384	0.258184
	6	8	3.849345	-0.631925	0.948408
	7	6	-0.349353	-1.184955	-1.423304
	8	6	-1.430629	-1.214836	-0.351221
	9	6	-2.470404	-0.26514	-0.358988
	10	6	-3.472784	-0.307804	0.614031
	11	6	-3.449941	-1.299152	1.595052
	12	6	-2.435153	-2.248873	1.610458
	13	6	-1.437236	-2.196819	0.637366
	14	8	-2.427458	0.666044	-1.359966
	15	6	-3.436139	1.666132	-1.413012
	16	6	1.330719	0.789332	0.33355
	17	6	1.187524	1.821085	-0.59318
5	18	6	0.83632	3.106305	-0.2151
	19	6	0.640854	3.377952	1.136809
	20	6	0.795499	2.368101	2.085725
	21	6	1.13728	1.080973	1.6843
	22	9	1.402146	1.56048	-1.902874
	23	1	3.611297	-2.998618	-0.40715
	24	1	-0.391422	-0.238386	-1.961699
	25	1	-0.527865	-1.976267	-2.157059
	26	1	-4.27102	0.421877	0.613572
	27	1	-4.234024	-1.3225	2.343531
	28	1	-2.417232	-3.023454	2.367878
	29	1	-0.642531	-2.935602	0.64082
	30	1	-3.191138	2.288728	-2.272019
	31	1	-4.428261	1.225226	-1.556868
	32	1	-3.43664	2.280841	-0.506715
	33	1	0.736009	3.871285	-0.974864
	34	1	0.373802	4.381488	1.446615
	35	1	0.651547	2.581703	3.137754
	36	1	1.266448	0.288261	2.409949

N	CN	AN	X	Y	Z
	1	7	-0.194317	-2.995451	0.895949
	2	7	0.780438	-2.317023	0.20124
	3	6	0.18044	-1.280923	-0.293567
	4	7	-1.170296	-1.262353	0.053641
	5	6	-1.430862	-2.407481	0.846921
	6	8	-2.480894	-2.756062	1.348209
	7	6	0.839341	-0.297858	-1.222505
	8	6	2.279072	0.000137	-0.869696
	9	6	2.581739	0.782179	0.260708
	10	6	3.906867	1.069043	0.588521
	11	6	4.940772	0.576508	-0.210496
	12	6	4.658904	-0.195368	-1.329931
	13	6	3.328956	-0.475699	-1.648161
	14	8	1.503108	1.224003	0.981459
	15	6	1.737016	1.977919	2.167103
	16	6	-2.155514	-0.272431	-0.224595
	17	6	-1.909875	1.062388	0.10567
6	18	6	-2.893979	1.995823	-0.174207
	19	6	-4.111965	1.656098	-0.740237
	20	6	-4.343867	0.314624	-1.039534
	21	6	-3.373195	-0.651916	-0.790919
	22	9	-2.654446	3.294052	0.136258
	23	1	0.027354	-3.842938	1.3904
	24	1	0.796607	-0.70846	-2.23667
	25	1	0.260034	0.62571	-1.238169
	26	1	4.145387	1.670058	1.455347
	27	1	5.96749	0.804013	0.053144
	28	1	5.459865	-0.579714	-1.949939
	29	1	3.100489	-1.083466	-2.51738
	30	1	2.31476	1.399985	2.895121
	31	1	0.754307	2.198868	2.580893
	32	1	2.255223	2.916582	1.946379
	33	1	-0.981104	1.364638	0.571263
	34	1	-4.851663	2.422891	-0.931834
	35	1	-5.291878	0.020995	-1.474096
	36	1	-3.558448	-1.693635	-1.014378

N	CN	AN	X	Y	Z	N	CN	AN	X	Y	Z
1	7		-0.080948	3.009595	0.682785	1	7		-0.791091	-4.239624	0.353605
2	7		-0.999848	2.221284	0.02779	2	7		-1.575701	-3.604012	-0.583015
3	6		-0.33442	1.174233	-0.346401	3	6		-1.059995	-2.417395	-0.694099
4	7		1.001045	1.253914	0.042964	4	7		0.041287	-2.259362	0.138015
5	6		1.181645	2.478577	0.729347	5	6		0.235366	-3.467701	0.842759
6	8		2.19829	2.922803	1.225025	6	8		1.091159	-3.739488	1.660483
7	6		-0.909082	0.068412	-1.187964	7	6		-1.628578	-1.346703	-1.570292
8	6		-2.359762	-0.231366	-0.887383	8	6		-2.36101	-0.251242	-0.805564
9	6		-2.711721	-0.887405	0.306822	9	6		-2.010783	1.081409	-0.984281
10	6		-4.047215	-1.17285	0.590808	10	6		-2.698346	2.098686	-0.308981
11	6		-5.042774	-0.804455	-0.316601	11	6		-3.745716	1.776841	0.55526
12	6		-4.711982	-0.15801	-1.500253	12	6		-4.091589	0.433794	0.731036
13	6		-3.371961	0.12178	-1.773642	13	6		-3.413654	-0.576211	0.062496
14	8		-1.668097	-1.212665	1.133849	14	8		-2.265475	3.369023	-0.562675
15	6		-1.958648	-1.808113	2.393724	15	6		-2.92661	4.451809	0.076755
16	6		2.040118	0.290676	-0.114496	16	6		0.897032	-1.121279	0.255581
17	6		1.883258	-1.0032	0.386387	17	6		1.763397	-0.79257	-0.788793
18	6		2.904217	-1.937952	0.236519	18	6		2.598803	0.3124	-0.696913
19	6		4.076471	-1.54538	-0.390107	19	6		2.579586	1.103883	0.472787
20	6		4.264639	-0.260353	-0.874537	20	6		1.732877	0.746733	1.523604
21	6		3.232187	0.662426	-0.737819	21	6		0.890288	-0.358261	1.414697
22	9		5.075798	-2.449132	-0.529132	22	8		3.404534	2.187255	0.480681
23	1		-0.357672	3.889578	1.083815	23	6		3.383562	3.050834	1.611705
24	1		-0.811639	0.354502	-2.240508	24	8		3.367826	0.640444	-1.782317
25	1		-0.305817	-0.830491	-1.055036	25	6		4.789299	0.538023	-1.615751
26	1		-4.323428	-1.676952	1.506919	26	1		-0.972883	-5.195472	0.608449
27	1		-6.07808	-1.029409	-0.0865	27	1		-0.837654	-0.900233	-2.177447
28	1		-5.48308	0.129739	-2.204718	28	1		-2.319975	-1.847483	-2.253102
29	1		-3.105819	0.632223	-2.693305	29	1		-1.197995	1.362991	-1.644087
30	1		-2.59313	-1.156562	3.002709	30	1		-4.291331	2.544031	1.087679
31	1		-0.999055	-1.941431	2.891179	31	1		-4.907433	0.183491	1.400309
32	1		-2.441937	-2.783104	2.27259	32	1		-3.69325	-1.61347	0.20759
33	1		0.963644	-1.274426	0.890054	33	1		-2.423856	5.353552	-0.269258
34	1		2.804763	-2.949365	0.609705	34	1		-3.984603	4.49703	-0.203698
35	1		5.200872	0.005992	-1.348293	35	1		-2.842021	4.385269	1.167082
36	1		3.355084	1.675115	-1.098609	36	1		1.803721	-1.393433	-1.689319
						37	1		1.708583	1.335836	2.430066
						38	1		0.229621	-0.621684	2.230484
						39	1		4.09078	3.847598	1.387846
						40	1		2.38812	3.480444	1.763697
						41	1		3.700843	2.527664	2.519831
						42	1		5.221048	0.78674	-2.58445
						43	1		5.150366	1.237315	-0.859873
						44	1		5.068535	-0.485368	-1.343448

N	CN	AN	X	Y	Z
	1	7	-0.526311	-2.831163	0.890121
	2	7	0.43946	-1.917157	0.534135
	3	6	-0.221249	-0.868243	0.156483
	4	7	-1.596181	-1.069945	0.249567
	5	6	-1.813586	-2.38399	0.723158
	6	8	-2.868274	-2.951177	0.92549
	7	6	-2.646541	-0.160077	-0.080892
	8	6	-2.795005	1.023418	0.641941
	9	6	-4.684178	1.612274	-0.71671
	10	6	-3.528494	-0.473603	-1.113282
	11	6	-3.811991	1.929885	0.3299
	12	6	-4.549319	0.419862	-1.424144
	13	6	-3.988876	3.195914	1.133266
	14	6	0.390028	0.407231	-0.348575
	15	6	1.880653	0.314206	-0.597811
	16	6	2.779366	0.702056	0.388116
	17	6	4.159983	0.618446	0.171557
	18	6	4.645654	0.145076	-1.048598
	19	6	3.736925	-0.239154	-2.037751
9	20	6	2.367778	-0.157639	-1.823578
	21	8	4.944328	1.026147	1.212679
	22	6	6.355901	0.948362	1.070854
	23	1	-0.265459	-3.751743	1.200396
	24	1	-2.119044	1.23112	1.46437
	25	1	-5.480431	2.302589	-0.975198
	26	1	-3.416498	-1.404992	-1.653411
	27	1	-5.240552	0.186059	-2.225747
	28	1	-4.408789	3.998351	0.52261
	29	1	-3.039727	3.544495	1.546408
	30	1	-4.672008	3.031663	1.973551
	31	1	-0.128342	0.691553	-1.270532
	32	1	0.184297	1.209158	0.367533
	33	1	2.433202	1.069643	1.347528
	34	1	5.707524	0.074118	-1.241003
	35	1	4.113799	-0.604202	-2.986765
	36	1	1.676276	-0.462849	-2.601067
	37	1	6.684411	-0.082743	0.900933
	38	1	6.769625	1.307571	2.011798
	39	1	6.712206	1.584152	0.252888

N	CN	AN	X	Y	Z
	1	7	0.825115	2.745039	0.669181
	2	7	-0.206934	1.87874	0.384081
	3	6	0.369541	0.759289	0.083735
	4	7	1.758565	0.869258	0.156851
	5	6	2.074344	2.196471	0.536827
	6	8	3.170525	2.694115	0.692873
	7	6	-0.331294	-0.505688	-0.316283
	8	6	-1.80984	-0.327524	-0.590806
	9	6	-2.743333	-0.636785	0.390268
	10	6	-4.113829	-0.478603	0.149313
	11	6	-4.553146	-0.007719	-1.089046
	12	6	-3.609164	0.298498	-2.072715
	13	6	-2.250729	0.14204	-1.835134
	14	8	-4.935565	-0.81515	1.186669
	15	6	-6.338377	-0.665562	1.018231
	16	6	2.739792	-0.125052	-0.090913
	17	6	2.83704	-1.254522	0.721772
	18	6	3.795394	-2.232244	0.513923
10	19	6	4.706643	-2.067781	-0.526509
	20	6	4.646506	-0.937263	-1.340147
	21	6	3.666598	0.026489	-1.124158
	22	9	1.968347	-1.399267	1.748768
	23	1	0.632409	3.699815	0.920543
	24	1	0.167568	-0.904514	-1.206824
	25	1	-0.185076	-1.249063	0.473001
	26	1	-2.432668	-1.00096	1.362955
	27	1	-5.60613	0.120141	-1.299992
	28	1	-3.950301	0.661782	-3.035832
	29	1	-1.53149	0.387609	-2.608627
	30	1	-6.786185	-0.981199	1.959177
	31	1	-6.608434	0.3775	0.820575
	32	1	-6.714374	-1.29969	0.207832
	33	1	3.823891	-3.092571	1.170815
	34	1	5.465955	-2.822085	-0.695272
	35	1	5.361607	-0.804797	-2.142768
	36	1	3.614313	0.914193	-1.741776



N	CN	AN	X	Y	Z
1	7	0.870562	2.79466	0.307826	
2	7	-0.145565	1.864504	0.310004	
3	6	0.442328	0.726128	0.12388	
4	7	1.822643	0.885017	-0.0076	
5	6	2.118223	2.265698	0.103219	
6	8	3.199691	2.812211	0.028417	
7	6	-0.242631	-0.606057	0.024947	
8	6	-1.752886	-0.526983	0.049155	
9	6	-2.45172	-0.523136	1.262843	
10	6	-3.835405	-0.448759	1.295086	
11	6	-4.562699	-0.376659	0.10104	
12	6	-3.883992	-0.383367	-1.119026	
13	6	-2.489417	-0.457991	-1.130019	
14	8	-5.920145	-0.308372	0.233664	
15	6	-6.713597	-0.219866	-0.941395	
16	6	2.81321	-0.107953	-0.221244	
17	6	3.060217	-1.094637	0.733445	
18	6	4.031169	-2.06594	0.556076	
19	6	4.803222	-2.039385	-0.602758	
20	6	4.594217	-1.049862	-1.562375	
21	6	3.602978	-0.092222	-1.372746	
22	9	2.32853	-1.103727	1.872152	
23	1	0.665087	3.772162	0.42677	
24	1	0.093928	-1.093792	-0.896859	
25	1	0.111223	-1.236598	0.84645	
26	1	-1.903543	-0.575367	2.197808	
27	1	-4.37619	-0.446266	2.233789	
28	1	-4.419066	-0.333404	-2.05772	
29	1	-1.975347	-0.460777	-2.086103	
30	1	-7.746367	-0.169788	-0.600164	
31	1	-6.478026	0.682426	-1.516356	
32	1	-6.585553	-1.101874	-1.578599	
33	1	4.177987	-2.812896	1.326139	
34	1	5.571233	-2.789369	-0.749987	
35	1	5.201918	-1.022663	-2.45853	
36	1	3.436788	0.687709	-2.105017	

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N	CN	AN	X	Y	Z
1	7	-0.637134	2.907703	-0.515242	
2	7	0.320628	1.920062	-0.543905	
3	6	-0.322418	0.822351	-0.300155	
4	7	-1.682733	1.064545	-0.102705	
5	6	-1.899677	2.459049	-0.223657	
6	8	-2.938572	3.074782	-0.100298	
7	6	0.30287	-0.540938	-0.200373	
8	6	1.815264	-0.522209	-0.162539	
9	6	2.565559	-0.525509	-1.344775	
10	6	3.951161	-0.505799	-1.316737	
11	6	4.628241	-0.482896	-0.091543	
12	6	3.897147	-0.483731	1.098116	
13	6	2.501789	-0.503357	1.048417	
14	8	5.991213	-0.466015	-0.164695	
15	6	6.736302	-0.431999	1.04474	
16	6	-2.71707	0.131503	0.192041	
17	6	-2.95805	-0.935827	-0.675134	
18	6	-3.969281	-1.826951	-0.354872	
19	6	-4.762872	-1.684708	0.771659	
20	6	-4.522349	-0.597714	1.610389	
21	6	-3.502665	0.30834	1.332193	
22	9	-4.195318	-2.868557	-1.190535	
23	1	-0.378561	3.870713	-0.648913	
24	1	-0.091271	-1.031284	0.69588	
25	1	-0.035707	-1.15198	-1.043959	
26	1	2.057421	-0.538994	-2.303452	
27	1	4.531788	-0.508809	-2.231288	
28	1	4.392384	-0.471748	2.059615	
29	1	1.94715	-0.503307	1.98154	
30	1	7.783877	-0.416609	0.74845	
31	1	6.511568	0.467761	1.627822	
32	1	6.546445	-1.320466	1.656927	
33	1	-2.392171	-1.06645	-1.587704	
34	1	-5.546551	-2.403417	0.974403	
35	1	-5.135704	-0.458449	2.492499	
36	1	-3.322953	1.156134	1.9793	

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N	CN	AN	X	Y	Z
	1	7	1.204598	2.77444	1.093316
	2	7	0.208535	1.876799	0.784868
	3	6	0.826549	0.834645	0.327362
	4	7	2.208986	1.027184	0.319856
	5	6	2.470731	2.329282	0.812086
	6	8	3.54195	2.885046	0.943956
	7	6	3.226888	0.131819	-0.115227
	8	6	3.33972	-1.130291	0.470968
	9	6	4.3376	-1.977924	0.018107
	10	6	5.238846	-1.612766	-0.968588
	11	6	5.12473	-0.338649	-1.522158
	12	6	4.122957	0.534245	-1.106823
	13	9	4.439478	-3.206576	0.578996
	14	6	0.15914	-0.414394	-0.175734
	15	6	-1.342131	-0.292158	-0.320245
	16	6	-2.188708	-0.597926	0.749479
	17	6	-3.568676	-0.486979	0.641524
	18	6	-4.139701	-0.045998	-0.571231
	19	6	-3.300616	0.245266	-1.646768
13	20	6	-1.916292	0.12119	-1.518115
	21	8	-5.499119	0.069616	-0.594935
	22	6	-6.114946	0.594731	-1.763866
	23	8	-4.335718	-0.736186	1.75137
	24	6	-5.203658	-1.873669	1.683684
	25	1	0.974298	3.685713	1.452041
	26	1	2.68586	-1.445958	1.272862
	27	1	6.006734	-2.308192	-1.28248
	28	1	5.823777	-0.025213	-2.288207
	29	1	4.040572	1.525481	-1.531753
	30	1	0.609588	-0.676662	-1.138888
	31	1	0.397299	-1.244036	0.497944
	32	1	-1.787085	-0.918176	1.704636
	33	1	-3.714596	0.578948	-2.588782
	34	1	-1.286488	0.359775	-2.368706
	35	1	-5.946764	-0.052126	-2.631837
	36	1	-5.752358	1.604199	-1.984356
	37	1	-7.180824	0.633816	-1.545115
	38	1	-5.952785	-1.756334	0.898354
	39	1	-5.695265	-1.933712	2.6542
	40	1	-4.623596	-2.787643	1.512979

N	CN	AN	X	Y	Z
	1	7	1.419556	2.565569	1.212283
	2	7	0.376193	1.752142	0.829129
	3	6	0.938309	0.72006	0.286481
	4	7	2.328913	0.837415	0.29641
	5	6	2.660783	2.073341	0.903275
	6	8	3.762107	2.550749	1.08519
	7	6	3.297506	-0.07013	-0.204261
	8	6	3.453135	-1.33712	0.357926
	9	6	4.399376	-2.237311	-0.102737
	10	6	5.239228	-1.853091	-1.145226
	11	6	5.121385	-0.583764	-1.709786
	12	6	4.154233	0.300562	-1.242711
	13	9	2.654502	-1.699216	1.388353
	14	6	0.218797	-0.453729	-0.311977
	15	6	-1.279951	-0.271906	-0.40959
	16	6	-2.113853	-0.653545	0.645856
	17	6	-3.491192	-0.488752	0.582041
	18	6	-4.072284	0.086969	-0.56771
	19	6	-3.246702	0.455339	-1.629817
14	20	6	-1.864997	0.275114	-1.547043
	21	8	-5.42773	0.247256	-0.547514
	22	6	-6.048648	0.905602	-1.643769
	23	8	-4.244759	-0.821849	1.679531
	24	6	-5.14616	-1.923111	1.51996
	25	1	1.237857	3.448963	1.657823
	26	1	4.474633	-3.210682	0.365639
	27	1	5.988639	-2.545481	-1.509908
	28	1	5.781799	-0.281354	-2.513236
	29	1	4.05838	1.29284	-1.665045
	30	1	0.638788	-0.638385	-1.307049
	31	1	0.45049	-1.342156	0.28377
	32	1	-1.702089	-1.078041	1.554884
	33	1	-3.668732	0.892632	-2.524682
	34	1	-1.245048	0.576919	-2.384728
	35	1	-7.107844	0.957782	-1.396885
	36	1	-5.655593	1.919556	-1.772703
	37	1	-5.921184	0.343028	2.488551
	38	1	-5.625748	-2.061374	2.488551
	39	1	-5.902671	-1.711045	0.761805
	40	1	-4.595558	-2.832563	1.253875

N	CN	AN	X	Y	Z
1	7	-1.200583	-2.725267	1.278596	
2	7	-0.199992	-1.881655	0.851439	
3	6	-0.819799	-0.885822	0.300614	
4	7	-2.201659	-1.054139	0.350657	
5	6	-2.468821	-2.286935	0.988669	
6	8	-3.543791	-2.805368	1.214249	
7	6	-3.215606	-0.181805	-0.150718	
8	6	-3.383466	1.084233	0.411147	
9	6	-5.182918	1.519613	-1.116073	
10	6	-4.043848	-0.611417	-1.185234	
11	6	-4.364403	1.955867	-0.068174	
12	6	-5.030195	0.247699	-1.661938	
13	6	-4.564059	3.315404	0.557326	
14	6	-0.158267	0.293431	-0.354143	
15	6	1.34999	0.195632	-0.41781	
16	6	2.141166	0.709331	0.614006	
17	6	3.527009	0.624786	0.582454	
18	6	4.161735	-0.002987	-0.509986	
19	6	3.378271	-0.503259	-1.550055	
20	6	1.987174	-0.402129	-1.500421	
21	8	5.523873	-0.079358	-0.459781	
22	6	6.201761	-0.778345	-1.495588	
23	8	4.236804	1.088371	1.661789	
24	6	5.087377	2.216545	1.427931	
25	1	-0.974129	-3.592282	1.735497	
26	1	-2.750762	1.384141	1.23953	
27	1	-5.951737	2.180374	-1.503338	
28	1	-3.919053	-1.604083	-1.598691	
29	1	-5.680226	-0.076512	-2.466564	
30	1	-4.836387	4.061485	-0.193076	
31	1	-3.660821	3.659284	1.065634	
32	1	-5.369521	3.288862	1.298961	
33	1	-0.573021	0.397818	-1.362894	
34	1	-0.448918	1.204736	0.178175	
35	1	1.689689	1.178295	1.481531	
36	1	3.841624	-0.983571	-2.401371	
37	1	1.401579	-0.807259	-2.318798	
38	1	6.056944	-0.295015	-2.468031	
39	1	5.871984	-1.820962	-1.553253	
40	1	7.257757	-0.747682	-1.231954	
41	1	5.873698	1.979431	0.708788	
42	1	5.532608	2.461466	2.391829	
43	1	4.500631	3.070689	1.071065	

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N	CN	AN	X	Y	Z
1	7	0.219427	-3.116421	-0.115634	
2	7	-1.014588	-2.527652	-0.014634	
3	6	-0.782602	-1.247004	-0.014549	
4	7	0.586373	-0.98731	-0.102355	
5	6	1.265227	-2.227688	-0.171801	
6	8	2.455793	-2.426752	-0.276719	
7	6	-1.852635	-0.24309	0.078712	
8	6	-3.094118	-0.526489	-0.509317	
9	6	-4.142594	0.381092	-0.408541	
10	6	-3.967707	1.583329	0.277069	
11	6	-2.73848	1.868684	0.867888	
12	6	-1.685222	0.963142	0.771612	
13	6	1.263613	0.251241	-0.269424	
14	6	2.113659	0.721236	0.730948	
15	6	2.822742	1.903663	0.590999	
16	6	2.672502	2.644478	-0.578735	
17	6	1.824359	2.197291	-1.591204	
18	6	1.131653	1.000142	-1.439027	
19	9	2.231156	0.018336	1.873485	
20	1	0.308302	-4.11866	-0.104506	
21	1	-3.223692	-1.461391	-1.04006	
22	1	-5.096823	0.151566	-0.86898	
23	1	-4.78511	2.291411	0.352354	
24	1	-2.598529	2.795397	1.412551	
25	1	-0.742741	1.190391	1.252504	
26	1	3.475313	2.225227	1.393004	
27	1	3.222565	3.570409	-0.697982	
28	1	1.711498	2.772025	-2.502256	
29	1	0.48162	0.632132	-2.223658	

N	CN	AN	X	Y	Z
	1	7	-0.245921	-3.292387	0.330267
	2	7	-1.373521	-2.514604	0.28464
	3	6	-0.944927	-1.306941	0.056428
	4	7	0.446488	-1.281017	-0.064841
	5	6	0.92084	-2.6065	0.102031
	6	8	2.063798	-3.010194	0.06251
	7	6	-1.854089	-0.162236	-0.106452
	8	6	-1.607924	0.850928	-1.04256
	9	6	-2.519403	1.890479	-1.2047
	10	6	-3.6821	1.932309	-0.437281
	11	6	-3.93462	0.923737	0.492277
	12	6	-3.02788	-0.117633	0.658783
	13	6	1.325135	-0.159836	-0.126048
	14	6	1.196768	0.873855	0.803597
17	15	6	2.074351	1.941426	0.71796
	16	6	3.081293	2.01021	-0.231974
	17	6	3.204847	0.955908	-1.134625
	18	6	2.33072	-0.127473	-1.092486
	19	9	1.945967	2.951809	1.61059
	20	1	-0.318604	-4.288584	0.453212
	21	1	-0.714492	0.82252	-1.653549
	22	1	-2.321667	2.666544	-1.935162
	23	1	-4.387682	2.745516	-0.563651
	24	1	-4.837381	0.950219	1.09178
	25	1	-3.219164	-0.904865	1.37742
	26	1	0.437978	0.85623	1.574413
	27	1	3.746873	2.863695	-0.252156
	28	1	3.990126	0.980449	-1.880573
	29	1	2.432538	-0.949788	-1.787277

N	CN	AN	X	Y	Z
	1	7	0.96659	3.204765	0.092035
	2	7	1.935864	2.235604	0.078777
	3	6	1.288181	1.109285	-0.006384
	4	7	-0.090099	1.323634	-0.062155
	5	6	-0.31394	2.72076	-0.010181
	6	8	-1.370276	3.317018	-0.040447
	7	6	1.970078	-0.191851	-0.083214
	8	6	1.490545	-1.232456	-0.889876
	9	6	2.192719	-2.431314	-0.977384
	10	6	3.376803	-2.60679	-0.263382
	11	6	3.861322	-1.572732	0.537413
	12	6	3.16436	-0.372632	0.628759
	13	6	-1.155324	0.377718	0.021983
	14	6	-1.19295	-0.54943	1.064527
18	15	6	-2.238391	-1.464028	1.146823
	16	6	-3.241644	-1.412551	0.191387
	17	6	-3.238591	-0.485232	-0.83883
	18	6	-2.18062	0.415146	-0.923489
	19	9	-4.263789	-2.296883	0.271242
	20	1	1.219653	4.1786	0.110836
	21	1	0.579279	-1.104207	-1.460124
	22	1	1.815569	-3.22721	-1.6093
	23	1	3.919493	-3.542706	-0.331903
	24	1	4.782085	-1.702003	1.094756
	25	1	3.53665	0.434996	1.246659
	26	1	-0.40628	-0.558777	1.808465
	27	1	-2.286746	-2.196909	1.942051
	28	1	-4.048975	-0.472816	-1.556466
	29	1	-2.15619	1.15546	-1.712092