Hydrolysis pathways and kinetics of chlorantraniliprole and cyantraniliprole: Density Functional Theory Investigation

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Text S1. $\Delta G^{\ddagger}$ correction.

During the DFT calculations, the aqueous molar standard state was considered for all reactions. Due to the change in standard state from 1 atm to 1 M aqueous standard state, the calculated $\Delta G^{\ddagger}$ was corrected by adding 7.9 kJ·mol^{-1} for the reaction type of A → B + C, and reducing 7.9 kJ·mol^{-1} for the reaction type of A + B → C.[1]

Table S1. Experimental k_B values of CLAP and CNAP.

Name	k_B **(mol^{-1}·L·s^{-1})**
CLAP	7.99×10^{-2}
CNAP	9.44×10^{-1}

Table S2. Comparison of logk_{B1} (mol^{-1}·L·s^{-1}) calculated by B3LYP and M062X functionals and experimental logk_B for CLAP and CNAP, respectively.

Name	Methods	$\log k_{B1\text{-}DFT}$	$\log k_{B\text{-}1exp}$
CLAP	B3LYP	-1.25	-1.10
	M06-2X	4.16	
CNAP	B3LYP	-0.12	-0.03
	M06-2X	4.74	

Table S3. Comparison between $\log k_{B1}$ calculated with different types of implicit solvation models and experimental $\log k_B$ for CLAP and CNAP.

Name	Methods	$\log k_{B1\text{-}DFT}$	$\log k_{B\text{-}1exp}$
CLAP	IEFPCM/B3LYP/6-311++G(3df,2pd)	-1.25	-1.10
	SMD/B3LYP/6-311++G(3df,2pd)	-6.28	
CNAP	IEFPCM/B3LYP/6-311++G(3df,2pd)	-0.12	-0.03
	SMD/B3LYP/6-311++G(3df,2pd)	-5.05	

Table S4. The product branching ratio for each feasible hydrolysis pathway of CLAP and CNAP.

Name	Pathway	Product Branching ratio (%)
CLAP	Amide bond on benzene	3.34×10^{-10}
	Amide bond between benzene and pyrazole	99.99
	C-Cl bond on benzene	1.09×10^{-3}
	C-Cl bond on pyridine	7.52×10^{-3}
	C-Br bond on pyrazole	1.01×10^{-3}
CNAP	Amide bond on benzene	9.12×10^{-10}
	Amide bond between benzene and pyrazole	99.99
	C-Cl bond on pyridine	6.46×10^{-4}

Cyano group	4.53×10^{-9}
C-Br bond on pyrazole	2.92×10^{-4}

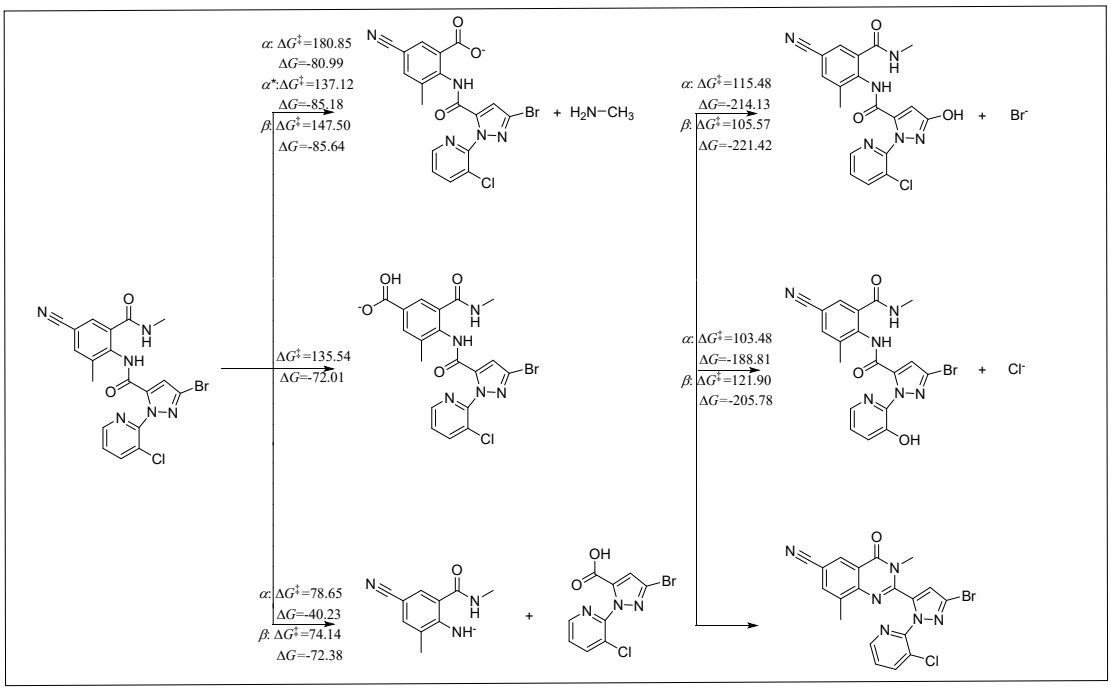


Figure S1. Potential hydrolysis pathways and the corresponding Gibbs free energies of reaction (ΔG, kJ·mol^{-1}) and Gibbs free energies of activation ($\Delta G^{\ddagger}$, kJ·mol^{-1}) for CNAP calculated at IEFPCM/B3LYP/6-311++G(3df,2pd) //IEFPCM/B3LYP/6-311++G(d,p) level.

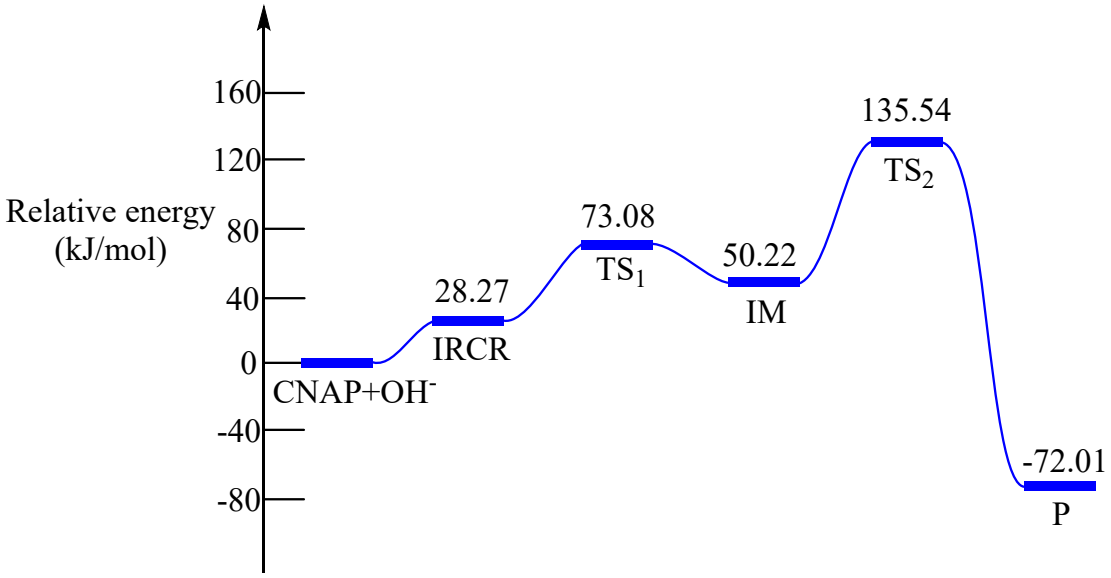


Figure S2. Schematic free energy surfaces for hydrolysis of C-N bond on pyrazole of CNAP calculated at IEFPCM/B3LYP/6-311++G(d,p) level. [The total energy of the reactants and OH^- is set to zero (reference state). The symbols "IRCR, TS, IM, P" refer to pre-reactive complexes, transition states, intermediates, and products involved in the reaction, respectively.]

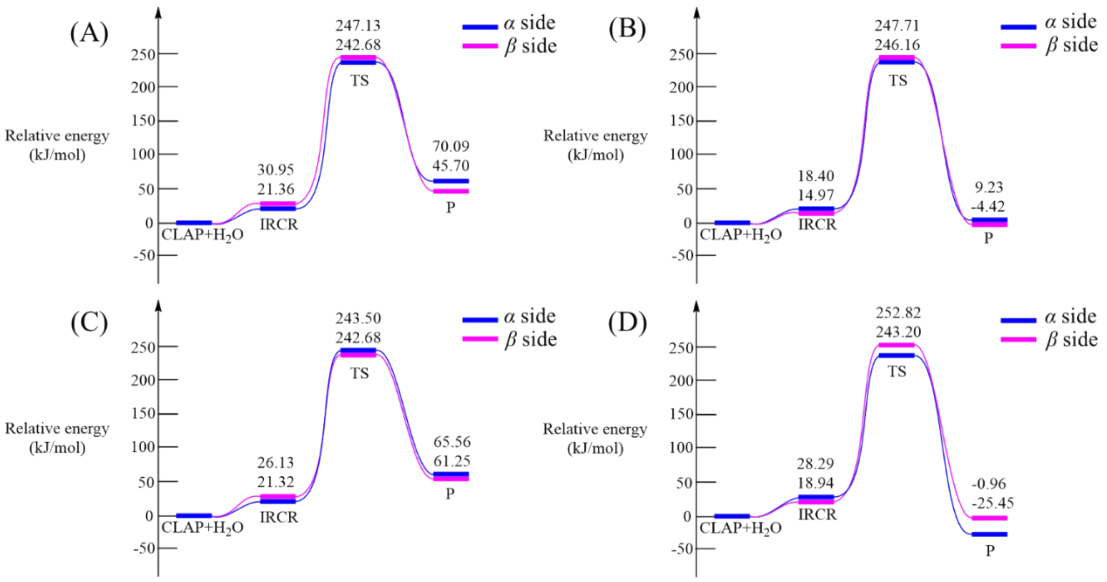


Figure S3. Schematic free energy surfaces for neutral hydrolysis of the amide bond on benzene of CLAP (A) and CNAP (C), and the amide bond between benzene and pyrazole of CLAP (B) and CNAP (D) calculated at IEFPCM/B3LYP/6-311++G(3df,2pd) //IEFPCM/B3LYP/6-311++G(d,p) level. [The total energy of the reactants and H_2O is set to zero (reference state). The symbols "IRCR, TS, P" refer to pre-reactive complexes, transition states, and products involved in the reaction, respectively. The α and β sides are shown in Figure 1.]

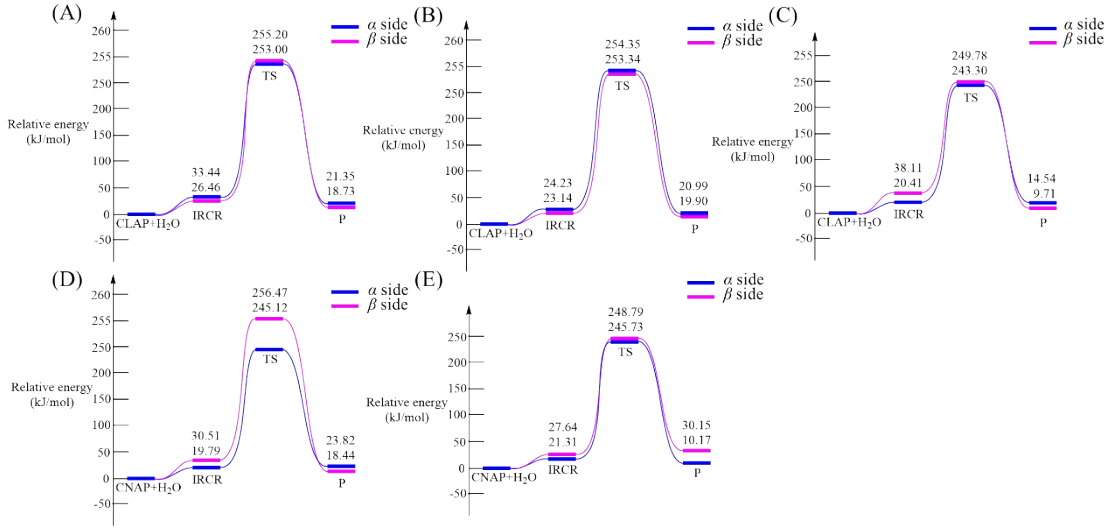


Figure S4. Schematic free energy surfaces for neutral hydrolysis of (A) C-Br bond on pyrazole of CLAP; (B) C-Cl bond on benzene of CLAP; (C) C-Cl bond on pyridine of CLAP; (D) C-Br bond on pyrazole of CNAP; and (E) C-Cl bond on pyridine of CNAP calculated at IEFPCM/B3LYP/6-311++G(d,p) level. [The total energy of the reactants and H_2O is set to zero (reference state). The symbols "IRCR, TS, P" refer to pre-reactive complexes, transition states, and products involved in the reaction, respectively. The α and β sides are shown in Figure 1.]

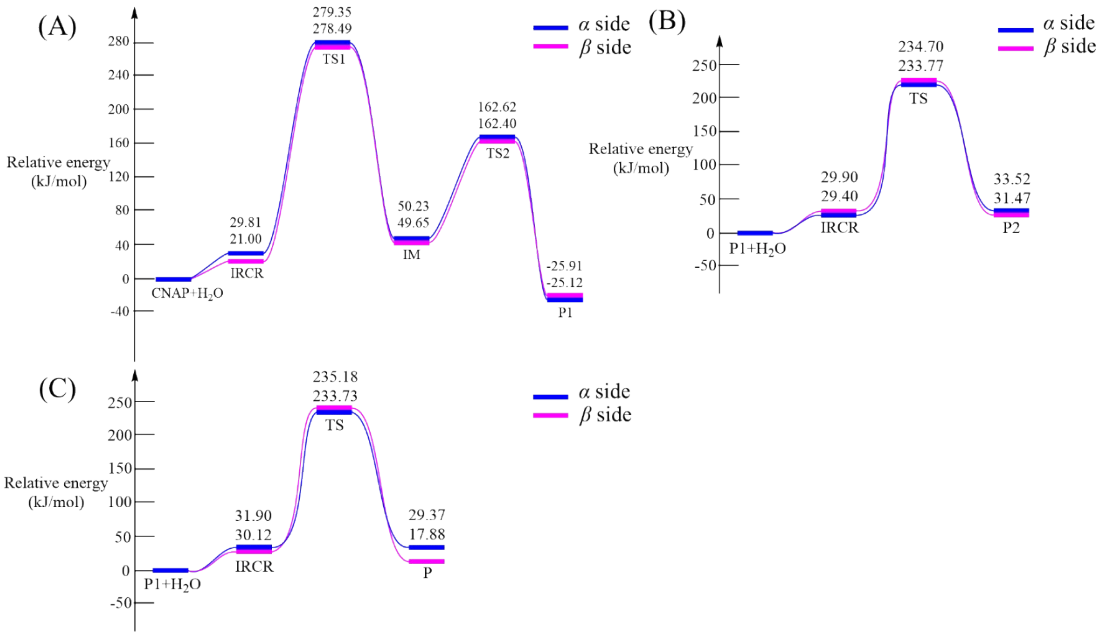


Figure S5. Schematic free energy surfaces for neutral hydrolysis of C-N bond on pyrazole of CNAP calculated at IEFPCM/B3LYP/6-311++G(d,p) level. (A) is the first step of neutral hydrolysis of CNAP, producing the intermediate product P1. (B) is the second step where the product P1, formed via nucleophilic attack at the α side, undergoes further neutral hydrolysis. (C) is the second step where the product P1, formed via nucleophilic attack at the β side, undergoes further neutral hydrolysis. [The total energy of the reactants and H_2O is set to zero (reference state). The symbols "IRCR, TS, IM, P" refer to pre-reactive complexes, transition states, intermediates, and products involved in the reaction, respectively. The α and β sides are shown in Figure 1.]

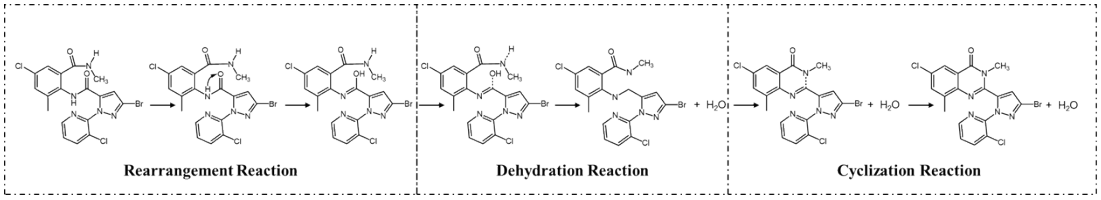


Figure S6. The rearrangement–dehydration–cyclization reaction pathway of CLAP.

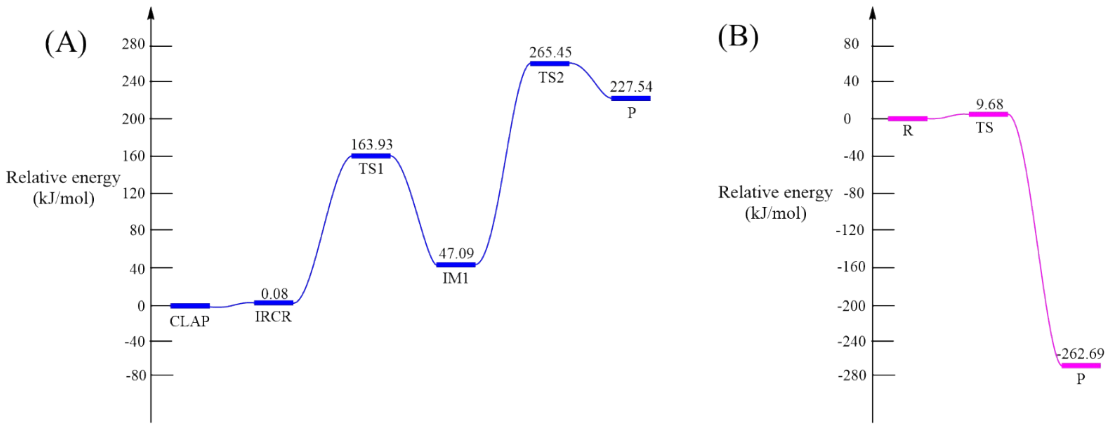


Figure S7. The potential energy surface of the rearrangement–dehydration–cyclization reaction of CLAP. (A) is the rearrangement–dehydration reaction of CLAP, (B) is the cyclization reaction of CLPA. [The total energy of the reactants is set to zero (reference state). The symbols "IRCR, TS, IM, P" refer to pre-reactive complexes, transition states, intermediates, and products involved in the reaction, respectively.]

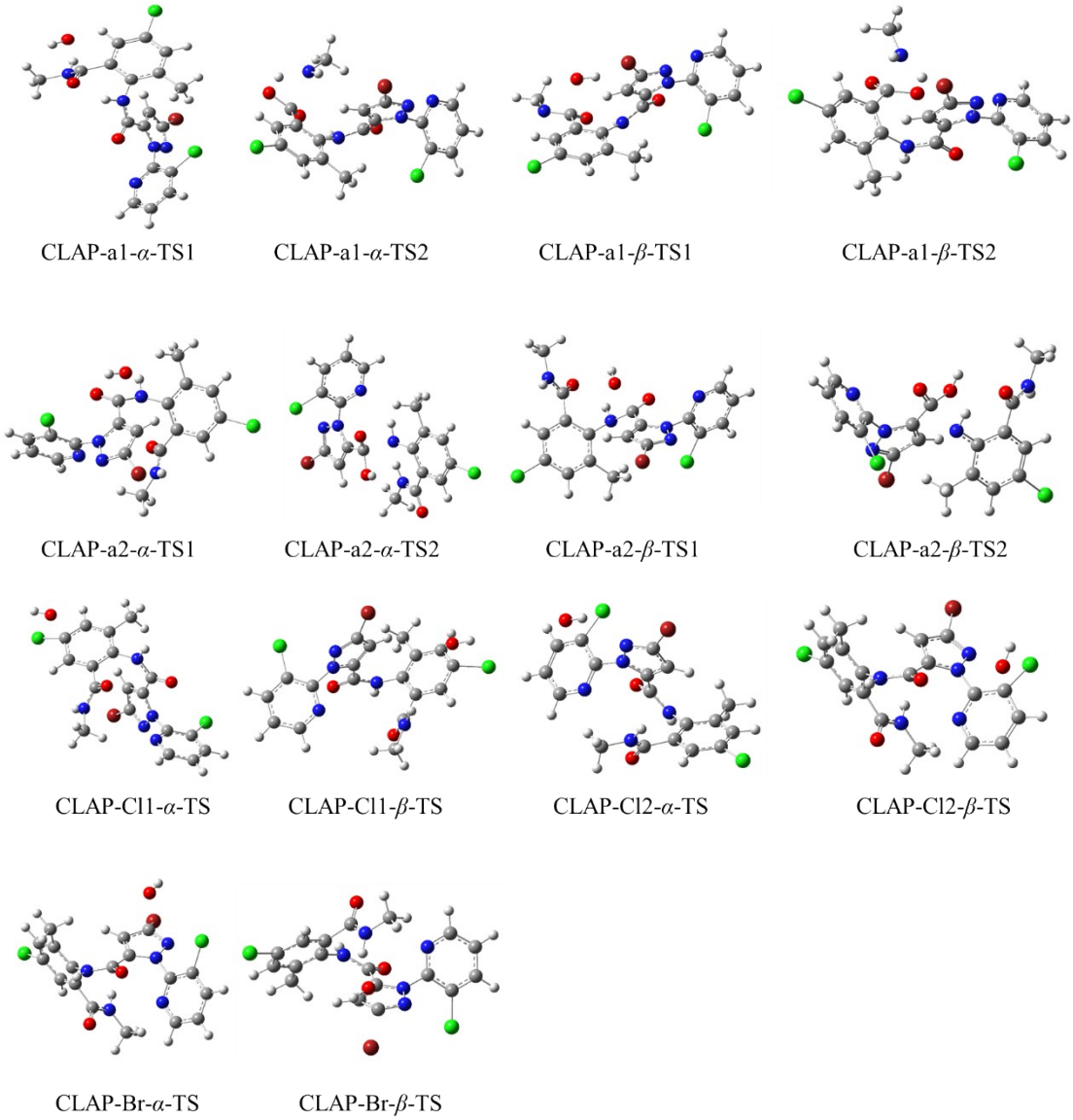


Figure S8. Structures of transition states (TS) of base-catalyzed hydrolysis of CLAP. [The symbols "a1, a2, Cl1, Cl2 and Br" refer to amide bond on benzene, amide bond between benzene and pyrazole, C-Cl bond on benzene, C-Cl bond on pyridine and C-Br bond on pyrazole, respectively. The α and β sides are shown in Figure 1.]

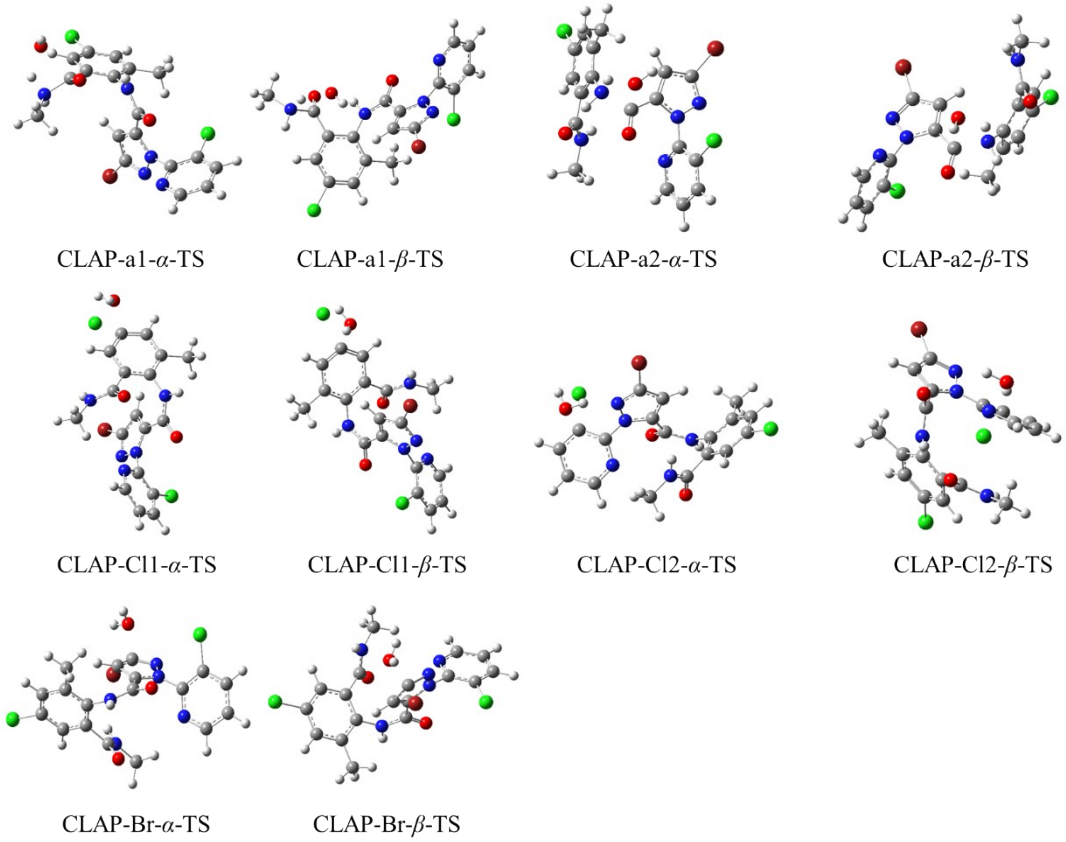
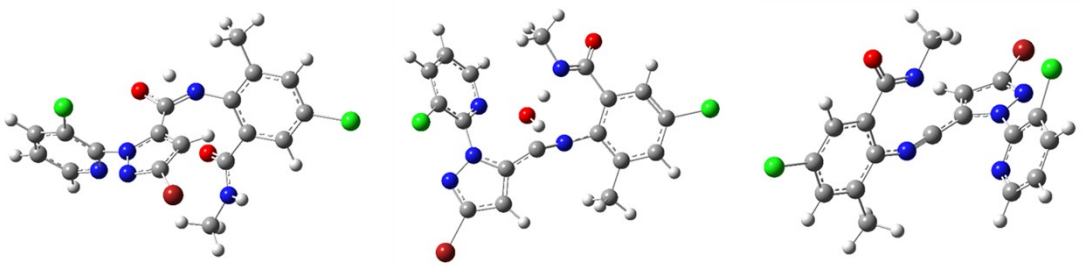


Figure S9. Structures of transition states (TS) of neutral hydrolysis of CLAP. [The symbols "a1, a2, Cl1, Cl2 and Br" refer to amide bond on benzene, amide bond between benzene and pyrazole, C-Cl bond on benzene, C-Cl bond on pyridine and C-Br bond on pyrazole, respectively. The α and β sides are shown in Figure 1.]



CLAP-Cyclization-TS1 CLAP-Cyclization-TS2 CLAP-Cyclization-TS3

Figure S10. Structures of transition states (TS) of the rearrangement–dehydration–cyclization reaction of CLAP.

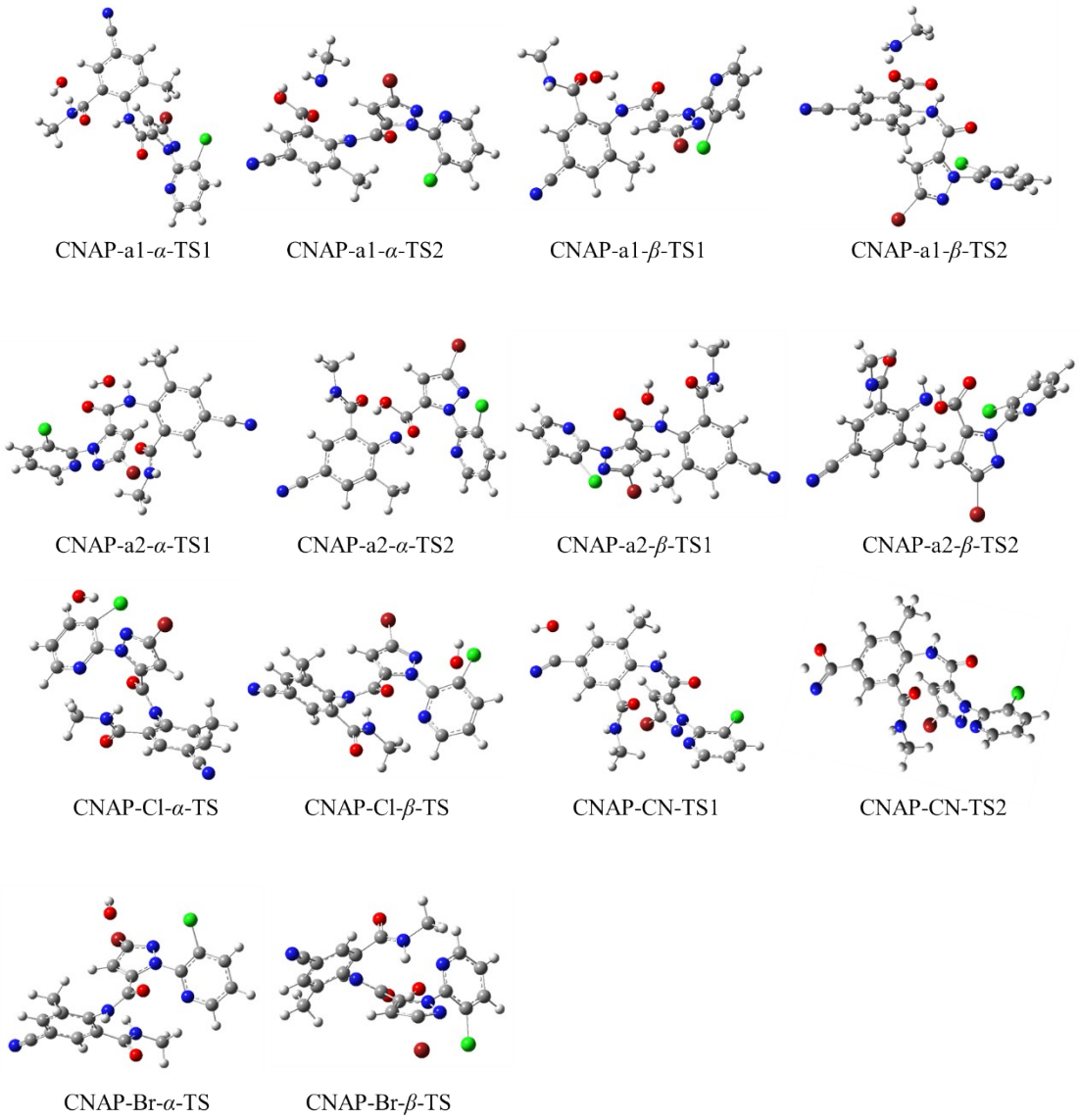


Figure S11. Structures of transition states (TS) of base-catalyzed hydrolysis of CNAP. [The symbols "a1, a2, Cl, CN and Br" refer to amide bond on benzene, amide bond between benzene and pyrazole, C-Cl bond on benzene, Cyano group and C-Br bond on pyrazole, respectively. The α and β sides are shown in Figure 1.]

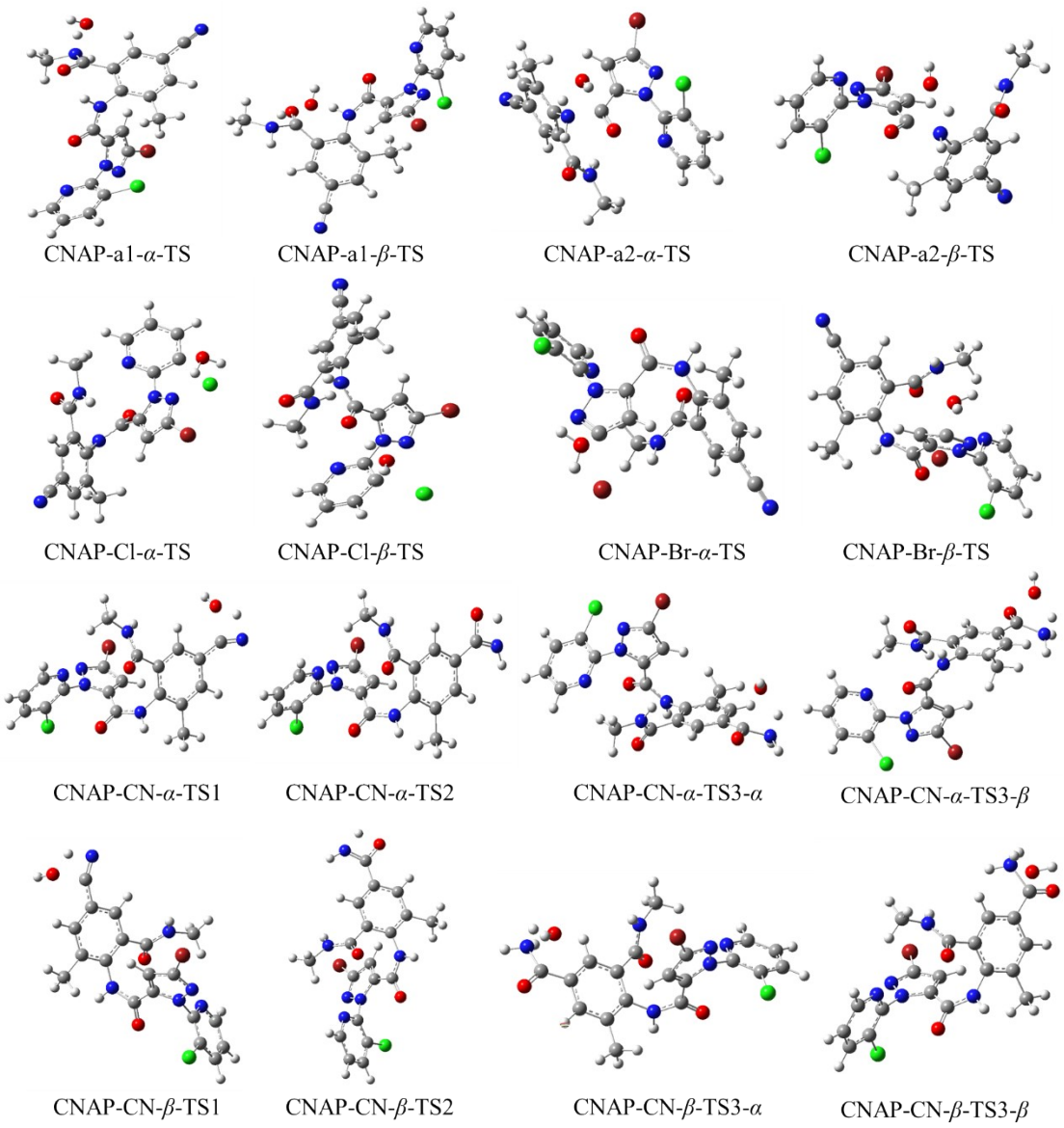


Figure S12. Structures of transition states (TS) of neutral hydrolysis of CNAP. [The symbols "a1, a2, Cl, CN and Br" refer to amide bond on benzene, amide bond between benzene and pyrazole, C-Cl bond on benzene, Cyano group and C-Br bond on pyrazole, respectively. The α and β sides are shown in Figure 1.]

Cartesian Coordinates of Optimized Structures

Amide bond on benzene of CLAP - *α* side -TS1.xyz

	x	y	z
C	-2.78222	0.99146	2.07822
C	-1.69928	0.1306	1.88543
C	-1.76753	-0.80902	0.83713
C	-2.94651	-0.96672	0.07964
C	-4.01445	-0.09626	0.29762
C	-3.90706	0.88308	1.27183
H	-2.74989	1.72652	2.87277
H	-4.92475	-0.23003	-0.2675
Cl	-5.26248	1.9902	1.53599
C	-0.51412	0.22101	2.81376
H	0.27267	0.86354	2.40909
H	-0.81889	0.64093	3.77382
H	-0.07397	-0.76197	2.99054
C	-3.03896	-2.08124	-0.96706
O	-2.46551	-3.18163	-0.75168
N	-3.08133	-1.57204	-2.27302
H	-3.70734	-0.78276	-2.36186
C	-3.19634	-2.51713	-3.37808
H	-3.15866	-1.9642	-4.31796
H	-2.36025	-3.21574	-3.35185
H	-4.12982	-3.093	-3.34195
N	-0.68339	-1.70214	0.58909
H	-1.01082	-2.64637	0.36714
C	0.5803	-1.47218	0.13727
O	1.36166	-2.40883	-0.04641
C	1.0202	-0.08791	-0.19434
C	0.32282	1.05435	-0.55693
N	2.35357	0.21459	-0.33976
C	1.32382	1.97843	-0.8932
H	-0.74176	1.19832	-0.58904
N	2.54406	1.4834	-0.76437
Br	1.07564	3.75992	-1.47885
C	3.51633	-0.61424	-0.1848
C	4.03801	-0.90177	1.07783
N	4.08884	-1.02117	-1.30864
C	5.18609	-1.68173	1.16332
C	5.19732	-1.76224	-1.22787
C	5.77579	-2.12489	-0.01434
H	5.60764	-1.92498	2.13
H	5.636	-2.07585	-2.16879
H	6.67102	-2.73301	0.00967
Cl	3.28654	-0.3003	2.53656
O	-4.99011	-2.48441	-0.62783
H	-4.93335	-3.40806	-0.89628

Amide bond on benzene of CLAP - α side -TS2.xyz

	x	y	z
C	-3.02231	0.67427	2.05613
C	-1.86703	-0.0915	1.85353
C	-1.84995	-1.01431	0.79416
C	-3.00806	-1.24897	0.01537
C	-4.14967	-0.47908	0.24862
C	-4.13129	0.48458	1.24693
H	-3.05213	1.39628	2.8625
H	-5.03532	-0.65305	-0.34506
Cl	-5.57741	1.46479	1.52413
C	-0.7031	0.08283	2.79645
H	0.0159	0.81701	2.4232
H	-1.05581	0.43244	3.76816
H	-0.1664	-0.85631	2.94123
C	-3.07393	-2.37721	-0.9853
O	-2.43826	-3.42607	-0.78167
N	-2.31718	-1.19462	-2.70447
H	-1.97424	-0.2623	-2.47792
C	-1.28729	-1.92402	-3.42274
H	-0.32086	-1.97765	-2.89046
H	-1.61471	-2.95891	-3.58144
H	-1.06692	-1.51217	-4.42314
N	-0.70435	-1.81621	0.53147
H	-0.95822	-2.77312	0.27417
C	0.55658	-1.48843	0.13159
O	1.40009	-2.36723	-0.05971
C	0.9182	-0.06835	-0.13592
C	0.16005	1.04453	-0.46625
N	2.23329	0.31971	-0.23968
C	1.1087	2.04039	-0.74286
H	-0.91034	1.12752	-0.51035
N	2.35401	1.61436	-0.60792
Br	0.76395	3.82731	-1.25878
C	3.4439	-0.43839	-0.08783
C	3.95168	-0.74792	1.17543
N	4.0723	-0.75213	-1.21163
C	5.14994	-1.44838	1.25916
C	5.22858	-1.41655	-1.13188
C	5.80046	-1.79292	0.0805
H	5.56266	-1.70605	2.22593
H	5.71234	-1.65482	-2.07277
H	6.73645	-2.33621	0.10349
Cl	3.12141	-0.27051	2.63728
O	-4.19819	-2.3955	-1.77992
H	-3.78688	-1.77203	-2.49844

Amide bond on benzene of CLAP - β side -TS1.xyz

	x	y	z
C	-2.81318	1.12077	2.02183
C	-1.72783	0.26265	1.8056
C	-1.82506	-0.70274	0.78851
C	-3.0319	-0.89133	0.07235
C	-4.10729	-0.04298	0.3377
C	-3.97148	0.96866	1.27945
H	-2.75374	1.87796	2.79359
H	-5.05057	-0.18422	-0.16978
Cl	-5.3371	2.05328	1.57867
C	-0.52041	0.38465	2.70149
H	0.22095	1.07782	2.29499
H	-0.81812	0.76136	3.68167
H	-0.02754	-0.57893	2.83985
C	-3.20153	-2.08529	-0.86437
O	-2.64292	-3.17032	-0.54889
N	-4.43281	-2.12753	-1.53501
H	-4.59991	-1.27049	-2.04612
C	-4.70122	-3.306	-2.35436
H	-5.67421	-3.17785	-2.83203
H	-3.94312	-3.46657	-3.13008
H	-4.74128	-4.19514	-1.72514
N	-0.76606	-1.61786	0.53342
H	-1.13431	-2.55254	0.31385
C	0.52103	-1.44017	0.12858
O	1.26967	-2.40989	-0.02174
C	1.02601	-0.0801	-0.20931
C	0.38245	1.0878	-0.58878
N	2.37268	0.1634	-0.34313
C	1.42537	1.96515	-0.92144
H	-0.67501	1.2746	-0.63299
N	2.62199	1.41896	-0.77598
Br	1.2613	3.75095	-1.52333
C	3.49681	-0.71349	-0.16901
C	4.00097	-0.9995	1.10103
N	4.0531	-1.16816	-1.28267
C	5.11067	-1.83081	1.20644
C	5.1249	-1.95915	-1.18284
C	5.68179	-2.32483	0.03989
H	5.51745	-2.07447	2.17931
H	5.55139	-2.31153	-2.11562
H	6.54708	-2.97409	0.07922
Cl	3.27396	-0.33346	2.54415
O	-2.17794	-1.23735	-2.36492
H	-1.24464	-1.34702	-2.15058

Amide bond on benzene of CLAP - β side -TS2.xyz

	x	y	z
C	3.80144	0.52743	-1.85919
C	2.54359	0.02659	-2.1855
C	1.91999	-0.88872	-1.30843
C	2.56184	-1.32739	-0.1381
C	3.83884	-0.82431	0.15244
C	4.4268	0.09534	-0.69179
H	4.29308	1.23684	-2.51245
H	4.34454	-1.16224	1.04612
Cl	6.02488	0.7374	-0.29224
C	1.87741	0.44893	-3.47242
H	0.89651	0.89623	-3.29243
H	2.49268	1.17789	-4.00098
H	1.72009	-0.40771	-4.13401
C	2.03616	-2.40027	0.79981
O	2.78648	-3.33938	1.08301
N	1.68256	-1.04418	2.53014
H	1.97541	-0.08525	2.34714
C	2.40673	-1.54725	3.68174
H	3.50723	-1.54072	3.55589
H	2.20206	-0.99777	4.61757
H	2.12519	-2.59063	3.87016
N	0.65979	-1.43649	-1.72777
H	0.69777	-2.26907	-2.3047
C	-0.60469	-1.14541	-1.33292
O	-1.55968	-1.83434	-1.69549
C	-0.84946	0.06627	-0.50021
C	-0.11173	1.21395	-0.25178
N	-2.06196	0.2514	0.11734
C	-0.96594	2.01383	0.52281
H	0.88388	1.44944	-0.57949
N	-2.13481	1.44042	0.75626
Br	-0.59598	3.73639	1.21278
C	-3.18263	-0.63697	0.24097
C	-4.31794	-0.45788	-0.55217
N	-3.09748	-1.56693	1.17973
C	-5.40551	-1.30104	-0.35791
C	-4.13963	-2.38463	1.36117
C	-5.31286	-2.28663	0.61877
H	-6.29733	-1.18822	-0.96061
H	-4.03082	-3.13843	2.13314
H	-6.13734	-2.96421	0.8003
Cl	-4.37699	0.77677	-1.78744
O	0.66467	-2.54163	0.90036
H	0.56924	-1.8684	1.66493

Amide bond between benzene and pyrazole of CLAP - *α* side -TS1.xyz

	x	y	z
C	4.30032	-1.02141	-1.09804
C	3.07797	-1.65045	-1.35379
C	2.04633	-1.56172	-0.39439
C	2.28947	-0.91073	0.82975
C	3.50541	-0.25798	1.05473
C	4.49187	-0.31657	0.08183
H	5.09505	-1.07485	-1.83195
H	3.68872	0.2507	1.99235
Cl	6.03478	0.49578	0.36547
C	2.88072	-2.41409	-2.63702
H	1.95981	-2.08778	-3.1282
H	3.73189	-2.27148	-3.30483
H	2.79344	-3.48981	-2.44218
C	1.33802	-1.00503	2.00282
O	1.05059	-2.09051	2.51164
N	0.91601	0.17284	2.50736
H	1.11603	1.01523	1.9902
C	0.07145	0.26316	3.69291
H	-0.02355	1.31249	3.96823
H	-0.92155	-0.14969	3.49915
H	0.52538	-0.28208	4.52246
N	0.79318	-2.18549	-0.63237
H	0.85647	-3.10095	-1.05957
C	-0.42393	-1.58468	-1.01931
O	-1.42472	-2.31435	-1.12292
C	-0.62332	-0.13262	-0.66489
C	0.13211	1.0138	-0.85497
N	-1.78004	0.2753	-0.05225
C	-0.65786	2.04323	-0.3251
H	1.08444	1.09228	-1.34558
N	-1.81276	1.61815	0.16287
Br	-0.23472	3.89265	-0.27424
C	-2.89434	-0.49388	0.41624
C	-4.08707	-0.53139	-0.31145
N	-2.75274	-1.09267	1.59007
C	-5.1657	-1.23754	0.20649
C	-3.78645	-1.78153	2.08457
C	-5.01076	-1.87933	1.43071
H	-6.09879	-1.28648	-0.33993
H	-3.628	-2.26487	3.04259
H	-5.82584	-2.44213	1.86763
Cl	-4.23102	0.26273	-1.86295
O	0.06707	-1.13177	-3.00622
H	-0.79656	-0.82897	-3.31112

Amide bond between benzene and pyrazole of CLAP - *α* side -TS2.xyz

	x	y	z
C	4.52641	1.43442	-0.27953
C	3.16604	1.37117	-0.55874
C	2.46208	0.12963	-0.44904
C	3.2163	-1.03414	-0.1054
C	4.5813	-0.93008	0.19688
C	5.21774	0.29117	0.1176
H	5.0488	2.3807	-0.36067
H	5.1202	-1.82839	0.46609
Cl	6.94763	0.41162	0.50005
C	2.44316	2.62296	-0.99675
H	1.60357	2.84839	-0.33618
H	3.12097	3.47831	-0.9993
H	2.04046	2.51782	-2.01109
C	2.68448	-2.445	-0.13968
O	3.34229	-3.39094	0.32929
N	1.51172	-2.63592	-0.77116
H	0.99007	-1.77935	-0.9871
C	0.90145	-3.94753	-0.88312
H	1.56241	-4.64684	-1.40151
H	0.66837	-4.37203	0.09936
H	-0.0229	-3.85283	-1.45226
N	1.09632	0.04744	-0.64748
H	0.7491	0.90416	-1.06765
C	0.1294	0.19718	1.00326
O	0.21672	1.38262	1.40078
C	-1.193	-0.32294	0.49759
C	-1.74874	-1.58844	0.55415
N	-2.12426	0.48196	-0.09568
C	-3.01288	-1.43483	-0.04076
H	-1.30787	-2.47727	0.96851
N	-3.25607	-0.19884	-0.4388
Br	-4.32297	-2.78366	-0.29549
C	-2.06626	1.87702	-0.40547
C	-2.76242	2.80711	0.37174
N	-1.37666	2.22037	-1.48539
C	-2.73429	4.14596	-0.00007
C	-1.33925	3.50985	-1.83689
C	-2.00738	4.50473	-1.12977
H	-3.26383	4.88564	0.58642
H	-0.75778	3.75045	-2.72011
H	-1.95988	5.53694	-1.45255
Cl	-3.63325	2.32236	1.80799
O	0.71999	-0.81212	1.77511
H	1.39359	-0.36612	2.30563

Amide bond between benzene and pyrazole of CLAP - β side -TS1.xyz

	x	y	z
C	-2.99185	1.22632	1.76812
C	-1.86544	0.39911	1.70367
C	-1.88662	-0.72632	0.85397
C	-3.07478	-1.04904	0.15793
C	-4.19512	-0.21883	0.25182
C	-4.12954	0.92268	1.03674
H	-2.98378	2.09092	2.42054
H	-5.11442	-0.47483	-0.25824
Cl	-5.5416	1.9769	1.1495
C	-0.68654	0.70766	2.59163
H	0.06207	1.31269	2.07472
H	-1.01292	1.26208	3.47336
H	-0.19385	-0.2114	2.91154
C	-3.19923	-2.3425	-0.60146
O	-2.74632	-3.40148	-0.1476
N	-3.89553	-2.295	-1.75604
H	-4.10564	-1.39282	-2.154
C	-4.10805	-3.47653	-2.58115
H	-4.79649	-3.21823	-3.38418
H	-3.17054	-3.83558	-3.01542
H	-4.5427	-4.27883	-1.98371
N	-0.76489	-1.59256	0.79057
H	-1.05649	-2.56402	0.73456
C	0.41136	-1.4487	0.01724
O	1.22678	-2.38495	0.06214
C	0.90503	-0.07026	-0.31638
C	0.27402	1.10992	-0.67666
N	2.25036	0.19612	-0.34807
C	1.32296	2.01107	-0.9025
H	-0.77986	1.28232	-0.79217
N	2.51937	1.47948	-0.71468
Br	1.16878	3.82637	-1.43407
C	3.37638	-0.66677	-0.14111
C	3.87585	-0.90701	1.14143
N	3.96126	-1.13882	-1.23397
C	5.00036	-1.71056	1.28539
C	5.04613	-1.90727	-1.09788
C	5.59543	-2.22765	0.1402
H	5.39968	-1.9179	2.26981
H	5.49193	-2.2767	-2.01516
H	6.47309	-2.85779	0.20812
Cl	3.11602	-0.21785	2.55808
O	-0.39159	-1.53372	-1.95557
H	-0.56952	-2.48205	-1.9488

Amide bond between benzene and pyrazole of CLAP - β side -TS2.xyz

	x	y	z
C	-2.96246	1.52404	1.44158
C	-1.85123	0.68912	1.46661
C	-1.89913	-0.60739	0.85815
C	-3.14555	-1.00629	0.27269
C	-4.25522	-0.14727	0.27688
C	-4.1505	1.1084	0.84327
H	-2.91528	2.49396	1.92332
H	-5.20127	-0.47307	-0.13731
Cl	-5.55765	2.1888	0.85539
C	-0.63274	1.11787	2.24476
H	0.27392	1.09907	1.64247
H	-0.76463	2.12674	2.64206
H	-0.46167	0.43622	3.08462
C	-3.31332	-2.36766	-0.32509
O	-2.79282	-3.38355	0.16115
N	-4.09426	-2.44931	-1.43171
H	-4.37818	-1.59796	-1.88963
C	-4.36363	-3.71452	-2.1004
H	-5.08186	-3.53664	-2.89963
H	-3.45408	-4.14495	-2.52948
H	-4.78577	-4.43587	-1.39839
N	-0.76202	-1.38499	0.87186
H	-1.03954	-2.34907	0.70829
C	0.36275	-1.4533	-0.72196
O	1.05844	-2.47573	-0.54515
C	0.99162	-0.08982	-0.72893
C	0.47483	1.13993	-1.09634
N	2.28608	0.13152	-0.34336
C	1.53798	2.03404	-0.88931
H	-0.52188	1.35306	-1.43881
N	2.63624	1.44661	-0.44699
Br	1.51959	3.90979	-1.17438
C	3.34324	-0.80969	-0.11206
C	3.73175	-1.1615	1.1821
N	3.97209	-1.25678	-1.19227
C	4.7925	-2.04596	1.34741
C	4.99012	-2.10669	-1.03524
C	5.43149	-2.53407	0.21441
H	5.10646	-2.33908	2.34088
H	5.47284	-2.4529	-1.94282
H	6.26059	-3.22488	0.30015
Cl	2.91824	-0.51846	2.58887
O	-0.61047	-1.46782	-1.74314
H	-0.82828	-2.40114	-1.87182

Amide bond on benzene of CNAP - α side -TS1.xyz

	x	y	z
C	-3.97641	0.97841	1.37315
C	-2.80465	1.05236	2.138
C	-1.7408	0.18774	1.90061
C	-1.85673	-0.73864	0.83981
C	-3.06394	-0.87745	0.11959
C	-4.11084	-0.00255	0.38565
H	-2.7349	1.77451	2.94253
H	-5.03906	-0.12043	-0.15424
C	-0.52972	0.24211	2.79758
H	-0.10202	-0.75108	2.94591
H	0.25671	0.87964	2.38561
H	-0.80387	0.64777	3.77265
C	-5.05549	1.87753	1.63557
N	-5.92748	2.60855	1.84618
C	-3.19959	-1.97442	-0.93939
O	-2.63057	-3.08264	-0.75874
N	-3.29889	-1.45263	-2.23239
H	-3.91578	-0.65352	-2.28855
C	-3.45906	-2.38135	-3.34566
H	-2.62155	-3.0785	-3.36612
H	-4.38969	-2.95859	-3.27785
H	-3.46233	-1.8135	-4.27716
N	-0.80453	-1.64553	0.54657
H	-1.16788	-2.56741	0.27873
C	0.47731	-1.44543	0.11992
C	0.95952	-0.07273	-0.19324
C	0.29446	1.09328	-0.54031
N	2.30092	0.19316	-0.33609
C	1.32094	1.99321	-0.8647
H	-0.76567	1.26792	-0.57141
O	1.22643	-2.40454	-0.06879
N	2.52652	1.46093	-0.74417
Br	1.12415	3.78864	-1.425
C	3.43801	-0.67502	-0.20401
C	3.96717	-0.98921	1.04883
N	3.97775	-1.09508	-1.33912
C	5.08641	-1.81229	1.11217
C	5.05871	-1.87744	-1.27963
C	5.64101	-2.26961	-0.07698
H	5.5129	-2.07763	2.07083
H	5.47145	-2.20087	-2.22892
H	6.51288	-2.91117	-0.07032
Cl	3.26022	-0.36868	2.52159
O	-5.158	-2.36512	-0.51292
H	-5.12086	-3.29054	-0.77898

Amide bond on benzene of CNAP - α side -TS2.xyz

	x	y	z
C	-4.00585	-0.627	1.76984
C	-2.74918	-0.85816	2.34042
C	-1.66743	-1.25731	1.5565
C	-1.84816	-1.38372	0.16462
C	-3.12037	-1.1518	-0.42127
C	-4.19169	-0.79487	0.39547
H	-2.62232	-0.76494	3.41193
H	-5.17061	-0.64355	-0.03752
C	-0.36506	-1.59023	2.2364
H	0.12727	-2.4417	1.7622
H	0.33266	-0.75079	2.20862
H	-0.54008	-1.83803	3.28425
C	-5.10817	-0.25171	2.59751
N	-5.99967	0.05433	3.26864
C	-3.36168	-1.38758	-1.87624
O	-2.72244	-2.20175	-2.52847
N	-2.632	1.0993	-1.95656
H	-3.45653	1.65919	-1.70591
C	-2.35466	1.32082	-3.36871
H	-1.38344	0.87362	-3.62608
H	-3.08614	0.86965	-4.07543
H	-2.28454	2.38566	-3.66466
N	-0.80107	-1.85252	-0.66388
H	-1.11037	-2.5056	-1.3798
C	0.49597	-1.44194	-0.8484
C	0.87616	-0.07885	-0.40653
C	0.0957	1.06242	-0.32652
N	2.17339	0.29506	-0.13417
C	1.01972	2.06473	0.01196
H	-0.9546	1.15364	-0.62214
O	1.29496	-2.15796	-1.44965
N	2.26177	1.61939	0.12954
Br	0.65138	3.90323	0.2927
C	3.39982	-0.43528	-0.28945
C	3.9947	-1.09576	0.78624
N	3.95437	-0.38401	-1.49425
C	5.19756	-1.76567	0.57756
C	5.11037	-1.01973	-1.69386
C	5.7633	-1.73211	-0.68969
H	5.67622	-2.28996	1.39448
H	5.53044	-0.9543	-2.69162
H	6.69771	-2.23969	-0.89255
Cl	3.28389	-1.07704	2.38193
O	-4.53107	-0.90798	-2.40186
H	-4.49551	0.04664	-2.20379

Amide bond on benzene of CNAP - α side -TS2-H.xyz

	x	y	z
C	-4.20758	0.52772	1.3782
C	-3.04739	0.6835	2.14358
C	-1.90691	-0.07647	1.88111
C	-1.93844	-0.97768	0.79915
C	-3.12932	-1.19325	0.05927
C	-4.25203	-0.42584	0.35362
H	-3.03986	1.38448	2.96936
H	-5.15784	-0.58248	-0.21472
C	-0.71026	0.06241	2.78799
H	-0.17559	-0.88377	2.88743
H	0.00074	0.80385	2.41504
H	-1.02892	0.38262	3.78123
C	-5.36392	1.31549	1.66816
N	-6.30016	1.95406	1.90191
C	-3.23019	-2.28853	-0.97466
O	-2.57594	-3.33819	-0.83447
N	-2.5509	-1.0571	-2.67251
H	-2.26517	-0.10603	-2.4446
C	-1.49903	-1.71194	-3.42959
H	-0.49872	-1.62514	-2.97221
H	-1.7191	-2.78406	-3.50624
H	-1.40059	-1.34054	-4.46459
N	-0.82065	-1.78343	0.4739
H	-1.10962	-2.71436	0.15349
C	0.45705	-1.47453	0.09814
C	0.85153	-0.05933	-0.13736
C	0.11531	1.07427	-0.44548
N	2.17414	0.30381	-0.23428
C	1.08342	2.05652	-0.70238
H	-0.95336	1.17891	-0.49088
O	1.27438	-2.37047	-0.11352
N	2.32002	1.60225	-0.57712
Br	0.77443	3.85939	-1.18236
C	3.36786	-0.48632	-0.11157
C	3.88397	-0.83012	1.13903
N	3.97134	-0.79829	-1.24941
C	5.06366	-1.56455	1.1941
C	5.1099	-1.49496	-1.19716
C	5.6878	-1.90713	0.00082
H	5.48248	-1.8497	2.15046
H	5.57388	-1.73055	-2.14861
H	6.6085	-2.47642	0.00144
Cl	3.08768	-0.35373	2.61976
O	-4.3851	-2.28986	-1.72041
H	-3.98824	-1.65877	-2.44993

Amide bond on benzene of CNAP - β side -TS1.xyz

	x	y	z
C	-4.03208	1.06316	1.37838
C	-2.83126	1.17764	2.08298
C	-1.76714	0.31282	1.8273
C	-1.9108	-0.64082	0.8
C	-3.1435	-0.80777	0.11724
C	-4.19402	0.04873	0.42468
H	-2.73576	1.92256	2.86366
H	-5.15213	-0.07619	-0.05953
C	-0.53686	0.39758	2.69586
H	-0.06418	-0.57874	2.81437
H	0.21132	1.07793	2.28154
H	-0.80554	0.76914	3.68612
C	-5.11574	1.94801	1.66695
N	-5.99309	2.66618	1.89877
C	-3.3537	-1.98541	-0.82947
O	-2.79082	-3.07811	-0.55488
N	-4.59668	-2.00253	-1.47034
H	-4.77033	-1.13664	-1.96394
C	-4.90943	-3.16993	-2.28954
H	-4.17872	-3.33609	-3.08964
H	-4.94377	-4.06316	-1.66588
H	-5.89445	-3.02208	-2.73537
N	-0.88248	-1.56614	0.50057
H	-1.28201	-2.48095	0.24263
C	0.41635	-1.41549	0.10821
C	0.95711	-0.06605	-0.20986
C	0.34216	1.12268	-0.57116
N	2.30953	0.14639	-0.33924
C	1.40615	1.98001	-0.88866
H	-0.7103	1.33624	-0.6151
O	1.13312	-2.40418	-0.056
N	2.58886	1.40186	-0.75197
Br	1.28675	3.77897	-1.45971
C	3.41106	-0.76338	-0.18815
C	3.91576	-1.08546	1.07279
N	3.94559	-1.21425	-1.31389
C	5.00233	-1.94952	1.15503
C	4.99519	-2.03671	-1.23623
C	5.55058	-2.43895	-0.02424
H	5.4092	-2.22136	2.12037
H	5.40456	-2.38466	-2.17828
H	6.39754	-3.11278	-0.00293
Cl	3.21854	-0.42431	2.5325
O	-2.3471	-1.09583	-2.34887
H	-1.41352	-1.28614	-2.20278

Amide bond on benzene of CNAP - β side -TS2.xyz

	x	y	z
C	-3.81441	1.4234	1.03905
C	-2.69141	1.23409	1.85539
C	-1.74216	0.26328	1.54984
C	-1.91623	-0.50672	0.37748
C	-3.11993	-0.42328	-0.3731
C	-4.03383	0.58098	-0.05251
H	-2.56475	1.84102	2.74357
H	-4.92361	0.6894	-0.65527
C	-0.59302	0.04326	2.5022
H	-0.28715	-1.00424	2.52069
H	0.28358	0.63772	2.23477
H	-0.88928	0.3311	3.51221
C	-4.75578	2.45282	1.34722
N	-5.51622	3.28859	1.59692
C	-3.45962	-1.39588	-1.47872
O	-2.64281	-2.23726	-1.88528
N	-5.10635	-2.39257	-0.3371
H	-5.19768	-2.05962	0.62165
C	-4.91883	-3.83108	-0.3264
H	-4.02189	-4.15611	0.23363
H	-5.76915	-4.38938	0.10234
H	-4.79519	-4.19663	-1.35266
N	-0.95408	-1.46696	-0.01032
H	-1.37649	-2.23559	-0.54216
C	0.38536	-1.36315	-0.28469
C	1.04865	-0.03316	-0.3327
C	0.55498	1.24086	-0.56678
N	2.41898	0.08263	-0.31183
C	1.70179	2.04366	-0.66158
H	-0.47104	1.5456	-0.66788
O	1.03218	-2.36883	-0.57537
N	2.82257	1.35646	-0.50983
Br	1.76334	3.90827	-0.96968
C	3.43446	-0.92997	-0.2233
C	3.79338	-1.49238	1.00265
N	4.03961	-1.23937	-1.36128
C	4.80358	-2.44815	1.02745
C	5.01649	-2.14978	-1.3369
C	5.42538	-2.78676	-0.1679
H	5.09666	-2.90481	1.9639
H	5.48712	-2.3761	-2.28734
H	6.21694	-3.52482	-0.19045
Cl	3.01135	-1.01778	2.49117
O	-4.52877	-1.0337	-2.26821
H	-5.22734	-1.50031	-1.66342

Amide bond between benzene and pyrazole of CNAP - α side -TS1.xyz

	x	y	z
C	4.59353	-0.35527	0.13532
C	4.3979	-1.05959	-1.05995
C	3.18083	-1.67105	-1.34321
C	2.12801	-1.57751	-0.40065
C	2.34448	-0.91973	0.83226
C	3.563	-0.29371	1.08039
H	5.20136	-1.11277	-1.78486
H	3.73077	0.20708	2.02549
C	2.98203	-2.40171	-2.64608
H	2.90826	-3.48413	-2.48551
H	2.05671	-2.0728	-3.12815
H	3.82684	-2.23055	-3.31459
C	5.84436	0.28016	0.39746
N	6.85832	0.79676	0.60838
C	1.36073	-0.99458	1.98029
O	0.96502	-2.07469	2.42168
N	1.02931	0.18732	2.54132
H	1.30759	1.03819	2.07712
C	0.17367	0.28195	3.71895
H	-0.8378	-0.06573	3.49628
H	0.58243	-0.31922	4.53345
H	0.13547	1.32405	4.03258
N	0.9019	-2.20214	-0.67901
H	0.9793	-3.0204	-1.26849
C	-0.3705	-1.61644	-0.89656
C	-0.54031	-0.15465	-0.59814
C	0.24236	0.96673	-0.82873
N	-1.69215	0.30237	-0.01149
C	-0.52841	2.03297	-0.34805
H	1.2014	1.00849	-1.31158
O	-1.3634	-2.35254	-0.89891
N	-1.69628	1.65178	0.14681
Br	-0.06359	3.87187	-0.36285
C	-2.84235	-0.41866	0.44991
C	-3.99296	-0.49426	-0.33965
N	-2.77441	-0.93092	1.66981
C	-5.10937	-1.14868	0.16562
C	-3.84551	-1.56829	2.15419
C	-5.0324	-1.70064	1.44008
H	-6.01135	-1.22636	-0.42766
H	-3.74882	-1.98075	3.15268
H	-5.87917	-2.22047	1.86989
Cl	-4.03615	0.19093	-1.94753
O	-0.0252	-1.24858	-2.98505
H	-0.90546	-0.95771	-3.25211

Amide bond between benzene and pyrazole of CNAP - α side -TS2.xyz

	x	y	z
C	5.34194	0.55451	-0.16826
C	4.60764	1.6889	-0.5761
C	3.23741	1.6485	-0.73086
C	2.50442	0.43048	-0.47187
C	3.27632	-0.73575	-0.12873
C	4.65292	-0.64983	0.03753
H	5.13537	2.61813	-0.7623
H	5.21504	-1.54198	0.287
C	2.50009	2.88935	-1.17146
H	1.96269	2.72668	-2.11269
H	1.75978	3.20798	-0.4315
H	3.19623	3.71516	-1.32604
C	6.74786	0.62168	-0.00116
N	7.89945	0.67997	0.1376
C	2.68389	-2.11957	-0.10939
O	2.0173	-2.57013	-1.04559
N	3.03694	-2.89476	0.94677
H	3.4413	-2.44451	1.75258
C	2.58872	-4.2724	1.0825
H	1.50566	-4.33458	1.22792
H	2.84768	-4.84491	0.1903
H	3.08709	-4.71668	1.94336
N	1.15552	0.39046	-0.54922
H	0.78236	1.28604	-0.84751
C	0.11334	0.19677	1.03444
C	-1.12863	-0.3787	0.39957
C	-1.55924	-1.68631	0.26982
N	-2.11498	0.40793	-0.12539
C	-2.81181	-1.57369	-0.3575
H	-1.04416	-2.57752	0.58128
O	0.06206	1.32943	1.56442
N	-3.16249	-0.32375	-0.60321
Br	-3.97138	-2.99353	-0.84588
C	-2.18987	1.83209	-0.23458
C	-3.01659	2.56654	0.62067
N	-1.48768	2.39561	-1.20871
C	-3.11039	3.9419	0.44424
C	-1.56711	3.72047	-1.37044
C	-2.36975	4.53157	-0.57403
H	-3.74224	4.53255	1.09493
H	-0.97067	4.14344	-2.17135
H	-2.4139	5.59989	-0.74329
Cl	-3.89794	1.79649	1.91949
O	0.77704	-0.83122	1.70598
H	1.35539	-0.3887	2.34189

Amide bond between benzene and pyrazole of CNAP - β side -TS1.xyz

	x	y	z
C	-4.16837	1.0216	1.16732
C	-2.97931	1.26831	1.86286
C	-1.88043	0.42046	1.74347
C	-1.96482	-0.68975	0.87168
C	-3.18638	-0.96857	0.20681
C	-4.27414	-0.1136	0.35648
H	-2.92327	2.11605	2.53527
H	-5.21327	-0.3343	-0.13442
C	-0.66638	0.67095	2.60078
H	-0.19296	-0.27043	2.8827
H	0.08386	1.26747	2.07741
H	-0.9501	1.21039	3.50613
C	-5.28394	1.90003	1.31899
N	-6.18614	2.61434	1.4395
C	-3.35954	-2.23618	-0.58696
O	-2.915	-3.31608	-0.17594
N	-4.08016	-2.13871	-1.72182
H	-4.28648	-1.22132	-2.08581
C	-4.34274	-3.29168	-2.57337
H	-4.77088	-4.10307	-1.98376
H	-5.05337	-2.99752	-3.34392
H	-3.42691	-3.65316	-3.04955
N	-0.88434	-1.58706	0.75401
H	-1.21563	-2.54006	0.62806
C	0.31955	-1.44289	0.01845
C	0.82691	-0.07197	-0.31373
C	0.20712	1.11436	-0.67316
N	2.17545	0.18062	-0.34634
C	1.26469	2.00525	-0.89894
H	-0.84476	1.29798	-0.78969
O	1.11544	-2.39084	0.05889
N	2.45564	1.46067	-0.71255
Br	1.12842	3.8218	-1.42851
C	3.29348	-0.69662	-0.15268
C	3.80461	-0.94507	1.12341
N	3.85743	-1.17632	-1.25311
C	4.91962	-1.76465	1.25259
C	4.93288	-1.95995	-1.13125
C	5.49309	-2.28879	0.09988
H	5.32807	-1.97852	2.23184
H	5.36186	-2.33498	-2.05422
H	6.36267	-2.93113	0.15651
Cl	3.07259	-0.24709	2.54992
O	-0.4987	-1.5059	-1.98506
H	-0.70179	-2.44927	-1.98381

Amide bond between benzene and pyrazole of CNAP - β side -TS2.xyz

	x	y	z
C	-4.19456	1.27225	0.91833
C	-2.96212	1.61601	1.50675
C	-1.88311	0.74867	1.49137
C	-1.99306	-0.52536	0.84448
C	-3.2659	-0.87575	0.28127
C	-4.33536	0.01372	0.32333
H	-2.87035	2.56902	2.01572
H	-5.29589	-0.2717	-0.08848
C	-0.64157	1.10367	2.2705
H	-0.47924	0.37376	3.06989
H	0.25684	1.09621	1.65653
H	-0.74334	2.09269	2.72204
C	-5.29247	2.17489	0.962
N	-6.18554	2.91364	0.99639
C	-3.48726	-2.22839	-0.32846
O	-3.03405	-3.26531	0.1765
N	-4.23762	-2.26284	-1.4545
H	-4.46838	-1.39455	-1.91098
C	-4.55635	-3.50901	-2.13839
H	-5.05893	-4.20066	-1.45985
H	-5.22065	-3.28488	-2.97158
H	-3.65552	-3.99598	-2.52204
N	-0.89197	-1.35125	0.80552
H	-1.21479	-2.30269	0.64757
C	0.19005	-1.38725	-0.68958
C	0.89163	-0.05021	-0.69199
C	0.43998	1.20866	-1.04541
N	2.20351	0.09522	-0.3315
C	1.55646	2.03992	-0.85661
H	-0.54761	1.48072	-1.37282
O	0.86796	-2.43841	-0.57367
N	2.6272	1.38799	-0.43822
Br	1.64271	3.91455	-1.13741
C	3.21082	-0.90386	-0.11803
C	3.57803	-1.30053	1.16918
N	3.82233	-1.3561	-1.20566
C	4.5931	-2.23947	1.31869
C	4.79789	-2.25705	-1.06407
C	5.2119	-2.73375	0.1771
H	4.88881	-2.56835	2.30658
H	5.2681	-2.6053	-1.97743
H	6.00591	-3.46602	0.25018
Cl	2.79465	-0.64333	2.58662
O	-0.76269	-1.33648	-1.74838
H	-0.95268	-2.26251	-1.95109

C-Br bond on pyrazole of CLAP - α side -TS.xyz

	x	y	z
C	-4.25858	-0.15315	1.4546
C	-3.05465	-0.62907	1.98208
C	-2.12583	-1.23162	1.1149
C	-2.41298	-1.37606	-0.25144
C	-3.61027	-0.87219	-0.7657
C	-4.51598	-0.2684	0.09582
H	-4.98517	0.31478	2.10679
H	-3.84439	-0.98025	-1.81658
Cl	-6.03342	0.35122	-0.54972
C	-2.76935	-0.49167	3.45617
H	-1.81219	0.00495	3.63187
H	-3.55318	0.0846	3.94804
H	-2.71715	-1.47094	3.94217
C	-1.50843	-2.15391	-1.17952
O	-1.17277	-3.31221	-0.92838
N	-1.16179	-1.51519	-2.31566
H	-1.39193	-0.53777	-2.4101
C	-0.3459	-2.14154	-3.34902
H	-0.3483	-1.49792	-4.22721
H	0.68279	-2.28013	-3.0077
H	-0.76197	-3.11359	-3.61779
N	-0.9042	-1.72224	1.668
H	-0.97196	-2.51947	2.28986
C	0.37922	-1.26821	1.54006
O	1.30451	-1.87373	2.08378
C	0.63283	-0.01953	0.78015
C	-0.13071	1.10862	0.60289
N	1.89587	0.26264	0.29589
C	0.75703	2.07092	0.02034
H	-1.13486	1.29205	0.94008
N	1.92622	1.52465	-0.28835
Br	0.09039	3.42679	-1.30595
C	2.90082	-0.65932	-0.07747
C	4.23839	-0.4577	0.29446
N	2.5285	-1.70921	-0.80707
C	5.20307	-1.36304	-0.12844
C	3.4526	-2.59671	-1.18595
C	4.80397	-2.45896	-0.88689
H	6.23967	-1.22003	0.14881
H	3.09633	-3.44279	-1.76449
H	5.525	-3.18999	-1.22975
Cl	4.71394	0.87213	1.33069
O	0.92608	3.36893	1.521
H	0.97847	4.24258	1.11465

C-Br bond on pyrazole of CLAP - β side -TS.xyz

	x	y	z
C	-4.33657	-0.38202	1.37804
C	-3.14712	-0.89766	1.90034
C	-2.14758	-1.33597	1.01181
C	-2.34768	-1.27166	-0.37596
C	-3.52768	-0.71985	-0.87906
C	-4.50677	-0.28687	0.00426
H	-5.11586	-0.04061	2.04755
H	-3.6841	-0.6552	-1.94781
Cl	-6.00321	0.39321	-0.63493
C	-2.94749	-0.96526	3.39384
H	-2.0188	-0.4724	3.69239
H	-3.77556	-0.48447	3.91508
H	-2.89039	-2.00091	3.74466
C	-1.3862	-1.87999	-1.37509
O	-1.21515	-3.10675	-1.39177
N	-0.83917	-1.03332	-2.25857
H	-0.8496	-0.00894	-2.09594
C	0.033	-1.52338	-3.31858
H	0.27731	-0.6872	-3.97272
H	0.95814	-1.94136	-2.91242
H	-0.47063	-2.29649	-3.90283
N	-0.93938	-1.85506	1.57183
H	-1.03875	-2.62567	2.22249
C	0.33802	-1.35811	1.54932
O	1.23718	-1.92655	2.16832
C	0.5925	-0.12578	0.76585
C	-0.19349	0.98059	0.55903
N	1.80177	0.11309	0.15398
C	0.56536	1.81604	-0.32129
H	-1.18689	1.16726	0.92416
N	1.79305	1.34206	-0.5021
Br	0.42942	3.85313	-0.11799
C	2.88379	-0.76695	-0.06046
C	4.19416	-0.4105	0.29671
N	2.61086	-1.9409	-0.62748
C	5.23448	-1.28769	0.01757
C	3.60786	-2.79802	-0.86201
C	4.9386	-2.50961	-0.57769
H	6.25037	-1.02463	0.28346
H	3.32928	-3.74636	-1.30995
H	5.72166	-3.2217	-0.80476
Cl	4.54767	1.07719	1.15205
O	-0.37432	1.74567	-1.9764
H	-1.04661	2.43844	-1.94969

C-Cl bond on benzene of CLAP - α side -TS.xyz

	x	y	z
C	-3.90872	0.18525	1.45669
C	-2.70845	-0.29961	1.96418
C	-1.87343	-1.08195	1.14289
C	-2.25529	-1.34846	-0.18541
C	-3.44984	-0.84426	-0.6902
C	-4.34971	-0.17039	0.16404
H	-4.5463	0.79985	2.0801
H	-3.74287	-1.04881	-1.71158
Cl	-5.45608	1.04854	-0.66012
C	-2.30238	0.03584	3.38046
H	-1.32224	0.51943	3.41866
H	-3.03072	0.70413	3.84206
H	-2.23506	-0.86587	3.99738
C	-1.40844	-2.21556	-1.08032
O	-1.01048	-3.33169	-0.73236
N	-1.14371	-1.70473	-2.30366
H	-1.44166	-0.76318	-2.50588
C	-0.39012	-2.43529	-3.31387
H	-0.38297	-1.84786	-4.23073
H	0.64053	-2.6043	-2.9916
H	-0.8545	-3.40288	-3.51553
N	-0.62928	-1.56344	1.66964
H	-0.654	-2.39042	2.25606
C	0.63469	-1.14688	1.42136
O	1.61619	-1.74615	1.86912
C	0.83809	0.08822	0.60746
C	0.06913	1.22373	0.40495
N	2.04366	0.32701	-0.00372
C	0.90153	2.07403	-0.3409
H	-0.9313	1.41666	0.74848
N	2.08297	1.53918	-0.60263
Br	0.48596	3.81254	-0.96202
C	3.15381	-0.55884	-0.1981
C	4.3554	-0.35502	0.48377
N	2.98183	-1.52935	-1.0836
C	5.42065	-1.2094	0.22337
C	4.00161	-2.35947	-1.32392
C	5.23919	-2.23362	-0.69925
H	6.36302	-1.07719	0.73898
H	3.82089	-3.14678	-2.04742
H	6.04343	-2.92149	-0.92694
Cl	4.52645	0.91619	1.67032
O	-5.79138	-1.50288	0.48812
H	-6.60007	-1.13541	0.1106

C-Cl bond on benzene of CLAP - β side -TS.xyz

	x	y	z
C	-3.89783	0.25013	1.48418
C	-2.67952	-0.18781	1.99232
C	-1.86033	-1.02145	1.20715
C	-2.31288	-1.4521	-0.05451
C	-3.52807	-1.00076	-0.55861
C	-4.28665	-0.05257	0.16154
H	-4.54055	0.87373	2.09317
H	-3.8932	-1.35956	-1.51193
Cl	-6.10143	-0.11403	-0.1325
C	-2.2567	0.21906	3.38501
H	-1.32505	0.79268	3.37123
H	-3.0241	0.83522	3.85575
H	-2.08238	-0.65304	4.02212
C	-1.54456	-2.47869	-0.84532
O	-1.15223	-3.5394	-0.34891
N	-1.3426	-2.17394	-2.14678
H	-1.63183	-1.26684	-2.47834
C	-0.67352	-3.0801	-3.07012
H	-0.68302	-2.6316	-4.0622
H	0.36238	-3.25668	-2.76996
H	-1.19006	-4.04162	-3.1097
N	-0.60906	-1.47984	1.73906
H	-0.62337	-2.29663	2.34006
C	0.651	-1.07104	1.46057
O	1.63799	-1.65146	1.92146
C	0.84652	0.12959	0.59517
C	0.07941	1.25891	0.35618
N	2.04677	0.33982	-0.03722
C	0.90734	2.07694	-0.43023
H	-0.916	1.46887	0.70331
N	2.08398	1.52778	-0.68294
Br	0.49458	3.79318	-1.11193
C	3.15003	-0.55804	-0.21279
C	4.36412	-0.33026	0.4388
N	2.95997	-1.56406	-1.05396
C	5.42288	-1.19725	0.19417
C	3.97357	-2.40624	-1.27824
C	5.22268	-2.25791	-0.68223
H	6.37476	-1.04652	0.68671
H	3.77814	-3.22212	-1.9653
H	6.02145	-2.95637	-0.89651
Cl	4.55878	0.98703	1.57016
O	-4.01908	1.64755	-0.8479
H	-4.88401	1.91375	-1.18367

C-Cl bond on pyridine of CLAP - α side -TS.xyz

	x	y	z
C	-4.44455	-0.05458	1.33217
C	-3.25517	-0.51595	1.90309
C	-2.29615	-1.12233	1.07189
C	-2.54017	-1.28825	-0.30059
C	-3.7236	-0.79721	-0.85759
C	-4.6587	-0.18735	-0.03267
H	-5.19392	0.41659	1.95549
H	-3.92511	-0.92165	-1.9134
Cl	-6.15799	0.41583	-0.73241
C	-3.01748	-0.36079	3.38393
H	-2.07029	0.14521	3.58607
H	-3.82134	0.21326	3.84495
H	-2.97324	-1.33469	3.88151
C	-1.60545	-2.07934	-1.18729
O	-1.27116	-3.22956	-0.89999
N	-1.22642	-1.46078	-2.32363
H	-1.46951	-0.49015	-2.45005
C	-0.36423	-2.0976	-3.31334
H	-0.33716	-1.46819	-4.20144
H	0.64943	-2.21889	-2.92387
H	-0.76202	-3.07717	-3.58281
N	-1.08869	-1.59341	1.67183
H	-1.17613	-2.35135	2.33935
C	0.20315	-1.17556	1.52409
O	1.11927	-1.75962	2.09622
C	0.46212	0.04479	0.70716
C	-0.27485	1.21372	0.57838
N	1.65486	0.25675	0.0648
C	0.56348	2.0616	-0.15909
H	-1.25018	1.43453	0.97393
N	1.71305	1.4926	-0.48347
Br	0.19451	3.84198	-0.69136
C	2.72952	-0.67141	-0.1519
C	4.03847	-0.3604	0.29771
N	2.42496	-1.75841	-0.8396
C	4.96912	-1.42203	0.23158
C	3.36366	-2.69303	-1.02561
C	4.64369	-2.56359	-0.47652
H	5.93861	-1.30532	0.69848
H	3.0728	-3.57541	-1.5849
H	5.36476	-3.36668	-0.58064
Cl	4.20322	0.75812	1.70576
O	4.79719	0.95154	-1.08342
H	4.1126	1.6331	-1.07652

C-Cl bond on pyridine of CLAP - β side -TS.xyz

	x	y	z
C	-4.45784	-0.05494	1.21678
C	-3.29447	-0.53312	1.82598
C	-2.31102	-1.14271	1.02527
C	-2.51093	-1.29843	-0.3546
C	-3.66736	-0.78973	-0.95116
C	-4.62433	-0.17471	-0.15594
H	-5.2241	0.41927	1.81679
H	-3.83061	-0.90448	-2.01473
Cl	-6.0908	0.45142	-0.90424
C	-3.10989	-0.39043	3.3158
H	-2.17617	0.12376	3.55681
H	-3.9349	0.17145	3.75385
H	-3.07219	-1.36814	3.80615
C	-1.56475	-2.10522	-1.21392
O	-1.3224	-3.28565	-0.95955
N	-1.07529	-1.46515	-2.29423
H	-1.25914	-0.47875	-2.39672
C	-0.19351	-2.1162	-3.25618
H	-0.02349	-1.4316	-4.08542
H	0.76379	-2.36934	-2.79517
H	-0.65565	-3.02897	-3.63643
N	-1.12992	-1.63209	1.66401
H	-1.25884	-2.38238	2.33351
C	0.16364	-1.17852	1.65001
O	1.01657	-1.7422	2.32639
C	0.46104	0.04706	0.85065
C	-0.30483	1.19788	0.73254
N	1.64952	0.29443	0.19953
C	0.49785	2.06605	-0.01804
H	-1.27922	1.39212	1.14349
N	1.65309	1.52603	-0.36174
Br	0.07477	3.83499	-0.55161
C	2.71456	-0.63146	-0.08748
C	4.09159	-0.30007	0.08232
N	2.29438	-1.83705	-0.44244
C	5.00124	-1.30045	-0.33541
C	3.17415	-2.80193	-0.71309
C	4.54958	-2.55916	-0.6807
H	6.05855	-1.06982	-0.32734
H	2.77153	-3.76647	-1.00274
H	5.25276	-3.33813	-0.95313
Cl	4.69694	1.39709	-0.19384
O	4.42795	-0.23694	2.07304
H	4.53872	0.69368	2.30305

C-Br bond on pyrazole of CNAP - α side -TS.xyz

	x	y	z
C	-4.64682	-0.31336	0.03889
C	-4.4203	-0.3513	1.41871
C	-3.21807	-0.8353	1.93128
C	-2.23748	-1.2973	1.03144
C	-2.47511	-1.3003	-0.35488
C	-3.67278	-0.78784	-0.84683
H	-5.18233	0.01282	2.09656
H	-3.86657	-0.788	-1.91179
C	-2.97752	-0.85217	3.41884
H	-2.92693	-1.87659	3.80175
H	-2.03301	-0.36546	3.67281
H	-3.78404	-0.34083	3.94435
C	-5.88218	0.19827	-0.46772
N	-6.88096	0.61271	-0.87707
C	-1.52631	-1.95957	-1.33094
O	-1.19362	-3.13785	-1.1983
N	-1.14659	-1.19508	-2.37381
H	-1.37155	-0.21167	-2.35989
C	-0.28477	-1.69728	-3.43806
H	0.72374	-1.88953	-3.06486
H	-0.69372	-2.6224	-3.84722
H	-0.24048	-0.94852	-4.2272
N	-1.02278	-1.79847	1.5743
H	-1.10553	-2.57264	2.22296
C	0.27325	-1.36183	1.45353
C	0.54001	-0.08385	0.7545
C	-0.21866	1.05707	0.64699
N	1.80269	0.22038	0.28593
C	0.67253	2.04818	0.12283
H	-1.22053	1.22367	1.0001
O	1.18384	-2.00285	1.97616
N	1.8396	1.51419	-0.21856
Br	0.01199	3.48307	-1.11889
C	2.82478	-0.67522	-0.10423
C	4.15307	-0.47672	0.3022
N	2.47717	-1.699	-0.88118
C	5.13408	-1.35611	-0.13793
C	3.41637	-2.56289	-1.27654
C	4.76043	-2.4248	-0.94644
H	6.16366	-1.21516	0.16527
H	3.07874	-3.38855	-1.89446
H	5.49499	-3.13522	-1.30354
Cl	4.59766	0.81192	1.40221
O	0.84759	3.24973	1.69957
H	0.91012	4.14635	1.34828

C-Br bond on pyrazole of CNAP - β side -TS.xyz

	x	y	z
C	-4.62553	-0.28625	-0.04434
C	-4.47163	-0.42842	1.33899
C	-3.28985	-0.93411	1.87612
C	-2.25624	-1.31903	0.99778
C	-2.42195	-1.22253	-0.39603
C	-3.59771	-0.68184	-0.90812
H	-5.27218	-0.12406	2.00179
H	-3.72751	-0.59568	-1.97925
C	-3.12452	-1.0472	3.37053
H	-3.06157	-2.09293	3.6895
H	-2.21146	-0.5499	3.70719
H	-3.97281	-0.59637	3.88566
C	-5.83753	0.25267	-0.57694
N	-6.81813	0.68893	-1.00785
C	-1.44085	-1.81381	-1.3878
O	-1.2537	-3.03794	-1.39928
N	-0.90525	-0.96109	-2.2712
H	-0.92191	0.06328	-2.10444
C	-0.02481	-1.44217	-3.32876
H	0.90037	-1.85537	-2.91843
H	-0.52098	-2.21655	-3.91773
H	0.21672	-0.60227	-3.97906
N	-1.05944	-1.82669	1.57611
H	-1.17284	-2.55851	2.26799
C	0.2362	-1.36862	1.51903
C	0.50544	-0.1382	0.74217
C	-0.26444	0.98532	0.56354
N	1.71161	0.09141	0.12287
C	0.50065	1.82494	-0.30648
H	-1.25047	1.18265	0.94341
O	1.12575	-1.96242	2.12438
N	1.71885	1.33217	-0.50671
Br	0.4026	3.85782	-0.06264
C	2.79568	-0.78909	-0.08437
C	4.09955	-0.44271	0.30447
N	2.5299	-1.95248	-0.67542
C	5.14249	-1.31879	0.03103
C	3.52863	-2.80895	-0.90495
C	4.85448	-2.5294	-0.59034
H	6.15375	-1.06377	0.32127
H	3.25592	-3.74891	-1.3736
H	5.63969	-3.24017	-0.81405
Cl	4.44091	1.02868	1.19185
O	-0.44906	1.80415	-1.95634
H	-1.11654	2.50039	-1.90729

C-Cl bond on pyridine of CNAP - α side -TS.xyz

	x	y	z
C	-4.78248	-0.20645	-0.06489
C	-4.58274	-0.17784	1.31929
C	-3.39491	-0.64471	1.87912
C	-2.40139	-1.15634	1.02156
C	-2.61246	-1.22862	-0.36746
C	-3.79664	-0.73255	-0.90694
H	-5.35449	0.22514	1.96323
H	-3.97155	-0.78651	-1.97376
C	-3.18457	-0.59146	3.37034
H	-3.15985	-1.59656	3.80357
H	-2.2374	-0.10847	3.62145
H	-3.9932	-0.0426	3.85287
C	-6.00324	0.29011	-0.61997
N	-6.98978	0.69326	-1.06814
C	-1.65013	-1.94693	-1.28757
O	-1.31023	-3.10995	-1.06821
N	-1.26019	-1.25267	-2.37433
H	-1.50754	-0.27718	-2.44165
C	-0.38317	-1.82171	-3.39261
H	0.61326	-2.00528	-2.9844
H	-0.7963	-2.76142	-3.76319
H	-0.31212	-1.11474	-4.21749
N	-1.19821	-1.63211	1.61266
H	-1.2935	-2.37279	2.29826
C	0.10569	-1.24283	1.44732
C	0.37495	0.00227	0.67659
C	-0.36178	1.17557	0.58936
N	1.57209	0.23897	0.05151
C	0.48031	2.05112	-0.10978
H	-1.33841	1.38156	0.99008
O	1.01202	-1.86734	1.98715
N	1.63284	1.49456	-0.44703
Br	0.11454	3.84962	-0.57767
C	2.6591	-0.67296	-0.17544
C	3.95258	-0.37184	0.32349
N	2.38208	-1.73199	-0.91569
C	4.89177	-1.42535	0.24314
C	3.33238	-2.65261	-1.11222
C	4.59464	-2.53892	-0.5198
H	5.84617	-1.32256	0.74318
H	3.06433	-3.51271	-1.71584
H	5.32347	-3.33353	-0.63447
Cl	4.06902	0.68949	1.78064
O	4.73512	0.99987	-0.98364
H	4.04033	1.67093	-0.97061

C-Cl bond on pyridine of CNAP - β side -TS.xyz

	x	y	z
C	-4.73338	-0.1817	-0.2187
C	-4.59949	-0.18034	1.17378
C	-3.44679	-0.67492	1.78139
C	-2.41869	-1.18492	0.96336
C	-2.5689	-1.23581	-0.43342
C	-3.71756	-0.7121	-1.0213
H	-5.39513	0.22323	1.78759
H	-3.84138	-0.7477	-2.09607
C	-3.31344	-0.65424	3.28262
H	-3.32217	-1.66841	3.69479
H	-2.37709	-0.1868	3.59586
H	-4.14104	-0.10679	3.73359
C	-5.91755	0.34527	-0.82287
N	-6.87431	0.77296	-1.31116
C	-1.58818	-1.96898	-1.32136
O	-1.34902	-3.16376	-1.14556
N	-1.07551	-1.24989	-2.33801
H	-1.26606	-0.26026	-2.37714
C	-0.17136	-1.82737	-3.32624
H	0.75752	-2.15316	-2.85394
H	-0.63971	-2.68276	-3.81702
H	0.05135	-1.06721	-4.07293
N	-1.2472	-1.68376	1.60066
H	-1.39156	-2.41288	2.29017
C	0.05605	-1.24225	1.59822
C	0.36457	0.00295	0.83718
C	-0.40017	1.15815	0.75513
N	1.55947	0.27373	0.2073
C	0.40951	2.05299	0.04499
H	-1.37709	1.3386	1.16685
O	0.89431	-1.82888	2.27027
N	1.56811	1.52474	-0.30688
Br	-0.0071	3.84044	-0.42704
C	2.63167	-0.6387	-0.09587
C	4.00556	-0.30599	0.09443
N	2.22028	-1.83724	-0.48191
C	4.92317	-1.29254	-0.33824
C	3.10625	-2.79186	-0.76797
C	4.48025	-2.54452	-0.71758
H	5.97938	-1.05801	-0.31458
H	2.71011	-3.75085	-1.08383
H	5.18916	-3.31401	-1.00176
Cl	4.60904	1.3982	-0.12884
O	4.31396	-0.29593	2.09273
H	4.41944	0.62807	2.3503

References

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