

Electronic Supplementary Information for

Degradation of Pesticides Diazinon and Diazoxon by Phosphotriesterase: Insight into Divergent Mechanisms from QM/MM and MD Simulations

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Contents

Table S1	2
Fig.S1	3
Fig.S2	3
Fig.S3	4
Fig. S4	4
Fig. S5	5
Fig. S6	5
Fig. S7	6
Fig. S8	6
Cartesian coordinates of QM region from QM/MM calculations.....	7

Table S1. The distances between zinc ions and the first shell residues for enzyme-DIN and enzyme-DON systems (Å).

	DIN	DON
Zn _α -N _{His55}	2.50 ± 0.24	2.32 ± 0.30
Zn _α -N _{His57}	2.24 ± 0.13	2.05 ± 0.10
Zn _α -O _{Lys169}	1.83 ± 0.05	1.80 ± 0.05
Zn _α -O _{Asp301}	1.80 ± 0.04	1.78 ± 0.04
Zn _α -O _μ	1.76 ± 0.04	1.73 ± 0.03
Zn _α -O _{H2O}	1.94 ± 0.07	
Zn _β -O _{Lys169}	1.76 ± 0.04	1.78 ± 0.04
Zn _β -N _{His201}	2.42 ± 0.20	2.61 ± 0.22
Zn _β -N _{His230}	2.01 ± 0.08	2.30 ± 0.18
Zn _β -O _μ	1.72 ± 0.03	1.73 ± 0.03
Zn _β -S _{DIN/O_{DON}}	3.30 ± 0.21	1.85 ± 0.06
Zn _β -O _{H2O}	1.87 ± 0.06	1.93 ± 0.07

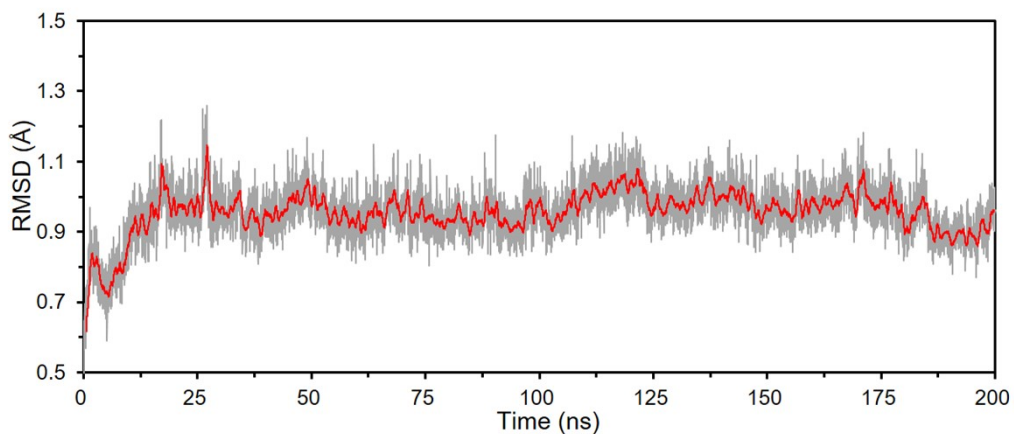


Fig. S1 RMSD values of enzyme-DIN system for 200 ns MM MD simulations, the atoms were used to compute the RMSD includes residues 1-329@CA, C, N.

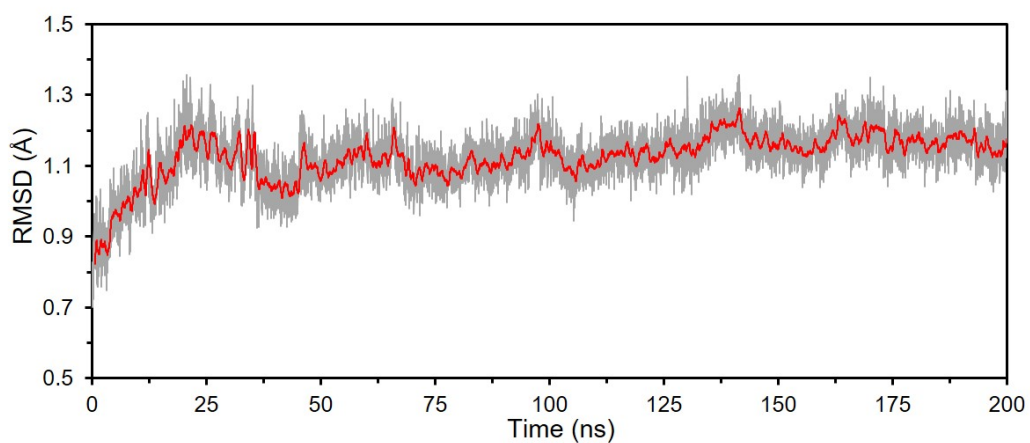


Fig. S2 RMSD values of enzyme-DON system for 200 ns MM MD simulations, the atoms were used to compute the RMSD includes residues 1-329@CA, C, N.

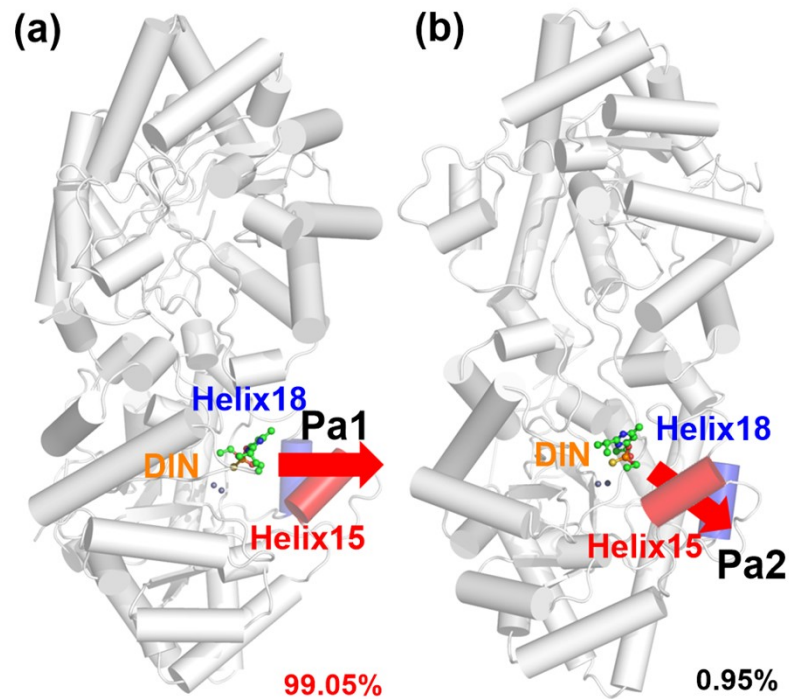


Fig. S3 Possible channels for DIN delivery to the active site are predicted by RAMD-MD simulations. (a) represents for pathway 1 (Pa1) and (b) represents for pathway 2 (Pa2).

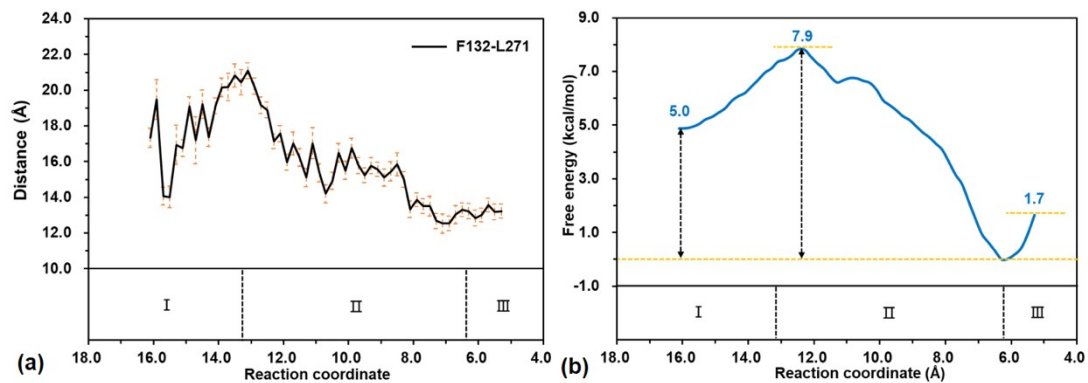


Fig. S4 (A) The distance fluctuation of the delivery channel characterized by the distance between Phe132@CZ and Leu271@CG. (B) Free energy profile for the process of DIN enters into the active site.

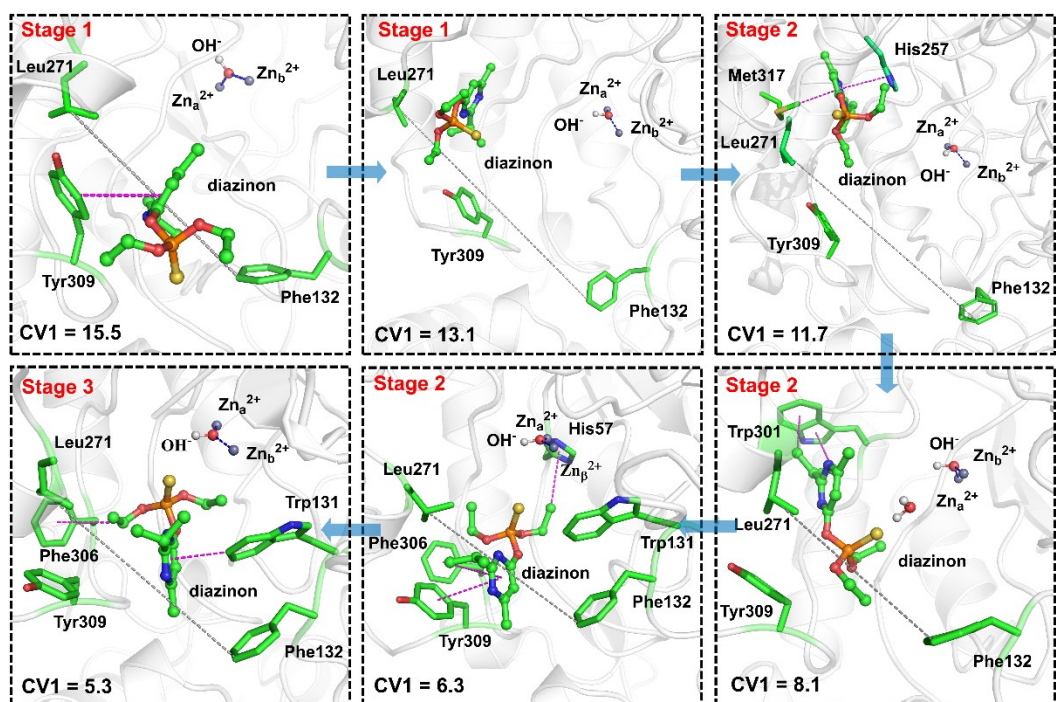


Fig. S5 Representative structures and conformational changes of the delivery channel in the DIN transportation.

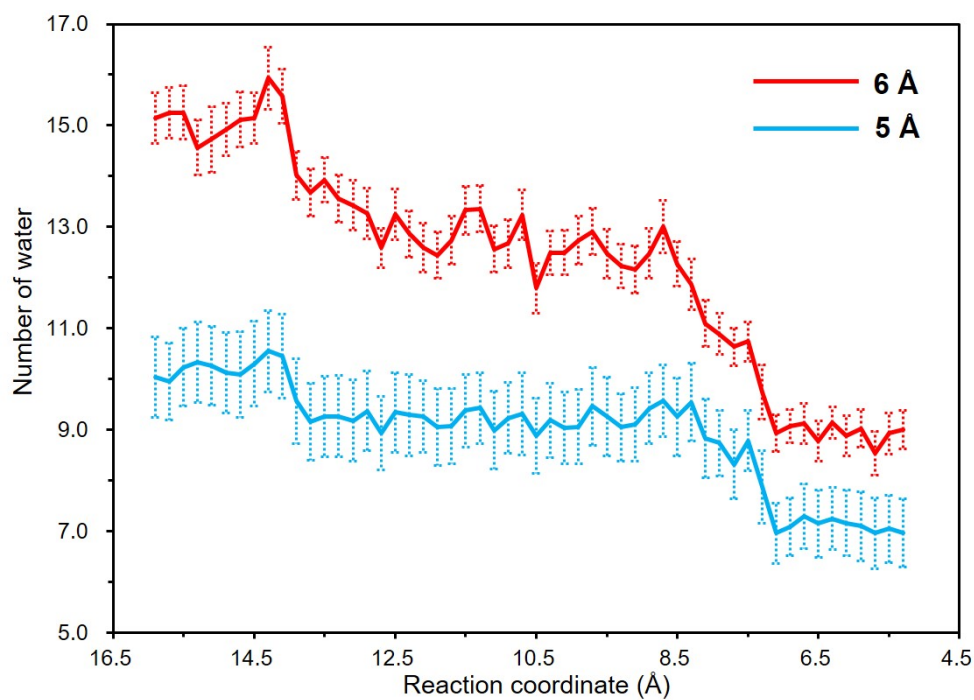


Fig. S6 Statistics analysis of water molecules around two zinc ions within 5 Å (blue) and 6 Å (red) during the delivery of DIN from the bulk water to the active site PTE enzyme.

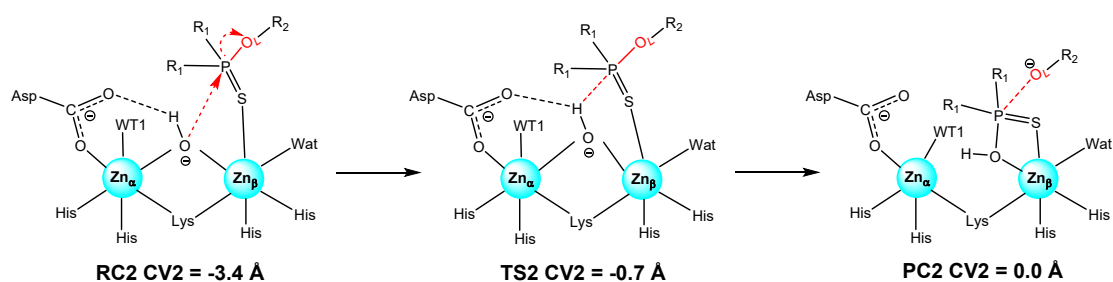
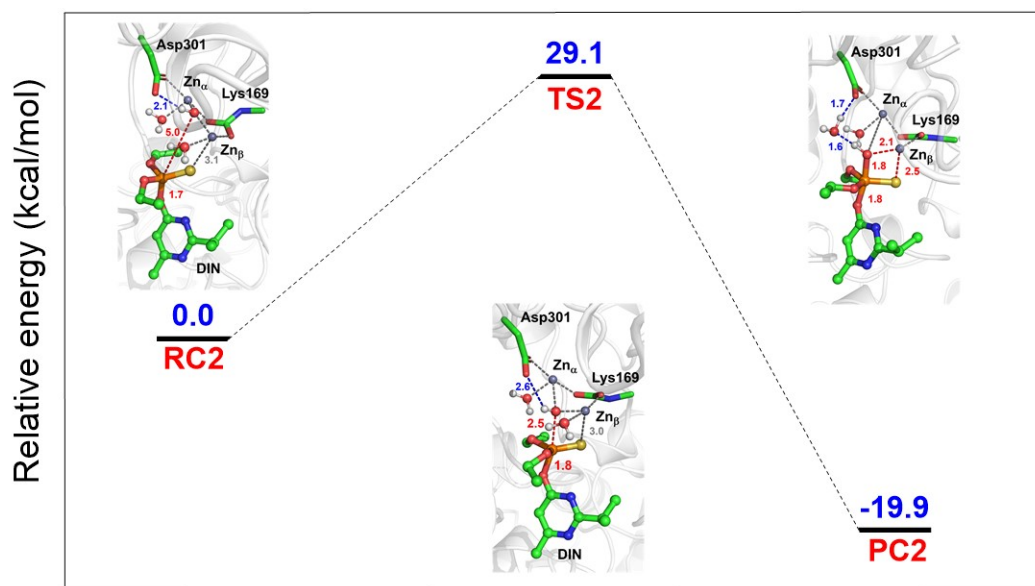


Fig. S7 QM/MM (B3LYP/TZVP) relative energies (in kcal/mol) and representative structures for the degradation of DIN Model A (RC = reactant complex, TS = transition state, PC = product).

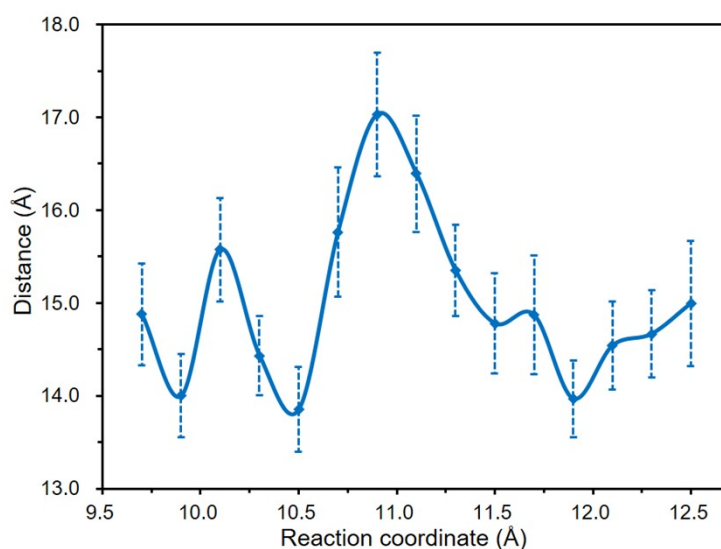


Fig. S8 The distance fluctuation during the release of LEG characterized by the distance between Phe132@CZ and Leu271@CG.

Cartesian coordinates of QM region from QM/MM calculations

RC1

c	54.852621	41.032149	51.150802	n	52.993789	45.251538	45.672527
h	55.678718	41.721615	51.383986	c	51.776430	44.585874	45.620943
h	55.303261	40.052834	50.921187	o	51.323088	44.363858	44.456685
c	54.112592	41.569621	49.960836	o	51.233752	44.247664	46.706561
n	54.812744	42.218612	48.953430	h	53.121470	45.740999	47.700625
h	55.819952	42.092484	48.757381	h	54.315772	46.549466	46.642084
c	53.931471	42.614484	48.008423	h	53.320075	45.530917	44.754237
h	54.212856	43.160890	47.110851	c	52.520671	46.065489	42.255576
n	52.700980	42.257610	48.341480	h	52.045621	45.908353	43.230220
c	52.793595	41.609579	49.557025	h	52.271646	47.076320	41.910537
h	51.909346	41.209920	50.045446	c	51.941259	45.071272	41.294677
c	46.642706	40.894279	50.180968	n	51.670143	43.741257	41.591588
h	46.589730	39.862688	49.813621	c	51.067127	43.223051	40.531471
h	45.654416	41.361384	50.034218	h	50.694794	42.206213	40.465414
c	47.692746	41.628918	49.421016	n	50.938409	44.148216	39.557625
n	47.835879	43.010155	49.432147	h	50.492619	44.024954	38.645472
h	47.303666	43.655693	50.005695	c	51.487626	45.324229	40.018838
c	48.862833	43.347951	48.614447	h	51.514266	46.227297	39.417454
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h	48.449129	49.222738	46.282310	h	55.853545	40.663804	45.372517
h	46.881000	49.388397	45.505181	c	54.149329	41.777795	44.789913
c	48.186411	48.020114	44.510276	h	53.520852	41.655208	45.661855
c	49.352655	47.299778	44.349771	n	53.772273	42.367636	43.665724
h	50.345997	47.508175	44.736670	c	54.823033	42.228169	42.784324
n	49.137309	46.178391	43.574537	h	54.762518	42.583798	41.757863
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TS1a

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n 53.093620 45.181552 45.667233
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o 51.477459 44.296750 44.381573
o 51.291390 44.176013 46.623027

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c	52.519332	46.181456	42.207441	c	48.072485	38.781086	45.827698
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c	51.951500	45.238581	41.192413	p	49.429551	41.356028	44.328934
n	51.758368	43.880668	41.405807	o	47.842449	40.999567	43.492327
c	51.144313	43.399365	40.332762	o	48.613908	41.896978	45.618251
h	50.824040	42.371759	40.195853	o	49.806819	42.355482	43.226404
n	50.943067	44.374998	39.428575	n	47.524510	39.768389	39.638082
h	50.479533	44.276375	38.520662	c	48.675728	39.735932	40.313169
c	51.449176	45.545264	39.948041	c	49.887148	39.125176	39.633257
h	51.415975	46.480614	39.400559	c	49.630424	37.646224	39.318440
c	57.080335	40.872137	42.836614	c	50.324586	39.918772	38.398198
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c	55.792453	41.379648	43.405892	c	46.518512	40.716770	41.582428
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c	28.141815	48.096737	62.708352	o	29.028721	43.124812	56.836486
n	28.213283	46.908077	61.989180	s	29.137609	45.177886	59.066014
c	29.338511	46.304235	62.332761	c	30.574873	41.703639	59.937253
h	29.689834	45.362291	61.928296	c	30.643143	42.534826	61.203636
n	30.004143	47.039391	63.246478	n	34.728354	44.527092	59.728873
h	30.899869	46.824500	63.677580	c	34.801090	43.621315	58.732010
c	29.270869	48.179895	63.496089	c	36.126998	42.941387	58.531935
h	29.613835	48.949750	64.181436	c	33.688810	43.312883	57.940579
c	24.540846	45.635249	65.999351	c	32.483620	43.933076	58.302984
h	25.007137	46.494409	66.500515	n	32.424250	44.837775	59.262190
h	25.067583	44.732248	66.343260	c	33.552881	45.136579	59.919756
c	24.644291	45.759674	64.514564	c	33.477020	46.218960	60.974962
n	23.661693	45.420037	63.599330	c	33.206074	45.575330	62.347490
h	22.682353	45.160482	63.799516	c	32.444494	47.292215	60.626685
c	24.137888	45.652583	62.360936	h	27.799372	45.634791	56.424937
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c	25.712950	46.173596	63.753585	h	27.743945	43.374483	55.304023
h	26.706822	46.463188	64.083408	h	29.475367	43.541360	54.878611
c	22.040085	40.874911	64.679906	h	30.986963	43.556198	60.987353
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c	23.002328	41.650917	63.840350	h	31.570260	41.605369	59.470334
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TS2

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n	29.828030	46.920654	63.034100	n	34.251826	44.609648	59.692647
h	30.732690	46.676116	63.425303	c	34.155384	43.738641	58.664154
c	29.139097	48.083017	63.303267	c	35.408131	42.980972	58.318094
h	29.527029	48.845520	63.972209	c	32.954648	43.554630	57.976714
c	24.505838	45.589359	65.813629	c	31.823933	44.247687	58.464513
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c	24.535787	45.607355	64.316896	c	33.242181	46.313980	61.121039
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c	23.922505	45.321393	62.204945	h	27.576124	45.910730	55.646444
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PC2

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TS3a

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IM3

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TS3b

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n 29.989180 47.094934 63.113678
h 30.906938 46.882098 63.500107
c 29.253363 48.222419 63.407760

h	29.612145	48.983693	64.094273	c	34.385649	43.797141	57.746706
c	24.534434	45.658092	65.888684	c	33.211385	44.636849	57.683231
h	24.991989	46.552354	66.332559	n	32.969676	45.421254	58.798598
h	25.086827	44.789467	66.274140	c	33.799863	45.372617	59.825937
c	24.619103	45.690325	64.395270	c	33.515124	46.312976	60.995673
n	23.620931	45.309306	63.514808	c	33.250722	45.514308	62.282114
h	22.642109	45.079024	63.751588	c	32.394410	47.304873	60.694971
c	24.090147	45.436843	62.257139	h	27.236385	46.140401	55.974137
h	23.509132	45.172424	61.380980	h	27.388550	46.094150	54.199488
n	25.336792	45.874666	62.272739	h	28.765952	46.645481	55.208812
c	25.688591	46.024689	63.595568	h	27.607439	43.786890	55.060078
h	26.689800	46.322633	63.892328	h	29.173353	44.319241	54.389187
c	22.050569	40.876327	64.650496	h	30.852246	44.221996	60.347860
h	21.774326	41.377809	65.590144	h	32.077586	42.945108	60.360691
h	22.506746	39.915864	64.937039	h	30.406291	42.560964	60.881084
c	23.100121	41.632782	63.903399	h	31.178285	43.433017	58.005268
n	24.302842	41.963344	64.514382	h	30.921147	41.746749	58.522036
h	24.525664	41.860774	65.519671	h	36.588250	42.382425	58.073946
c	25.165216	42.460304	63.625298	h	36.150383	42.109510	59.787086
h	26.182290	42.788105	63.820922	h	37.231829	43.447309	59.365542
n	24.549980	42.461872	62.445926	h	34.624180	43.168679	56.886669
h	24.981687	42.752428	61.570985	h	32.311179	44.942103	62.190698
c	23.265069	41.975272	62.582806	h	34.059331	44.792748	62.467180
h	22.592527	41.908601	61.736391	h	33.168652	46.175656	63.162573
c	21.585992	42.548810	59.076497	h	31.453054	46.772549	60.495801
h	21.079443	43.355131	59.635491	h	32.611193	47.887698	59.792449
h	21.591332	41.678930	59.741630	h	32.241549	48.000856	61.534743
c	23.002561	43.017980	58.814363	h	34.450619	46.880891	61.127967
o	23.291287	43.687095	57.782106	o	25.377508	44.784582	59.384207
o	23.850178	42.759290	59.732147	h	24.846781	43.980852	59.668066
zn	24.296241	45.621303	57.758511	o	27.002828	43.754575	57.724897
zn	26.733910	45.986966	60.700198	h	26.544803	43.047229	57.120565
c	28.435819	44.506873	55.181428	h	26.079069	44.379744	58.794746
c	27.929824	45.934706	55.146344	o	27.234332	43.995790	61.370522
o	29.220703	42.872823	58.526535	h	27.821634	43.840012	62.150723
p	28.547781	44.157098	57.865497	h	27.221969	43.208638	60.780072
o	32.416678	44.645525	56.715215	o	26.481502	41.880756	59.895839
o	29.147497	44.179391	56.393277	h	25.542945	41.961465	59.642841
s	28.677672	45.831924	58.894453	h	26.550266	41.063436	60.449229
c	30.669270	42.794039	58.743020	o	25.545206	42.259808	56.364233
c	31.012900	43.149942	60.174209	h	25.743232	41.301184	56.528902
n	34.887919	44.591575	59.959553	h	24.657402	42.445003	56.728492
c	35.158438	43.793949	58.890902	o	28.608147	43.755266	63.621979
c	36.348920	42.881717	59.024762	h	28.204622	43.743299	64.535436

h 29.575507 43.762524 63.803206
h 18.567714 47.035881 58.366479
h 22.137876 45.133234 51.965431
h 30.193342 53.299483 58.007220
h 25.421861 50.964355 58.293376
h 26.424231 49.472885 63.358628
h 23.509122 45.603477 66.254499
h 21.142679 40.685135 64.078441
h 20.947320 42.332408 58.220147