Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.
This journal is © The Royal Society of Chemistry 2024

Text S1

Calculation of transmission coefficient κ

The value of κ can be calculated by Skodje-Truhlar method:

$$\alpha = \frac{2\pi}{\hbar \nu^{\neq}} \times c$$

$$\beta = \frac{1}{k_B T}$$

$$\text{When } \beta < \alpha,\ \kappa = \frac{\beta\pi}{\alpha}\sin\left(\frac{\beta\pi}{\alpha}\right) - \frac{\beta}{\alpha-\beta}\exp((\beta-\alpha)\times(\Delta U - V)\times(1000/N_A))$$

$$\text{When } \alpha < \beta,\ \kappa = \frac{\beta}{\beta-\alpha}\exp((\beta-\alpha)\times(\Delta U - V)\times(1000/N_A))$$

where $\nu^{\neq}$ is imaginary frequency of transition state, c is the speed of light (3×10^8 m s^{-1}) ΔU is standard internal energy difference between transition state (U_{TS}^0) and reactants (U_R^0) calculated at 0 K, N_A is Avogado constant, V (kJ/mol) is zero for exothermic reactions and is the difference between internal energy of products and reactants at 0 K for endothermic reactions, in addition, $\hbar$, k_B and T are mentioned in manuscript.

Text S2

Quantum Chemical Linear Free Energy Relationship (LFER) for Estimation of pK_a Values

Based on the proton theory of acids and bases, acid is a donor of protons. The stronger the ability to provide protons, the stronger the acidity. Quantum chemical calculations were performed with the Gaussian 09 software package. The bond dissociation energies (BDEs) of X-H(X=N/O/C) in organic compounds were calculated at the M06-2X/cc-pVTZ level in conjunction with the SMD implicit solvation model. All structures were confirmed as minima by frequency calculations. BDEs values were computed by evaluating the enthalpies difference.

$$BDE = H(H^+) + H(R{-}X^-) - H(R{-}X{-}H)$$

The correlation between the BDEs and experimental pK_a values of amines was established and illustrated in Figure S1 and Table S1. The squared correlation coefficient for the above system is $R^2 = 0.982$. Based on the obtained quantum chemical LFER,[1-3] the calculated pK_a and BDEs of tyrosine, chlorinated tyrosine and *N*-Acetyl-*L*-Tyrosine were listed in Table S1.

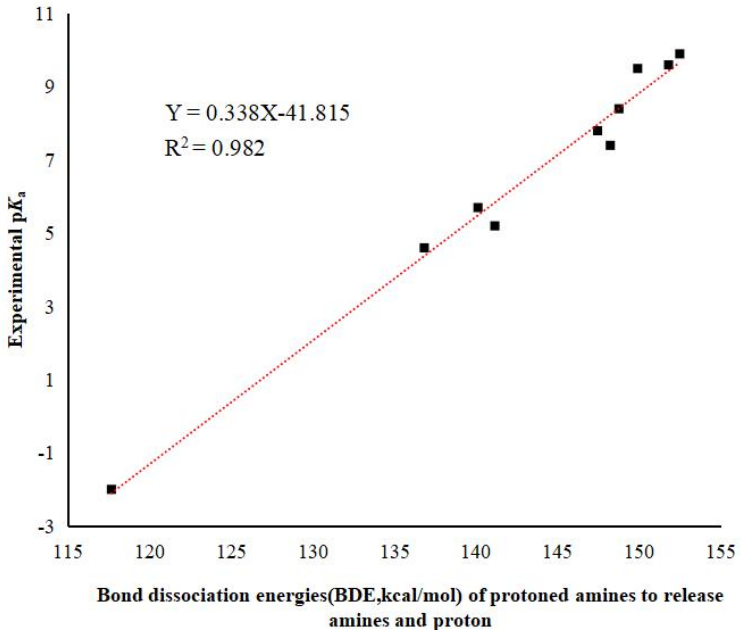


Figure S1. The correlation between the experimental pK_a values and BDEs for 10 amines.

Table S1. The experimental pK_a values (pK_a (exp.)), BDEs (in kcal/mol) of N-H bonds and calculated pK_a values (pK_a (calc.)) of 10 amines.

Amines	pK_a (exp.)	BDE	pK_a (calc.)	Amines	pK_a (exp.)	BDE	pK_a (calc.)
$CN\text{-}N(CH_2CH_3)_2$	–2.0	117.6	–2.1	$(C_2H_5OH)_3N$	7.8	147.5	8.0
$C_6H_5\text{-}NH_2$	4.6	136.8	4.4	Morpholine	8.4	148.8	8.5
$C_6H_5\text{-}N\text{-}(CH_3)_2$	5.2	141.2	5.9	$CH_2OH\text{-}CH_2\text{-}NH_2$	9.5	149.9	8.9
$CF_3\text{-}CH_2\text{-}NH_2$	5.7	140.1	5.5	Glycine	9.6	151.8	9.5
4-Methylmorpholine	7.4	148.3	8.3	Alanine	9.9	152.5	9.7

Table S2. The BDE (in kcal/mol) of N-H bonds, pK_a(calc.) values of amino group in Tyr, Tyr-Am and their iodinated products calculated by using LFER and the fraction of $-NH_3^+$ (f(C)) and $-NH_2$ (f(N)).

Heterolytic reaction	BDE	pK_a(calc.)	f(C)	f(N)
$Tyr^+ \rightarrow Tyr + H^+$	150.4	9.7	0.9980	0.0020
$1\text{-I-}Tyr^+ \rightarrow 1\text{-I-}Tyr + H^+$	147.3	8.6	0.9755	0.0245
$3\text{-I-}Tyr^+ \rightarrow 3\text{-I-}Tyr + H^+$	150.5	9.8	0.9984	0.0016
$5\text{-I-}Tyr^+ \rightarrow 5\text{-I-}Tyr + H^+$	151.0	9.9	0.9987	0.0013
$1,3\text{-di-I-}Tyr^+ \rightarrow 1,3\text{-di-I-}Tyr + H^+$	149.3	9.4	0.9960	0.0040
$3,3\text{-di-I-}Tyr^+ \rightarrow 3,3\text{-di-I-}Tyr + H^+$	149.2	9.3	0.0095	0.0050
$3,5\text{-di-I-}Tyr^+ \rightarrow 3,5\text{-di-I-}Tyr + H^+$	150.2	9.7	0.9980	0.0020
$1,3,5\text{-tri-I-}Tyr^+ \rightarrow 1,3,5\text{-tri-I-}Tyr + H^+$	148.9	9.2	0.937	0.0063
$3,3,5\text{-tri-I-}Tyr^+ \rightarrow 3,3,5\text{-tri-I-}Tyr + H^+$	150.9	10.0	0.9989	0.0011
$Tyr\text{-}Am^+ \rightarrow Tyr\text{-}Am + H^+$	145.5	8.0	0.9091	0.0909

The correlation between the BDEs and experimental pK_a values of O-H bonds of substituted phenols was established and illustrated in Figure S2 and Table S3. the squared correlation coefficient for the above system is R^2 = 0.992. The calculated pK_a and BDEs of tyrosine, *N*-Acetyl-*L*-Tyrosine and their chlorinated products were listed in Table S2.

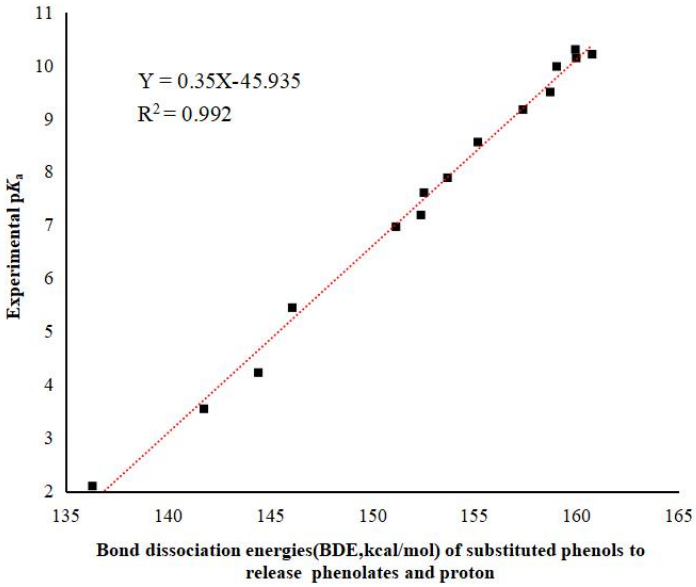


Figure S2. The correlation between the experimental pK_a values and BDE for 15 substituted phenols.

Table S3. The experimental pK_a values (pK_a (exp.)), BDEs (in kcal/mol) of O-H bonds and calculated pK_a values (pK_a (calc.)) of 15 substituted phenols.

Substituted phenols	pK_a (exp.)	BDE	pK_a (calc.)	Substituted phenols	pK_a (exp.)	BDE	pK_a (calc.)
2-Cl-4,6-di-nitrophenol	2.1	136.3	1.9	2-Chlorophenol	8.6	155.2	8.5
2,6-di-Cl-4-nitrophenol	3.6	141.7	3.8	4-Bromophenol	9.2	157.4	9.3
4-methyl-2,6-di-nitrophenol	4.2	144.4	4.7	4-Acetaminophenol	9.5	158.7	9.8
2-Cl-4-nitrophenol	5.5	146.1	5.3	Phenol	10.0	159.0	9.9
2,6-di-Cl-phenol	7.0	151.2	7.1	4-tBuphenol	10.1	160.0	10.3
2,6-di-Cl-4-methylphenol	7.2	152.4	7.6	4-Methoxyphenol	10.2	160.8	10.5
4-Formylphenol	7.6	152.5	7.6	4-Ipropphenol	10.3	160.0	10.2
2,4-di-Cl-phenol	7.9	153.7	8.0				

Table S4. The BDE (in kcal/mol) of O-H bonds, pK_a(calc.) values of Tyr, Tyr-Am, and NacTyr and their iodinated products calculated by using LFER and the fraction of the neutral form (f(N)) and the anion form (f(A)).

Organic Compounds	BDE	pK_a(calc.)	f(N)	f(A)
Tyr	160.7	10.2	0.9994	0.0006
3-I-Tyr	154.4	8.1	0.9264	0.0736
3,5-di-I-Tyr	151.0	6.9	0.4427	0.5573
Tyr-Am	159.6	10.0	0.9990	0.0010
3-I-Tyr-Am	153.7	7.9	0.8882	0.1118
3,5-di-I-Tyr-Am	150.2	6.6	0.2847	0.7153
NacTyr	160.2	10.1	0.9992	0.0008
3-I- NacTyr	155.7	8.6	0.9755	0.0245
3,5-di-I- NacTyr	149.4	6.4	0.2008	0.7992

Text S3

Calculation of the relative contribution of different iodinating agents to HOI during the iodination of Tyr.

In the actual water system under conditions of pH=7 and the concentrations of Br^-, I^-, and NH_2Cl being 900 μg/L, 30 μg/L, and 2.6 μmol, respectively, the relative fractions of the iodinating agents were calculated based on the equilibrium constants of their conversion between different iodination reagents as below. For agent IX including I_2, ICl, and IBr, their K_{eq} are 1.8×10^{12}, 1.2×10^{3}, and 1.8×10^{6}, respectively, and their relative fractions were calculated from eqs. (1)

$$Rf(IX)=\frac{[IX]_{max}}{[HOI]}=\frac{[X^-]_{max}\,[H^+]}{[H_2O]}K_{eq}(IX)=1.8\times10^{-9}\,K_{eq}(IX)[X^-]_{max} \quad (1)$$

$$K_{eq}(IX)=\frac{[IX][H_2O]}{[HOI][H^+][X^-]} \quad (2)$$

For NHClI, H_2OI^+, and NH_2ClI^+, their K_{eq} are 2.0×10^{3}, 0.5, and 0.5, respectively, their relative fractions were calculated from eqs. (3) and (4), (5) and (6), as well as (7) and (8), respectively.

$$Rf(NHClI)=\frac{[NHClI]}{[HOI]}=\frac{[NH_2Cl]}{[H_2O]}K_{eq}(NHClI)=1/55.6\,K_{eq}(NHClI)[X^-] \quad (3)$$

$$K_{eq}(NHClI)=\frac{[NHClI][H_2O]}{[HOI][NH_2Cl]} \quad (4)$$

$$Rf(H_2OI^+)=\frac{[H_2OI^+]}{[HOI]}=[H^+]\,K_{eq}(H_2OI^+)=10^{-7}\,K_{eq}(H_2OI^+) \quad (5)$$

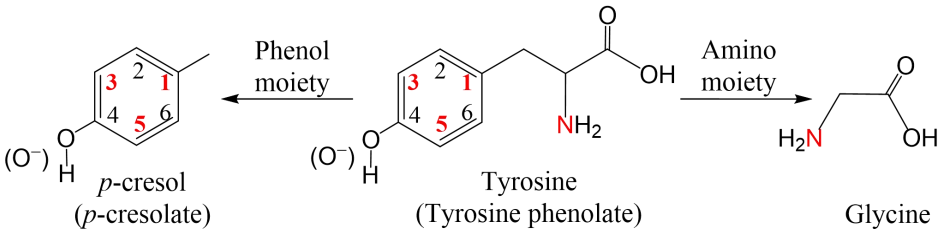
$$K_{eq}(H_2OI^+)=\frac{[H_2OI^+]}{[HOI][H^+]} \quad (6)$$

$$Rf(NH_2ClI^+)=\frac{[NH_2ClI^+]}{[NHClI]}\,\frac{[NHClI]}{[HOI]}=[H^+]\,K_{eq}(NH_2ClI^+)Rf(NHClI) \quad (7)$$

$$K_{eq}(NH_2ClI^+)=\frac{[NH_2ClI^+]}{[NHClI][H^+]} \quad (8)$$

The contribution of each iodinating agent during iodination was calculated according to eq. (9) with the contribution of HOI was set to be 1.

$$p(IA)=\frac{Rfk_{obs\text{-}est}(IA)}{k_{obs\text{-}est}(HOI)+Rfk_{obs\text{-}est}(IA)} \quad (9)$$



Scheme S1. Structures of *p*-cresol and glycine representing the respective phenol and amino moieties of Tyr.

Table S5. The activation free energies and reaction enthalpy changes ($\Delta G^{\neq}/\Delta H$, at 298 K and 1 atm, in kcal/mol) of each step in iodination of the *p*-cresol and *p*-cresolate via the concerted, classic S_EAr(cs), and modified S_EAr(ms) mechanisms.

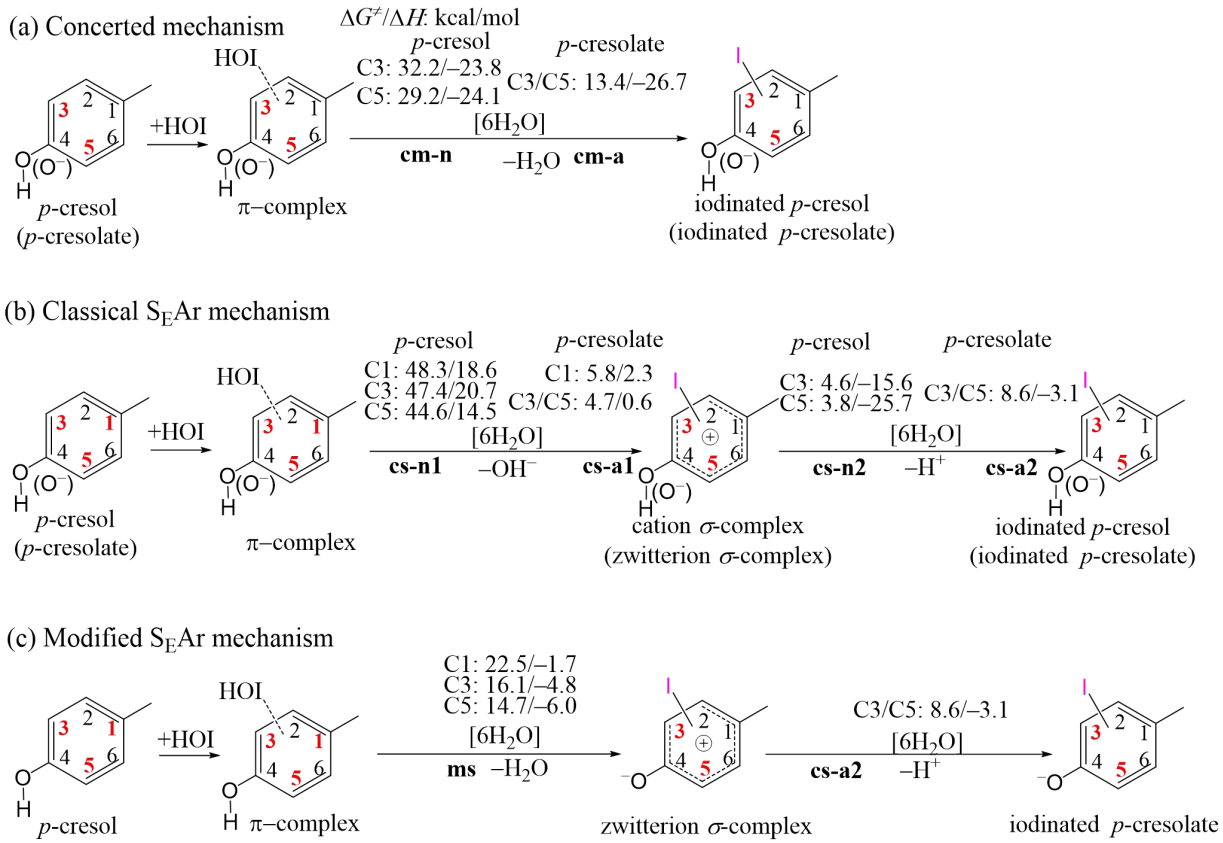
Reactive site	*p*-cresol				*p*-cresolate		
	Concerted	Classic S_EAr		Modified S_EAr	Concerted	Classic S_EAr	
		cs-n1	cs-n2	ms		cs-a1	cs-a2
C1	——	48.3/18.6	——	22.5/–1.7	——	5.8/2.3	——
C3	32.3/–23.8	47.4/20.7	4.6/–15.6	16.1/–4.8	13.4/–26.7	4.7/0.6	8.6/–3.1
C5	29.2/–24.1	44.6/14.5	3.8/–25.7	14.7/–6.0	13.4/–26.7	4.7/0.6	8.6/–3.1

Table S6. The activation free energies ($\Delta G^{\neq}/\Delta H$ at 298 K and 1 atm, in kcal/mol) and the estimated rate constants (k_{est}, in M^{-1} s^{-1}) during iodination of *ortho*-C3 in the *p*-cresol and *p*-cresolate by HOI.

	$\Delta G^{\neq}$	k_{est}	k_{expt}
p-cresol	14.7	1.1×10^{2}	$(3\pm1)\times10^{2}$
p-cresolate	4.7	2.4×10^{9}	$(7\pm3)\times10^{8}$

Table S7. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) in iodination of *ortho*-C3 in *p*-cresol/cresolate by HOI *via*. the modified and classic S_EAr mechanisms respectively assisted by 1–7 explicit water molecules.

	1	2	3	4	5	6	7
ms	28.4	17.5	16.9	17.5	15.8	15.6	15.1
cs-a1	2.6	0.8	1.6	3.7	4.6	4.7	4.3



Scheme S2. Iodination mechanisms of *p*-cresol by HOI through (a) concerted, (b) classic S_EAr (cs), and (c) modified S_EAr (ms) mechanism.

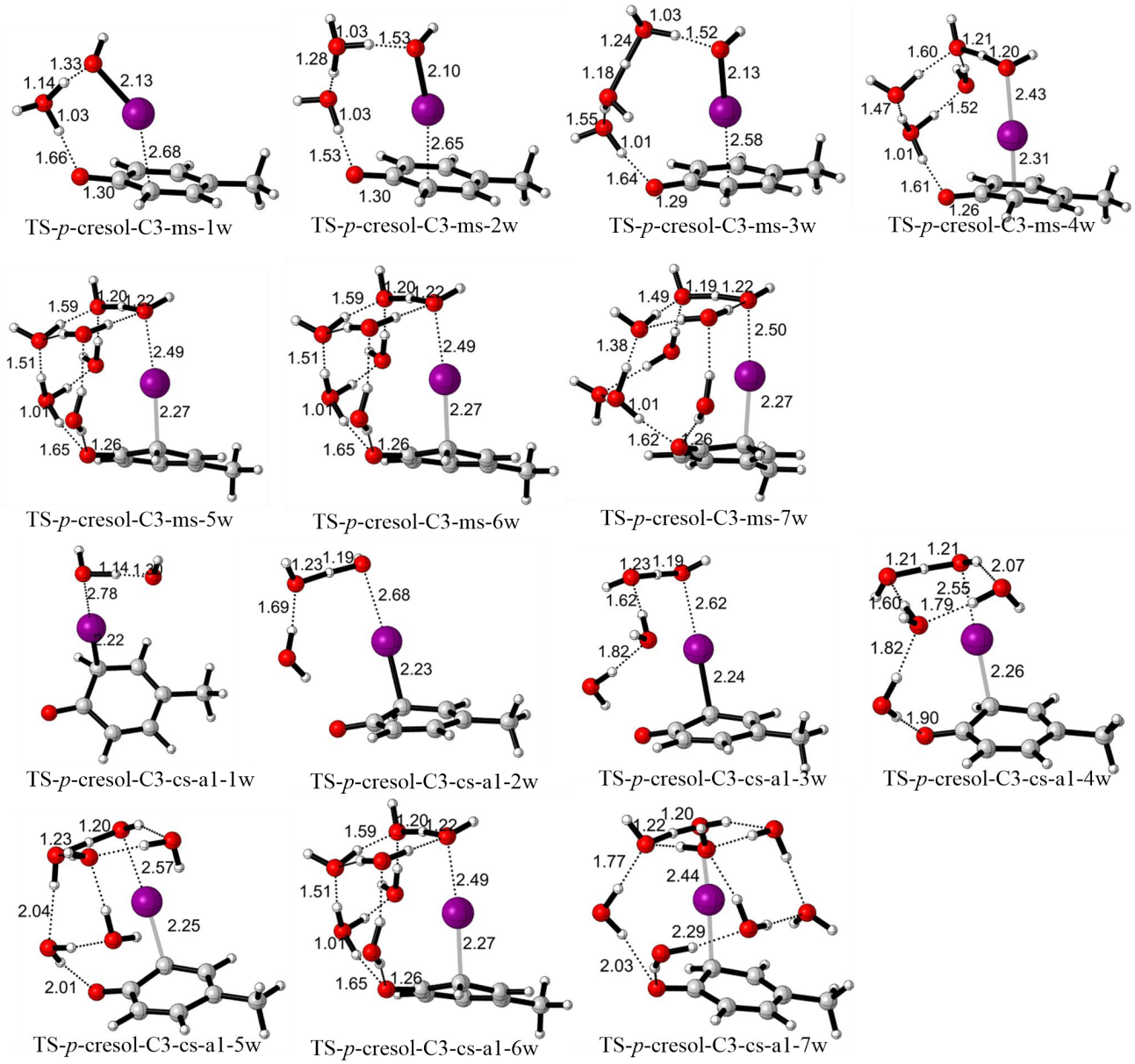


Figure S3. The structures of the transition states in step ms for *p*-cresol (TS-*p*-cresol-C3-ms-nw) and in step cs-a1 for *p*-cresolate (TS-*p*-cresol-C3-cs-a1-nw) during iodination of C3 in *p*-cresol by HOI assisted with 1-7 water molecules.

Table S8. The activation free energies, reaction enthalpy changes ($\Delta G^{\neq}/\Delta H$, in kcal/mol) and the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) at pH=7.0 of iodination of Gly by HOI.

$\Delta G^{\neq}$	ΔH	$k_{obs\text{-}est}$	k_{expt}
15.1	0.6	0.1	<0.1

The pK_a of H-N bond of -NH_3^+ of amino group in Tyr is 9.7 with f(N)=0.998 and f(A)=0.002 at pH=7.0.

Table S9. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) in iodination of the phenol moiety in Tyr by HOI *via*. the concerted, classic S_EAr (cs), and modified S_EAr (ms) mechanisms with the attack from the same and opposite sides.

Reactive site	Neutral phenol						Phenolate			
	Concerted		Classic S_EAr		Modified S_EAr		Concerted		Classic S_EAr	
	Same	Opp.	Same	Opp.	Same	Opp.	Same	Opp.	Same	Opp.
C1	——	——	——	53.4	25.1	24.1	——	——	12.8	8.6
C3	30.8	30.4	50.7	50.6	18.2	16.6	20.6	16.4	7.8	7.4
C5	29.7	28.3	——	44.0	16.0	15.9	17.4	16.1	7.6	6.9

Table S10. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in iodination of the neutral phenol and phenolate moieties in Tyr via the concerted, classic S_EAr(cs), and modified S_EAr(ms) mechanisms.

Reactive site	Neutral phenol				Phenolate		
	Concerted	Classic S_EAr		Modified S_EAr	Concerted	Classic S_EAr	
		cs-n1	cs-n2	ms		cs-a1	cs-a2
C1	——	53.4	——	24.1	——	8.6	——
C3	30.4	50.6	5.3	16.6	16.4	7.4	7.5
C5	28.3	44.0	3.9	15.9	16.1	6.9	10.2

Table S11. The calculated rate constants (k_{est}, in M^{-1} s^{-1}) during the iodination of neutral phenol and phenolate moieties in Tyr by HOI, their contributions (c, in %) to estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of Tyr and the reaction enthalpy changes of the overall reactions ($\Delta H_{obs\text{-}est}$, in kcal/mol).

Reactive site	Neutral phenol		Phenolate		$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
	k_{est}	c	k_{est}	c		
C1	1.4×10^{-5}	0%	3.3×10^{6}	100%	2.0×10^{3}	7.7
C3	4.6	0%	2.5×10^{7}	100%	1.5×10^{4}	–29.2
C5	14.2	0%	5.8×10^{7}	100%	3.5×10^{4}	–29.3

The pK_a of O−H moiety in Tyr is 10.2 with f(N)=0.9994 and f(A)=0.0006 at pH=7.0.

c (Neutral phenol, %) = (k_{est}(Neutral phenol)× f(N))/$k_{obs\text{-}est}$ ×100%; c (Phenolate, %)= (k_{est}(Phenolate)× f(A))/$k_{obs\text{-}est}$ ×100%.

Table S12. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in iodination of the neutral phenol and phenolate moieties in 3-I-Tyr via respective modified and classic S_EAr mechanisms.

Reactive site	Neutral phenol	Phenolate	
	ms	cs-a1	cs-a2
C1	22.9	11.3	——
C3	21.2	14.4	——
C5	17.1	8.4	10.3

Table S13. The calculated rate constants (k_{est}, in M^{-1} s^{-1}) during the iodination of neutral phenol and phenolate moieties in 3-I-Tyr by HOI, their contributions (c, in %) to estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of 3-I-Tyr and the reaction enthalpy changes of the overall reactions ($\Delta H_{obs\text{-}est}$, in kcal/mol).

Reactive site	Neutral phenol		Phenolate		$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
	k_{est}	c	k_{est}	c		
C1	1.1×10^{-4}	0%	3.5×10^{4}	100%	2.1×10^{3}	11.2
C3	2.0×10^{-3}	0%	1.9×10^{2}	100%	11.0	15.6
C5	2.0	0%	4.6×10^{6}	100%	1.1×10^{4}	–28.4

The pK_a of O−H moiety in 3-I-Tyr is 8.1 with f(N)=0.9264 and f(A)=0.0736 at pH=7.0.

c (Neutral phenol, %) = (k_{est}(Neutral phenol)× f(N))/$k_{obs\text{-}est}$ ×100%; c (Phenolate, %)= (k_{est}(Phenolate)× f(A))/$k_{obs\text{-}est}$ ×100%.

Table S14. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of iodination of the neutral phenol and phenolate moieties in 3,5-di-I-Tyr via respective modified and classic S_EAr mechanisms.

Reactive site	Neutral phenol	Phenolate
C1	——	15.1
C3	18.0	16.9
C5	16.9	14.2

Table S15. The calculated rate constants (k_{est}, in M^{-1} s^{-1}) during the iodination of neutral phenol and phenolate moieties in 3,5-di-I-Tyr by HOI, their contributions (c, in %) to estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of 3,5-di-I-Tyr and the reaction enthalpy changes of the overall reactions ($\Delta H_{obs\text{-}est}$, in kcal/mol).

Reactive site	Neutral phenol		Phenolate		$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
	k_{est}	c	k_{est}	c		
C1	5.7×10^{-5}	0%	57.0	100%	31.7	14.7
C3	0.2	0%	2.7	100%	1.5	19.0
C5	——	——	2.6×10^{2}	100%	1.4×10^{2}	16.4

The pK_a of O−H moiety in 3,5-di-Tyr is 6.9 with f(N)=0.4427 and f(A)=0.5573 at pH=7.0.

c (Neutral phenol, %) = (k_{est}(Neutral phenol)× f(N))/$k_{obs\text{-}est}$ ×100%; c (Phenolate, %)= (k_{est}(Phenolate)× f(A))/$k_{obs\text{-}est}$ ×100%.

--: transition state was not found.

Table S16. The activation free energies, reaction enthalpy changes ($\Delta G^{\neq}/\Delta H_{obs\text{-}est}$ at 298 K and 1 atm, in kcal/mol) and the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of iodination of amino groups in (iodo-)Tyr and Tyr-Am by HOI.

Reactant	$\Delta G^{\neq}/\Delta H_{obs\text{-}est}$	$k_{obs\text{-}est}$	Reactant	$\Delta G^{\neq}/\Delta H_{obs\text{-}est}$	$k_{obs\text{-}est}$
Tyr	16.4/–5.0	1.2×10^{-2}	3,5-di-I-Tyr	18.1/–5.2	7.0×10^{-4}
3-I-Tyr	16.8/–5.0	6.5×10^{-3}	Tyr-Am	19.0/–5.0	7.5×10^{-3}

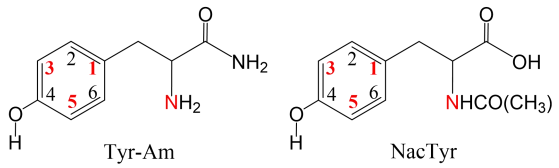


Figure S4. The structures of Tyr-Am and NacTyr

Table S17. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in iodination of the neutral phenol and phenolate moieties in Tyr-Am via respective modified and classic S_EAr mechanisms.

Reactive site	Neutral phenol	Phenolate	
	ms	cs-a1	cs-a2
C1	22.4	10.6	——
C3	17.5	8.9	6.9
C5	15.3	7.5	8.7

Table S18. The calculated rate constants (k_{est}, in M^{-1} s^{-1}) during the iodination of neutral phenol and phenolate moieties in Tyr-Am by HOI, their contributions (c, in %) to estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of Tyr-Am by HOI and the reaction enthalpy changes of the overall reactions ($\Delta H_{obs\text{-}est}$, in kcal/mol).

Reactive site	Neutral phenol		Phenolate		$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
	k_{est}	c	k_{est}	c		
C1	2.4×10^{-4}	0%	1.1×10^{5}	100%	1.1×10^{2}	10.0
C3	1.0	0%	2.0×10^{6}	100%	2.0×10^{3}	–29.0
C5	40.7	0%	2.1×10^{7}	100%	2.1×10^{4}	–29.2

The pK_a of O–H moiety in Tyr-Am is 10.0 with f(N)=0.9990 and f(A)=0.0010 at pH=7.0.

c (Neutral phenol, %) = (k_{est}(Neutral phenol)× f(N))/$k_{obs\text{-}est}$ ×100%; c (Phenolate, %)= (k_{est}(Phenolate)× f(A))/$k_{obs\text{-}est}$ ×100%.

Table S19. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in iodination of the phenolate moieties in 3-I-Tyr-Am *via.* the classic S_EAr mechanisms, the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}), and the estimated reaction enthalpy changes ($\Delta H_{obs\text{-}est}$, in kcal/mol) of phenol moieties in 3-I-Tyr-Am.

Reactive site	cs-a1	cs-a2	$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
C1	12.7	——	3.6×10^{2}	13.4
C3	17.1	——	0.2	16.9
C5	9.6	9.2	6.8×10^{4}	–28.4

The pK_a of O–H moiety in 3-I-Tyr-Am is 7.9 with f(N)=0.8882 and f(A)=0.1118 at pH=7.0.

Table S20. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of the iodination of the phenolate moieties, the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}), and the estimated reaction enthalpy changes ($\Delta H_{obs\text{-}est}$, in kcal/mol) of phenol moieties in 3,5-di-I-Tyr-Am.

Reactive site	cs-a1	$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
C1	14.7	79.8	16.9
C3	17.7	0.5	19.7
C5	14.6	1.9×10^{2}	17.7

The pK_a of O−H moiety in 3,5-di-I-Tyr-Am is 7.9 with f(N)=0.2847 and f(A)=0.7153 at pH=7.0.

Table S21 The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in the iodination of each reactive C-site in the neutral and anion forms of NacTyr.

Reactive site	Neutral phenol	Phenolate	
	ms	cs-a1	cs-a2
C1	18.4	6.1	——
C3	15.2	6.3	10.5
C5	15.0	3.2	8.6

Table S22. The calculated rate constants (k_{est}, in M^{-1} s^{-1}) during the iodination of neutral phenol and phenolate moieties in NacTyr by HOI, their contributions (c, in %) to estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}) of NacTyr and the reaction enthalpy changes of the overall reactions ($\Delta H_{obs\text{-}est}$, in kcal/mol).

Reactive site	Neutral phenol		Phenolate		$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
	k_{est}	c	k_{est}	c		
C1	0.2	0%	2.2×10^{8}	100%	1.8×10^{5}	4.1
C3	45.9	0%	1.6×10^{8}	100%	1.3×10^{5}	–29.5
C5	63.2	0%	$1.0\times10^{9*}$	100%	8.0×10^{5}	–30.0

The pK_a of O−H moiety in NacTyr is 10.1 with f(N)=0.9992 and f(A)=0.0008 at pH=7.0.

c (Neutral phenol, %) = (k_{est}(Neutral phenol)× f(N))/$k_{obs\text{-}est}$ ×100%; c (Phenolate, %)= (k_{est}(Phenolate)× f(A))/$k_{obs\text{-}est}$ ×100%.

Table S23. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step in iodination of the phenolate moiety, the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}), and the estimated reaction enthalpy changes ($\Delta H_{obs\text{-}est}$, in kcal/mol) of phenol moieties in 3-I-NacTyr.

Reactive site	cs-a1	cs-a2	$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
C1	9.2	——	2.9×10^{4}	7.7
C3	12.6	——	94.5	12.6
C5	8.5	11.5	1.0×10^{5}	–29.1

The pK_a of O−H moiety in 3-I-NacTyr is 8.6 with f(N)=0.9755 and f(A)=0.0245 at pH=7.0.

Table S24. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of the iodination of the phenolate moiety, the estimated apparent rate constants ($k_{obs\text{-}est}$, in M^{-1} s^{-1}), and the estimated reaction enthalpy changes ($\Delta H_{obs\text{-}est}$, in kcal/mol) of phenol moieties in 3,5-di-NacTyr.

Reactive site	cs-a1	$k_{obs\text{-}est}$	$\Delta H_{obs\text{-}est}$
C1	9.6	4.9×10^5	10.9
C3	15.5	23.1	16.1
C5	13.1	1.3×10^3	14.9

The pK_a of O−H moiety in 3,5-di-I-NacTyr is 6.4 with f(N)=0.2008 and f(A)=0.7992 at pH=7.0.

Table S25. The activation free energies of iodination of *ortho*-C3 site ($\Delta G^{\neq}$, in kcal/mol) in the phenolic moiety in Tyr by different iodinated agents

Iodinating agents	Neutral phenol	Phenolate	Iodinating agents	Neutral phenol	Phenolate
HOI	16.6	7.4	I_2	19.6	0.1**
H_2OI^+	4.2*	——	IBr	(9.5)	——
NHClI	17.7	12.8	ICl	7.8 (6.6)	——
NH_2ClI^+	8.9	——			

* *via.* the concerted mechanism assisted with one water molecule.
**assisted with one water molecule.
——: transition states of these reactions were not found.
():data calculated at M05(D3)/6-311G(d) with 5 water molecules assisted

Table S26. Estimated apparent rate constants of each iodinating agent (IA) ($k_{obs\text{-}est}$ (IA), in M^{-1} s^{-1}) in σ-complex formation (step ms/cs-a1) for the *ortho*-C3 in the phenol ring of Tyr (R) along with the fraction of each IA relative to HOI (Rf) and $k_{obs\text{-}est}$ in real water ($k_{obs\text{-}est}$ (water) , in M^{-1} s^{-1}) and the contributions (p, in %) under the typical experimental conditions of pH=7 and concentrations of [Br^-]: 900 μg/L, [I^-]: 30 μg/L, [NH_2Cl]: 2.6 μmol.

IA	$k_{obs\text{-}est}$ (IA)	Rf	$k_{obs\text{-}est}$ (water)	p	IA	$k_{obs\text{-}est}$ (IA)	Rf	$k_{obs\text{-}est}$ (water)	p
HOI	10^4	1.0	10^4	97%	I_2	10^6	10^{-3}	10^3	3%
H_2OI^+	10^9	10^{-8}	10^1	0%	IBr	(10^6)	10^{-8}	(10^{-2})	(0%)
NHClI	10^0	10^{-4}	10^{-4}	0%	ICl	10^7	10^{-10}	10^{-3}	0%
NH_2ClI^+	10^6	10^{-12}	10^{-6}	0%					

():data calculated at M05(D3)/6-311G(d) with 5 water molecules assisted

Table S27. The activation free energies ($\Delta G^{\neq}$, in kcal/mol) of each step during halogenation of *ortho*-C3 of the phenolate moiety and amino N in Tyr by HOCl, HOBr, and HOI.

Agent	*ortho*-C3		Amino N
	cs-a1	cs-a2	
HOCl	10.3	6.1	1.7
HOBr	5.0	10.2	10.7
HOI	7.4	7.5	16.4

Table S28. The volume (in bohr^3/mol) of HOX and APT charge of X as well as the reaction free energy changes (ΔG, in kcal/mol) in step cs-a1 for iodination of the phenolate moiety in Tyr

	HOCl	HOBr	HOI
Volume	342	382	493
APT-X	0.037	0.072	0.288
ΔG^*	–8.0	–1.8	10.0

* $\Delta G = \sum G$ (product) – $\sum G$ (reactant)

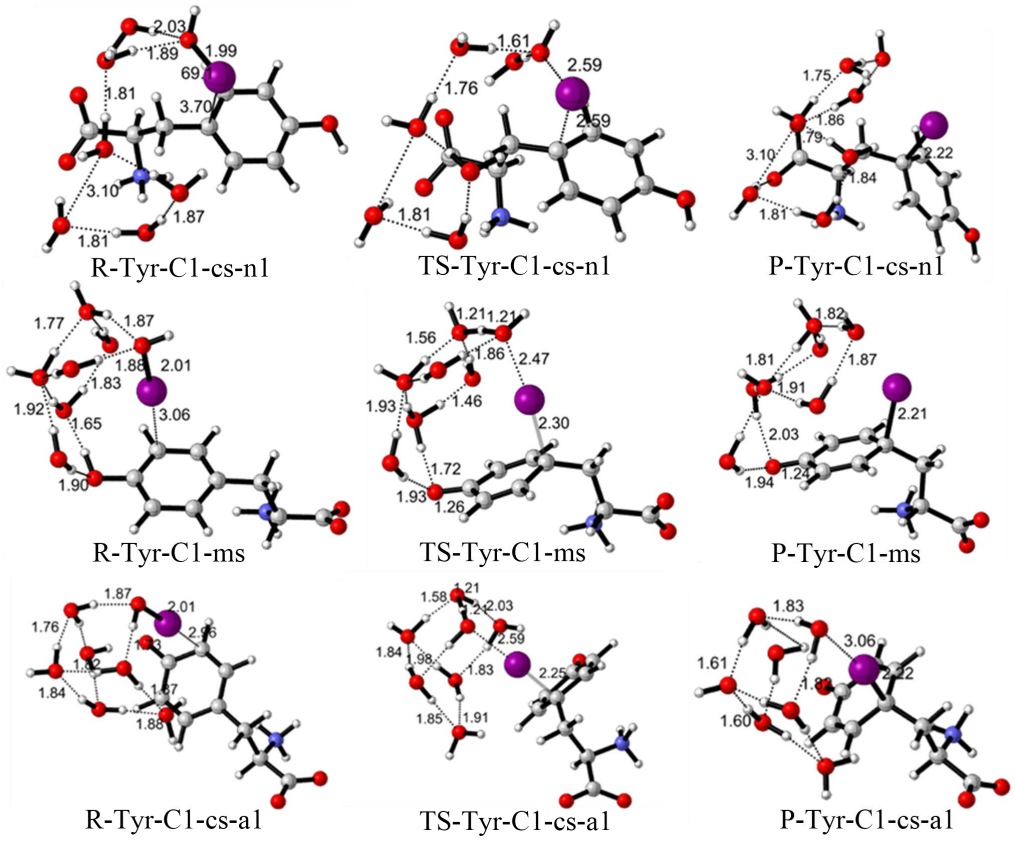


Figure S5. The structures of the reactants, transition states, and products of all mechanisms for *para*-C1 of Tyr.

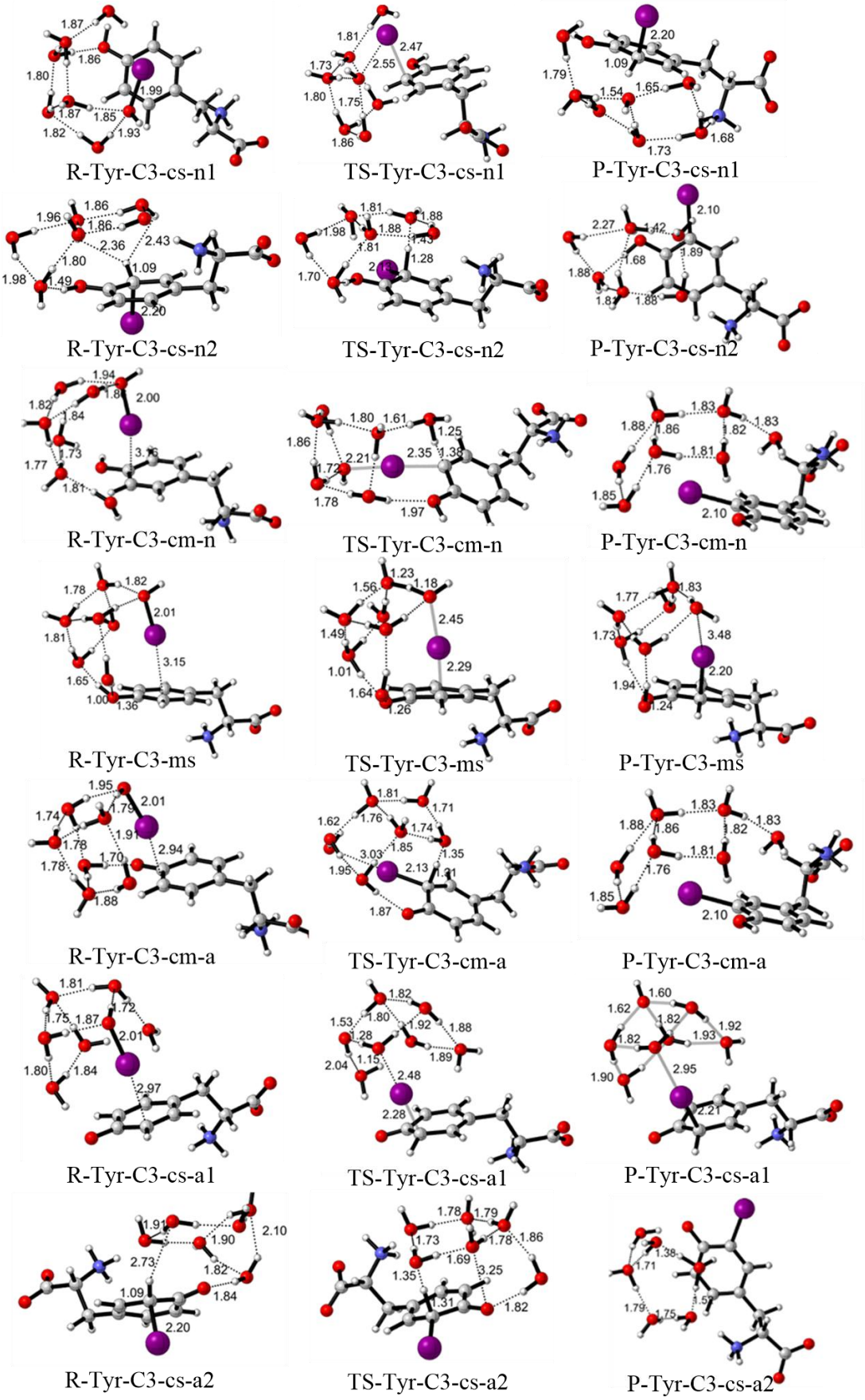


Figure S6. The structures of the reactants, transition states, and products of all mechanisms for *ortho*-C3 of Tyr.

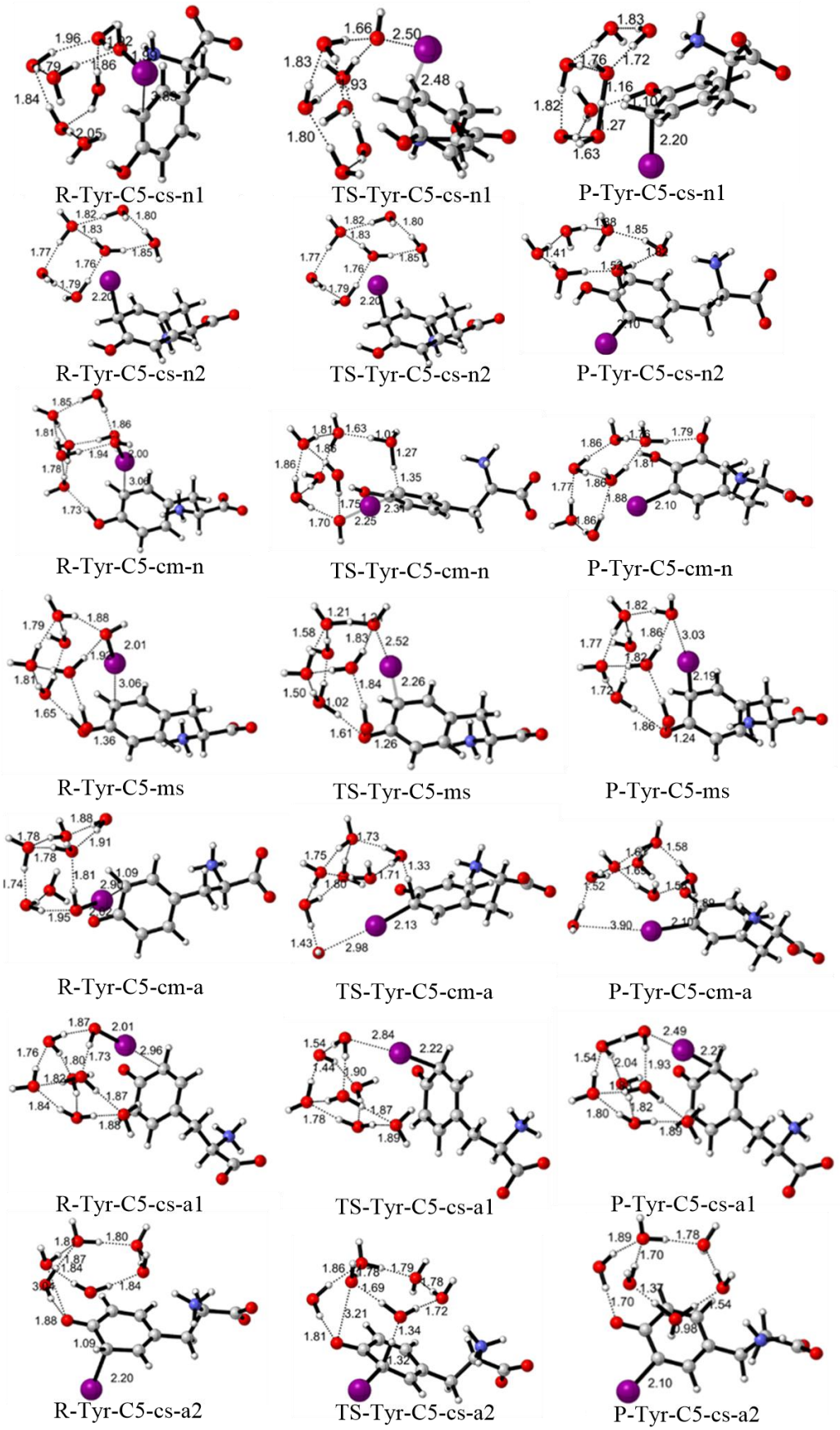


Figure S7. The structures of the reactants, transition states, and products of all mechanisms for *ortho*-C5 of Tyr.

Coordinates (xyz) for the key structures of the reaction of Tyr

Tyr-C1-cs-n1

Reactant:

C	3.20607500	2.72205400	0.13820500
C	2.30510800	2.75253000	-0.92478100
C	1.09164600	2.07296900	-0.81228700
C	1.68215100	1.35338800	1.40326900
C	2.89677600	2.02454100	1.30804000
H	2.55502800	3.29877200	-1.83078800
O	1.31385100	-2.01004900	1.20627100
H	-0.45258800	-2.66995200	1.14162300
H	1.86752300	-2.68606000	1.63977800
H	3.61129100	2.01118900	2.12590700
I	1.77509000	-2.03081600	-0.73399600
O	-1.31934600	-3.04379200	0.87992800
H	-1.09201100	-3.82851400	0.35449100
H	1.44531300	0.80415400	2.31253400
O	-4.75695200	0.59727000	-1.65080000
H	-4.54924000	0.64636600	-0.69211600
H	-5.49905700	1.20872900	-1.78084700
O	-2.46247100	-1.40775500	-1.07549300
H	-3.13060200	-1.98328100	-1.48130800
H	-2.04116900	-1.95571200	-0.37207300
O	-2.40132700	2.00191100	-2.16294800
H	-3.24784100	1.50538700	-2.08531200
H	-1.74535700	1.32712100	-2.44450700
O	-0.34200500	-1.10088500	3.49987600
H	-1.16939800	-0.88848100	3.01027200
H	0.32827700	-1.23552100	2.80667800
O	-0.80200400	-0.21233700	-2.94320000
H	-1.32670900	-0.75802000	-2.31123800
H	0.07904800	-0.14589900	-2.53703600
H	0.39126700	2.09088900	-1.64565200
O	4.41804300	3.36645600	0.08557000
H	4.51192700	3.81319600	-0.77276100
C	0.76432600	1.36313200	0.34554900
C	-0.54478200	0.62442300	0.45880500
H	-0.95956900	0.44058500	-0.53555800
H	-0.39132800	-0.35123000	0.92652300
C	-1.59518200	1.37819300	1.27742300
H	-1.19874700	1.65248600	2.25961900
N	-1.94161200	2.64107800	0.56402200
C	-2.86298300	0.53529000	1.47863100

H	-2.77185300	3.07852200	0.97714000
H	-1.16425500	3.30923700	0.60857400
H	-2.14403100	2.44259700	-0.44594200
O	-3.93732100	0.96560000	0.98400800
O	-2.71711800	-0.52391700	2.13785200

TS:

0 1

C	3.07091100	2.31326000	0.37057000
C	2.17517800	2.40247300	-0.73483800
C	1.06923400	1.60784400	-0.75914400
C	1.69801200	0.65063200	1.41570500
C	2.81636400	1.45192200	1.44941100
H	2.39008900	3.10653900	-1.53354100
O	0.85839300	-2.17975000	1.35784900
H	-0.36264200	-2.86127200	0.56863900
H	1.50418500	-2.89819000	1.45428600
H	3.50747700	1.42973000	2.28491200
I	2.02371600	-1.34518200	-0.80460900
O	-1.15299600	-3.26651800	0.08031400
H	-0.76932900	-3.72589700	-0.68348500
H	1.46999500	-0.00927900	2.24636400
O	-4.83951600	0.87443700	-1.47837700
H	-4.60715300	0.89044400	-0.52447000
H	-5.49232600	1.58361700	-1.59092300
O	-2.80020100	-1.45408400	-1.16345700
H	-3.50214100	-1.98444700	-1.57336400
H	-2.23337200	-2.10176200	-0.67344700
O	-2.34013500	1.98220000	-2.05138900
H	-3.23516600	1.58906900	-1.93240800
H	-1.79426100	1.24874200	-2.41070400
O	-0.59084000	-1.46598000	3.52369900
H	-1.40803500	-1.15343800	3.07989300
H	-0.00105300	-1.75430900	2.77652600
O	-1.05424300	-0.35035400	-3.01111000
H	-1.66393300	-0.84833300	-2.41582300
H	-0.17467200	-0.45405100	-2.60731800
H	0.37514200	1.66450100	-1.59530100
O	4.17289100	3.05327400	0.42363900
H	4.26761100	3.61191500	-0.37074700
C	0.79837600	0.65416100	0.28890700
C	-0.62947700	0.18707700	0.45501600
H	-1.09750100	0.08928800	-0.52755600
H	-0.65056100	-0.78493800	0.94048800

C	**-1.47928400**	**1.13408200**	**1.30904000**
H	**-1.00928100**	**1.31238800**	**2.28107200**
N	**-1.63621100**	**2.45519000**	**0.63483300**
C	**-2.87542000**	**0.52169800**	**1.54303300**
H	**-2.39926200**	**2.98356100**	**1.07209200**
H	**-0.78056100**	**3.01789000**	**0.69894300**
H	**-1.88452600**	**2.32366400**	**-0.37864600**
O	**-3.86666300**	**1.16625600**	**1.11254800**
O	**-2.90113500**	**-0.57273500**	**2.15488200**

Product:

C	**3.03956500**	**2.33519400**	**0.41918000**
C	**2.25560500**	**2.34005500**	**-0.77468600**
C	**1.29645000**	**1.39495000**	**-0.92656400**
C	**1.89953300**	**0.41557600**	**1.28948900**
C	**2.85158700**	**1.36341800**	**1.44838000**
H	**2.43908600**	**3.10229000**	**-1.52534900**
O	**0.19172600**	**-2.97824300**	**2.03412500**
H	**-0.72536300**	**-3.09835500**	**0.87176000**
H	**0.09188400**	**-3.80871300**	**2.52409600**
H	**3.48025500**	**1.41552200**	**2.33032200**
I	**1.81937500**	**-1.44439900**	**-0.97539700**
O	**-1.34942800**	**-3.19628800**	**0.03494200**
H	**-0.74904900**	**-3.16022500**	**-0.72787000**
H	**1.71946300**	**-0.32973000**	**2.06132200**
O	**-4.66191000**	**1.33187300**	**-1.34462200**
H	**-4.36071400**	**1.33708100**	**-0.41032900**
H	**-5.22290400**	**2.11896800**	**-1.43205700**
O	**-3.01982600**	**-1.25165200**	**-0.89610300**
H	**-3.83884300**	**-1.68670800**	**-1.18210200**
H	**-2.47904600**	**-1.95917900**	**-0.45940300**
O	**-2.06292100**	**2.00377200**	**-2.12394400**
H	**-3.00660600**	**1.79512000**	**-1.93501700**
H	**-1.69117500**	**1.15659100**	**-2.45916300**
O	**-0.40677500**	**-1.07171600**	**3.72525000**
H	**-1.21252900**	**-0.70572700**	**3.30809500**
H	**-0.14665300**	**-1.82098000**	**3.09418300**
O	**-1.38488900**	**-0.55800400**	**-3.01645000**
H	**-1.99046800**	**-0.90843700**	**-2.31876800**
H	**-0.49078500**	**-0.77760300**	**-2.70272800**
H	**0.66256900**	**1.38617800**	**-1.81221500**
O	**3.97021500**	**3.22146900**	**0.62862600**
H	**4.05528300**	**3.86357400**	**-0.10520200**
C	**1.04505500**	**0.34884200**	**0.08741700**

C	-0.43675000	0.09205400	0.40054500
H	-0.98091900	-0.05034200	-0.53714300
H	-0.51402500	-0.82918000	0.98478800
C	-1.10632700	1.20504600	1.21281300
H	-0.56605400	1.39138500	2.14629400
N	-1.14688100	2.48971700	0.45712700
C	-2.55564700	0.79966100	1.56812800
H	-1.84338400	3.11198600	0.88330100
H	-0.24144200	2.97180800	0.46788000
H	-1.44967800	2.33155400	-0.54113700
O	-3.47425900	1.55966900	1.16773700
O	-2.68593900	-0.24719400	2.24348800

Tyr-C1-ms

Reactant:

C	2.19895500	1.08032100	-1.35302600
C	1.09995200	1.92958300	-1.36430000
C	0.27090600	2.00604300	-0.23886400
C	0.54982700	1.22375600	0.88765400
C	1.66230100	0.37220200	0.87766100
C	2.49661700	0.28424700	-0.23618100
H	0.86577800	2.53388000	-2.23592300
O	-4.52151400	0.85327700	-0.24065000
H	-5.40263600	1.26222900	-0.22397800
O	-2.73711100	2.27843300	1.41294400
H	-3.38238900	1.88420500	0.78497500
O	-2.65775800	-2.42969800	-0.48328200
H	-4.56202300	0.09428000	0.39150000
H	-2.21120600	-3.29534900	-0.50208100
O	-4.37200700	-1.34233600	1.41370700
H	-3.93272000	-1.97742000	0.80876200
H	-5.20870600	-1.75532400	1.68194900
H	-2.54432400	1.54359900	2.03978700
H	-0.07635200	1.30627500	1.77284600
I	-1.27427000	-1.02943000	-0.08974800
O	-4.41659700	-1.15939300	-2.29380600
H	-3.79922600	-1.73306700	-1.79922900
H	-4.53742900	-0.39060100	-1.70289400
O	-2.58593100	0.05497000	3.10116300
H	-3.20601400	-0.49277500	2.57223800
H	-3.09681800	0.33028700	3.87952900
H	1.87064000	-0.23431100	1.75633600

O	**-0.79298900**	**2.85444400**	**-0.28173400**
H	**-1.44437800**	**2.65051300**	**0.45334200**
H	**2.83594600**	**1.02320000**	**-2.23331600**
C	**3.70705900**	**-0.61772400**	**-0.23771200**
H	**3.64564500**	**-1.33312700**	**0.59154700**
H	**3.75661000**	**-1.18978900**	**-1.16891200**
C	**5.02554100**	**0.15429800**	**-0.12379600**
H	**5.12211600**	**0.87497300**	**-0.93933300**
N	**5.03750600**	**0.93967100**	**1.14666200**
C	**6.23123300**	**-0.80125200**	**-0.13282900**
H	**5.91137800**	**1.46848200**	**1.24349900**
H	**4.25110600**	**1.59945400**	**1.18731300**
H	**4.97575600**	**0.31019300**	**1.95629100**
O	**6.88468600**	**-0.91135300**	**0.93532800**
O	**6.43461000**	**-1.40271300**	**-1.21603100**
O	**-2.70201800**	**1.94107600**	**-2.20294400**
H	**-3.29790900**	**1.51368500**	**-1.55869300**
H	**-1.98037300**	**2.30613500**	**-1.65476300**

TS:

C	**-1.10436500**	**0.78790600**	**1.38347200**
C	**-0.33188000**	**1.89308000**	**1.49357200**
C	**0.26032000**	**2.48717100**	**0.30801000**
C	**-0.21293100**	**2.03898700**	**-0.98893700**
C	**-0.99490800**	**0.93927600**	**-1.08335200**
C	**-1.38959700**	**0.14898300**	**0.09132300**
H	**-0.07490200**	**2.31949800**	**2.45855000**
O	**4.08050800**	**0.42248000**	**0.31991200**
H	**5.04531900**	**0.48197700**	**0.42528800**
O	**3.14229500**	**2.29758900**	**-1.15533500**
H	**3.58203800**	**1.64324400**	**-0.49145500**
O	**2.19421800**	**-2.97886900**	**-0.07794100**
H	**3.90514800**	**-0.32976100**	**-0.35522700**
H	**1.95582800**	**-3.77891600**	**-0.57332200**
O	**3.45196400**	**-1.40145200**	**-1.39110900**
H	**2.85387900**	**-2.25679600**	**-0.78423900**
H	**4.23626500**	**-1.79350600**	**-1.80568600**
H	**2.69721900**	**1.64040100**	**-1.85979200**
H	**0.13480200**	**2.57239000**	**-1.86900800**
I	**0.24942800**	**-1.46654900**	**0.01153000**
O	**3.31344100**	**-1.69982500**	**2.16676500**
H	**2.91264000**	**-2.27424800**	**1.48206500**
H	**3.56233000**	**-0.89064000**	**1.68078000**
O	**2.25425500**	**0.54754500**	**-2.71235800**

H	**2.70165900**	**-0.25515000**	**-2.29750600**
H	**2.66782500**	**0.66347200**	**-3.58450200**
H	**-1.31353300**	**0.57051900**	**-2.05764800**
O	**1.18628900**	**3.33854000**	**0.39907000**
H	**2.42626000**	**2.78876700**	**-0.65977400**
H	**-1.50599900**	**0.30513500**	**2.27283600**
C	**-2.73835200**	**-0.56391900**	**-0.00084700**
H	**-2.84514500**	**-1.01853900**	**-0.99307300**
H	**-2.78620700**	**-1.36381800**	**0.74184100**
C	**-3.93022300**	**0.35514700**	**0.27507500**
H	**-3.87843300**	**0.75350200**	**1.29290700**
N	**-3.93418700**	**1.54227800**	**-0.63413400**
C	**-5.27885500**	**-0.38084100**	**0.12099700**
H	**-4.86133400**	**1.98569200**	**-0.60112900**
H	**-3.22205300**	**2.23559800**	**-0.37486200**
H	**-3.77727200**	**1.26575400**	**-1.61200900**
O	**-6.15432900**	**0.18211400**	**-0.58388500**
O	**-5.37952500**	**-1.46937200**	**0.73488100**
O	**2.97807400**	**2.16991600**	**2.33518400**
H	**3.32248100**	**1.47637900**	**1.74213000**
H	**2.36801100**	**2.68613700**	**1.77334300**

Product:

C	**0.70302100**	**0.51417100**	**-1.16335400**
C	**0.00414900**	**1.66002200**	**-1.22029900**
C	**-0.35430200**	**2.38407500**	**0.00263400**
C	**0.10636200**	**1.83702000**	**1.28284100**
C	**0.81785200**	**0.69879800**	**1.33245400**
C	**1.16722500**	**-0.08677300**	**0.11625500**
H	**-0.32230600**	**2.08116500**	**-2.16675500**
O	**-3.54141200**	**0.94906800**	**-0.74537200**
H	**-4.47899600**	**0.96991200**	**-1.00286000**
O	**-3.23760200**	**2.37156200**	**1.54843500**
H	**-3.47607300**	**1.51202400**	**0.07162900**
O	**-2.87715400**	**-3.18776700**	**-1.25934600**
H	**-3.58238200**	**-0.61157100**	**0.17907600**
H	**-3.70036200**	**-3.51295900**	**-1.65724700**
O	**-3.58020400**	**-1.40211100**	**0.76833100**
H	**-3.16049900**	**-2.66360700**	**-0.47629900**
H	**-4.50973100**	**-1.53032000**	**1.02059700**
H	**-2.81586700**	**1.64420300**	**2.06340100**
H	**-0.14724400**	**2.39237900**	**2.18169400**
I	**-0.02912100**	**-1.93585100**	**0.33687500**
O	**-2.22436300**	**-0.77699500**	**-2.61928900**

H	-2.40180700	-1.64651700	-2.20186400
H	-2.54410900	-0.12247600	-1.96964000
O	-2.34017900	0.06436000	2.81658300
H	-2.76461400	-0.55151700	2.17732900
H	-2.87579300	-0.00037500	3.62354400
H	1.17241600	0.30331900	2.28270400
O	-1.03195900	3.42370200	-0.03528200
H	-2.51288100	2.96400400	1.27593000
H	0.97072500	-0.02058200	-2.07275300
C	2.63905000	-0.52920200	0.05752200
H	2.92203000	-0.98351500	1.01425400
H	2.74846400	-1.28599100	-0.72218500
C	3.61351000	0.59442100	-0.29151400
H	3.32747700	1.08248500	-1.22862400
N	3.64225700	1.66870300	0.74856600
C	5.06058400	0.06756800	-0.47008400
H	4.55656600	2.14120600	0.68916200
H	2.89084100	2.35675000	0.62741900
H	3.57199400	1.27876100	1.69703800
O	5.97090900	0.74370600	0.07304300
O	5.19023000	-0.96424300	-1.16689000
O	-2.84253300	3.31083400	-2.23969100
H	-3.09937600	2.43345600	-1.89328600
H	-2.15144300	3.59140900	-1.60951500

Tyr-C1-cs-a1

Reactant:

C	1.50148100	-0.32093300	1.41395400
C	0.50280000	-1.18011500	1.84017300
C	-0.00761900	-2.20984600	0.99479900
C	0.57529400	-2.30239100	-0.30238900
C	1.59386500	-1.42944400	-0.70867800
C	2.06580800	-0.41673900	0.12636600
O	-4.16096900	2.38477200	1.37883100
H	-4.90353300	2.86551400	1.77710900
O	-1.68106100	1.39939600	2.25337200
H	-2.52186800	1.85539900	2.03861000
O	-3.20219200	0.50178800	-1.88563600
H	-4.50769500	1.50354000	1.08876100
H	-3.00269300	1.42620400	-1.57643100
O	-4.70429300	-0.11683800	0.44359700
H	-4.28579700	0.03183600	-0.43132000

H	-4.02622200	-0.58638300	0.98545800
H	-1.07531200	1.61221300	1.51230000
H	0.24745000	-3.10355500	-0.96164100
I	-1.59230200	-0.57506700	-1.34542100
H	1.85285900	0.46086300	2.08756300
O	-2.83674900	-1.15355700	2.21716700
H	-2.20396800	-1.85494700	1.91490300
H	-2.31537400	-0.31943600	2.23045600
O	-2.54279500	2.91218800	-0.82406900
H	-1.63509200	2.74408400	-0.49961700
H	-3.11722300	2.86632300	-0.02862300
O	0.04274300	2.23149000	0.13663200
H	0.80397500	2.64444000	0.57775000
H	0.37654900	1.38172000	-0.20463500
H	2.01618500	-1.53812600	-1.70668300
H	0.08045600	-1.07684200	2.83756200
O	-0.97878200	-2.99258500	1.37783100
C	3.17309200	0.51541400	-0.30374700
H	3.35204700	0.41317300	-1.38157800
H	2.90485500	1.56007900	-0.11161000
C	4.48812600	0.25554800	0.43954700
H	4.35588300	0.40246200	1.51447300
N	4.88770500	-1.17076700	0.25179600
C	5.61593600	1.16811100	-0.06717100
H	5.04139300	-1.37290900	-0.74366100
H	5.76529200	-1.37638400	0.74104500
H	4.15837900	-1.80456000	0.60061400
O	6.58199200	0.62053500	-0.65699100
O	5.45270600	2.39550800	0.14511500

TS:

-1 1

C	-0.90899900	0.77192700	1.10322900
C	-0.82226200	2.06051500	1.48443700
C	-1.06442100	3.14909500	0.53314200
C	-1.43341800	2.77230900	-0.83429200
C	-1.52944800	1.47745800	-1.19741400
C	-1.22458700	0.35520100	-0.28132200
O	4.81605600	-0.45577800	1.20210600
H	5.62038900	-0.09212700	1.60366800
O	2.38637800	0.38801400	2.25523100
H	3.26860500	0.06329000	1.95911800
O	3.05362000	-1.30285500	-1.82931800
H	4.67646400	0.02472000	0.31299000

H	**3.16971400**	**-1.93962200**	**-1.09774000**
O	**4.23136200**	**0.66753900**	**-1.05465800**
H	**3.63558200**	**-0.30843500**	**-1.45616800**
H	**3.56445300**	**1.30178900**	**-0.73153800**
H	**1.78489400**	**-0.37488900**	**2.14091100**
H	**-1.63520800**	**3.57700000**	**-1.53531600**
I	**0.72669500**	**-0.43912500**	**-1.08538700**
H	**-0.74119200**	**-0.02479500**	**1.82654100**
O	**2.31569700**	**2.45767400**	**0.37281400**
H	**1.59084700**	**2.33309100**	**-0.26209400**
H	**2.20641600**	**1.71976500**	**1.01647700**
O	**3.32305500**	**-2.76598000**	**0.69666200**
H	**2.47597200**	**-2.55536300**	**1.14189500**
H	**3.93417900**	**-2.04918600**	**0.96604300**
O	**0.92414500**	**-2.08241500**	**2.03933700**
H	**0.66014100**	**-2.67853400**	**2.75915300**
H	**0.20200300**	**-2.12018300**	**1.38890200**
H	**-1.82855700**	**1.21154500**	**-2.21061700**
H	**-0.56637800**	**2.33736900**	**2.50345700**
O	**-0.96795700**	**4.33958300**	**0.87278400**
C	**-2.21510900**	**-0.81631300**	**-0.33945900**
H	**-2.40123000**	**-1.09195000**	**-1.38475900**
H	**-1.77482000**	**-1.68317400**	**0.16031000**
C	**-3.54314100**	**-0.53992300**	**0.36458600**
H	**-3.37309000**	**-0.24460000**	**1.40491800**
N	**-4.28520800**	**0.59127100**	**-0.27396800**
C	**-4.47105900**	**-1.77718700**	**0.38269200**
H	**-4.23423900**	**0.53758800**	**-1.29922300**
H	**-5.27983000**	**0.51421500**	**-0.02033300**
H	**-3.92742200**	**1.50821600**	**0.01700700**
O	**-5.67442400**	**-1.58402500**	**0.07285700**
O	**-3.94186000**	**-2.85544200**	**0.74044600**

Product:

C	**-0.87432000**	**0.74369300**	**1.06578100**
C	**-0.86301400**	**2.03090800**	**1.44686000**
C	**-1.15193900**	**3.10920500**	**0.49131300**
C	**-1.47777700**	**2.71861900**	**-0.88859700**
C	**-1.50199600**	**1.42663100**	**-1.25779700**
C	**-1.18372700**	**0.31023700**	**-0.32402700**
O	**4.63548900**	**-0.32895100**	**1.40010100**
H	**5.34953900**	**-0.25325900**	**2.04924500**
O	**2.31593100**	**0.55275000**	**2.17935500**
H	**3.24125300**	**0.21053600**	**1.92710800**

O	3.51816200	-1.54054700	-1.80097400
H	4.55601500	0.51905700	0.02945800
H	3.44267300	-1.98731900	-0.92657300
O	4.34231500	0.96751900	-0.84895800
H	3.79167300	-0.62309100	-1.57169700
H	3.58049400	1.54493000	-0.63523500
H	1.72518000	-0.21838500	2.08327200
H	-1.70744000	3.51625600	-1.58893600
I	0.70792400	-0.52893200	-1.11924100
H	-0.67118900	-0.04769300	1.78506200
O	2.18174400	2.50643400	0.22919600
H	1.47184300	2.32123200	-0.40790000
H	2.09518900	1.79722100	0.91403000
O	3.41996000	-2.55678200	0.80587100
H	2.52578800	-2.42620800	1.18125900
H	3.94476200	-1.74467600	1.10268300
O	0.90856400	-2.03315600	2.06580800
H	0.70382400	-2.66493800	2.77431400
H	0.22090100	-2.16939800	1.39173800
H	-1.76734900	1.14477200	-2.27542900
H	-0.63305000	2.32082800	2.46824900
O	-1.12794900	4.29689400	0.83373200
C	-2.20577100	-0.84004900	-0.35251700
H	-2.39901800	-1.13538400	-1.39069200
H	-1.78126500	-1.70157300	0.16896100
C	-3.52343500	-0.51617200	0.34902100
H	-3.34395400	-0.16898700	1.37144500
N	-4.27654000	0.57730600	-0.33889400
C	-4.45301600	-1.75156000	0.44619500
H	-4.21757000	0.48618900	-1.36125500
H	-5.27158500	0.48857800	-0.08785000
H	-3.93901900	1.51169300	-0.08168700
O	-5.66319600	-1.56589700	0.16007600
O	-3.91751200	-2.81291600	0.84017400

Tyr-C3-cs-n1

Reactant:

C	-1.47089900	1.67023400	-1.27578100
C	-0.38489100	2.54470800	-1.20802400
C	0.40171100	2.56752000	-0.05754200
C	0.11715800	1.72070600	1.01609700
C	-0.97473600	0.86313500	0.93220000

H	**-0.14917000**	**3.20686500**	**-2.03783700**
O	**0.67157300**	**-2.03277400**	**0.60902200**
H	**2.44055000**	**-2.17453300**	**1.14056300**
H	**0.27343900**	**-2.92259900**	**0.63138100**
I	**0.88483700**	**-1.51231400**	**-1.30310300**
H	**0.74743600**	**1.74634300**	**1.90171500**
O	**3.39550500**	**-2.01286500**	**1.29999700**
H	**3.82766600**	**-2.88066400**	**1.25001200**
H	**-2.07898000**	**1.64624700**	**-2.17730000**
H	**-1.19817600**	**0.20293800**	**1.76727800**
O	**1.47075800**	**3.41985700**	**0.07666600**
H	**1.64050900**	**3.88479800**	**-0.76156600**
O	**3.32075700**	**0.24041900**	**2.98294300**
H	**3.53327300**	**-0.56726200**	**2.47236000**
H	**3.41056800**	**0.97148400**	**2.32982600**
O	**4.28200900**	**-0.18853600**	**-0.59995300**
H	**5.24818500**	**-0.26340200**	**-0.65658400**
H	**3.99264200**	**-0.89277000**	**0.02633700**
O	**3.80725900**	**2.08308000**	**0.96809700**
H	**3.00583600**	**2.52845900**	**0.62942700**
H	**3.98663400**	**1.34815000**	**0.34149700**
O	**0.75788300**	**-0.83182300**	**3.24175400**
H	**1.61037500**	**-0.34549600**	**3.19830400**
H	**0.62020600**	**-1.15533900**	**2.33200200**
O	**2.68781100**	**1.50295100**	**-2.23779500**
H	**3.17948100**	**0.83492400**	**-1.71865200**
H	**1.75844900**	**1.37290100**	**-1.98500200**
C	**-1.77932000**	**0.81918000**	**-0.21314500**
C	**-2.94132200**	**-0.14158700**	**-0.28967900**
H	**-3.29621100**	**-0.22275800**	**-1.32447700**
H	**-2.62777200**	**-1.13950500**	**0.03293900**
C	**-4.11480900**	**0.26593700**	**0.60434800**
H	**-3.79616200**	**0.34006400**	**1.64753200**
N	**-4.59522900**	**1.62416200**	**0.20926400**
C	**-5.28498100**	**-0.72849700**	**0.50248000**
H	**-5.40929700**	**1.90063800**	**0.76888500**
H	**-3.85849600**	**2.32998300**	**0.32791400**
H	**-4.89070400**	**1.63033300**	**-0.77470600**
O	**-6.38375000**	**-0.28368900**	**0.08406900**
O	**-5.02324300**	**-1.90716000**	**0.84670200**

TS:

C	**1.64375700**	**-1.34362900**	**1.76561600**
C	**0.38319700**	**-1.22940200**	**2.34824100**

C	-0.58673100	-0.47867700	1.70308100
C	-0.31750300	0.11219800	0.41970100
C	1.02282700	0.03611300	-0.08780800
H	0.15791600	-1.71104600	3.29482600
O	-0.86782200	0.68690400	-2.18538700
H	-2.26766400	1.22264800	-1.89823400
H	-0.87840900	0.41650200	-3.11827500
I	-1.25801900	-1.58700100	-1.10316100
H	-0.97997700	0.91254100	0.09317600
O	-3.17544600	1.61927900	-1.61414800
H	-3.70672500	1.71958400	-2.41953800
H	2.39786800	-1.93985900	2.27512400
H	1.24264400	0.54837800	-1.01865900
O	-1.82018800	-0.30491200	2.17168200
H	-1.95233000	-0.77318200	3.01844100
O	-2.23655900	3.71310200	-0.06494800
H	-2.66311900	3.06644000	-0.67193000
H	-2.36447500	3.31892100	0.82546500
O	-4.38839200	0.70079900	0.63085000
H	-5.32451300	0.94807100	0.55832100
H	-3.97825300	0.96309800	-0.23266700
O	-2.92836700	2.37553600	2.29990900
H	-2.21142500	1.77293100	2.55870600
H	-3.52803800	1.79525800	1.77654300
O	0.18981600	3.06546200	-1.34887600
H	-0.56755900	3.37134300	-0.80608900
H	-0.12603900	2.20454900	-1.72357000
O	-4.15515100	-2.01585700	1.25048600
H	-4.23915100	-1.06676500	1.00920000
H	-3.19778100	-2.17686400	1.21577000
C	1.99130200	-0.70788500	0.55639300
C	3.38936200	-0.80965300	-0.00433400
H	3.92836600	-1.63386200	0.47721300
H	3.34937400	-1.01759900	-1.07669300
C	4.19152500	0.48123700	0.17024500
H	3.67428700	1.32088900	-0.30245400
N	4.30743000	0.81648800	1.62171900
C	5.60630300	0.36441000	-0.42869000
H	4.92592500	1.62434000	1.75544200
H	3.39355800	1.03184600	2.03711400
H	4.72182100	0.03346300	2.14246200
O	6.57448800	0.55163300	0.35019500
O	5.65418000	0.09502600	-1.65337000

Product:

C	0.77263900	-1.49754200	2.25626700
C	-0.56778800	-1.45318800	2.53510500
C	-1.41139300	-0.76792100	1.64373100
C	-0.89093400	-0.25622400	0.36490900
C	0.57456000	-0.27215400	0.20199800
H	-0.98210700	-1.89031500	3.43765200
O	0.02544700	1.16776600	-2.70359600
H	-0.73501000	1.58356700	-2.17894500
H	-0.08180300	1.49503200	-3.61071300
I	-1.65444300	-1.71225700	-1.10333500
H	-1.37424900	0.67055700	0.03995600
O	-1.87781100	2.29713500	-1.27873500
H	-2.28258800	2.95308700	-1.86737700
H	1.42705200	-2.00976000	2.95843500
H	0.94375300	0.19501000	-0.70776500
O	-2.67519100	-0.56581100	1.86355300
H	-2.97549300	-0.95655100	2.70971300
O	-0.06688100	3.49311900	0.22191800
H	-0.76618400	3.08457800	-0.38067400
H	-0.12438100	2.95851900	1.04038400
O	-3.16666400	2.27814400	0.93820300
H	-3.59836400	3.13507700	1.08308700
H	-2.68914200	2.34814100	0.02862500
O	-0.86929400	1.88479700	2.41778300
H	-0.83796100	2.41552800	3.22965100
H	-1.76176200	2.05373500	2.02798100
O	1.93416100	2.71234000	-1.44784000
H	1.28549200	3.07213800	-0.79174700
H	1.37732800	2.10267100	-1.98781200
O	-4.83035800	0.29466100	-0.08496400
H	-4.27703100	0.98655300	0.34342400
H	-4.24442100	-0.47892900	-0.12992600
C	1.38203500	-0.89312000	1.09782500
C	2.87775800	-1.05663900	0.96302000
H	3.34318600	-0.89355200	1.94394300
H	3.08697900	-2.09585200	0.68769800
C	3.55889700	-0.15842100	-0.05878300
H	3.10158700	-0.26362600	-1.04705200
N	3.45342700	1.27805600	0.33576000
C	5.05350000	-0.53195500	-0.20472200
H	4.41447100	1.65359400	0.37267500
H	2.88772000	1.83402600	-0.35803500
H	3.03193500	1.39634400	1.26288100

O	5.89528900	0.37415600	0.02592100
O	5.28715700	-1.71423000	-0.54920500

Tyr-C3-cs-n2

Reactant:

C	1.32196800	0.03572700	-0.57005000
C	0.49926300	0.41480700	-1.65666200
C	-0.83015900	0.08694100	-1.62310200
C	-0.67993500	-1.05841600	0.48029700
C	0.77942600	-0.84727000	0.48675400
H	0.92466400	0.97675200	-2.48129200
H	-1.45056500	0.38356300	-2.46735900
H	-1.09563500	-1.61900600	1.31374400
H	1.19304400	-0.60830500	1.46967000
O	2.54678100	0.40433600	-0.43735300
O	-0.28336100	1.53829500	2.65863100
H	-0.34440100	0.58808000	2.84468800
H	0.64958200	1.70037500	2.40037000
I	1.65934900	-2.81677400	0.06522900
O	4.70681200	3.02198400	0.37211800
H	3.94083100	2.72361000	0.89816700
H	4.45247300	2.82741900	-0.54708000
O	-1.34186000	2.77482600	0.42092400
H	-0.49194100	2.96020900	-0.03184600
H	-1.08314600	2.23197900	1.19923500
O	2.42140000	2.00819100	1.90988400
H	2.77949800	2.25560900	2.77980600
H	2.75868200	1.11225300	1.73298100
O	1.30140500	3.32418600	-0.37773000
H	1.68731000	2.90538100	0.42068100
H	1.37973700	4.27968200	-0.21800900
O	3.21106500	2.28192800	-1.98335800
H	2.47392900	2.85820100	-1.66291600
H	3.05761800	2.12467000	-2.93046900
H	2.85988300	1.08848500	-1.16282400
C	-1.46204400	-0.61903500	-0.53443800
C	-2.95289400	-0.84956000	-0.54384400
H	-3.29990500	-1.02463600	-1.56969500
H	-3.18565600	-1.73852000	0.04535800
C	-3.74629800	0.30993800	0.05886200
C	-5.25916000	0.00871200	0.15262600
O	-5.57071900	-1.10526900	0.63719000
O	-6.04202600	0.91473100	-0.23266000

N	**-3.54763400**	**1.56303400**	**-0.72527600**
H	**-3.52914300**	**1.37435200**	**-1.73451300**
H	**-4.35362400**	**2.17933700**	**-0.55573100**
H	**-2.66578700**	**2.05189200**	**-0.43936700**
H	**-3.38645800**	**0.51965900**	**1.07235200**

TS:

C	**1.01804900**	**0.19513100**	**-1.06319800**
C	**0.14192700**	**1.07824000**	**-1.72082100**
C	**-1.21266900**	**0.83199500**	**-1.70225600**
C	**-0.95601800**	**-1.14421600**	**-0.37859200**
C	**0.46633900**	**-0.89211600**	**-0.28802500**
H	**0.54808300**	**1.91838400**	**-2.27463100**
H	**-1.87033200**	**1.51360900**	**-2.23911400**
H	**-1.35331900**	**-2.00354300**	**0.15620500**
H	**0.50938500**	**-0.40119900**	**0.86315100**
O	**2.32231700**	**0.34945000**	**-1.08058200**
O	**0.64061800**	**0.06157500**	**2.24237500**
H	**0.67275900**	**-0.74623000**	**2.78641400**
H	**1.56519100**	**0.41737400**	**2.21393000**
I	**1.73214100**	**-2.57204500**	**0.04472700**
O	**4.93358900**	**2.92144900**	**0.38566400**
H	**4.35627300**	**2.30899300**	**0.88034700**
H	**4.48849200**	**3.00483800**	**-0.47735200**
O	**-1.07528400**	**2.15856800**	**1.40670500**
H	**-0.28816200**	**2.53398500**	**0.95635700**
H	**-0.72544400**	**1.35823100**	**1.84128700**
O	**3.12170200**	**0.97833100**	**1.57776000**
H	**3.77429800**	**0.57009800**	**2.17265400**
H	**3.13273100**	**0.44396800**	**0.75934200**
O	**1.44763000**	**3.08401400**	**0.52076800**
H	**2.01293500**	**2.47023000**	**1.03161000**
H	**1.54546400**	**3.94211400**	**0.96661400**
O	**2.99205900**	**2.77606500**	**-1.70766000**
H	**2.35790700**	**3.13766500**	**-1.04279500**
H	**2.67857800**	**3.07269000**	**-2.57818600**
H	**2.59926900**	**1.25248000**	**-1.45909000**
C	**-1.79377500**	**-0.27318600**	**-1.02048700**
C	**-3.29156700**	**-0.44841500**	**-0.98215300**
H	**-3.74308800**	**-0.02987000**	**-1.88951600**
H	**-3.54266100**	**-1.51037100**	**-0.94009800**
C	**-3.92383700**	**0.21582300**	**0.24275200**
C	**-5.45534000**	**0.02838000**	**0.28602800**
O	**-5.86547500**	**-1.15040900**	**0.15604000**

O	**-6.15143200**	**1.05937800**	**0.46871500**
N	**-3.60860100**	**1.67367600**	**0.27145200**
H	**-3.74459300**	**2.09845300**	**-0.65361700**
H	**-4.26745600**	**2.14213800**	**0.90515700**
H	**-2.63238900**	**1.86161600**	**0.59435600**
H	**-3.50164700**	**-0.21019400**	**1.15848700**

Product:

C	**0.99558700**	**0.26191400**	**-1.18140600**
C	**0.16930300**	**1.24500200**	**-1.72753900**
C	**-1.20993100**	**1.06369300**	**-1.74684300**
C	**-0.95502400**	**-1.07647200**	**-0.68296800**
C	**0.42922700**	**-0.91590600**	**-0.68082500**
H	**0.61420300**	**2.14824700**	**-2.13540900**
H	**-1.84182900**	**1.83677200**	**-2.17801100**
H	**-1.39021300**	**-1.98797000**	**-0.28080200**
H	**0.57311800**	**-1.15072700**	**2.36065300**
O	**2.35756000**	**0.42240300**	**-1.11628000**
O	**0.70139900**	**-0.19920600**	**2.53775000**
H	**0.76760800**	**-0.11077700**	**3.50601300**
H	**1.91139000**	**0.21988600**	**1.93191800**
I	**1.65008300**	**-2.47756500**	**0.00888300**
O	**5.05323500**	**2.40466000**	**0.38220900**
H	**4.42831400**	**2.12451200**	**1.06979700**
H	**4.48470700**	**2.65003800**	**-0.37259800**
O	**-0.92320600**	**1.90428700**	**1.55069900**
H	**-0.17103000**	**2.37274800**	**1.13064100**
H	**-0.53723200**	**1.06183200**	**1.85954200**
O	**2.80339600**	**0.58849800**	**1.46358200**
H	**3.54474600**	**0.01501000**	**1.74973400**
H	**2.71140800**	**0.47278100**	**0.45774500**
O	**1.48795000**	**3.15749000**	**0.70842100**
H	**2.09726100**	**2.64530400**	**1.27007000**
H	**1.45978200**	**4.03954400**	**1.11614800**
O	**3.03914600**	**2.95727100**	**-1.54411800**
H	**2.40286100**	**3.25027900**	**-0.85054700**
H	**2.74007700**	**3.35215100**	**-2.37952100**
H	**2.61817100**	**1.33598100**	**-1.42922100**
C	**-1.79090700**	**-0.08782900**	**-1.20978600**
C	**-3.28912400**	**-0.25144200**	**-1.14357300**
H	**-3.77110000**	**0.33903600**	**-1.93228500**
H	**-3.56553300**	**-1.29813400**	**-1.29093200**
C	**-3.85579800**	**0.18186900**	**0.21060200**
C	**-5.38491500**	**0.00077600**	**0.29424800**

O	-5.81634000	-1.14040300	-0.00148200
O	-6.06165300	0.99466800	0.66344500
N	-3.51257400	1.60958800	0.47678500
H	-3.68160700	2.18538600	-0.35675100
H	-4.12900600	1.97160400	1.21361800
H	-2.51738400	1.72603000	0.77174000
H	-3.39747800	-0.40269800	1.01489300

Tyr-C3-cm-n

Reactant:

C	-1.47159200	0.50127300	0.71519900
C	-2.23723400	1.50806200	-1.32739600
C	-1.26011100	2.49966500	-1.21749700
C	-0.38893400	2.48159500	-0.13371900
C	-0.48879000	1.48282500	0.84208600
H	0.19821100	1.48736200	1.68521100
O	3.24830800	2.34801900	0.34963100
H	2.35305700	2.59746400	0.05021000
O	0.67404100	-0.86055900	3.10783400
H	-0.06563100	-0.26064300	3.29089400
H	3.59575400	1.68867600	-0.29305000
O	2.91842500	0.64828500	2.44424200
H	3.20561800	1.10930800	3.24926200
H	2.96607000	1.32232800	1.71732800
H	1.40854000	-0.27571800	2.82075000
H	-1.16891700	3.27515600	-1.97340600
O	4.64161200	0.39108700	-1.09193700
H	4.07066800	-0.21264800	-1.60356500
H	4.82425400	-0.09236000	-0.25477500
O	2.62941100	-1.46400200	-1.92650700
H	2.18904300	-1.85286000	-2.70404300
O	4.91377100	-0.89474400	1.37335500
H	4.24134400	-0.37500200	1.87530400
H	5.76098500	-0.75696800	1.82587200
I	1.22369000	-0.60881900	-0.78568900
H	-2.91356700	1.52180400	-2.17922200
H	-1.54861300	-0.27761700	1.47111900
O	0.61062800	3.40759500	0.01912400
H	0.59255500	4.04627900	-0.71528600
O	4.03159400	-3.11324300	-0.10677900
H	3.54156100	-2.63439000	-0.80430200
H	4.35955800	-2.40609700	0.48490200

C	-2.35673200	0.49717500	-0.37264300
C	-3.43077300	-0.55726100	-0.48060300
H	-3.84421000	-0.56972400	-1.49635700
H	-3.01651200	-1.54874800	-0.27526300
C	-4.57468700	-0.33597600	0.51397600
H	-4.20372100	-0.37085500	1.54136800
N	-5.15304700	1.02768000	0.31603100
C	-5.68883800	-1.38248900	0.33696500
H	-5.97915000	1.16199400	0.90952900
H	-4.46868700	1.76153700	0.53516600
H	-5.45838900	1.15268100	-0.65719100
O	-6.81592400	-0.96543500	-0.03161800
O	-5.35660800	-2.57031300	0.57148500

TS:

0 1

C	-1.66391100	-0.12679400	-0.25309200
C	-2.79758100	1.79587300	-1.12213500
C	-1.62668400	2.54266600	-1.04938600
C	-0.46309400	1.93440500	-0.57593900
C	-0.44959400	0.58553600	-0.16609600
H	0.12345800	0.48890100	1.08063800
O	3.53715300	2.30205800	-0.12994600
H	2.63398100	2.20818500	-0.48724700
O	0.50200300	0.51358300	2.26961500
H	-0.00708300	1.22675400	2.69900100
H	4.04555700	1.52606600	-0.47242800
O	3.02877500	1.22097500	2.28894600
H	3.18300000	1.87117200	2.99463500
H	3.21080900	1.69685900	1.43225300
H	1.47189000	0.80516600	2.28299300
H	-1.61025900	3.58379900	-1.36079400
O	5.07828100	0.10530300	-0.78019100
H	4.45067700	-0.58001100	-1.12717100
H	5.22532900	-0.14933900	0.15570500
O	3.24357400	-1.75932400	-1.45829500
H	3.08657400	-2.08334800	-2.35960800
O	5.10267500	-0.58296200	1.95692000
H	4.39314500	0.04917000	2.21270900
H	5.86103900	-0.38484200	2.52868000
I	1.45630400	-0.64544600	-0.77962500
H	-3.70232200	2.26735800	-1.50061800
H	-1.67617400	-1.17079300	0.05937900
O	0.70481600	2.62645800	-0.47398600

H	0.57706500	3.55371200	-0.74134500
O	4.05769500	-2.98110100	0.84687100
H	3.75703000	-2.63901500	-0.02762800
H	4.44398500	-2.20282500	1.29442800
C	-2.83987100	0.45051600	-0.72119700
C	-4.12560300	-0.34020400	-0.76786000
H	-4.82797500	0.11620500	-1.47635700
H	-3.92843300	-1.36162400	-1.10492800
C	-4.80780700	-0.45088500	0.59905200
H	-4.12502400	-0.88365200	1.33434300
N	-5.16735500	0.91133800	1.09558600
C	-6.08509200	-1.30551000	0.51755000
H	-5.65709000	0.85487900	1.99564700
H	-4.33551600	1.50136600	1.21725200
H	-5.80271400	1.37725700	0.43623000
O	-7.18237800	-0.71607600	0.68514400
O	-5.90361000	-2.52337900	0.27240600

Product

C	-1.38147700	0.51406000	-0.99469700
C	-2.46865500	2.32486800	0.15115200
C	-1.22910500	2.83907800	0.52333300
C	-0.05730600	2.18396900	0.14712700
C	-0.13625900	1.00680900	-0.60649000
H	-1.20501000	-0.64107400	1.05016400
O	2.37754700	0.97911300	2.50099600
H	1.98691600	1.48271100	1.76102700
O	-1.35920800	-0.56750500	2.00989100
H	-1.14526900	0.36312700	2.20458500
H	3.89282800	0.31106500	1.77302800
O	1.20659300	-1.56083700	2.52664900
H	1.29389600	-1.89995200	3.43246300
H	1.91306600	0.11275000	2.50354600
H	0.25801800	-1.32622800	2.41852700
H	-1.15966900	3.74994500	1.11254500
O	4.63931200	-0.21596500	1.40558400
H	5.02576700	0.41059700	-0.18901000
H	4.23723700	-1.09134900	1.21535300
O	5.19082000	0.60941800	-1.14374900
H	6.15460000	0.57060500	-1.24877600
O	3.22393400	-2.61638200	0.90511200
H	2.42853200	-2.32052000	1.40139000
H	3.61604300	-3.32598800	1.43918500
I	1.60262800	-0.06160500	-1.08067000

H	-3.37408200	2.84148700	0.46028700
H	-1.43504700	-0.40052900	-1.58132900
O	1.17723800	2.65525300	0.49975600
H	1.08321100	3.47917100	1.01049800
O	4.12579000	-1.94417200	-1.71513100
H	4.53865000	-1.06262900	-1.58979500
H	3.82940300	-2.21535000	-0.82395000
C	-2.56298100	1.16060000	-0.61418200
C	-3.90302600	0.56144400	-0.96559900
H	-4.69346800	1.31160400	-0.84325700
H	-3.91480000	0.22990500	-2.00686300
C	-4.23935100	-0.65623200	-0.10271800
H	-3.48555600	-1.43821700	-0.24167200
N	-4.20678100	-0.29634100	1.34733500
C	-5.61760700	-1.26241500	-0.43882000
H	-4.79248800	-0.96565200	1.86388600
H	-3.24027400	-0.31431400	1.72158400
H	-4.60620900	0.63605300	1.50808400
O	-6.38809200	-1.50000200	0.52689400
O	-5.83437200	-1.48778200	-1.65374600

Tyr-C3-ms

Reactant:

C	-0.16351500	1.26895800	1.18838700
C	-0.75244000	1.86857400	0.07096000
C	-1.89915100	1.30759200	-0.48632800
C	-2.48328800	0.15453300	0.05107700
C	-1.88696700	-0.42849300	1.17351500
C	-0.73246400	0.11328500	1.74027000
H	-0.31321200	2.76663100	-0.35423400
H	-0.27129100	-0.33985000	2.61400500
O	4.72160100	1.38149500	-0.22634700
H	5.55656000	1.86354100	-0.33951100
O	2.38987400	2.89971700	-0.16334600
H	3.26116900	2.44853700	-0.09399400
O	3.06698500	-2.09062700	-0.89718300
H	4.51887000	0.97790500	-1.10364200
H	2.82026900	-2.94011100	-1.30591600
O	3.79918000	0.06930500	-2.45581800
H	3.63227000	-0.81455900	-2.05930900
H	4.37758500	-0.07862200	-3.22111100
H	1.98840800	2.51086000	-0.97544500

I	**1.41871000**	**-1.27432200**	**-0.09833000**
O	**4.76909900**	**-1.03150800**	**1.16389200**
H	**4.32666600**	**-1.60671700**	**0.51134200**
H	**4.86003700**	**-0.16985800**	**0.69963300**
H	**-2.34862500**	**1.77690400**	**-1.35910900**
O	**1.49643300**	**1.65009900**	**-2.49883900**
H	**2.28157400**	**1.06405300**	**-2.58016000**
H	**1.60301600**	**2.31203700**	**-3.20089200**
H	**-2.32199700**	**-1.32530600**	**1.60936700**
O	**0.96526700**	**1.77230000**	**1.76648900**
H	**1.49443500**	**2.27817600**	**1.08102300**
C	**-3.75461800**	**-0.41821300**	**-0.52749400**
H	**-3.89045700**	**-0.07586900**	**-1.56090000**
H	**-3.71134500**	**-1.51096300**	**-0.54003100**
C	**-4.99579900**	**-0.03396200**	**0.28460200**
H	**-4.89265000**	**-0.36428900**	**1.32120700**
N	**-5.13110300**	**1.45342300**	**0.32186500**
C	**-6.27519600**	**-0.63748200**	**-0.32027300**
H	**-5.97382600**	**1.73163700**	**0.83650700**
H	**-4.31716000**	**1.89315400**	**0.76865100**
H	**-5.22054800**	**1.83074200**	**-0.62949300**
O	**-7.11632300**	**0.16219600**	**-0.80309000**
O	**-6.35055400**	**-1.89041800**	**-0.28396200**
O	**2.90954300**	**0.05223100**	**3.01543500**
H	**2.23500200**	**0.54634500**	**2.50971200**
H	**3.48312900**	**-0.37633600**	**2.34461100**

TS:

C	**-0.00601000**	**1.32678500**	**-1.02129100**
C	**0.73616000**	**2.00292000**	**0.01330300**
C	**1.87535100**	**1.44765100**	**0.51443400**
C	**2.38426600**	**0.16584800**	**0.08870300**
C	**1.66944800**	**-0.53786700**	**-0.82851900**
C	**0.39186400**	**-0.05437900**	**-1.34097400**
H	**0.39312800**	**2.98279000**	**0.33314100**
H	**0.12559700**	**-0.37226100**	**-2.34877800**
O	**-4.61685300**	**1.19201200**	**0.43228000**
H	**-5.41462500**	**1.67296000**	**0.70937000**
O	**-2.58694100**	**2.69440400**	**0.34965200**
H	**-3.46336800**	**2.13081700**	**0.28666000**
O	**-3.12273500**	**-2.19339000**	**1.00662400**
H	**-4.30780600**	**0.63860500**	**1.23822900**
H	**-2.80613100**	**-2.93745600**	**1.54411900**
O	**-3.59458900**	**-0.23088200**	**2.31851100**

H	**-3.37593900**	**-1.28732000**	**1.71967700**
H	**-4.17675200**	**-0.39674700**	**3.07575600**
H	**-2.12193100**	**2.30843300**	**1.20379200**
I	**-1.20784800**	**-1.16442900**	**-0.12816000**
O	**-4.68227300**	**-1.15567200**	**-1.11357000**
H	**-4.17501200**	**-1.70192800**	**-0.47821900**
H	**-4.82978500**	**-0.31770100**	**-0.62696500**
H	**2.44040700**	**1.99366500**	**1.26845000**
O	**-1.68040600**	**1.58831100**	**2.44109400**
H	**-2.38517600**	**0.87241200**	**2.50704500**
H	**-1.83124600**	**2.18209000**	**3.19550200**
H	**2.01533900**	**-1.50913900**	**-1.17611800**
O	**-0.99513800**	**1.86504200**	**-1.59158400**
H	**-2.00786800**	**2.46057900**	**-0.44118300**
C	**3.69582200**	**-0.34321500**	**0.63970100**
H	**3.90972000**	**0.13400500**	**1.60417400**
H	**3.64093600**	**-1.42172700**	**0.80756500**
C	**4.88040400**	**-0.10461500**	**-0.30136900**
H	**4.70976300**	**-0.60093500**	**-1.26009300**
N	**5.01884300**	**1.35406800**	**-0.59597800**
C	**6.19805400**	**-0.61435600**	**0.31085900**
H	**5.87349200**	**1.53342100**	**-1.13492600**
H	**4.21825600**	**1.71272300**	**-1.12930900**
H	**5.09605000**	**1.89546200**	**0.27416800**
O	**7.09214600**	**0.23841800**	**0.54118900**
O	**6.24966000**	**-1.84940700**	**0.52948900**
O	**-3.03731600**	**0.34960800**	**-2.91046000**
H	**-2.31054500**	**0.77895200**	**-2.41561700**
H	**-3.48905300**	**-0.23560400**	**-2.26700100**

Product:

C	**-0.11336200**	**1.40320600**	**0.92146000**
C	**-0.93108800**	**2.04149800**	**-0.09785700**
C	**-2.03229800**	**1.41208500**	**-0.56977100**
C	**-2.44309400**	**0.07911100**	**-0.13765400**
C	**-1.64462200**	**-0.61288400**	**0.70071200**
C	**-0.36317900**	**-0.05789100**	**1.18611600**
H	**-0.66169000**	**3.04634500**	**-0.40868400**
H	**-0.12892700**	**-0.31957900**	**2.21910100**
O	**4.62539100**	**1.34464000**	**-0.47458400**
H	**5.41777800**	**1.83705500**	**-0.74228800**
O	**2.41484700**	**2.90151000**	**-0.67128200**
H	**3.87234300**	**1.98972400**	**-0.49810900**
O	**4.29621800**	**-2.63869000**	**-0.43012600**

H	4.12911500	0.11688200	-1.64532500
H	3.50448000	-3.16653300	-0.23863800
O	3.69573800	-0.56690100	-2.21316200
H	4.02303800	-1.99980600	-1.12676400
H	4.25968200	-0.64433600	-3.00020300
H	1.98534000	2.32946300	-1.34983300
I	1.24196600	-1.03810800	0.04984600
O	4.68684400	-0.61470600	1.50357800
H	4.48225800	-1.39444000	0.94310000
H	4.72792900	0.12955700	0.86484000
H	-2.65872400	1.91792300	-1.30322800
O	1.56990500	1.22603500	-2.72632200
H	2.26540400	0.53932000	-2.61444000
H	1.83840200	1.72759200	-3.51328400
H	-1.90422200	-1.61798300	1.02429600
O	0.77635000	2.00871800	1.53334400
H	1.91590400	2.74969600	0.15349500
C	-3.75825200	-0.47996900	-0.62415100
H	-3.98853000	-0.08929700	-1.62340600
H	-3.69618900	-1.56809000	-0.69535000
C	-4.92760800	-0.16625600	0.31287200
H	-4.73143400	-0.57082800	1.30951900
N	-5.08586800	1.31135900	0.48115100
C	-6.25632200	-0.74900000	-0.20868700
H	-5.97248300	1.51672200	0.95618400
H	-4.31975300	1.72143200	1.02806300
H	-5.12214300	1.78399000	-0.43104600
O	-7.20517000	0.05665400	-0.38236300
O	-6.26350700	-1.98813600	-0.40505500
O	2.65565100	0.47032800	3.10936700
H	2.04101000	0.95761200	2.52730600
H	3.29912200	0.03276300	2.50943600

Tyr-C3-cm-a

Reactant:

C	-1.47159200	0.50127300	0.71519900
C	-2.23723400	1.50806200	-1.32739600
C	-1.26011100	2.49966500	-1.21749700
C	-0.38893400	2.48159500	-0.13371900
C	-0.48879000	1.48282500	0.84208600
H	0.19821100	1.48736200	1.68521100
O	3.24830800	2.34801900	0.34963100

H	2.35305700	2.59746400	0.05021000
O	0.67404100	-0.86055900	3.10783400
H	-0.06563100	-0.26064300	3.29089400
H	3.59575400	1.68867600	-0.29305000
O	2.91842500	0.64828500	2.44424200
H	3.20561800	1.10930800	3.24926200
H	2.96607000	1.32232800	1.71732800
H	1.40854000	-0.27571800	2.82075000
H	-1.16891700	3.27515600	-1.97340600
O	4.64161200	0.39108700	-1.09193700
H	4.07066800	-0.21264800	-1.60356500
H	4.82425400	-0.09236000	-0.25477500
O	2.62941100	-1.46400200	-1.92650700
H	2.18904300	-1.85286000	-2.70404300
O	4.91377100	-0.89474400	1.37335500
H	4.24134400	-0.37500200	1.87530400
H	5.76098500	-0.75696800	1.82587200
I	1.22369000	-0.60881900	-0.78568900
H	-2.91356700	1.52180400	-2.17922200
H	-1.54861300	-0.27761700	1.47111900
O	0.61062800	3.40759500	0.01912400
H	0.59255500	4.04627900	-0.71528600
O	4.03159400	-3.11324300	-0.10677900
H	3.54156100	-2.63439000	-0.80430200
H	4.35955800	-2.40609700	0.48490200
C	-2.35673200	0.49717500	-0.37264300
C	-3.43077300	-0.55726100	-0.48060300
H	-3.84421000	-0.56972400	-1.49635700
H	-3.01651200	-1.54874800	-0.27526300
C	-4.57468700	-0.33597600	0.51397600
H	-4.20372100	-0.37085500	1.54136800
N	-5.15304700	1.02768000	0.31603100
C	-5.68883800	-1.38248900	0.33696500
H	-5.97915000	1.16199400	0.90952900
H	-4.46868700	1.76153700	0.53516600
H	-5.45838900	1.15268100	-0.65719100
O	-6.81592400	-0.96543500	-0.03161800
O	-5.35660800	-2.57031300	0.57148500

TS:

C	-1.66391100	-0.12679400	-0.25309200
C	-2.79758100	1.79587300	-1.12213500
C	-1.62668400	2.54266600	-1.04938600
C	-0.46309400	1.93440500	-0.57593900

C	-0.44959400	0.58553600	-0.16609600
H	0.12345800	0.48890100	1.08063800
O	3.53715300	2.30205800	-0.12994600
H	2.63398100	2.20818500	-0.48724700
O	0.50200300	0.51358300	2.26961500
H	-0.00708300	1.22675400	2.69900100
H	4.04555700	1.52606600	-0.47242800
O	3.02877500	1.22097500	2.28894600
H	3.18300000	1.87117200	2.99463500
H	3.21080900	1.69685900	1.43225300
H	1.47189000	0.80516600	2.28299300
H	-1.61025900	3.58379900	-1.36079400
O	5.07828100	0.10530300	-0.78019100
H	4.45067700	-0.58001100	-1.12717100
H	5.22532900	-0.14933900	0.15570500
O	3.24357400	-1.75932400	-1.45829500
H	3.08657400	-2.08334800	-2.35960800
O	5.10267500	-0.58296200	1.95692000
H	4.39314500	0.04917000	2.21270900
H	5.86103900	-0.38484200	2.52868000
I	1.45630400	-0.64544600	-0.77962500
H	-3.70232200	2.26735800	-1.50061800
H	-1.67617400	-1.17079300	0.05937900
O	0.70481600	2.62645800	-0.47398600
H	0.57706500	3.55371200	-0.74134500
O	4.05769500	-2.98110100	0.84687100
H	3.75703000	-2.63901500	-0.02762800
H	4.44398500	-2.20282500	1.29442800
C	-2.83987100	0.45051600	-0.72119700
C	-4.12560300	-0.34020400	-0.76786000
H	-4.82797500	0.11620500	-1.47635700
H	-3.92843300	-1.36162400	-1.10492800
C	-4.80780700	-0.45088500	0.59905200
H	-4.12502400	-0.88365200	1.33434300
N	-5.16735500	0.91133800	1.09558600
C	-6.08509200	-1.30551000	0.51755000
H	-5.65709000	0.85487900	1.99564700
H	-4.33551600	1.50136600	1.21725200
H	-5.80271400	1.37725700	0.43623000
O	-7.18237800	-0.71607600	0.68514400
O	-5.90361000	-2.52337900	0.27240600

Product:

C	-1.38147700	0.51406000	-0.99469700

C	-2.46865500	2.32486800	0.15115200
C	-1.22910500	2.83907800	0.52333300
C	-0.05730600	2.18396900	0.14712700
C	-0.13625900	1.00680900	-0.60649000
H	-1.20501000	-0.64107400	1.05016400
O	2.37754700	0.97911300	2.50099600
H	1.98691600	1.48271100	1.76102700
O	-1.35920800	-0.56750500	2.00989100
H	-1.14526900	0.36312700	2.20458500
H	3.89282800	0.31106500	1.77302800
O	1.20659300	-1.56083700	2.52664900
H	1.29389600	-1.89995200	3.43246300
H	1.91306600	0.11275000	2.50354600
H	0.25801800	-1.32622800	2.41852700
H	-1.15966900	3.74994500	1.11254500
O	4.63931200	-0.21596500	1.40558400
H	5.02576700	0.41059700	-0.18901000
H	4.23723700	-1.09134900	1.21535300
O	5.19082000	0.60941800	-1.14374900
H	6.15460000	0.57060500	-1.24877600
O	3.22393400	-2.61638200	0.90511200
H	2.42853200	-2.32052000	1.40139000
H	3.61604300	-3.32598800	1.43918500
I	1.60262800	-0.06160500	-1.08067000
H	-3.37408200	2.84148700	0.46028700
H	-1.43504700	-0.40052900	-1.58132900
O	1.17723800	2.65525300	0.49975600
H	1.08321100	3.47917100	1.01049800
O	4.12579000	-1.94417200	-1.71513100
H	4.53865000	-1.06262900	-1.58979500
H	3.82940300	-2.21535000	-0.82395000
C	-2.56298100	1.16060000	-0.61418200
C	-3.90302600	0.56144400	-0.96559900
H	-4.69346800	1.31160400	-0.84325700
H	-3.91480000	0.22990500	-2.00686300
C	-4.23935100	-0.65623200	-0.10271800
H	-3.48555600	-1.43821700	-0.24167200
N	-4.20678100	-0.29634100	1.34733500
C	-5.61760700	-1.26241500	-0.43882000
H	-4.79248800	-0.96565200	1.86388600
H	-3.24027400	-0.31431400	1.72158400
H	-4.60620900	0.63605300	1.50808400
O	-6.38809200	-1.50000200	0.52689400
O	-5.83437200	-1.48778200	-1.65374600

Tyr-C3-cs-a1

Reactant:

C	1.60996700	1.14260800	-0.98149500
C	2.04731300	0.42782200	0.13760100
C	1.45843200	0.73800800	1.37559000
C	0.46164700	1.69664700	1.49439300
C	-0.01558800	2.41660000	0.36361600
C	0.60294100	2.10787400	-0.88528700
H	0.29866500	2.67065500	-1.76565200
O	-4.20221000	-1.86119200	1.98377400
H	-4.97377700	-2.28455700	2.39197700
O	-1.69496900	-0.69900600	2.51724800
H	-2.53626500	-1.19630900	2.45783600
O	-3.16828700	-1.03178900	-1.68168500
H	-4.54032500	-1.11004200	1.43362500
H	-2.98216400	-1.82354000	-1.10740700
O	-4.70499000	0.24706600	0.33474200
H	-4.27220500	-0.15422200	-0.44890700
H	-4.03298200	0.85293600	0.72862900
H	-1.09689700	-1.12416300	1.86705300
H	0.01768500	1.90599200	2.46534400
I	-1.55992800	0.14890900	-1.45784800
H	1.78556700	0.19746200	2.26370300
H	2.05251700	0.93542000	-1.95524800
O	-0.98999800	3.28114000	0.45693200
O	-2.85930900	1.74665500	1.76626200
H	-2.22870300	2.33962000	1.28200600
H	-2.33506300	0.95152300	2.01131300
O	-2.57073300	-3.02318000	0.05707400
H	-1.66066600	-2.78395300	0.32423200
H	-3.14904300	-2.72344200	0.79392900
O	0.04364800	-2.12435400	0.74563100
H	0.78528200	-2.35017200	1.33198900
H	0.37172000	-1.39193000	0.19209500
C	3.14354600	-0.60569100	0.03009200
H	2.97346900	-1.26986600	-0.82296900
H	3.16160300	-1.22745100	0.93496400
C	4.53133700	0.01584300	-0.16269800
C	5.64025700	-1.04848300	-0.17314000
O	5.57329300	-1.89219900	-1.10152700
O	6.50180800	-0.99387700	0.74144000

H	**4.56738100**	**0.58748000**	**-1.09371500**
N	**4.79640000**	**0.98678100**	**0.94049300**
H	**4.74746100**	**0.51884500**	**1.85392800**
H	**5.73573300**	**1.39033700**	**0.85889200**
H	**4.10727000**	**1.74828000**	**0.93373000**

TS:

C	**-1.44957200**	**-0.88169400**	**-0.99466700**
C	**-2.02031200**	**-0.32453700**	**0.10266700**
C	**-1.50694500**	**-0.68751700**	**1.40958300**
C	**-0.51813800**	**-1.60031100**	**1.58973100**
C	**0.05903200**	**-2.29655000**	**0.45108200**
C	**-0.29897700**	**-1.78295500**	**-0.89390500**
H	**-0.21487900**	**-2.53217300**	**-1.68054200**
O	**4.11696300**	**2.08996600**	**1.68896200**
H	**4.80949100**	**2.32720200**	**2.32477700**
O	**1.73062800**	**0.87183200**	**2.39911300**
H	**2.56331000**	**1.36992400**	**2.22799500**
O	**3.52431100**	**0.94754700**	**-1.63107200**
H	**4.44617100**	**1.26783100**	**1.16075900**
H	**3.18205700**	**1.80588500**	**-1.30528800**
O	**4.73343100**	**0.04802800**	**0.27700100**
H	**4.10852500**	**0.51225200**	**-0.74140900**
H	**4.15615700**	**-0.62542500**	**0.68292000**
H	**1.08487100**	**1.22222800**	**1.75054400**
H	**-0.17060700**	**-1.87632700**	**2.58135200**
I	**1.50414400**	**-0.45268100**	**-1.31963600**
H	**-1.94823600**	**-0.20127600**	**2.27885700**
H	**-1.79998200**	**-0.62410300**	**-1.99232400**
O	**0.86278600**	**-3.23986000**	**0.59535600**
O	**2.92427800**	**-1.62036900**	**1.96990300**
H	**2.34643100**	**-2.24978700**	**1.49985600**
H	**2.38793600**	**-0.80017300**	**2.06528600**
O	**2.46876200**	**3.23590400**	**-0.23206900**
H	**1.57768300**	**2.93891300**	**0.03725200**
H	**3.05988700**	**2.97281100**	**0.50650100**
O	**-0.05397800**	**2.17493300**	**0.58863600**
H	**-0.89261300**	**2.43074700**	**1.00844400**
H	**-0.29542300**	**1.51412800**	**-0.08486300**
C	**-3.16378100**	**0.65825500**	**0.00008200**
H	**-3.01483900**	**1.32299500**	**-0.85480000**
H	**-3.20236500**	**1.28117900**	**0.90304700**
C	**-4.52627000**	**-0.01306300**	**-0.19473700**
C	**-5.66642700**	**1.02103000**	**-0.23056400**

O	**-5.59725100**	**1.87131800**	**-1.15160300**
O	**-6.55208200**	**0.93085700**	**0.65710700**
H	**-4.53453900**	**-0.59340500**	**-1.12090900**
N	**-4.78652700**	**-0.98108300**	**0.91381600**
H	**-4.68181800**	**-0.52670100**	**1.82954800**
H	**-5.74976700**	**-1.33184400**	**0.86490600**
H	**-4.14582500**	**-1.78241400**	**0.87575900**

Product:

C	**-1.44502100**	**-0.80514000**	**-1.01277600**
C	**-2.03773400**	**-0.28771000**	**0.08424600**
C	**-1.53420500**	**-0.65723000**	**1.40376200**
C	**-0.55188200**	**-1.56761500**	**1.59391800**
C	**0.03445300**	**-2.26044800**	**0.45319400**
C	**-0.28218300**	**-1.71274500**	**-0.91156900**
H	**-0.25634300**	**-2.49351300**	**-1.67236900**
O	**3.92574500**	**2.10175600**	**1.78243500**
H	**4.32143100**	**2.61232800**	**2.50327800**
O	**1.72921800**	**0.82543000**	**2.36815100**
H	**2.57954500**	**1.35246900**	**2.18852600**
O	**3.88960600**	**1.20471300**	**-1.69733500**
H	**4.57427500**	**0.76859200**	**1.12732900**
H	**3.39476000**	**1.93381500**	**-1.25727700**
O	**4.82731900**	**-0.06091500**	**0.61321800**
H	**4.27191300**	**0.69395700**	**-0.94662000**
H	**4.19164600**	**-0.73614800**	**0.92925400**
H	**1.08026300**	**1.15496900**	**1.71447100**
H	**-0.21081600**	**-1.84908100**	**2.58584600**
I	**1.49669000**	**-0.49001800**	**-1.37586200**
H	**-1.98718600**	**-0.17192300**	**2.26721100**
H	**-1.77648100**	**-0.53013900**	**-2.01165400**
O	**0.79305400**	**-3.22736600**	**0.58610200**
O	**2.89471600**	**-1.63713700**	**1.98939000**
H	**2.34029200**	**-2.26481700**	**1.49337200**
H	**2.35210000**	**-0.81441500**	**2.07563300**
O	**2.57768200**	**3.15437500**	**-0.17862300**
H	**1.65709400**	**2.88397300**	**-0.00240800**
H	**3.10387300**	**2.83279500**	**0.62510700**
O	**-0.04726300**	**2.17736900**	**0.53469100**
H	**-0.88245400**	**2.42250500**	**0.96747700**
H	**-0.29906500**	**1.54550000**	**-0.16159000**
C	**-3.19472100**	**0.67878200**	**-0.01353300**
H	**-3.06560000**	**1.32980900**	**-0.88169500**
H	**-3.22466900**	**1.31504600**	**0.88030500**

C	-4.55206000	-0.00949800	-0.17803400
C	-5.70323700	1.01382400	-0.22364000
O	-5.63430100	1.86571900	-1.14269700
O	-6.59793200	0.90962600	0.65318900
H	-4.56545100	-0.60689500	-1.09327700
N	-4.79730400	-0.95875100	0.95048100
H	-4.65688000	-0.49686700	1.85773500
H	-5.77047300	-1.28500900	0.93244200
H	-4.17843800	-1.77664500	0.90465400

Tyr-C3-cs-a2

Reactant:

C	-1.17735500	0.33051000	-0.46003200
C	-0.42688000	-0.19999500	-1.59210800
C	0.92278900	-0.12372900	-1.60216400
C	1.69774100	0.50271500	-0.53469900
C	1.05165700	1.13385800	0.46509500
C	-0.42522800	1.20437800	0.51497800
H	-0.98203200	-0.69624400	-2.38238400
H	1.47486000	-0.56081200	-2.43264600
H	1.59847800	1.62449200	1.26716500
H	-0.83142600	1.09208100	1.52141900
O	-2.37819100	0.10319700	-0.28915500
O	-1.89902200	-1.17463200	2.60049000
H	-2.72168600	-1.30744100	2.08130500
H	-1.16694400	-1.37911400	1.98533300
I	-0.99782600	3.25757800	-0.01228400
O	-3.84982800	-4.07401700	-0.04873400
H	-4.09405600	-4.81638900	0.52665900
H	-2.87659000	-4.11974100	-0.15507700
O	0.31092400	-2.09076100	1.01004500
H	-0.22749500	-2.53853300	0.31240800
H	0.45253300	-2.77637500	1.68529200
O	-4.33243200	-1.66634000	1.27205500
H	-4.92862000	-1.84030400	2.01767400
H	-4.18375100	-2.54521800	0.85460500
O	-1.24926300	-3.41193700	-0.83029600
H	-0.70856500	-3.93627300	-1.44268600
H	-1.82028900	-2.83809200	-1.39445200
O	-3.30474400	-1.95375000	-1.95031400
H	-3.92363600	-2.52108800	-1.45734600
H	-3.14731100	-1.17579500	-1.37374000
C	3.20076800	0.36560600	-0.54320200

H	**3.55890900**	**0.18289000**	**-1.56342300**
H	**3.66904200**	**1.28353800**	**-0.18092000**
C	**3.67863900**	**-0.77179100**	**0.36532500**
H	**3.40581400**	**-0.55879500**	**1.40312500**
N	**2.99257600**	**-2.04735700**	**0.00463000**
C	**5.20447600**	**-0.96700800**	**0.28289600**
H	**1.99287500**	**-2.04718600**	**0.30561100**
H	**3.03869400**	**-2.21637200**	**-1.00753500**
H	**3.47396000**	**-2.83584900**	**0.45195000**
O	**5.62229400**	**-2.10536100**	**-0.04858700**
O	**5.89580300**	**0.04350500**	**0.56196600**

TS:

C	**1.39589400**	**0.21108200**	**-0.94801500**
C	**0.39046400**	**1.14641600**	**-1.41479500**
C	**-0.93495100**	**0.82100200**	**-1.42292100**
C	**-1.43116100**	**-0.43598500**	**-0.93314300**
C	**-0.53303300**	**-1.30742000**	**-0.39185500**
C	**0.85992300**	**-0.94365500**	**-0.22582800**
H	**0.74114500**	**2.08032700**	**-1.84779600**
H	**-1.64915900**	**1.52943400**	**-1.84337100**
H	**-0.86742300**	**-2.26572200**	**-0.00033300**
H	**0.81376100**	**-0.36658500**	**0.94559600**
O	**2.62465400**	**0.43039000**	**-1.07844800**
O	**0.77355300**	**0.28304400**	**2.12892300**
H	**1.60683300**	**0.83376300**	**2.09862200**
H	**0.02451500**	**0.92268300**	**1.99680800**
I	**2.23257400**	**-2.52272000**	**0.14739600**
O	**2.15227300**	**3.85219000**	**0.27253100**
H	**2.43556100**	**4.68540000**	**0.68240500**
H	**1.17926300**	**3.93241700**	**0.15004400**
O	**-1.31603400**	**1.95906700**	**1.65811100**
H	**-1.03851000**	**2.69034100**	**1.05690400**
H	**-1.58445000**	**2.39185600**	**2.48588400**
O	**3.00654900**	**1.75235100**	**1.86490400**
H	**3.22777700**	**2.14861900**	**2.72297900**
H	**2.70005900**	**2.50437900**	**1.30496900**
O	**-0.59742000**	**3.97796900**	**-0.08386400**
H	**-0.99781100**	**4.84247300**	**0.10731500**
H	**-0.83853900**	**3.77936700**	**-1.00458600**
O	**3.41076400**	**2.91741500**	**-2.05824600**
H	**3.01867100**	**3.42899100**	**-1.32193100**
H	**3.16822500**	**1.99502100**	**-1.82207600**
C	**-2.89632700**	**-0.78828300**	**-1.04093300**

H	**-3.33356300**	**-0.31052900**	**-1.92736200**
H	**-3.00450200**	**-1.86876000**	**-1.16345300**
C	**-3.73025100**	**-0.39864100**	**0.18127600**
H	**-3.31147300**	**-0.85282100**	**1.08414700**
N	**-3.69325500**	**1.07810100**	**0.38805300**
C	**-5.19682900**	**-0.85167200**	**0.03689300**
H	**-2.80058000**	**1.39175600**	**0.82583600**
H	**-3.81817400**	**1.57357200**	**-0.50266900**
H	**-4.47712200**	**1.35892200**	**0.98841800**
O	**-6.08345700**	**0.03742900**	**0.10933300**
O	**-5.37219800**	**-2.08292000**	**-0.13684600**

Product:

C	**1.44690300**	**0.10789700**	**-0.91507300**
C	**0.53501700**	**1.11790500**	**-1.33833100**
C	**-0.83690200**	**0.90800700**	**-1.39270900**
C	**-1.41046100**	**-0.31205400**	**-1.00741600**
C	**-0.55066400**	**-1.31060700**	**-0.54056500**
C	**0.82731200**	**-1.10505200**	**-0.48543100**
H	**0.95396300**	**2.07149500**	**-1.65438600**
H	**-1.48283500**	**1.70771200**	**-1.75540100**
H	**-0.96369100**	**-2.26787400**	**-0.22922400**
H	**0.63932600**	**-0.11991800**	**1.50401000**
O	**2.73235000**	**0.28550800**	**-0.90635800**
O	**0.66016700**	**0.60741600**	**2.16595300**
H	**1.59694300**	**1.13646900**	**2.02609100**
H	**-0.09768900**	**1.25786100**	**1.90819200**
I	**2.07674800**	**-2.64594500**	**0.21888200**
O	**2.32979300**	**3.87013500**	**0.13845900**
H	**2.63211700**	**4.69287300**	**0.55651300**
H	**1.36503200**	**3.98834300**	**-0.01890700**
O	**-1.22693400**	**2.21362700**	**1.54961100**
H	**-0.93216600**	**2.88850400**	**0.88770100**
H	**-1.48491000**	**2.71190100**	**2.34421500**
O	**2.77940700**	**1.83478900**	**1.86284800**
H	**2.99305900**	**2.25867600**	**2.71223200**
H	**2.61006600**	**2.58034100**	**1.22383500**
O	**-0.40260100**	**4.08449000**	**-0.27259900**
H	**-0.76991100**	**4.97048200**	**-0.11567000**
H	**-0.62852900**	**3.87040400**	**-1.19392700**
O	**3.65553500**	**2.56843900**	**-1.99574100**
H	**3.26796300**	**3.21612300**	**-1.37614800**
H	**3.31776100**	**1.70305900**	**-1.63964300**
C	**-2.89295300**	**-0.57755200**	**-1.12031200**

H	-3.33160400	0.05472000	-1.90349900
H	-3.05952100	-1.61849600	-1.41202600
C	-3.68327100	-0.35431000	0.17252200
H	-3.22565400	-0.90072300	1.00156500
N	-3.65834400	1.09106600	0.53837600
C	-5.14613700	-0.80784200	0.01524900
H	-2.71506800	1.41595500	0.82926900
H	-3.97101900	1.66386300	-0.25411400
H	-4.31144400	1.27487600	1.30770200
O	-6.03477900	0.08086000	0.06430500
O	-5.31725000	-2.03993200	-0.16214900

Tyr-C5-cs-n1

Reactant:

C	-2.31234300	0.58900300	2.33679800
C	-1.28600100	1.39992200	2.80717300
C	-0.01692600	1.31948300	2.22539700
C	0.21113900	0.43240900	1.17206700
C	-0.82501400	-0.38863900	0.72616400
H	-1.45168100	2.09730900	3.62323800
O	1.91162400	-1.15402400	-1.31752100
H	2.87911200	0.39731300	-1.67635100
H	2.01555700	-1.69911900	-2.11985400
I	2.94409100	-2.04063900	0.13983400
H	1.18880200	0.38808200	0.69948200
O	3.38318500	1.23663800	-1.70486800
H	3.38619900	1.53699000	-0.77323000
H	-3.29856800	0.66187700	2.79081200
H	-0.63825700	-1.08415900	-0.09019700
O	0.96239300	2.13233700	2.72924000
H	1.80531500	1.98719300	2.24348100
O	1.43943900	2.82113200	-2.86363100
H	2.21061300	2.29027400	-2.55322500
H	0.73346500	2.15534600	-2.96268900
O	3.19105900	1.72887200	1.10776700
H	3.96650700	2.22558500	1.42052500
H	3.39730000	0.79270000	1.29060700
O	1.05363200	3.44336800	-0.15363200
H	1.16072500	3.34212100	-1.12609500
H	1.70584500	2.82736700	0.22586500
O	-0.14827000	0.47441500	-2.45774300
H	-0.87814700	-0.15014300	-2.60465900

H	**0.47732400**	**-0.00401700**	**-1.87783900**
O	**-1.49502500**	**2.42138600**	**-0.92402000**
H	**-0.99389700**	**1.77620800**	**-1.47014500**
H	**-0.80531800**	**2.78983600**	**-0.33579700**
C	**-2.09838000**	**-0.32198600**	**1.29352400**
C	**-3.23852600**	**-1.15083000**	**0.75470100**
H	**-2.85640200**	**-1.91601200**	**0.06757700**
H	**-3.76635000**	**-1.66306300**	**1.56427800**
C	**-4.27458300**	**-0.29677100**	**0.01665300**
H	**-4.71391400**	**0.43985300**	**0.69454900**
N	**-3.60860900**	**0.47381500**	**-1.07390000**
C	**-5.39795000**	**-1.16066800**	**-0.58235900**
H	**-4.30598400**	**0.97890700**	**-1.63124300**
H	**-2.91209800**	**1.15719300**	**-0.71855100**
H	**-3.12389900**	**-0.16352400**	**-1.71803400**
O	**-5.52846000**	**-1.15488400**	**-1.83302300**
O	**-6.08549100**	**-1.80655200**	**0.24779100**

TS:

C	**-1.51159400**	**-0.97079400**	**1.92698600**
C	**-0.32662000**	**-0.66525000**	**2.57408500**
C	**0.74189800**	**-0.15663800**	**1.83495400**
C	**0.63007500**	**-0.01051600**	**0.40722500**
C	**-0.64514300**	**-0.28562100**	**-0.19895800**
H	**-0.21229800**	**-0.80623300**	**3.64356300**
O	**1.51739000**	**-0.21395800**	**-2.13945400**
H	**2.99167000**	**0.48577800**	**-1.86104000**
H	**1.62159500**	**-0.74029100**	**-2.94940500**
I	**1.87845800**	**-1.99470100**	**-0.41666600**
H	**1.31170000**	**0.69059500**	**-0.07487900**
O	**3.84116900**	**0.97285400**	**-1.64480400**
H	**4.05745100**	**0.70872200**	**-0.73047500**
H	**-2.33997400**	**-1.36612600**	**2.51172100**
H	**-0.75223100**	**-0.11234400**	**-1.26428900**
O	**1.86241200**	**0.13368100**	**2.47600900**
H	**2.60958300**	**0.45267400**	**1.88293300**
O	**2.28588800**	**3.08495100**	**-0.65695200**
H	**2.94259000**	**2.42266300**	**-0.97201600**
H	**1.48278100**	**2.86018500**	**-1.17741500**
O	**3.94716500**	**1.04173300**	**1.16244700**
H	**3.87044200**	**2.01236200**	**1.18488900**
H	**4.69960100**	**0.83350400**	**1.74262000**
O	**1.10926600**	**3.02511900**	**1.83643200**
H	**1.66340200**	**2.94833100**	**1.02351400**

H	1.41602900	2.32643900	2.43659000
O	0.17715100	2.05831800	-2.20431700
H	0.27963200	2.51406800	-3.05479800
H	0.66907900	1.18325100	-2.28917700
O	-1.17023000	2.76228500	0.18678800
H	-0.71228400	2.53026000	-0.64885200
H	-0.47173000	2.72228400	0.87500400
C	-1.69574900	-0.77968900	0.53475700
C	-3.04521700	-1.03991000	-0.08220300
H	-2.95317100	-1.14312300	-1.16991000
H	-3.46922500	-1.96844500	0.30984200
C	-4.04206600	0.07994800	0.22896900
H	-4.10808000	0.24603300	1.30806900
N	-3.56991100	1.35823400	-0.37614800
C	-5.44678300	-0.25122100	-0.30961300
H	-4.28069800	2.08849100	-0.25914800
H	-2.67329000	1.70752600	0.02482000
H	-3.43640900	1.24217600	-1.38811900
O	-5.92547700	0.51538900	-1.18291700
O	-5.98571800	-1.27401500	0.18115300

Product:

C	-1.40908900	-1.01231700	1.85830400
C	-0.22983400	-0.71212200	2.48515900
C	0.86578800	-0.27326600	1.71155100
C	0.77659100	-0.27387800	0.23023800
C	-0.55774900	-0.54362500	-0.33963500
H	-0.11798200	-0.77027800	3.56199300
O	0.92379600	0.59764000	-2.89453600
H	2.42402000	0.85840300	-2.30437300
H	1.00075600	0.87567500	-3.82039700
I	2.01897500	-1.98710400	-0.37982700
H	1.28921600	0.58281500	-0.22553000
O	3.32942200	1.14042400	-1.95818400
H	3.48920900	0.62797200	-1.14576000
H	-2.25142200	-1.33516200	2.46757000
H	-0.64824600	-0.44906100	-1.41807700
O	1.94105400	0.10186800	2.31561800
H	2.71079300	0.41552800	1.69386200
O	2.02152500	3.19162900	-0.60457100
H	2.62646200	2.54938100	-1.04067000
H	1.13553900	2.95216700	-0.97780300
O	3.84280100	0.92405500	0.85052100
H	3.84038600	1.89807100	0.89003500

H	4.67981500	0.65044800	1.26586300
O	1.40878400	3.08328200	2.05826500
H	1.77254800	3.04176400	1.13981800
H	1.75837600	2.30426700	2.51858400
O	-0.33184700	2.27316000	-1.67189000
H	-0.65237900	2.95519300	-2.28218300
H	0.24483600	1.48940400	-2.29648400
O	-1.05720500	2.38024400	0.93736400
H	-0.75409200	2.36317700	-0.00575400
H	-0.25476300	2.59451100	1.46170800
C	-1.60558000	-0.91187600	0.43431000
C	-2.97804900	-1.15321600	-0.13751400
H	-2.92565000	-1.15615300	-1.23207200
H	-3.36054600	-2.12562400	0.18603500
C	-3.98487800	-0.09357100	0.31667500
H	-4.09818500	-0.10657300	1.40480000
N	-3.49069300	1.26747900	-0.04140300
C	-5.37180900	-0.31471200	-0.31901100
H	-4.24160900	1.95483900	0.08808300
H	-2.66495000	1.55807700	0.51596500
H	-3.22427600	1.30723000	-1.03372600
O	-5.87232400	0.64822600	-0.95270900
O	-5.87863800	-1.44808200	-0.13378800

Tyr-C5-cs-n2

Reactant:

C	-0.12591400	2.74450800	0.18145500
C	1.01815300	3.05187400	-0.57142100
C	1.94516200	2.06362400	-0.79136700
C	0.70063000	0.39436600	0.40417100
C	-0.38480900	1.36365200	0.62522400
H	1.15813500	4.06381400	-0.93397600
H	2.83729600	2.30942800	-1.36424200
H	0.55248800	-0.60562800	0.80401700
H	-0.82615600	1.30984400	1.62506400
O	-0.95348500	3.70751700	0.47218200
O	-1.35663400	-0.67847300	2.75188500
H	-1.34331600	-1.09875000	3.62694000
H	-1.17297500	-1.41100900	2.11302000
I	-2.03369700	0.67514500	-0.65831800
O	-0.00747100	-2.24973500	-1.61534000
H	0.23629200	-1.31041000	-1.66067700

H	**-0.93850300**	**-2.28178000**	**-1.94022700**
O	**-4.04288000**	**-0.39390100**	**2.15099400**
H	**-4.13870100**	**0.39508900**	**1.59253700**
H	**-3.08675400**	**-0.41155500**	**2.39680100**
O	**-1.07397600**	**-2.72896000**	**0.94438400**
H	**-2.02217400**	**-2.71512200**	**0.68457400**
H	**-0.58645700**	**-2.51867500**	**0.11755500**
O	**-3.78043000**	**-2.40969500**	**0.29085400**
H	**-4.34372000**	**-3.16095200**	**0.53677600**
H	**-3.97051700**	**-1.69536100**	**0.94776600**
O	**-2.69636700**	**-2.41776300**	**-2.28938000**
H	**-3.11709600**	**-2.33472000**	**-1.40622100**
H	**-2.87711600**	**-1.57329800**	**-2.73307000**
H	**-1.72612800**	**3.40496700**	**0.99498700**
C	**1.81370400**	**0.71595700**	**-0.29907200**
C	**2.91649000**	**-0.27722200**	**-0.55930100**
H	**3.21505900**	**-0.22808100**	**-1.61044800**
H	**2.55856700**	**-1.29333800**	**-0.35611400**
C	**4.16687000**	**-0.00729300**	**0.27915100**
C	**5.31609400**	**-0.96511200**	**-0.09380700**
O	**5.70895800**	**-0.89722800**	**-1.28322100**
O	**5.75088600**	**-1.71556700**	**0.81452000**
N	**3.84941900**	**-0.17338200**	**1.72891800**
H	**3.50313600**	**-1.12293800**	**1.91428200**
H	**4.69314100**	**-0.04649200**	**2.29917400**
H	**3.13881500**	**0.49719600**	**2.04581400**
H	**4.50959500**	**1.02306800**	**0.14887300**

TS:

C	**-0.15351000**	**2.52409800**	**0.23150200**
C	**1.13095600**	**3.07185000**	**0.40216400**
C	**2.23293400**	**2.33938300**	**0.03260100**
C	**0.91273000**	**0.46637200**	**-0.66663200**
C	**-0.28438300**	**1.13809800**	**-0.17555800**
H	**1.21888900**	**4.08279900**	**0.78483600**
H	**3.21850400**	**2.78435500**	**0.15271400**
H	**0.80120200**	**-0.54314500**	**-1.05446900**
H	**-0.36126400**	**0.62610700**	**0.91219700**
O	**-1.17757200**	**3.27806500**	**0.55633500**
O	**-0.44038400**	**-0.13467400**	**2.26852400**
H	**0.45263300**	**-0.10391500**	**2.65313200**
H	**-0.59685800**	**-1.07675700**	**1.96427300**
I	**-2.13240900**	**0.53202600**	**-1.04906000**
O	**-1.00471900**	**-2.97474400**	**-1.34683800**

H	-0.69479000	-2.15521800	-1.76530200
H	-1.98827200	-2.89682600	-1.35132900
O	-3.09611400	0.78287000	2.50551500
H	-3.21185600	1.35253400	1.72656300
H	-2.13432900	0.60308700	2.53606200
O	-1.14131600	-2.54516600	1.40666400
H	-2.10781800	-2.36681800	1.46089000
H	-0.96199500	-2.65442000	0.44509600
O	-3.79533000	-1.69489600	1.50284300
H	-4.34771000	-2.15980100	2.15167100
H	-3.62509900	-0.79697800	1.87816600
O	-3.75389900	-2.68959800	-1.11027900
H	-3.81519800	-2.26102400	-0.22908600
H	-3.96051000	-1.98606600	-1.74643600
H	-2.04127200	2.86585900	0.34211800
C	2.14697300	1.02336900	-0.51964500
C	3.40386900	0.27757100	-0.88474900
H	4.09235500	0.94121600	-1.41498100
H	3.16241500	-0.56170000	-1.54691300
C	4.14647500	-0.25205500	0.34455000
C	5.45070700	-0.96879600	-0.05712800
O	6.30270300	-0.24916000	-0.63172500
O	5.54080100	-2.19141200	0.21673600
N	3.27635400	-1.20858900	1.09328100
H	2.96892200	-1.97509200	0.48164800
H	3.79637800	-1.63634400	1.86791100
H	2.44123000	-0.75019600	1.47839500
H	4.38378600	0.56147700	1.03524500

Product:

C	-0.87650800	0.37177900	-1.09764700
C	-0.04077100	1.39219700	-1.55506500
C	1.33403100	1.20455500	-1.60014100
C	1.06506200	-1.02524500	-0.74036500
C	-0.31803300	-0.84895600	-0.70180200
H	-0.49283300	2.33006700	-1.86545900
H	1.97291700	2.00968400	-1.95561800
H	1.49423100	-1.97136300	-0.42016400
H	-0.67416200	0.56638100	2.11513800
O	-2.20886400	0.65900100	-1.04123200
O	-1.45040600	0.09599600	2.49978300
H	-1.24696000	-0.85154400	2.40427100
H	-2.82496100	0.24611400	1.86127300
I	-1.54676200	-2.43347500	-0.07640500

O	-4.63262000	1.84013400	-0.09747600
H	-5.25479200	2.42739100	0.36501700
H	-4.00943600	2.43632100	-0.58941900
O	0.78923000	1.55032900	1.66997500
H	0.16535300	2.17412700	1.23330600
H	0.96964700	1.94920500	2.53844500
O	-3.81286900	0.19059300	1.55518700
H	-3.92168700	-0.68575000	1.13181200
H	-4.07699000	0.94099400	0.83242000
O	-1.50273000	2.82333600	0.75892200
H	-1.95555700	1.98438800	0.54560500
H	-1.93928800	3.14493000	1.56540500
O	-3.02690200	3.62452600	-1.43559600
H	-2.30249100	3.55725000	-0.77833200
H	-2.69578200	3.15267900	-2.21749900
H	-2.72985600	-0.13918500	-0.83505300
C	1.90589900	-0.00110500	-1.18099600
C	3.40336200	-0.16995700	-1.12421900
H	3.88771300	0.51902300	-1.82682300
H	3.69083000	-1.18803600	-1.39814400
C	3.95011600	0.09408100	0.28196800
H	3.52721300	-0.62225100	0.99260100
N	3.52834300	1.44856600	0.74586800
C	5.48596100	-0.00730300	0.33165500
H	4.08049900	1.71745500	1.56808600
H	2.51653200	1.48477300	0.98727300
H	3.71689000	2.15483300	0.02378900
O	6.11557600	0.99088500	0.76554400
O	5.97061300	-1.09524300	-0.06633900

Tyr-C5-cm-n

Reactant:

C	1.59317600	-0.10721900	0.55072700
C	2.54450900	1.91683500	-0.32091700
C	1.48306400	2.65198200	0.19138900
C	0.46006800	2.00316800	0.89170200
C	0.51986900	0.61701800	1.08525700
H	-0.24934200	0.11642700	1.67136800
O	-2.85918700	1.41527200	1.91827900
H	-3.34065200	1.85495300	2.63878700
O	-0.47616500	-2.70204500	1.61003200
H	0.28213800	-2.33578200	2.09112900

H	-3.49862400	1.35916800	1.16278100
O	-2.71399600	-1.27447800	2.42757900
H	-2.80258400	-1.42757500	3.38255400
H	-2.67444600	-0.29371800	2.31785600
H	-1.23697100	-2.14205600	1.87941400
H	1.42351400	3.72634600	0.04468500
O	-4.77693800	0.99760100	-0.02739200
H	-4.37985000	0.83767900	-0.90544300
H	-4.99272600	0.10189900	0.31766600
O	-3.19130100	0.10536000	-2.25247000
H	-2.95586700	0.37993300	-3.15728100
O	-5.07617600	-1.55403800	1.05130900
H	-4.27707700	-1.55089900	1.62938900
H	-5.82995600	-1.76607600	1.62415900
I	-1.52821200	0.14095100	-1.13314800
H	3.33154200	2.42978900	-0.86990700
H	1.63165000	-1.18480500	0.69315000
O	-0.57169000	2.76348600	1.35248900
H	-1.35232900	2.20643200	1.60158600
O	-4.41828800	-2.35556000	-1.57055200
H	-4.01129400	-1.53062400	-1.90100900
H	-4.68503200	-2.14920300	-0.65206800
C	2.61275300	0.52532200	-0.16082900
C	3.78629400	-0.25228000	-0.70553900
H	4.02068500	0.07066700	-1.72390700
H	3.54853300	-1.32254600	-0.74028300
C	5.05920900	-0.05767000	0.12413600
C	6.24023100	-0.85527100	-0.45618900
O	6.62499600	-0.49525900	-1.59581300
O	6.70292500	-1.79108200	0.24412500
N	4.81380600	-0.50255900	1.52898500
H	4.54982400	-1.49526600	1.55077500
H	5.66188200	-0.40423900	2.09792400
H	4.06041100	0.04074500	1.96727100
H	5.32668700	1.00087900	0.17425800

TS:

C	1.62546700	-0.10666300	-0.32493400
C	2.81391800	1.92246000	-0.76552500
C	1.65936900	2.66341500	-0.59312200
C	0.45357500	2.01038500	-0.28800300
C	0.41064800	0.60574700	-0.13207900
H	-0.07983400	0.29803200	1.09055900
O	-3.25645000	2.21792700	0.38020400

H	-3.74584400	3.04555500	0.51540700
O	-0.39949300	0.03995900	2.29514500
H	0.08381600	0.68189100	2.84806000
H	-3.86603000	1.60947200	-0.11716700
O	-2.95806600	0.62218100	2.54575600
H	-3.08645800	1.08718000	3.38955200
H	-3.08066300	1.30487600	1.83576500
H	-1.37948600	0.25085100	2.41182600
H	1.66387700	3.74384700	-0.70065500
O	-4.95555800	0.40721300	-0.74190200
H	-4.39254000	-0.26770700	-1.20927100
H	-5.19570100	-0.02031800	0.10694700
O	-3.31297400	-1.46232000	-1.76941400
H	-3.20974200	-1.54942000	-2.73030000
O	-5.16987500	-0.85466900	1.76896800
H	-4.42767800	-0.36878200	2.19406400
H	-5.87967600	-0.90472100	2.42860000
I	-1.46778500	-0.48258700	-0.93321900
H	3.74159700	2.43589700	-1.01089900
H	1.60694200	-1.18995200	-0.20751300
O	-0.62632500	2.80361300	-0.13261000
H	-1.47502300	2.32252000	0.02106600
O	-4.09369700	-3.03530300	0.31876000
H	-3.81635100	-2.56308900	-0.50131900
H	-4.48495800	-2.33683800	0.88123000
C	2.82025100	0.51641800	-0.63584300
C	4.10467000	-0.26029200	-0.79112900
H	3.88533800	-1.32427500	-0.94187700
H	4.66231700	0.09305500	-1.66307600
C	5.03110500	-0.11337800	0.41904600
H	5.27673300	0.93825300	0.58940900
N	4.32925300	-0.59191700	1.64762100
C	6.33275400	-0.91526300	0.24310500
H	4.94549600	-0.53380100	2.46572400
H	3.48185400	-0.04234100	1.83436400
H	4.05765700	-1.57781100	1.54645400
O	6.55618800	-1.83626800	1.06875600
O	7.05270700	-0.57093400	-0.72601100

Product:

C	1.59317600	-0.10721900	0.55072700
C	2.54450900	1.91683500	-0.32091700
C	1.48306400	2.65198200	0.19138900
C	0.46006800	2.00316800	0.89170200

C	0.51986900	0.61701800	1.08525700
H	-0.24934200	0.11642700	1.67136800
O	-2.85918700	1.41527200	1.91827900
H	-3.34065200	1.85495300	2.63878700
O	-0.47616500	-2.70204500	1.61003200
H	0.28213800	-2.33578200	2.09112900
H	-3.49862400	1.35916800	1.16278100
O	-2.71399600	-1.27447800	2.42757900
H	-2.80258400	-1.42757500	3.38255400
H	-2.67444600	-0.29371800	2.31785600
H	-1.23697100	-2.14205600	1.87941400
H	1.42351400	3.72634600	0.04468500
O	-4.77693800	0.99760100	-0.02739200
H	-4.37985000	0.83767900	-0.90544300
H	-4.99272600	0.10189900	0.31766600
O	-3.19130100	0.10536000	-2.25247000
H	-2.95586700	0.37993300	-3.15728100
O	-5.07617600	-1.55403800	1.05130900
H	-4.27707700	-1.55089900	1.62938900
H	-5.82995600	-1.76607600	1.62415900
I	-1.52821200	0.14095100	-1.13314800
H	3.33154200	2.42978900	-0.86990700
H	1.63165000	-1.18480500	0.69315000
O	-0.57169000	2.76348600	1.35248900
H	-1.35232900	2.20643200	1.60158600
O	-4.41828800	-2.35556000	-1.57055200
H	-4.01129400	-1.53062400	-1.90100900
H	-4.68503200	-2.14920300	-0.65206800
C	2.61275300	0.52532200	-0.16082900
C	3.78629400	-0.25228000	-0.70553900
H	4.02068500	0.07066700	-1.72390700
H	3.54853300	-1.32254600	-0.74028300
C	5.05920900	-0.05767000	0.12413600
C	6.24023100	-0.85527100	-0.45618900
O	6.62499600	-0.49525900	-1.59581300
O	6.70292500	-1.79108200	0.24412500
N	4.81380600	-0.50255900	1.52898500
H	4.54982400	-1.49526600	1.55077500
H	5.66188200	-0.40423900	2.09792400
H	4.06041100	0.04074500	1.96727100
H	5.32668700	1.00087900	0.17425800

Tyr-C5-ms

Reactant:

C	1.69980100	-0.28989400	0.89488800
C	2.55062300	0.23600300	-0.07560200
C	2.23187400	1.48544700	-0.63146600
C	1.09568700	2.18178300	-0.24275700
C	0.24646500	1.63827900	0.72985800
C	0.54838700	0.39670000	1.30221700
H	-0.09001900	-0.01198700	2.08141800
O	-4.78461800	0.61547700	0.83826800
H	-5.66409200	0.81979000	1.19526900
O	-2.61500900	0.99090200	2.53570500
H	-3.41655900	0.99327500	1.96448000
O	-2.97248000	-1.45184200	-1.79218700
H	-4.73004700	-0.36898500	0.80222500
H	-2.63569100	-2.01271600	-2.51421100
O	-4.32864900	-2.09492800	0.55694100
H	-4.00870000	-2.10488900	-0.36989800
H	-5.10237200	-2.68072000	0.58492800
H	-2.38467200	0.03523600	2.59473700
H	0.84573600	3.14123900	-0.68644800
I	-1.40362300	-0.76526700	-0.74203400
H	1.92723300	-1.25286500	1.34664000
O	-4.32403700	1.05488000	-1.87428000
H	-3.91296600	0.19301400	-2.08221200
H	-4.58986900	0.96470100	-0.93226300
O	-0.86588500	2.34271200	1.07202900
H	-1.47722800	1.79789300	1.65243900
H	2.88336900	1.91310000	-1.39078800
O	-2.35912900	-1.79717700	2.57457300
H	-3.01872600	-1.97350000	1.86926700
H	-2.80202400	-2.05375000	3.39953800
C	3.80790900	-0.48919400	-0.49159500
H	3.79167400	-1.51864900	-0.11370200
H	3.88282800	-0.53498300	-1.58189700
C	5.07890000	0.20232600	0.01022300
H	5.13623600	1.22487300	-0.37161000
N	5.03562200	0.30674200	1.49928400
C	6.34693100	-0.56468600	-0.40381200
H	5.88793400	0.74791600	1.86210100
H	4.22500300	0.85489600	1.81107800
H	4.97660500	-0.62659900	1.92455900
O	7.06279600	-1.03412000	0.51673300
O	6.54122200	-0.65781300	-1.64079400

O	**-2.28208700**	**2.92960300**	**-1.37171400**
H	**-2.94658200**	**2.22955600**	**-1.55329300**
H	**-1.85087500**	**2.67398900**	**-0.53348300**

TS:

C	**1.61725400**	**-0.56482300**	**0.45350000**
C	**2.53204400**	**0.22196500**	**-0.16179300**
C	**2.24817000**	**1.63649700**	**-0.29978800**
C	**1.12497900**	**2.22106600**	**0.19411200**
C	**0.15461100**	**1.43303600**	**0.91894100**
C	**0.33223500**	**-0.03565200**	**0.92152700**
H	**-0.06064100**	**-0.50850500**	**1.82303200**
O	**-4.72835100**	**0.71241100**	**0.61295800**
H	**-5.59928700**	**0.90443200**	**0.99932600**
O	**-2.91169900**	**0.66368000**	**2.38094900**
H	**-3.65806800**	**0.79741100**	**1.66717500**
O	**-3.18700800**	**-1.38868400**	**-1.99354000**
H	**-4.71365800**	**-0.28638300**	**0.39962400**
H	**-2.95822000**	**-2.19981500**	**-2.47426300**
O	**-4.41080700**	**-1.79315100**	**0.04027400**
H	**-3.84286700**	**-1.67009100**	**-1.01867300**
H	**-5.23021800**	**-2.29587900**	**-0.08521000**
H	**-2.79398700**	**-0.36217800**	**2.40312200**
H	**0.94553800**	**3.28765900**	**0.10001700**
I	**-1.21670200**	**-0.68913600**	**-0.59063700**
H	**1.79479900**	**-1.63056800**	**0.57927300**
O	**-4.01245700**	**1.26106000**	**-2.05012000**
H	**-3.66162700**	**0.35945900**	**-2.22189900**
H	**-4.42801200**	**1.17633800**	**-1.16673200**
O	**-0.83131300**	**1.97122100**	**1.48304500**
H	**-2.06209000**	**1.09633900**	**2.03022000**
H	**2.97952300**	**2.25278400**	**-0.82012700**
O	**-2.92394900**	**-1.89633400**	**2.27426500**
H	**-3.49191500**	**-1.96750600**	**1.45341200**
H	**-3.48397600**	**-2.20024800**	**3.00801400**
C	**3.84293900**	**-0.31435800**	**-0.67573500**
H	**3.82827200**	**-1.41067600**	**-0.66420800**
H	**4.00680600**	**0.00932400**	**-1.70821100**
C	**5.04111300**	**0.17537700**	**0.14110100**
H	**5.09326500**	**1.26770500**	**0.14216000**
N	**4.87885700**	**-0.24338900**	**1.56519400**
C	**6.36870400**	**-0.38684100**	**-0.40038200**
H	**5.70636500**	**0.01158100**	**2.11536200**
H	**4.05180000**	**0.19032100**	**1.99294400**

H	**4.77528900**	**-1.26340900**	**1.63332000**
O	**7.05590200**	**-1.09002200**	**0.38215700**
O	**6.63706200**	**-0.08502400**	**-1.58867600**
O	**-2.16986700**	**3.05969700**	**-0.91237000**
H	**-2.72458700**	**2.37061900**	**-1.33906500**
H	**-1.85168400**	**2.66279200**	**-0.08162400**

Product:

C	**1.57710900**	**-0.53836800**	**0.23055000**
C	**2.55044400**	**0.29381300**	**-0.19034500**
C	**2.34216100**	**1.73690500**	**-0.10503900**
C	**1.24153900**	**2.29585200**	**0.44771400**
C	**0.20845900**	**1.45155600**	**1.02574100**
C	**0.28953200**	**-0.02746000**	**0.75105900**
H	**-0.10060700**	**-0.60425900**	**1.59260300**
O	**-4.84292400**	**0.14946500**	**1.16141700**
H	**-5.64729800**	**0.22198900**	**1.69941700**
O	**-2.62580900**	**0.07046600**	**2.71497500**
H	**-4.07495000**	**0.19892700**	**1.78857400**
O	**-3.65851700**	**-0.97266000**	**-2.50704300**
H	**-4.58851100**	**-1.41388100**	**0.37222200**
H	**-4.28065900**	**-1.16267200**	**-3.22721900**
O	**-4.23416800**	**-2.21367300**	**-0.08746200**
H	**-3.94880700**	**-1.52721800**	**-1.74727200**
H	**-4.93574700**	**-2.88270600**	**-0.03340000**
H	**-2.34628100**	**-0.82207400**	**2.40633000**
H	**1.11518900**	**3.37116000**	**0.52520700**
I	**-1.22238500**	**-0.36057200**	**-0.80393000**
H	**1.69334300**	**-1.61757400**	**0.16725500**
O	**-4.42658200**	**1.44988300**	**-1.26356700**
H	**-4.08980100**	**0.69358200**	**-1.79102000**
H	**-4.64251000**	**1.05089000**	**-0.39269700**
O	**-0.72177100**	**1.91595400**	**1.69878500**
H	**-1.98735800**	**0.70146600**	**2.32198900**
H	**3.12381900**	**2.38143800**	**-0.50335100**
O	**-2.19471900**	**-2.54204200**	**1.82034500**
H	**-2.89293600**	**-2.53078200**	**1.12692600**
H	**-2.56526000**	**-3.07565900**	**2.54177100**
C	**3.86008000**	**-0.20740800**	**-0.74069600**
H	**3.79914600**	**-1.28399500**	**-0.93824700**
H	**4.08308300**	**0.29734000**	**-1.68615200**
C	**5.04010400**	**0.06313400**	**0.19585600**
H	**5.10802500**	**1.12542000**	**0.44562800**
N	**4.83475300**	**-0.66650000**	**1.48199900**

C	6.37211200	-0.39017700	-0.43096600
H	5.62335200	-0.51111500	2.11976100
H	3.97071100	-0.36818900	1.95064000
H	4.77827600	-1.67865100	1.31473900
O	6.99655600	-1.31079700	0.15306400
O	6.70368600	0.20978800	-1.48212200
O	-2.49937300	3.22289700	-0.29098700
H	-3.11525600	2.55184200	-0.66248200
H	-1.99610800	2.75920100	0.40062600

Tyr-C5-cm-a

Reactant:

C	0.37497300	2.30918000	0.38882600
C	1.41154400	2.64268800	-0.53275400
C	2.43514500	1.75696700	-0.82499100
C	1.49663900	0.12764000	0.65750200
C	0.44579000	1.00631900	0.96411200
H	1.38195300	3.62231700	-1.00404800
H	1.51756300	-0.85315500	1.13165900
H	-0.28923100	0.73079000	1.71784500
O	-4.84563900	-1.17698200	1.09292300
H	-5.71974700	-1.33175500	1.48542400
O	-1.52423000	-2.94081900	1.36235900
H	-2.12043200	-2.97113900	0.58723000
H	-4.91100000	-0.33043500	0.58045800
O	-2.59503100	-0.58047500	2.54873900
H	-2.70894000	-0.63026100	3.51173900
H	-3.47187900	-0.82070900	2.16580100
H	-1.77738000	-2.11479200	1.82409800
O	-4.65175100	1.11874800	-0.35475700
H	-4.17348200	0.68826900	-1.09314900
H	-3.95703900	1.51699000	0.22325500
O	-3.02488000	-0.50067000	-2.13176500
H	-3.30835200	-1.38193400	-1.78842400
O	-0.59074400	3.13932800	0.66556000
O	-2.89695900	2.08507100	1.59780400
H	-2.68735200	1.20282300	1.97060100
H	-2.03050700	2.43679700	1.25131200
I	-1.41863800	-0.01769000	-1.00751500
C	2.50088300	0.47569900	-0.24289200
H	3.20925800	2.05481800	-1.53140800
C	3.65312500	-0.45148700	-0.54212400

H	**3.40627800**	**-1.47587500**	**-0.23525900**
H	**3.87269500**	**-0.47000700**	**-1.61422900**
C	**4.94776000**	**-0.02854800**	**0.16444400**
H	**5.23347800**	**0.98295400**	**-0.13319300**
N	**4.71560900**	**0.00516800**	**1.63906600**
C	**6.09544400**	**-1.00510100**	**-0.13854200**
H	**5.53335600**	**0.37490000**	**2.13582000**
H	**3.90065500**	**0.58630900**	**1.87263500**
H	**4.55224600**	**-0.94621100**	**1.99094100**
O	**6.46310000**	**-1.76787500**	**0.79150700**
O	**6.54467400**	**-0.96617400**	**-1.31092200**
O	**-3.53707900**	**-2.79404900**	**-0.68552300**
H	**-4.14497100**	**-2.34729400**	**-0.05010900**
H	**-4.02811700**	**-3.55098300**	**-1.04308100**

TS:

C	**0.00498400**	**-2.02951000**	**0.79762600**
C	**-1.26711800**	**-2.54778900**	**1.26316200**
C	**-2.44961000**	**-2.11409000**	**0.74181400**
C	**-1.35302900**	**-0.56056300**	**-0.72387700**
C	**-0.08468400**	**-0.88884800**	**-0.10862700**
H	**-1.23723000**	**-3.34291000**	**2.00304800**
H	**-1.36901600**	**0.21941300**	**-1.48334300**
H	**-0.06643200**	**0.06852200**	**0.79956600**
O	**3.45758200**	**2.44519000**	**0.75574100**
H	**4.03935100**	**3.17456800**	**1.02345600**
O	**-0.04080800**	**1.10970100**	**1.63340900**
H	**0.18171200**	**1.87103100**	**1.02528500**
H	**4.06136000**	**1.70928200**	**0.41862900**
O	**2.40061100**	**0.97523500**	**2.79495300**
H	**2.49228200**	**1.36748300**	**3.67811200**
H	**2.82359000**	**1.60919000**	**2.16233700**
H	**0.78940100**	**0.99321500**	**2.17030200**
O	**4.93975500**	**0.42087400**	**-0.04271100**
H	**4.65453600**	**0.34622700**	**-1.07134300**
H	**4.46953000**	**-0.28894200**	**0.44133900**
O	**4.29849500**	**0.28143300**	**-2.45017600**
H	**4.01294700**	**1.17252600**	**-2.70303600**
O	**1.09384100**	**-2.49921700**	**1.22036400**
O	**3.60419200**	**-1.36300500**	**1.79697800**
H	**2.78827300**	**-1.75808200**	**1.42176800**
H	**3.27058300**	**-0.57804200**	**2.27956900**
I	**1.69101600**	**-0.39869200**	**-1.17797300**
C	**-2.52117100**	**-1.10735500**	**-0.28012200**

H	**-3.38029100**	**-2.55283100**	**1.09852700**
C	**-3.86396400**	**-0.63087200**	**-0.77035100**
H	**-3.74754200**	**-0.06586100**	**-1.70307400**
H	**-4.52730600**	**-1.47765700**	**-0.96981300**
C	**-4.56914100**	**0.25680000**	**0.26182200**
H	**-4.71341400**	**-0.28456200**	**1.20060700**
N	**-3.70774000**	**1.43579100**	**0.57770400**
C	**-5.93219200**	**0.75184400**	**-0.25139500**
H	**-4.17452600**	**2.06129400**	**1.24329500**
H	**-2.80509500**	**1.14727100**	**0.97596600**
H	**-3.52284700**	**1.98397500**	**-0.27146100**
O	**-6.06869200**	**1.98984000**	**-0.42163000**
O	**-6.78607000**	**-0.14390200**	**-0.46388200**
O	**0.85398000**	**3.04935600**	**-0.00794200**
H	**1.80828900**	**2.88064700**	**0.17108700**
H	**0.67464900**	**3.92262200**	**0.37666100**

Product:

C	**0.37805600**	**-1.64805100**	**1.43161600**
C	**-0.83693500**	**-1.80107300**	**2.16236500**
C	**-2.08541400**	**-1.63584700**	**1.57798000**
C	**-1.04981100**	**-1.13541400**	**-0.52356700**
C	**0.20502100**	**-1.29334500**	**0.06363000**
H	**-0.75472700**	**-2.06186900**	**3.21484900**
H	**-1.12229800**	**-0.86725100**	**-1.57533300**
H	**-0.79083200**	**0.57819200**	**1.70099800**
O	**2.23413000**	**2.86244200**	**-0.79598800**
H	**2.31561400**	**3.77064400**	**-1.12854800**
O	**-0.97325000**	**1.49548200**	**1.42624500**
H	**-0.47155400**	**1.60993300**	**-0.40006600**
H	**3.69993300**	**1.92495900**	**-0.14547400**
O	**1.41965300**	**2.76803200**	**1.84586400**
H	**1.53307100**	**3.59953700**	**2.33315900**
H	**1.76418400**	**2.92842900**	**0.93535000**
H	**-0.16887700**	**2.00726500**	**1.68004200**
O	**4.41157400**	**1.48002600**	**0.35859100**
H	**5.05969900**	**0.21779200**	**-0.71247900**
H	**3.93482700**	**1.01518600**	**1.08630700**
O	**5.49297800**	**-0.42688100**	**-1.32039500**
H	**5.01377300**	**-1.25945000**	**-1.18549300**
O	**1.54065100**	**-1.81565500**	**1.99398000**
O	**2.91431200**	**0.46656200**	**2.45594400**
H	**2.39629300**	**-0.35208400**	**2.23572400**
H	**2.29207000**	**1.21755700**	**2.36198100**

I	1.93645000	-0.96260000	-1.08316600
C	-2.21900000	-1.30288300	0.22207000
H	-2.97872600	-1.76438200	2.18725400
C	-3.57979700	-1.08729000	-0.39506200
H	-3.49229300	-1.02237300	-1.48698100
H	-4.24553200	-1.92495300	-0.16703700
C	-4.27203400	0.17998700	0.11498100
H	-4.40056000	0.13413100	1.20028800
N	-3.41553000	1.37115700	-0.16046700
C	-5.65109800	0.38931800	-0.53568900
H	-3.96260200	2.23059000	-0.03863900
H	-2.58364900	1.40850700	0.45581600
H	-3.08539500	1.36520200	-1.13386200
O	-5.83466800	1.46197200	-1.16674700
O	-6.47820700	-0.54170900	-0.37059200
O	-0.29322100	1.92633500	-1.31279100
H	1.35675600	2.53255900	-1.11025900
H	-0.83782200	2.72632000	-1.39936300

Tyr-C5-cs-a1

Reactant:

C	1.59387700	-1.42938900	-0.70865500
C	2.06581000	-0.41670500	0.12641800
C	1.50147000	-0.32093200	1.41400400
C	0.50278500	-1.18012400	1.84019100
C	-0.00762100	-2.20983800	0.99478900
C	0.57530600	-2.30235200	-0.30239600
H	0.24747500	-3.10350400	-0.96166700
O	-4.16102600	2.38478000	1.37864900
H	-4.90327400	2.86502900	1.77810900
O	-1.68123900	1.39939300	2.25337900
H	-2.52207200	1.85529100	2.03844500
O	-3.20217500	0.50179900	-1.88563600
H	-4.50773900	1.50350400	1.08869900
H	-3.00266600	1.42621800	-1.57645600
O	-4.70431600	-0.11689700	0.44355400
H	-4.28580400	0.03180200	-0.43135200
H	-4.02624500	-0.58643400	0.98542300
H	-1.07540900	1.61219000	1.51236700
H	0.08042700	-1.07687200	2.83757800
I	-1.59228300	-0.57505200	-1.34541400
H	1.85284200	0.46084900	2.08763300

H	**2.01620400**	**-1.53804400**	**-1.70666000**
O	**-0.97878500**	**-2.99258800**	**1.37779100**
O	**-2.83678900**	**-1.15359800**	**2.21714300**
H	**-2.20399500**	**-1.85497200**	**1.91487300**
H	**-2.31543100**	**-0.31946600**	**2.23045200**
O	**-2.54269800**	**2.91224000**	**-0.82417000**
H	**-1.63503500**	**2.74409600**	**-0.49962200**
H	**-3.11719200**	**2.86650400**	**-0.02877700**
O	**0.04270600**	**2.23147800**	**0.13677200**
H	**0.80395000**	**2.64442900**	**0.57786800**
H	**0.37652600**	**1.38174700**	**-0.20457800**
C	**3.17309400**	**0.51546400**	**-0.30366000**
H	**3.35199000**	**0.41333000**	**-1.38151100**
H	**2.90489000**	**1.56011500**	**-0.11140100**
C	**4.48816100**	**0.25549500**	**0.43954000**
H	**4.35597000**	**0.40230000**	**1.51448800**
N	**4.88770800**	**-1.17080900**	**0.25162400**
C	**5.61596700**	**1.16808800**	**-0.06713400**
H	**5.04130500**	**-1.37286600**	**-0.74386500**
H	**5.76533500**	**-1.37647400**	**0.74077800**
H	**4.15840600**	**-1.80462500**	**0.60045000**
O	**6.58201500**	**0.62054800**	**-0.65699900**
O	**5.45274400**	**2.39547300**	**0.14523400**

TS:

C	**1.45275400**	**-1.09370200**	**-0.76881200**
C	**2.05007800**	**-0.25487100**	**0.11181800**
C	**1.56376100**	**-0.21619000**	**1.48075300**
C	**0.57822000**	**-1.02852400**	**1.93507700**
C	**-0.01519000**	**-2.02826300**	**1.05752100**
C	**0.30284900**	**-1.92274200**	**-0.38885400**
H	**0.21863100**	**-2.87297800**	**-0.91548000**
O	**-4.18438500**	**2.44537300**	**1.05311800**
H	**-4.81319700**	**2.78768100**	**1.70715000**
O	**-1.76534900**	**1.50577600**	**2.04771700**
H	**-2.60227100**	**1.91764200**	**1.72969200**
O	**-3.59060800**	**0.42273700**	**-1.80538300**
H	**-4.49158500**	**1.49847200**	**0.79575500**
H	**-3.25660700**	**1.34009100**	**-1.73016400**
O	**-4.75012700**	**0.06031500**	**0.29644400**
H	**-4.15690400**	**0.23389700**	**-0.80719800**
H	**-4.15170900**	**-0.45837700**	**0.86614700**
H	**-1.11797600**	**1.64832100**	**1.32609800**
H	**0.24563600**	**-1.00217000**	**2.96899100**

I	**-1.52573300**	**-0.80281200**	**-1.14133100**
H	**2.02338200**	**0.49972100**	**2.16099800**
H	**1.78548800**	**-1.13841900**	**-1.80378900**
O	**-0.79736000**	**-2.89678600**	**1.48930900**
O	**-2.90645700**	**-1.02584800**	**2.37424200**
H	**-2.30175500**	**-1.74676300**	**2.11815900**
H	**-2.39299700**	**-0.19742900**	**2.23314800**
O	**-2.51610800**	**3.01428500**	**-1.10716700**
H	**-1.62651000**	**2.80039100**	**-0.76385200**
H	**-3.10684200**	**2.98081000**	**-0.32559800**
O	**0.02355700**	**2.24171800**	**-0.05539200**
H	**0.84615600**	**2.62457200**	**0.29296000**
H	**0.29470800**	**1.43130300**	**-0.52270400**
C	**3.21174600**	**0.62760300**	**-0.26486500**
H	**3.31210700**	**0.67994500**	**-1.35556900**
H	**3.05073600**	**1.64471900**	**0.10849600**
C	**4.53140200**	**0.13306900**	**0.33597400**
H	**4.44720000**	**0.02491200**	**1.42037500**
N	**4.84346900**	**-1.22076800**	**-0.21106800**
C	**5.69214500**	**1.08841700**	**0.00568900**
H	**5.04468700**	**-1.15705000**	**-1.21663700**
H	**5.67681500**	**-1.61810300**	**0.23683800**
H	**4.05946200**	**-1.87153700**	**-0.07423500**
O	**6.58283200**	**0.66231100**	**-0.77169500**
O	**5.62479500**	**2.22211900**	**0.54038700**

Product:

C	**1.44685500**	**-1.04977100**	**-0.78009000**
C	**2.06698000**	**-0.24009600**	**0.10569600**
C	**1.59708100**	**-0.20117600**	**1.48721300**
C	**0.61503900**	**-1.00461800**	**1.95389600**
C	**0.00841600**	**-2.00341800**	**1.07930700**
C	**0.29981200**	**-1.88906900**	**-0.38833000**
H	**0.24658300**	**-2.85486900**	**-0.89116800**
O	**-4.16562600**	**2.40100000**	**1.11073600**
H	**-4.75884500**	**2.74134300**	**1.79776000**
O	**-1.72366200**	**1.49089100**	**2.02460700**
H	**-2.58032900**	**1.88870100**	**1.73372800**
O	**-3.86201400**	**0.57191200**	**-1.88042500**
H	**-4.48989700**	**1.42079100**	**0.85930900**
H	**-3.39619100**	**1.42384300**	**-1.75320700**
O	**-4.80965900**	**0.08077500**	**0.45368300**
H	**-4.25497700**	**0.35411300**	**-0.95577000**
H	**-4.15668500**	**-0.44153100**	**0.95209600**

H	-1.10625300	1.62725100	1.27624100
H	0.28826800	-0.97600300	2.98915200
I	-1.50903100	-0.85660400	-1.16747600
H	2.07197000	0.51329300	2.15789800
H	1.75608100	-1.07594300	-1.82215300
O	-0.74025100	-2.88698200	1.51633100
O	-2.85736900	-1.01401700	2.46426700
H	-2.27741300	-1.75570600	2.21788900
H	-2.33221300	-0.20241000	2.27541200
O	-2.58335700	3.00983100	-1.08384100
H	-1.68321000	2.77365400	-0.78865200
H	-3.14254600	2.95350600	-0.27901000
O	-0.00997200	2.23621000	-0.13636200
H	0.81015700	2.63824000	0.19585200
H	0.27105400	1.43977900	-0.62049900
C	3.22806800	0.64102700	-0.27293500
H	3.32710400	0.69349200	-1.36369200
H	3.06571900	1.65765300	0.10210300
C	4.54673900	0.14308000	0.32567500
H	4.46286300	0.02069200	1.40861300
N	4.86694700	-1.20168700	-0.23974800
C	5.70442100	1.10810600	0.00961600
H	5.05696800	-1.12407500	-1.24652100
H	5.71024500	-1.59368500	0.19451400
H	4.09419500	-1.86541400	-0.10235700
O	6.60435000	0.69060700	-0.76148000
O	5.62842300	2.23611200	0.55456200

Tyr-C5-cs-a2

Reactant:

C	-1.56812400	0.37364700	0.06427600
C	-0.59628100	0.79125100	-0.94286300
C	0.57673100	0.13234100	-1.07074000
C	0.95013300	-1.00882000	-0.23871000
C	0.06623100	-1.48869100	0.65770800
C	-1.29876900	-0.92765700	0.78403300
H	-0.84236500	1.65620900	-1.55341700
H	1.29617300	0.46162400	-1.81885600
H	0.31204700	-2.34136000	1.28602200
H	-1.66032200	-0.87992800	1.81102700
O	-2.58942000	1.01839500	0.31106300
O	0.01831500	1.41677500	2.28886500

H	-0.67753400	2.09714400	2.15991200
H	0.74199200	1.70291200	1.69382700
I	-2.66363400	-2.38183800	-0.13977600
O	-0.71469900	4.42036700	-0.59956500
H	-0.61355600	5.38380100	-0.65823000
H	0.07062800	4.03713900	-1.05226400
O	2.17100900	2.31736100	0.71337900
H	1.95825500	2.57598000	-0.21055800
H	2.51509800	3.11954100	1.13822500
O	-1.78135100	3.52443200	1.82028500
H	-1.53551700	4.16674600	2.50480800
H	-1.36952800	3.86297800	0.99459600
O	1.48348000	3.25333400	-1.82446700
H	2.10304400	3.88468400	-2.22593100
H	1.19593600	2.67598300	-2.55155500
O	-3.14829500	3.24519800	-1.36913800
H	-2.31999200	3.74500100	-1.21748400
H	-3.03623900	2.45045200	-0.80973600
C	2.30985600	-1.62832500	-0.43078600
H	2.43533300	-1.92378400	-1.47733100
H	2.39363100	-2.53099400	0.18530900
C	3.46115000	-0.68327700	-0.08996900
C	4.83993400	-1.35107400	-0.27740800
O	5.03205600	-1.90247700	-1.38728400
O	5.65228100	-1.26700300	0.67997200
H	3.43505800	0.20372500	-0.73158300
N	3.33842600	-0.19260500	1.31446600
H	4.28718300	-0.10396800	1.70649000
H	2.82011300	-0.85271500	1.90625200
H	2.86198700	0.72708100	1.32923300

TS:

C	-1.40706300	0.30145200	-0.97935300
C	-0.30896900	1.12909700	-1.44602400
C	0.97554100	0.67285900	-1.43583100
C	1.34047600	-0.61707700	-0.91658500
C	0.35964600	-1.38412300	-0.36315900
C	-0.99734800	-0.88805800	-0.23465600
H	-0.56098900	2.08620500	-1.89638600
H	1.76210300	1.29547400	-1.86178800
H	0.59679100	-2.35963900	0.05547300
H	-0.95786700	-0.28982000	0.93827300
O	-2.60661500	0.64125600	-1.12779500
O	-0.94230300	0.36968700	2.09911500

H	-1.64799500	1.06785100	1.97939300
H	-0.07685600	0.85721400	2.05582300
I	-2.51851500	-2.33156400	0.11370600
O	-1.36223500	4.12546000	0.17868400
H	-1.48201500	5.02183300	0.53136400
H	-0.38982500	3.98844200	0.11391500
O	1.45937500	1.59963700	1.86593400
H	1.46273300	2.30073300	1.17237400
H	1.70107800	2.04871900	2.69292500
O	-2.79671500	2.26098900	1.63866800
H	-3.01934100	2.67933900	2.48594000
H	-2.28355800	2.94079100	1.14162100
O	1.36613300	3.64618500	0.01123100
H	1.90197400	4.41397000	0.27166500
H	1.62254500	3.45304000	-0.90619900
O	-3.04675700	3.27919800	-1.91741600
H	-2.44935300	3.71165700	-1.27470900
H	-2.93858700	2.32418200	-1.71242000
C	2.77224300	-1.08142000	-1.01444900
H	3.13887600	-0.94861200	-2.03651500
H	2.83582700	-2.14957200	-0.77372100
C	3.71681600	-0.31111700	-0.09236400
C	5.18584200	-0.75812700	-0.23661400
O	5.64406400	-0.76735600	-1.40502200
O	5.80242400	-1.04882800	0.82104100
H	3.67182100	0.76144700	-0.31049300
N	3.29069000	-0.47315500	1.32768400
H	4.11969100	-0.38741500	1.93042200
H	2.89398800	-1.40567600	1.49190700
H	2.58332000	0.24406700	1.58961800

Product:

C	-1.44412700	0.24037200	-0.95406200
C	-0.37462400	1.09283200	-1.36726200
C	0.94523000	0.67157200	-1.38820400
C	1.31555600	-0.61885200	-0.97527400
C	0.30495500	-1.46374400	-0.51796100
C	-1.03002200	-1.04645900	-0.50040700
H	-0.63319800	2.09578600	-1.70231000
H	1.71599900	1.35387600	-1.74530100
H	0.55726800	-2.46741400	-0.18281400
H	-0.69651200	-0.05571600	1.42471400
O	-2.68366700	0.62298100	-0.97412200
O	-0.60704200	0.64185200	2.11389200

H	-1.41585200	1.35758800	1.95262000
H	0.27129400	1.13556800	1.91497300
I	-2.51398600	-2.37560700	0.17905900
O	-1.49420600	4.20993000	0.13927300
H	-1.63247300	5.07993500	0.54763500
H	-0.52286300	4.12547900	0.00046900
O	1.59982400	1.87630600	1.65049600
H	1.49740500	2.54811100	0.93141900
H	1.84554300	2.37233300	2.44993000
O	-2.42426500	2.26081400	1.75594500
H	-2.61712900	2.68206400	2.61178600
H	-2.07868100	2.98791300	1.16752600
O	1.21823300	3.82196800	-0.24656600
H	1.76492800	4.60947200	-0.08753700
H	1.37682200	3.58250700	-1.17533100
O	-3.18295600	3.11701500	-1.86288200
H	-2.61981000	3.65548500	-1.27428600
H	-2.99639100	2.18545600	-1.56812800
C	2.75007800	-1.08622900	-1.05543900
H	3.14024300	-0.94990700	-2.06843400
H	2.80536000	-2.15746100	-0.82453300
C	3.69036900	-0.33668900	-0.11151400
C	5.14320900	-0.84415400	-0.19630400
O	5.65260600	-0.85444000	-1.34362600
O	5.69768200	-1.18503300	0.88105600
H	3.69272600	0.73275700	-0.34552800
N	3.20855100	-0.46097300	1.29584400
H	4.02273000	-0.43837000	1.92463100
H	2.73070500	-1.35642000	1.44975200
H	2.55990500	0.31189500	1.52855100

Tyr+hoi-n

Reactant:

O	-2.04573500	-1.69942100	-1.68000700
H	-2.18511300	-1.94494900	-2.61143500
O	-1.70866700	-3.45648200	0.40168100
H	-1.91208000	-2.81110200	1.11895500
H	-1.84183300	-2.93033800	-0.42835200
O	1.01727900	-3.37857200	0.84835000
H	0.04986300	-3.44719400	0.62804200
H	1.22213300	-4.19956000	1.32717900
I	-0.14229700	-0.63677600	-1.52700800

O	0.65191000	-1.47298500	2.83025700
H	0.77551200	-1.94708700	3.66989600
H	0.85847200	-2.14465900	2.12976700
O	-2.08548100	-1.49399100	2.40668100
H	-2.47697400	-1.93041000	3.18151500
H	-1.11628100	-1.41578300	2.60671600
O	-3.72518900	-0.58551700	0.22121000
H	-3.19345900	-0.93198100	-0.53518800
H	-3.17012600	-0.78352600	1.00356200
H	2.63654600	-0.05812100	-1.76163200
N	1.93547300	0.46135900	-1.22683400
H	1.86926500	1.38542600	-1.65896600
C	0.10290100	3.11574300	-0.32588400
C	0.60385300	2.28405200	0.68583000
C	-0.31231000	1.69886000	1.57319200
C	-1.68416200	1.92052300	1.45013700
C	-2.16110800	2.73824200	0.41899900
C	-1.26833800	3.34667500	-0.46646900
H	-1.64947100	3.98342400	-1.26006100
H	-2.38476300	1.45236700	2.13633800
H	0.04907100	1.04164000	2.35936000
H	0.79266700	3.58220400	-1.02617500
O	-3.51179800	2.98162700	0.23463600
C	2.07763000	1.95489300	0.77029500
H	2.66424800	2.71305400	0.23575800
H	2.41148800	1.95213200	1.81187200
C	2.41241500	0.56842300	0.17897500
C	3.92641900	0.26096700	0.28746500
O	4.56518100	0.00677200	-0.77770000
O	4.41078500	0.27209800	1.45768100
H	-4.03023600	2.43467800	0.85087200
H	1.89440500	-0.19909900	0.76366900

TS:

O	1.95235600	-3.08154100	-0.52862400
H	2.04758700	-3.90886600	-1.03004200
O	3.68076800	-1.35174700	-1.39749000
H	4.26960500	-1.31121000	-0.62556200
H	2.64355200	-2.41596500	-0.92671600
O	2.72554400	1.04686600	-1.44804800
H	3.12085600	0.08065600	-1.45388600
H	3.42656700	1.63795400	-1.76813900
I	0.06905400	-0.87510200	-0.74347000
O	2.67986000	1.28519800	1.29244900

H	2.71740100	2.22815100	1.52537900
H	2.67326000	1.26267800	0.29936300
O	4.64872400	-0.49551200	2.01555300
H	5.29240600	-0.53244500	1.28840900
H	3.98804800	0.19027700	1.74081600
O	3.12138600	-2.87859900	2.02766200
H	2.70568100	-2.98863400	1.14108000
H	3.65117800	-2.05030400	1.96475200
H	0.88729100	1.48220300	-1.28325100
N	-0.07791100	1.25237100	-0.97271000
H	-0.71543100	1.45058700	-1.75219600
C	-3.44587700	0.55784600	-0.74575500
C	-2.77044100	1.04847800	0.38091200
C	-2.81986100	0.29625200	1.56417800
C	-3.51249200	-0.91348200	1.62465200
C	-4.17398100	-1.38615300	0.48432600
C	-4.14627300	-0.65011900	-0.70313700
H	-4.66552500	-1.02673500	-1.57993100
H	-3.54269000	-1.49146200	2.54550300
H	-2.29798800	0.65457800	2.44877500
H	-3.41736000	1.12275000	-1.67488000
O	-4.87724700	-2.57781500	0.48286800
C	-1.95454700	2.31932800	0.31111300
H	-2.25337300	2.91332200	-0.56175700
H	-2.12404800	2.93345100	1.20110200
C	-0.43581700	2.07442800	0.23722100
C	0.32888500	3.42048200	0.17844300
O	0.85074000	3.75954600	-0.92189000
O	0.34084900	4.07449500	1.25823400
H	-4.83028600	-2.98785200	1.36460700
H	-0.09264900	1.52118500	1.11201400

Product:

O	-0.00002200	4.18092800	-0.50960300
H	-0.02757800	5.08849400	-0.16278600
O	-2.18937300	2.99681300	0.67506800
H	-1.69122200	2.48189500	1.35266000
H	-0.83538800	3.75913600	-0.17857200
O	-3.47336500	0.73061200	-0.42756900
H	-2.65641500	2.30463100	0.15773900
H	-4.31369200	0.44773200	-0.82467600
I	0.06921100	0.66239300	-1.62565800
O	-3.23125100	-0.06684800	2.25966700
H	-3.02189000	-1.02120800	2.11203800

H	-3.40289100	0.26222300	1.34452100
O	-0.89855200	1.32754300	2.57039200
H	-0.98575300	1.79563900	3.41798100
H	-1.69899600	0.73630300	2.51761600
O	1.40250300	2.69534100	1.47546100
H	0.99115600	3.22712600	0.75646400
H	0.68701600	2.09224000	1.76196300
H	-2.77233000	0.10862000	-0.78393500
N	-1.32077500	-0.85851000	-1.14593500
H	-1.31446900	-1.48112500	-1.95718700
C	2.55595500	-1.99259900	-0.66289700
C	1.52004700	-1.89253100	0.27669200
C	1.75331600	-1.13645600	1.43563700
C	2.96810100	-0.48136900	1.64425500
C	3.98075900	-0.58489300	0.68394000
C	3.77990200	-1.34753400	-0.47013800
H	4.57446400	-1.42431800	-1.20733100
H	3.13065100	0.11004800	2.54214600
H	0.97078100	-1.04158400	2.18449400
H	2.39945900	-2.56987900	-1.57117400
O	5.20554600	0.04538800	0.83190100
C	0.19139000	-2.58265200	0.05738000
H	0.20156300	-3.13613100	-0.88892500
H	0.04198800	-3.32169900	0.85640600
C	-1.05303500	-1.65757700	0.06684600
C	-2.29308300	-2.57260600	0.25636700
O	-2.73245700	-3.18282500	-0.75794800
O	-2.75029800	-2.67739600	1.43846500
H	5.21923500	0.54218900	1.66892500
H	-1.00040400	-0.96472500	0.90787500

Tyr+ICl-cs-ms

Reactant:

C	0.22586900	1.87097500	-0.21031900
C	0.84215300	1.78065800	1.04266300
C	1.95846200	0.96704900	1.20273400
C	2.49131700	0.23440400	0.13191400
C	1.87761200	0.34498100	-1.11572300
C	0.74334000	1.14552700	-1.29531500
H	0.44290700	2.34793300	1.87862700
H	0.28602400	1.25262100	-2.27549700
O	-4.43282900	0.64486700	0.88575500

H	-5.29013700	0.95839700	1.21705300
O	-2.34747900	2.28483000	1.73855600
H	-3.12672600	1.79613100	1.38733100
H	-4.18822700	-0.11118700	1.46648900
O	-3.47872900	-1.30964100	2.61203600
H	-3.36543600	-2.18346100	2.20116900
H	-4.03228400	-1.46314200	3.39568800
H	-1.84719600	1.59946600	2.24063400
I	-1.32558400	-0.87796500	-0.58921000
H	2.42779000	0.89617500	2.18150000
H	2.27209300	-0.21015900	-1.96394600
O	-0.87221900	2.65488500	-0.41071700
H	-1.44332100	2.62826400	0.41781600
O	-1.16220800	0.15433100	3.11711900
H	-1.15146500	0.40009200	4.05615900
H	-1.94014300	-0.43734600	3.01654400
O	-4.60098400	0.47221500	-1.92381600
H	-3.81587600	0.99203500	-2.20083100
H	-4.54402600	0.44055500	-0.94675500
Cl	-3.00490800	-2.57749700	-0.35458600
C	3.72104100	-0.62408500	0.30938500
H	3.91433900	-0.79174400	1.37596200
H	3.57455800	-1.60054100	-0.16087400
C	4.96995700	-0.00868400	-0.32814700
C	6.20727000	-0.90296600	-0.13223500
O	7.15278300	-0.43432900	0.55041100
O	6.14707500	-2.03371100	-0.67452200
O	-2.38022600	2.00126600	-2.71646600
H	-1.89054500	2.24589100	-1.90274900
H	-2.75930400	2.83294100	-3.04300000
N	5.23638800	1.32973200	0.27934400
H	5.39064200	1.24089100	1.29120100
H	6.08424300	1.74937000	-0.11830600
H	4.45080100	1.97365200	0.12659900
H	4.81233200	0.15973900	-1.39672100

TS:

C	-0.06268800	-1.55865600	-0.64930400
C	-0.76033300	-1.95314700	0.52558400
C	-1.91494700	-1.30313100	0.89423900
C	-2.45478400	-0.21123400	0.15598000
C	-1.77473700	0.21117000	-0.95958900
C	-0.53265300	-0.38889200	-1.34830900
H	-0.39053000	-2.80279900	1.09209200

H	-0.17354900	-0.23662400	-2.36382600
O	4.59537800	-1.34823000	0.39952200
H	5.44445700	-1.79096000	0.56249800
O	2.44127900	-2.85817400	0.73924800
H	3.30459700	-2.37905400	0.54740700
H	4.44825200	-0.74327700	1.16619700
O	3.77481800	0.28650600	2.44269000
H	3.55575200	1.14228500	2.02042800
H	4.38459000	0.49873100	3.16837500
H	2.08302300	-2.38998000	1.56176400
I	1.08284500	1.14221600	-0.29322200
H	-2.44804600	-1.63975100	1.78154700
H	-2.15362100	1.03786600	-1.55669300
O	0.98504800	-2.19628900	-1.07702900
H	1.73762200	-2.60705600	-0.11669000
O	1.64380300	-1.43912100	2.81517900
H	1.75338500	-1.93952300	3.64036700
H	2.37348600	-0.77754500	2.81077300
O	4.52141600	0.27454800	-1.91607500
H	3.74845100	-0.10948100	-2.38338200
H	4.60156100	-0.26349900	-1.10249200
Cl	2.87133600	2.80345900	0.68261000
C	-3.75853800	0.42736900	0.57261200
H	-3.98894700	0.16674600	1.61268600
H	-3.68466600	1.51647300	0.51113400
C	-4.93727700	0.01289300	-0.31351300
C	-6.24946500	0.66025200	0.16408400
O	-7.13304100	-0.10500200	0.62584200
O	-6.30387100	1.90997500	0.05666000
O	2.34692700	-0.97528500	-3.19659600
H	1.89465000	-1.44090000	-2.45810700
H	2.79211300	-1.67383700	-3.70215800
N	-5.09022400	-1.47333000	-0.28989700
H	-5.21841200	-1.80872800	0.67278600
H	-5.91844300	-1.76270200	-0.82193300
H	-4.26813500	-1.94152300	-0.68960400
H	-4.75106500	0.29104300	-1.35372500

Product

C	-0.13584400	-1.63084500	-0.50658900
C	-0.92290000	-1.94247100	0.66552500
C	-2.03722000	-1.21961400	0.94541300
C	-2.48592500	-0.09689900	0.13990000
C	-1.72422600	0.29516400	-0.90657000

C	-0.44639300	-0.36262000	-1.22401000
H	-0.62787900	-2.79790100	1.26612400
H	-0.21676700	-0.41957300	-2.28896400
O	4.45152800	-1.33659900	0.68462700
H	5.28403100	-1.76932800	0.93921200
O	2.38510400	-2.73940100	1.21398800
H	3.25676400	-2.25190200	0.94793100
H	4.30102700	-0.60840900	1.34092900
O	3.61552400	0.57905000	2.41590700
H	3.53000000	1.39763600	1.86727600
H	4.19854300	0.81350000	3.15658500
H	1.93393800	-2.08965000	1.90108800
I	1.15078400	1.00830100	-0.47550500
H	-2.63908100	-1.49249000	1.81104800
H	-2.01487900	1.14127800	-1.52501300
O	0.79737100	-2.36776700	-0.89573200
H	1.80218200	-2.75714600	0.40060800
O	1.44571800	-1.04047200	2.83656900
H	1.46630600	-1.39892400	3.74015600
H	2.16813800	-0.36621000	2.79767300
O	4.54693600	-0.25052200	-1.94253900
H	3.73800100	-0.62319900	-2.35455700
H	4.53423400	-0.58697100	-1.02464000
Cl	3.35450700	2.97864900	0.49166800
C	-3.78652200	0.59043800	0.48283700
H	-3.99329200	0.48805900	1.55534100
H	-3.71469800	1.65692500	0.25699900
C	-4.98662300	0.05610900	-0.30467600
C	-6.29105500	0.76781500	0.10300300
O	-7.20441800	0.05454100	0.58917700
O	-6.31296600	2.00771500	-0.08912200
O	2.26764600	-1.42495700	-3.11599300
H	1.76864500	-1.79108300	-2.35447100
H	2.64778900	-2.19665800	-3.56513600
N	-5.15021100	-1.41272300	-0.07692500
H	-5.20178000	-1.62599500	0.92714500
H	-6.02744600	-1.74234500	-0.49626300
H	-4.37537600	-1.94945100	-0.48346300
H	-4.82438600	0.18674600	-1.37780100

Tyr+I_2-ms

Reactant:

C	1.14067500	2.01952700	-0.76936900
C	1.42274700	1.62059500	0.54025200
C	2.41941900	0.66742700	0.77102500
C	3.14368000	0.10715000	-0.28112000
C	2.85735100	0.53538900	-1.58626500
C	1.86763800	1.47759200	-1.83608600
H	0.87699300	2.05601900	1.37180600
H	1.63877700	1.79371700	-2.84973900
O	-3.88200200	1.86708600	0.57962500
H	-4.65438200	2.40701500	0.81433800
O	-1.51078500	3.29030500	0.98530300
H	-2.35604200	2.85346100	0.73399400
H	-3.75099500	1.24938000	1.33536200
O	-3.26537800	0.25809000	2.76352900
H	-3.12247800	-0.65279200	2.45158700
H	-3.92836200	0.18744000	3.47016200
H	-1.20288100	2.76891200	1.76285200
I	-1.05775800	-0.40528200	0.05697000
H	2.62710500	0.35676800	1.79283200
H	3.41360900	0.11351700	-2.42073300
O	0.15889800	2.92505500	-1.05524100
H	-0.43793600	3.06657500	-0.26162900
I	-3.15065700	-2.09653700	-0.17873700
O	-0.87353000	1.65928400	3.16077600
H	-0.96440800	2.19879500	3.96263300
H	-1.69661100	1.12460400	3.11840500
O	-3.90635300	1.10354300	-2.13219700
H	-3.00500400	1.32549300	-2.45096600
H	-3.89688600	1.30702500	-1.17470400
C	4.24378600	-0.89445800	-0.02606900
H	4.15001900	-1.30847700	0.98529600
H	4.18045300	-1.72504500	-0.73503700
C	5.64089900	-0.28527600	-0.18168900
C	6.73970400	-1.31754300	0.12382200
O	7.44097600	-1.12410700	1.14887100
O	6.81930500	-2.27495100	-0.68449500
N	5.78792100	0.87277000	0.75029700
H	5.66276000	0.56880400	1.72381500
H	6.72596000	1.28235300	0.68221300
H	5.09589700	1.60507100	0.54871800
H	5.77842600	0.10683000	-1.19232800
O	-1.36182200	1.74390700	-3.11703200
H	-1.53296400	2.42477300	-3.78733200
H	-0.88038100	2.20862500	-2.40009600

TS:

C	**0.90120700**	**1.95381800**	**-0.57218900**
C	**1.67737600**	**2.15098400**	**0.62236100**
C	**2.66920800**	**1.27261000**	**0.94993500**
C	**2.97855100**	**0.10574600**	**0.16365400**
C	**2.22094500**	**-0.14834900**	**-0.93806400**
C	**1.09081700**	**0.69188000**	**-1.29601200**
H	**1.49153400**	**3.04305500**	**1.21319700**
H	**0.81880500**	**0.72368300**	**-2.35002400**
O	**-3.57731000**	**2.15513700**	**0.60576000**
H	**-4.38708900**	**2.63782400**	**0.84425400**
O	**-1.44549100**	**3.55423700**	**0.99110200**
H	**-2.32951600**	**3.07550500**	**0.78617100**
H	**-3.43219100**	**1.49276600**	**1.32582900**
O	**-2.74936500**	**0.45744400**	**2.59537200**
H	**-2.61027400**	**-0.38139400**	**2.11307500**
H	**-3.39331700**	**0.24719500**	**3.29204800**
H	**-1.06898300**	**3.05223100**	**1.81729900**
I	**-0.77159000**	**-0.50090500**	**-0.51341200**
H	**3.26861000**	**1.46163300**	**1.83896100**
H	**2.42126300**	**-1.01733400**	**-1.56113200**
O	**0.05779600**	**2.81078000**	**-0.97438100**
H	**-0.82156100**	**3.35681500**	**0.20794700**
I	**-3.34050300**	**-2.19150000**	**0.24591100**
O	**-0.65339200**	**2.18417200**	**2.99724100**
H	**-0.77236100**	**2.68911800**	**3.81910400**
H	**-1.36252700**	**1.49850100**	**3.00072200**
O	**-3.86941700**	**1.13989800**	**-2.04219900**
H	**-3.02760900**	**1.42952000**	**-2.45599800**
H	**-3.78495100**	**1.40558200**	**-1.10502200**
C	**4.14060200**	**-0.77943700**	**0.54876400**
H	**4.39047000**	**-0.63475900**	**1.60700300**
H	**3.87493000**	**-1.83064900**	**0.41094900**
C	**5.39393800**	**-0.52937200**	**-0.29413400**
C	**6.55241900**	**-1.45084300**	**0.12896900**
O	**7.58635800**	**-0.90140200**	**0.58566200**
O	**6.34567700**	**-2.67990800**	**-0.02080900**
N	**5.83109500**	**0.89275900**	**-0.15521700**
H	**5.96952300**	**1.13611200**	**0.83357200**
H	**6.72963700**	**1.04128800**	**-0.62787500**
H	**5.14210300**	**1.54143100**	**-0.55374000**
H	**5.17717500**	**-0.68570200**	**-1.35400100**
O	**-1.47356300**	**2.06898100**	**-3.19504300**

H	**-1.75148200**	**2.88702000**	**-3.63680200**
H	**-0.93962600**	**2.36181800**	**-2.42279700**

Product

C	**1.08432300**	**2.00384600**	**-0.45594200**
C	**1.92047700**	**2.16211700**	**0.71348600**
C	**2.86617500**	**1.23178000**	**1.00082800**
C	**3.07844000**	**0.03389000**	**0.20470600**
C	**2.25549900**	**-0.20719500**	**-0.84002300**
C	**1.13991300**	**0.69470500**	**-1.17129200**
H	**1.80225900**	**3.06407200**	**1.30648200**
H	**0.94986200**	**0.80380700**	**-2.24018100**
O	**-3.46719000**	**2.25869200**	**0.73293000**
H	**-4.23744200**	**2.77923000**	**1.01889700**
O	**-1.27515300**	**3.46268100**	**1.24071700**
H	**-2.18491000**	**3.04694000**	**0.97681400**
H	**-3.37532700**	**1.52013700**	**1.38613900**
O	**-2.78179800**	**0.28316100**	**2.49332200**
H	**-2.80584600**	**-0.50756200**	**1.91463600**
H	**-3.40907100**	**0.09421800**	**3.21110700**
H	**-0.88675600**	**2.79468900**	**1.94955000**
I	**-0.71977600**	**-0.32834300**	**-0.48934200**
H	**3.51335700**	**1.38463300**	**1.86291400**
H	**2.37318400**	**-1.09804900**	**-1.45263800**
O	**0.31402700**	**2.90542800**	**-0.85015300**
H	**-0.68231900**	**3.41492000**	**0.43886000**
I	**-3.71827000**	**-2.18448900**	**0.11539300**
O	**-0.48998100**	**1.73398000**	**2.90965400**
H	**-0.49290400**	**2.10971700**	**3.80647400**
H	**-1.25787900**	**1.11386400**	**2.87662500**
O	**-3.78266800**	**1.46330600**	**-1.98753600**
H	**-2.91862400**	**1.72373500**	**-2.37360400**
H	**-3.70124400**	**1.67593400**	**-1.03698100**
C	**4.21826400**	**-0.89714300**	**0.54533000**
H	**4.49622400**	**-0.78552100**	**1.60050800**
H	**3.90998200**	**-1.93385500**	**0.38979500**
C	**5.45997800**	**-0.67686000**	**-0.32188400**
C	**6.58806300**	**-1.65977600**	**0.04534000**
O	**7.66674400**	**-1.16546100**	**0.45950600**
O	**6.31599600**	**-2.87556100**	**-0.10657400**
N	**5.96721800**	**0.71990800**	**-0.16175800**
H	**6.11656700**	**0.94284600**	**0.83036000**
H	**6.87449300**	**0.82491900**	**-0.62992900**
H	**5.31641800**	**1.41063400**	**-0.55357500**

H	5.21034900	-0.79732000	-1.37920400
O	-1.31738800	2.28311600	-3.07431200
H	-1.52588000	3.12257100	-3.51427600
H	-0.76606100	2.52926900	-2.30090400

Tyr+NHClI-ms

Reactant:

C	-0.56704600	-1.89228900	-0.62859300
C	-1.10677200	-1.92576100	0.66036300
C	-2.17979100	-1.09525400	0.97935100
C	-2.18558000	-0.21143600	-1.25467600
C	-1.11070400	-1.03194900	-1.59006700
H	-0.68719300	-2.59857700	1.40321100
H	-0.68016200	-1.01177700	-2.58770400
O	4.34658400	-1.62487500	0.45981000
H	5.15889400	-2.13385100	0.61552700
O	2.02361300	-3.01140000	1.14701600
H	2.87028100	-2.61135600	0.84572000
H	4.26892100	-1.00180400	1.22087100
O	3.72680800	0.22530100	2.40776700
H	3.59541300	0.94637900	1.74434100
H	4.38755300	0.55025900	3.04035600
H	1.67502100	-2.36186600	1.80149600
I	1.34396100	0.76696200	-0.28247400
O	4.33699200	0.00621100	-1.76288700
H	5.16468300	-0.01889800	-2.26872200
H	4.47129700	-0.60163900	-0.99783600
H	-2.59375900	-1.12445800	1.98487400
O	1.30653100	-1.04130600	2.99732200
H	2.14018500	-0.53277300	2.88272000
H	1.38748500	-1.46221800	3.86841800
H	-2.59798000	0.45843800	-2.00637300
O	0.49187300	-2.67792200	-0.98768700
H	1.04193500	-2.89231200	-0.17660800
N	3.11525800	1.76421000	0.16449200
H	3.72700600	1.53054100	-0.63172900
Cl	2.95749700	3.50168900	0.14424000
O	2.34615400	-1.67276900	-2.93693900
H	1.72416100	-1.92214600	-2.22512000
H	2.98542000	-1.05334100	-2.52808900
C	-2.73235500	-0.22521300	0.03394500
C	-3.91956800	0.64396300	0.37460200

H	-4.08118100	0.65247400	1.45943000
H	-3.74755900	1.67576300	0.05493300
C	-5.20568000	0.17701200	-0.31329700
C	-6.41374800	1.04050900	0.08887600
O	-7.35410300	0.46773600	0.69535300
O	-6.33773500	2.25432200	-0.22339800
N	-5.47859900	-1.24560000	0.05091500
H	-5.59587700	-1.34268200	1.06695300
H	-6.34652700	-1.57624900	-0.38488600
H	-4.70853500	-1.85789800	-0.24460100
H	-5.08972900	0.20211800	-1.39988600

TS:

C	-0.45602500	-2.03201000	-0.63079900
C	-1.11136700	-2.12304700	0.62365600
C	-2.16239800	-1.27516900	0.95157300
C	-1.99116100	-0.19264000	-1.17833200
C	-0.92765400	-1.03156100	-1.52456700
H	-0.77558200	-2.87690200	1.33223600
H	-0.46947600	-0.95699000	-2.50858000
O	4.22115000	-1.52677300	0.93603200
H	4.96706800	-2.03999400	1.29449600
O	2.06805200	-2.84465600	1.22737800
H	3.37352900	-2.11862600	1.00040600
H	3.99022200	-0.49577400	1.67054500
O	3.65352000	0.45616600	2.20301700
H	3.42913100	1.11969000	1.42310800
H	4.39440300	0.82446200	2.72115900
H	1.61747400	-2.20834100	1.82944900
I	1.23452100	0.77622300	-0.46422600
O	4.35782700	-0.13634700	-1.51860500
H	5.19085900	-0.24576100	-2.00463300
H	4.45320600	-0.68050200	-0.70870600
H	-2.64107400	-1.37432800	1.92490900
O	1.16330200	-0.84320400	2.95397600
H	1.96740400	-0.29638100	2.86786600
H	1.20045700	-1.20174200	3.85563100
H	-2.32642100	0.55825500	-1.89250700
O	0.55616200	-2.81291000	-0.94057600
H	1.51746100	-2.86260300	0.38549900
N	2.98299000	1.79377800	0.09306900
H	3.65421500	1.57796200	-0.65768000
Cl	2.82727400	3.52513100	0.14424800
O	2.43778500	-1.93728700	-2.71794500

H	**1.74444000**	**-2.18861600**	**-2.05678700**
H	**3.01316100**	**-1.28022800**	**-2.27849300**
C	**-2.62162300**	**-0.28916300**	**0.06466100**
C	**-3.79278900**	**0.59656900**	**0.41494300**
H	**-3.97510400**	**0.57069600**	**1.49676600**
H	**-3.59450700**	**1.63583900**	**0.13701700**
C	**-5.08097900**	**0.18548400**	**-0.30703300**
C	**-6.27595900**	**1.05161400**	**0.12328700**
O	**-7.22089400**	**0.47593800**	**0.72065400**
O	**-6.18523100**	**2.27338200**	**-0.15382700**
N	**-5.38171600**	**-1.24690700**	**-0.00838800**
H	**-5.51470200**	**-1.38449700**	**1.00101900**
H	**-6.24712600**	**-1.54619300**	**-0.47053300**
H	**-4.61453600**	**-1.85570000**	**-0.31844700**
H	**-4.95033800**	**0.25618300**	**-1.38992200**

Product

C	**-0.44042000**	**-1.94791700**	**-0.66032500**
C	**-1.27129800**	**-2.24804700**	**0.49034000**
C	**-2.29120300**	**-1.42027300**	**0.82982100**
C	**-1.79223500**	**0.17629100**	**-0.91050900**
C	**-0.59701500**	**-0.59972500**	**-1.27875900**
H	**-1.07940400**	**-3.17224500**	**1.02756100**
H	**-0.37376800**	**-0.61034100**	**-2.34658200**
O	**4.14542100**	**-1.11702000**	**0.96895600**
H	**4.95672600**	**-1.56538100**	**1.26033200**
O	**2.10043300**	**-2.88981600**	**1.24855300**
H	**3.43507700**	**-1.81020300**	**1.00173800**
H	**3.55447700**	**-0.10384100**	**2.31124100**
O	**3.06221000**	**0.50652400**	**2.90996900**
H	**3.50459400**	**1.84433000**	**1.34467400**
H	**3.50267700**	**0.43915300**	**3.77214600**
H	**1.53978800**	**-2.30803200**	**1.81429500**
I	**1.15087100**	**0.52625400**	**-0.46362400**
O	**4.44584100**	**-0.26959100**	**-1.64336000**
H	**5.26168700**	**-0.64522600**	**-2.01113200**
H	**4.38076600**	**-0.63585000**	**-0.73054200**
H	**-2.92428400**	**-1.67894900**	**1.67738800**
O	**0.79300200**	**-1.10916500**	**2.94464700**
H	**1.55281200**	**-0.48438200**	**3.00459000**
H	**0.76334900**	**-1.55289600**	**3.80748900**
H	**-1.98152900**	**1.09276000**	**-1.46543000**
O	**0.40158600**	**-2.75686900**	**-1.09526900**
H	**1.62023000**	**-2.96274300**	**0.40174800**

N	3.37159200	1.89118100	0.32986500
H	4.19582900	1.48168000	-0.11795900
Cl	3.36541900	3.57636400	-0.10193300
O	2.50320800	-1.95532900	-2.86980600
H	1.78261900	-2.13850500	-2.23438200
H	3.10867400	-1.33152600	-2.41624300
C	-2.59848200	-0.19562900	0.10945000
C	-3.80807400	0.62036300	0.50206900
H	-4.05957300	0.44134600	1.55478200
H	-3.59037100	1.68521800	0.38881200
C	-5.04240300	0.33424400	-0.35701000
C	-6.23438000	1.21973100	0.05259900
O	-7.26304600	0.63712600	0.47883200
O	-6.05797500	2.45527900	-0.07996200
N	-5.44123000	-1.10064100	-0.23091100
H	-5.56912500	-1.35847900	0.75566200
H	-6.33811100	-1.26666500	-0.70111100
H	-4.73948300	-1.72837200	-0.64004900
H	-4.81685800	0.50243300	-1.41326900

Tyr+I2-cs-a1

Reactant:

H	-1.61009300	2.65376300	2.46243200
C	-1.74723300	2.14364900	1.51134000
C	-1.36328700	2.01107800	-0.87116900
C	-2.09938300	0.82168600	-0.90952300
H	-2.22786700	0.31002700	-1.86307900
C	-2.46241800	0.95814200	1.45333300
C	-1.17740800	2.73768200	0.34276800
H	-0.95643900	2.42922000	-1.78967500
I	3.72066900	-0.69223300	0.05247100
I	1.31621700	0.53043600	-0.34232500
O	6.36149500	-2.04098500	0.44805100
H	6.85931900	-1.47001900	-0.15868700
H	6.15911300	-2.83227700	-0.07630500
H	-2.88444400	0.54636400	2.36977300
O	-0.52451700	3.86178800	0.38778000
C	-3.49973700	-0.98423700	0.19028300
H	-3.30062700	-1.53568900	-0.73769100
H	-3.26790400	-1.65003200	1.02742400
C	-5.00417400	-0.68963200	0.26752600
H	-5.24804900	-0.18892200	1.20760700
N	-5.37880700	0.25219100	-0.82906400

C	-5.83579300	-1.97367300	0.12727200
H	-5.21526600	-0.18509600	-1.74405200
H	-6.37399800	0.49643900	-0.78462500
H	-4.82470800	1.11626900	-0.77720300
O	-6.49908200	-2.11670700	-0.93193400
O	-5.75267300	-2.78361200	1.08411300
C	-2.65958400	0.26797000	0.24245800

TS:

H	-1.64674000	2.68760500	2.43622400
C	-1.75193500	2.14985800	1.49659900
C	-1.27462200	1.94240300	-0.86876800
C	-2.03471500	0.76169100	-0.90081000
H	-2.13782400	0.22775300	-1.84493100
C	-2.47385700	0.97194200	1.44393600
C	-1.14005600	2.71191300	0.32960600
H	-0.86075200	2.34736300	-1.78975400
I	3.69999600	-0.67276200	0.06991600
I	1.27514500	0.55366100	-0.33796800
O	6.53267600	-2.17218000	0.38386300
H	6.82910700	-1.47751700	-0.22526100
H	6.05806500	-2.80136600	-0.18235500
H	-2.93119700	0.58790500	2.35537000
O	-0.49872300	3.83625800	0.36376400
C	-3.48843300	-0.99674400	0.20022700
H	-3.28528700	-1.56135600	-0.71875100
H	-3.26886700	-1.65324000	1.04800900
C	-4.99062200	-0.68841600	0.26064300
H	-5.23930400	-0.17447100	1.19232200
N	-5.34750600	0.24282200	-0.85069500
C	-5.83110100	-1.96772100	0.12873700
H	-5.18301500	-0.20863900	-1.75861400
H	-6.34019400	0.49855400	-0.81619100
H	-4.78373800	1.10107800	-0.80668500
O	-6.49213000	-2.11477300	-0.93122100
O	-5.75672500	-2.76971400	1.09284900
C	-2.63815700	0.24878000	0.24286700

Product

H	-1.61009300	2.65376300	2.46243200
C	-1.74723300	2.14364900	1.51134000
C	-1.36328700	2.01107800	-0.87116900
C	-2.09938300	0.82168600	-0.90952300
H	-2.22786700	0.31002700	-1.86307900

C	-2.46241800	0.95814200	1.45333300
C	-1.17740800	2.73768200	0.34276800
H	-0.95643900	2.42922000	-1.78967500
I	3.72066900	-0.69223300	0.05247100
I	1.31621700	0.53043600	-0.34232500
O	6.36149500	-2.04098500	0.44805100
H	6.85931900	-1.47001900	-0.15868700
H	6.15911300	-2.83227700	-0.07630500
H	-2.88444400	0.54636400	2.36977300
O	-0.52451700	3.86178800	0.38778000
C	-3.49973700	-0.98423700	0.19028300
H	-3.30062700	-1.53568900	-0.73769100
H	-3.26790400	-1.65003200	1.02742400
C	-5.00417400	-0.68963200	0.26752600
H	-5.24804900	-0.18892200	1.20760700
N	-5.37880700	0.25219100	-0.82906400
C	-5.83579300	-1.97367300	0.12727200
H	-5.21526600	-0.18509600	-1.74405200
H	-6.37399800	0.49643900	-0.78462500
H	-4.82470800	1.11626900	-0.77720300
O	-6.49908200	-2.11670700	-0.93193400
O	-5.75267300	-2.78361200	1.08411300
C	-2.65958400	0.26797000	0.24245800

Tyr+H_2OI

Reactant:

C	0.97213600	1.84285600	-0.39728500
C	0.09073300	1.95405100	-1.47379200
C	-1.04141200	1.16583100	-1.49044200
C	-0.48269700	0.10187500	0.57160700
C	0.75384900	0.84341200	0.61808600
H	0.28716000	2.67603700	-2.25749100
H	-0.67954900	-0.59171400	1.38243100
O	2.03523500	2.60998800	-0.24292300
H	2.16471800	3.22232200	-0.98313900
H	-1.73031100	1.27138600	-2.32347800
C	-1.35548700	0.22790600	-0.47383000
C	-2.63234200	-0.57334400	-0.52533600
H	-3.02071500	-0.60378300	-1.54727700
H	-2.43847600	-1.59958500	-0.21549600
C	-3.70917400	-0.02737000	0.40461400
H	-3.32763600	0.04014900	1.42568500

N	**-4.09404400**	**1.36152600**	**0.01016000**
C	**-4.99100100**	**-0.89423000**	**0.43288000**
H	**-4.98862900**	**1.58411800**	**0.45680400**
H	**-3.39185400**	**2.05524200**	**0.27483600**
H	**-4.24429900**	**1.42581700**	**-1.00036700**
O	**-6.07581200**	**-0.27376000**	**0.38673700**
O	**-4.80945500**	**-2.12226000**	**0.52870900**
O	**3.51654900**	**1.84064700**	**2.20580900**
H	**3.22201100**	**2.27311800**	**1.39503100**
O	**3.89809100**	**-2.49213600**	**-0.67196500**
H	**3.93122700**	**-3.14796200**	**0.03637500**
H	**3.55807600**	**0.90452100**	**1.98078700**
I	**2.24923800**	**-0.79931500**	**-0.06108900**
H	**4.76825000**	**-2.07406100**	**-0.69734000**
H	**1.19423900**	**1.05164000**	**1.58929700**

TS:

C	**0.87493200**	**1.93720700**	**-0.41981200**
C	**-0.27268800**	**2.57231600**	**-0.90943500**
C	**-1.41877400**	**1.83722800**	**-1.10727900**
C	**-0.39964000**	**-0.17168400**	**-0.32237500**
C	**0.81063300**	**0.55615800**	**-0.02061800**
H	**-0.23065100**	**3.62667400**	**-1.15791000**
H	**-0.42611300**	**-1.22810000**	**-0.07425200**
O	**2.01679700**	**2.56748700**	**-0.23709800**
H	**1.94605100**	**3.51381600**	**-0.43620800**
H	**-2.29453900**	**2.34053800**	**-1.50685000**
C	**-1.50906400**	**0.44955900**	**-0.82061100**
C	**-2.79969300**	**-0.30255700**	**-1.03100300**
H	**-3.41579200**	**0.20755400**	**-1.77718100**
H	**-2.59091300**	**-1.30517100**	**-1.40230300**
C	**-3.60079500**	**-0.46854700**	**0.25538600**
H	**-2.99745300**	**-0.97725400**	**1.01022800**
N	**-3.95934500**	**0.86199000**	**0.83398200**
C	**-4.90535600**	**-1.27646900**	**0.05628100**
H	**-4.71543400**	**0.72596400**	**1.51126700**
H	**-3.16662800**	**1.32000500**	**1.28810200**
H	**-4.32089400**	**1.48793900**	**0.10924300**
O	**-5.93128600**	**-0.80812200**	**0.59652300**
O	**-4.79173800**	**-2.32692500**	**-0.60219300**
H	**0.72359100**	**0.69523600**	**1.19575700**
O	**0.73419500**	**0.81451000**	**2.67837200**
H	**0.57640800**	**1.74354500**	**2.88928900**
O	**5.02109000**	**-2.09344800**	**-0.12152100**

H	5.29668500	-1.95521100	-1.03417200
H	1.64501500	0.62480300	2.93772600
I	2.64092400	-0.56416300	-0.03566700
H	4.64732900	-2.98091700	-0.09612200

Product

C	0.97859900	1.97694400	-0.37588700
C	-0.19676100	2.69376000	-0.59577400
C	-1.39105000	2.03018600	-0.85135300
C	-0.26492400	-0.07829000	-0.67378700
C	0.93536900	0.57668000	-0.40305300
H	-0.16288800	3.77835300	-0.56754300
H	-0.28373100	-1.16310900	-0.70498400
O	2.16614700	2.58751600	-0.12521300
H	2.06364100	3.54772000	-0.15899200
H	-2.29298700	2.60853300	-1.02538000
C	-1.44320300	0.63812700	-0.90407400
C	-2.73811200	-0.09404900	-1.14915600
H	-3.44539300	0.55329500	-1.67625900
H	-2.56578000	-0.97188900	-1.77147300
C	-3.38564200	-0.58842100	0.13983800
H	-2.69066300	-1.22759900	0.68934700
N	-3.70799400	0.55639200	1.04599400
C	-4.68685600	-1.39254600	-0.09753200
H	-4.45478200	0.24939500	1.67844200
H	-2.89902000	0.87268700	1.58427700
H	-4.07337600	1.35197800	0.51617600
O	-5.64863000	-1.12032800	0.65564400
O	-4.63690700	-2.25015800	-0.99877400
H	-0.38336400	0.40594200	1.57892200
O	-0.79141200	0.90097800	2.32285200
H	-0.63332800	1.85678800	2.20065600
O	5.10027100	-2.32054300	0.42678500
H	5.49075900	-1.94175300	-0.36782500
H	-0.40665800	0.60697100	3.16960700
I	2.67520500	-0.53453100	-0.02585000
H	4.54736900	-3.04598700	0.11742700

Tyr+NH_2ClI^+-n

Reactant:

C	0.20013200	2.23169200	-0.30507700
C	-0.66824800	2.18343800	-1.39274200

C	-1.65781000	1.21447000	-1.42690700
C	-0.95122900	0.31122700	0.66867000
C	0.10448400	1.25605100	0.72035700
H	-0.57336000	2.91256800	-2.18946800
H	-1.04653700	-0.39669600	1.48570400
O	1.15820900	3.16076500	-0.17455600
H	1.19543300	3.74866300	-0.94272000
H	-2.33300600	1.18921900	-2.27705100
C	-1.81968800	0.26252300	-0.40513100
C	-2.93612900	-0.74976200	-0.45311800
H	-3.30075900	-0.86028900	-1.47845800
H	-2.57852400	-1.72495300	-0.12333500
C	-4.10341800	-0.37759300	0.45360700
H	-3.76416400	-0.28057500	1.48715400
N	-4.65886200	0.95565800	0.07062900
C	-5.25622500	-1.40789600	0.41816500
H	-5.58310300	1.05499300	0.49992000
H	-4.05613800	1.72862100	0.35879400
H	-4.79479200	1.01594400	-0.94227400
O	-6.41275600	-0.93739700	0.34712600
O	-4.91407800	-2.60319400	0.48909600
H	0.64668100	1.42778400	1.64462600
O	2.92335300	2.54243900	2.05128100
H	2.46624200	2.91356100	1.28544600
H	3.19110300	-2.50155800	-1.28403000
H	3.04356900	1.61091100	1.83788100
I	1.89469800	-0.31593200	-0.16136100
H	4.09371600	-1.16240900	-1.63986400
N	3.59667500	-1.64905100	-0.89025100
Cl	4.75887600	-2.11314400	0.30568600

TS

C	0.08137300	2.35633900	-0.08165800
C	-1.16771800	2.91949200	-0.36625600
C	-2.22201200	2.09598800	-0.68905200
C	-0.89748900	0.12593400	-0.45891600
H	-1.27986100	3.99768900	-0.34976400
H	-0.77000800	-0.95226800	-0.46977500
O	1.13845500	3.08365200	0.21927300
H	0.92618200	4.02861800	0.26969100
H	-3.18303200	2.54877300	-0.91375000
C	-2.11115600	0.68285000	-0.74772300
C	-3.31096000	-0.17404000	-1.07007400
H	-4.11386300	0.44373300	-1.48149500

H	-3.05264000	-0.92191400	-1.81913300
C	-3.82705700	-0.92502500	0.15100600
H	-3.05185900	-1.58777800	0.54170800
N	-4.15610800	0.02482900	1.25711700
C	-5.08498600	-1.77969400	-0.13571600
H	-4.79367900	-0.45447900	1.90167100
H	-3.32636900	0.34662100	1.75887600
H	-4.65266000	0.84547800	0.89905700
O	-5.96585000	-1.76969200	0.75261500
O	-5.08002200	-2.40973900	-1.20898100
C	0.22385800	0.92610800	-0.02787400
H	0.17230400	0.76066300	1.18454200
O	0.14195100	0.52852400	2.66089300
H	-0.00767900	1.38676700	3.07739400
H	4.85998400	-1.59254300	-1.56575400
H	1.03510700	0.25666100	2.90728600
I	2.18876700	0.10089400	-0.33522900
H	5.51692300	-0.46999600	-0.58323000
N	4.72460000	-1.10178700	-0.68361500
Cl	4.92692000	-2.31025700	0.56249900

Product

C	0.18039300	2.39571900	0.07240900
C	-1.10097200	2.94066000	0.13449300
C	-2.20573300	2.19050400	-0.25131300
C	-0.77512900	0.34093400	-0.77510000
H	-1.22042500	3.96016300	0.48713100
H	-0.64058700	-0.67717900	-1.12690500
O	1.28384200	3.09514900	0.44471100
H	1.03347600	3.98024100	0.74047200
H	-3.19504000	2.63309700	-0.19335300
C	-2.06127000	0.88397300	-0.71539500
C	-3.25542900	0.03837100	-1.07826300
H	-4.11671800	0.67426800	-1.30377600
H	-3.04512600	-0.56135700	-1.96363800
C	-3.63361200	-0.93230400	0.03552700
H	-2.78800900	-1.58187100	0.27344100
N	-3.95735100	-0.19035700	1.29209100
C	-4.84238500	-1.83145900	-0.31632400
H	-4.55162800	-0.79746100	1.86687700
H	-3.12003300	0.08022400	1.81304700
H	-4.49864700	0.65427700	1.09004100
O	-5.70359800	-1.97384200	0.58046200
O	-4.82287600	-2.34427400	-1.45069800

C	0.34044400	1.07745800	-0.37811300
H	-0.58276700	0.23911200	1.49733700
O	-1.02878100	0.24630000	2.37441400
H	-0.96777700	1.13857100	2.76435300
H	5.18911500	-1.74798000	-1.21294900
H	-0.60878800	-0.40226500	2.96937500
I	2.25398000	0.20889400	-0.44809000
H	5.68582200	-0.74565700	-0.03340300
N	4.87389900	-1.25335000	-0.38031700
Cl	4.57904700	-2.50714300	0.80821700

Tyr+HOCl-n

Reactant:

O	3.54075700	0.09010900	1.30995200
H	2.86815400	0.70475000	1.64768700
H	3.38928800	0.04810500	0.33343500
O	2.74034400	-2.58940900	1.64316200
H	2.68679300	-2.83061200	0.68849200
H	2.98961800	-1.63527100	1.62831300
O	-0.07352500	-2.78561200	1.92018700
H	-0.28638800	-2.81937700	0.95584600
H	0.90685400	-2.68348800	1.92663800
N	0.68278100	1.10575400	-1.12865900
H	0.17270800	1.54265300	-1.90052100
C	-2.74917900	1.38794400	-0.96055600
C	-1.97644400	1.56300700	0.19525600
C	-2.25081100	0.75002000	1.30469400
C	-3.25613100	-0.21669500	1.26439500
C	-4.00909100	-0.37964600	0.09507100
C	-3.76205000	0.42659400	-1.01926600
H	-4.35538400	0.29362900	-1.91972900
H	-3.45646800	-0.84528200	2.12907500
H	-1.65928900	0.86219100	2.21080700
H	-2.55099000	2.00416600	-1.83492100
O	-5.01677300	-1.32449100	-0.00851000
C	-0.83194600	2.55001100	0.23252900
H	-0.92880800	3.27489400	-0.58558600
H	-0.84200300	3.11108500	1.17212800
C	0.55423300	1.88069600	0.13122500
C	1.67919500	2.94150600	0.24146400
O	2.36823500	3.19228400	-0.78952700
O	1.80399100	3.48112400	1.37881900

H	-5.08535700	-1.82732500	0.82239700
H	0.67641500	1.16982000	0.95353100
Cl	0.11322200	-0.79528300	-1.00852400
O	-0.25782500	-2.83036700	-0.83508900
H	-0.92119000	-3.00872000	-1.52481700
O	2.40793200	-3.04191800	-1.10882100
H	2.73327400	-3.84387600	-1.54978700
H	1.40789400	-3.09336700	-1.11864000
O	3.27542400	-0.36363900	-1.43256500
H	2.98675700	-1.30699200	-1.39083600
H	4.20029200	-0.39325300	-1.73020700
H	1.66845900	1.01053600	-1.39751700

TS:

O	3.55832400	0.23265800	1.29849900
H	2.85523300	0.79054600	1.67045300
H	3.35800600	0.17246500	0.33116300
O	2.90142100	-2.51140500	1.55459000
H	2.78846800	-2.68994700	0.57691400
H	3.10915400	-1.54979700	1.59174800
O	0.14030800	-2.86023400	1.93268300
H	-0.07600100	-2.96648400	0.97888400
H	1.11417400	-2.69652600	1.91412400
N	0.63660000	1.06956700	-1.07010000
H	0.13210900	1.49433200	-1.85765400
C	-2.79383700	1.30548400	-0.96158900
C	-2.05248700	1.51032200	0.21008700
C	-2.33392000	0.70612600	1.32398700
C	-3.31677600	-0.28269800	1.27230700
C	-4.03850900	-0.47641800	0.08748000
C	-3.78321600	0.32137300	-1.03131900
H	-4.35238800	0.16426900	-1.94330900
H	-3.52480700	-0.90405200	2.14029300
H	-1.76641900	0.84352400	2.24183200
H	-2.58808500	1.91547100	-1.83859700
O	-5.02236200	-1.44293100	-0.02836100
C	-0.92765100	2.51896300	0.25455300
H	-1.02465300	3.23362000	-0.57201800
H	-0.95594300	3.08912600	1.18813000
C	0.47265200	1.88157500	0.18488600
C	1.58065800	2.96547200	0.21615300
O	2.24796700	3.15150900	-0.84134700
O	1.70049500	3.57581200	1.31288600

H	**-5.10027300**	**-1.93907700**	**0.80569600**
H	**0.62445100**	**1.19402900**	**1.01992000**
Cl	**0.13452200**	**-0.68484300**	**-0.95592800**
O	**0.04716400**	**-3.08836200**	**-0.84974000**
H	**-0.39050000**	**-3.33021300**	**-1.68290800**
O	**2.45512800**	**-2.85034100**	**-1.10304800**
H	**2.88482100**	**-3.62690800**	**-1.49593000**
H	**1.23050300**	**-3.03910300**	**-1.03819500**
O	**3.15463400**	**-0.24443300**	**-1.41722500**
H	**2.94923300**	**-1.22544700**	**-1.37664700**
H	**4.04483200**	**-0.16962300**	**-1.79868000**
H	**1.63889600**	**0.99578700**	**-1.32452600**

Product:

O	**-4.34882200**	**0.03193800**	**0.72184600**
H	**-3.68908800**	**-0.41277200**	**1.29983900**
H	**-3.99972500**	**-0.13395800**	**-0.18555900**
O	**-3.44831700**	**2.67204600**	**0.72161900**
H	**-3.03818700**	**2.67764100**	**-0.17297900**
H	**-3.80841700**	**1.75357200**	**0.79867000**
O	**-0.91987000**	**2.43262900**	**1.95261700**
H	**-0.37903900**	**2.41098700**	**1.13076600**
H	**-1.84286300**	**2.50768500**	**1.61267700**
N	**-0.72921600**	**-1.57251100**	**-1.09288700**
H	**-0.58009100**	**-2.57382200**	**-1.24192400**
C	**3.08882300**	**-1.47331700**	**-0.03389200**
C	**2.01927000**	**-0.96705500**	**0.71791700**
C	**2.12814600**	**0.33685200**	**1.22351500**
C	**3.25093500**	**1.12713700**	**0.96374000**
C	**4.29770300**	**0.60406100**	**0.19690800**
C	**4.22299100**	**-0.70223800**	**-0.29675800**
H	**5.04514500**	**-1.10017600**	**-0.88532400**
H	**3.31714200**	**2.14074400**	**1.35231100**
H	**1.31868800**	**0.75035700**	**1.82019100**
H	**3.02945800**	**-2.48205000**	**-0.43563800**
O	**5.43645300**	**1.33564800**	**-0.09795400**
C	**0.78041800**	**-1.79245100**	**0.98921400**
H	**0.93119300**	**-2.82935300**	**0.66594900**
H	**0.60405400**	**-1.81725800**	**2.07224400**
C	**-0.52840200**	**-1.27101600**	**0.34159200**
C	**-1.71765000**	**-1.95568600**	**1.06643200**
O	**-2.06350700**	**-3.10102500**	**0.66379200**
O	**-2.22777100**	**-1.32031700**	**2.03950100**
H	**5.36410900**	**2.22658100**	**0.28770000**

H	-0.61733900	-0.18946700	0.46448900
Cl	0.47388400	-0.79026900	-2.16970700
O	0.36536500	2.45090800	-0.58880500
H	0.80232100	1.58203600	-0.58970500
O	-2.14550100	2.26266700	-1.74697200
H	-2.29328200	2.71955800	-2.59180800
H	-0.49034900	2.31569300	-1.06447700
O	-3.09751200	-0.30639700	-1.76599700
H	-2.48583000	1.33881600	-1.87029900
H	-3.51278100	-0.68536000	-2.55858400
H	-2.28418200	-0.85982100	-1.58250500

Tyr+HOBr-n

Reactant:

O	2.39622800	-1.81268800	-1.84770100
H	2.60030700	-1.92047600	-2.79364400
O	4.18527000	-1.19116800	0.11942800
H	3.75539500	-1.68339900	0.85739500
H	3.62010600	-1.40032300	-0.66916400
O	3.31010900	1.26108600	1.06582700
H	3.64735600	0.41810500	0.66351400
H	4.00308300	1.52697000	1.69360500
O	1.40341700	-0.00317100	2.63534700
H	1.52907700	0.29691700	3.55110900
H	2.03462700	0.54287900	2.09864200
O	2.66430200	-2.39867300	2.15814000
H	3.10049700	-2.73688100	2.95764500
H	2.18840900	-1.57071200	2.43132800
O	1.52230800	-3.74241900	-0.07143100
H	1.78789400	-3.10600300	-0.77950000
H	1.87780400	-3.34311400	0.75150000
H	-0.08120200	2.18859500	-1.92677100
N	-0.35934200	1.39629900	-1.33947300
H	-1.27234600	1.06030700	-1.65119000
C	-3.70215800	0.76832400	-0.53244900
C	-2.71600200	0.89836700	0.45682700
C	-2.52445500	-0.17442600	1.34301700
C	-3.29188800	-1.33644700	1.25286700
C	-4.27336400	-1.44039800	0.25841900
C	-4.48049500	-0.38876100	-0.63749700
H	-5.24393000	-0.48048200	-1.40508900
H	-3.13637800	-2.15973300	1.94663400

H	**-1.75959600**	**-0.10276700**	**2.11317300**
H	**-3.86794900**	**1.58399800**	**-1.23285500**
O	**-5.06868200**	**-2.56471600**	**0.11856000**
C	**-1.84199500**	**2.13080200**	**0.54155800**
H	**-2.26742000**	**2.94086600**	**-0.06272800**
H	**-1.78055200**	**2.48425200**	**1.57602600**
C	**-0.39352200**	**1.85657200**	**0.07184000**
C	**0.47879000**	**3.12067300**	**0.24140700**
O	**0.85380000**	**3.72826800**	**-0.80607100**
O	**0.72506500**	**3.46423300**	**1.43342700**
H	**-4.84097300**	**-3.21998800**	**0.80149400**
H	**0.03223300**	**1.06960900**	**0.69942000**
Br	**1.06071300**	**-0.24848500**	**-1.67612500**

TS:

O	**1.07539600**	**-3.13587300**	**-0.99471100**
H	**0.82972700**	**-3.69306600**	**-1.75200300**
O	**3.28029200**	**-1.81024300**	**-1.57706700**
H	**3.95680300**	**-2.11812900**	**-0.95150100**
H	**1.94609400**	**-2.65869000**	**-1.24931700**
O	**2.99061200**	**0.59101100**	**-1.12029700**
H	**3.13420400**	**-0.52784800**	**-1.34122000**
H	**3.73909500**	**1.07573100**	**-1.50402200**
O	**2.97209600**	**0.71197500**	**1.57379500**
H	**3.70477900**	**1.27849800**	**1.86797300**
H	**3.02311400**	**0.71742200**	**0.57407400**
O	**3.65249000**	**-1.89532400**	**2.14018400**
H	**4.17487900**	**-2.18870900**	**1.37473900**
H	**3.41076200**	**-0.95505100**	**1.93187100**
O	**1.32422300**	**-3.44867800**	**1.78839700**
H	**1.17203800**	**-3.40596900**	**0.81813000**
H	**2.12174400**	**-2.88650800**	**1.93086600**
H	**1.41926800**	**1.29118400**	**-1.15059300**
N	**0.37358900**	**1.28383400**	**-0.99002400**
H	**-0.09509900**	**1.68690600**	**-1.80988500**
C	**-3.15915400**	**0.87660200**	**-0.82152100**
C	**-2.40959800**	**1.22705300**	**0.30974000**
C	**-2.50959700**	**0.41637300**	**1.45010500**
C	**-3.31974800**	**-0.71900400**	**1.46172800**
C	**-4.05133200**	**-1.05538200**	**0.31572700**
C	**-3.97913300**	**-0.25426800**	**-0.82686600**
H	**-4.55533100**	**-0.52293800**	**-1.70791700**
H	**-3.38670800**	**-1.34430700**	**2.34915600**
H	**-1.93448200**	**0.66768900**	**2.33868600**

H	**-3.09519100**	**1.49025900**	**-1.71753100**
O	**-4.87044700**	**-2.17043100**	**0.26488300**
C	**-1.47714100**	**2.41684400**	**0.29177100**
H	**-1.69843800**	**3.05862200**	**-0.57012300**
H	**-1.61449900**	**3.02175700**	**1.19389700**
C	**0.01800200**	**2.05059500**	**0.25171500**
C	**0.88473200**	**3.33736800**	**0.28575300**
O	**1.45183500**	**3.69104600**	**-0.78732500**
O	**0.91696200**	**3.93122800**	**1.39740900**
H	**-4.83295700**	**-2.64740600**	**1.11291600**
H	**0.29093900**	**1.42045500**	**1.09992600**
Br	**0.09555100**	**-0.66404300**	**-0.96282900**

Product

O	**-2.75869700**	**-2.94083800**	**0.40434000**
H	**-2.81111500**	**-3.75389000**	**0.93403400**
O	**-4.24473500**	**-0.96450100**	**1.66307800**
H	**-4.80255900**	**-0.82221600**	**0.87812400**
H	**-3.21441600**	**-2.25014200**	**0.94786900**
O	**-2.54003300**	**1.23094700**	**1.52445000**
H	**-3.63955000**	**-0.18735900**	**1.67543900**
H	**-2.91771700**	**2.10159600**	**1.31364800**
O	**-2.73592700**	**0.25001500**	**-1.19190200**
H	**-2.26501700**	**1.01025000**	**-1.60668300**
H	**-2.69630300**	**0.46986000**	**-0.23479000**
O	**-5.38920500**	**-0.19598800**	**-1.67658300**
H	**-5.88964700**	**0.18352200**	**-0.93508200**
H	**-4.44197500**	**0.04921100**	**-1.50534400**
O	**-5.05306000**	**-2.97379200**	**-1.30572200**
H	**-4.24370600**	**-3.02098700**	**-0.74864000**
H	**-5.21311100**	**-2.00786000**	**-1.42052400**
H	**-1.54992700**	**1.34335900**	**1.43200900**
N	**0.18856500**	**1.40575600**	**1.08137600**
H	**0.71556400**	**2.15753000**	**1.53427800**
C	**3.87109500**	**0.63487600**	**-0.04264600**
C	**2.73014000**	**0.61734300**	**-0.85628700**
C	**2.48565300**	**-0.53027800**	**-1.62513500**
C	**3.33827800**	**-1.63449700**	**-1.57440400**
C	**4.46427700**	**-1.59752400**	**-0.74314100**
C	**4.73786300**	**-0.45878300**	**0.01966000**
H	**5.61813200**	**-0.43907200**	**0.65648300**
H	**3.13668700**	**-2.51980400**	**-2.17359400**
H	**1.61008200**	**-0.56808000**	**-2.26978200**
H	**4.08201300**	**1.51289700**	**0.56363500**

O	5.34863000	-2.66043100	-0.64495100
C	1.78274200	1.79533700	-0.90923500
H	2.19632000	2.64256200	-0.34898500
H	1.67555900	2.12348700	-1.95179000
C	0.35238200	1.52175600	-0.38520300
C	-0.54274900	2.71998800	-0.80944700
O	-0.46189700	3.77749800	-0.12480200
O	-1.25951900	2.55405800	-1.84466700
H	5.05083500	-3.39369800	-1.21192000
H	-0.05122900	0.61200100	-0.83192400
Br	0.90767400	-0.23167200	1.85322900

Tyr+HOCl-C3-cs-a1

Reactant:

H	0.50824900	1.23083600	-1.74288600
O	2.62141600	0.53392200	2.50438500
H	2.12085000	0.96610100	3.22502500
Cl	1.56107700	0.48596800	1.16497500
O	3.17221500	0.80611900	-2.52847800
H	2.93855300	1.59056900	-1.98648500
H	2.49621400	0.10440300	-2.30642800
O	4.59931500	1.90543200	0.93525100
H	4.07603200	1.59042400	1.69442700
H	4.77693900	1.09111300	0.40357200
O	2.82715500	3.05308500	-0.86443200
H	3.41887700	2.69351800	-0.16079400
H	1.92971100	3.00100600	-0.49928300
C	-0.07521200	0.45334700	-1.25297200
C	-0.39911400	-1.86614000	-0.66235000
C	-2.03296900	-0.19877200	0.04219800
C	-1.57715900	-1.52421200	-0.00715400
H	-0.06062600	-2.89976500	-0.68203600
H	-2.15942500	-2.30326900	0.48372400
H	-1.59031600	1.81587000	-0.57463900
O	1.52037400	-1.20215600	-1.91546200
C	0.39078000	-0.88534700	-1.30830000
C	-1.26211700	0.77735900	-0.59713200
O	2.68826200	-2.37680700	2.55401700
H	2.77012200	-1.43927000	2.80147100
H	2.81106500	-2.38425400	1.57900100
O	3.15621200	-2.33685500	-0.18575600
H	3.46045300	-3.17875000	-0.55973000

H	**2.50351700**	**-1.95866700**	**-0.85232900**
O	**4.96298400**	**-0.26404900**	**-0.72073300**
H	**4.42729900**	**-1.02947600**	**-0.41559700**
H	**4.41450900**	**0.12420900**	**-1.44460600**
C	**-3.34090100**	**0.15556200**	**0.70733800**
H	**-3.63240800**	**-0.63105100**	**1.41497700**
H	**-3.25281900**	**1.09084400**	**1.26830600**
C	**-4.48140000**	**0.35181200**	**-0.29921900**
H	**-4.24007600**	**1.15622500**	**-0.99808300**
N	**-4.64221500**	**-0.88916300**	**-1.11494800**
H	**-4.89742400**	**-1.68192900**	**-0.51358100**
H	**-5.39198700**	**-0.78207600**	**-1.80664100**
C	**-5.80951900**	**0.66146000**	**0.40931300**
O	**-6.70058900**	**-0.22511500**	**0.37533900**
O	**-5.86886700**	**1.77765800**	**0.98219400**
H	**-3.77225600**	**-1.12421800**	**-1.60824900**

TS:

H	**0.61950600**	**1.01872500**	**-1.55335900**
O	**2.60120100**	**0.87775100**	**2.39701800**
H	**2.08788600**	**1.46603300**	**2.97701600**
Cl	**1.37830200**	**0.59878100**	**0.86226600**
O	**3.17976000**	**0.52956900**	**-2.59320200**
H	**2.94120000**	**1.36884000**	**-2.14005700**
H	**2.52962300**	**-0.14150200**	**-2.27355700**
O	**4.47527400**	**1.97747000**	**0.75599500**
H	**3.83208200**	**1.64975900**	**1.43123700**
H	**4.75700400**	**1.16390300**	**0.27669200**
O	**2.79552100**	**2.93667300**	**-1.20102700**
H	**3.38161100**	**2.64503600**	**-0.45825100**
H	**1.89679700**	**2.91393300**	**-0.83522100**
C	**0.10456200**	**0.31279300**	**-0.90530000**
C	**-0.43296200**	**-2.03951900**	**-0.44043300**
C	**-2.02369400**	**-0.26117800**	**0.15455700**
C	**-1.61076100**	**-1.63290900**	**0.12704800**
H	**-0.15631500**	**-3.08972100**	**-0.47297100**
H	**-2.27156400**	**-2.37710000**	**0.56976300**
H	**-1.46131200**	**1.72614300**	**-0.38732400**
O	**1.51102600**	**-1.45181300**	**-1.66290900**
C	**0.44722300**	**-1.08718700**	**-1.06020300**
C	**-1.18388500**	**0.67346800**	**-0.38868700**
O	**2.60216900**	**-1.85861100**	**2.82351200**
H	**2.58610800**	**-0.87539100**	**2.79971700**
H	**2.83949200**	**-2.10922100**	**1.90668500**

O	3.37482100	-2.35128600	0.15463300
H	3.68080400	-3.24309400	-0.07490900
H	2.67706900	-2.12962000	-0.50640800
O	5.08012500	-0.29176100	-0.74291700
H	4.58662500	-1.03651400	-0.33714200
H	4.49724500	-0.00255800	-1.48352200
C	-3.36899000	0.11862600	0.72615000
H	-3.72550400	-0.66454600	1.40676900
H	-3.29279100	1.04684200	1.29909500
C	-4.43477100	0.35312300	-0.34991600
H	-4.12666900	1.15532800	-1.02454400
N	-4.58821600	-0.87461600	-1.18808500
H	-4.84032700	-1.68120500	-0.60386800
H	-5.34117900	-0.75574600	-1.87490900
C	-5.79351500	0.69938800	0.28279400
O	-6.70879900	-0.15649000	0.18260800
O	-5.84952800	1.81013300	0.86563100
H	-3.72282900	-1.09798100	-1.69366300

Product

H	-0.25012000	0.31799400	-1.26393000
O	-3.44012800	-3.05275800	1.10675600
H	-2.47291600	-3.05023800	1.15995600
Cl	-1.52022800	-0.52320000	0.52266700
O	-2.72311500	1.41947000	-2.30047400
H	-2.37584300	0.50490800	-2.42496300
H	-2.27232000	1.77364500	-1.51061600
O	-4.14815800	-2.04037200	-1.15175300
H	-3.82615300	-2.42898400	-0.25624000
H	-4.48232900	-1.14000700	-0.95002100
O	-2.09770900	-1.24700900	-2.72511800
H	-2.78803800	-1.60352400	-2.10191300
H	-1.24564200	-1.55008300	-2.37442800
C	-0.11515500	0.36992300	-0.17207900
C	0.97798100	2.51622700	0.65523500
C	2.22737000	0.37125400	0.63534700
C	2.11005300	1.81211700	0.87372300
H	0.90539400	3.57687400	0.87314400
H	2.98479100	2.32695900	1.26864900
H	1.21498600	-1.38093100	-0.00514700
O	-1.29638600	2.43736400	0.04784400
C	-0.22276400	1.84783800	0.18736400
C	1.16414100	-0.30993600	0.17822000
O	-4.39716300	-0.96789600	2.35041100

H	-3.97275100	-1.74115500	1.84609800
H	-4.07123400	-0.13972600	1.95547100
O	-3.73820400	1.69985700	1.43024500
H	-4.18467600	2.53537100	1.64200000
H	-2.92135700	1.95201400	0.95794800
O	-4.99188600	0.64148400	-0.86668000
H	-4.68596600	0.95992200	0.00850500
H	-4.28390300	0.95257700	-1.47459600
C	3.54823100	-0.31226100	0.89698500
H	4.07695100	0.18557700	1.71911600
H	3.37275200	-1.34930100	1.19055400
C	4.45853200	-0.35221900	-0.33004900
H	3.94321200	-0.83636000	-1.16495300
N	4.79740900	1.02989800	-0.79132900
H	5.08162200	1.62385200	-0.00194900
H	5.60108500	0.98297500	-1.43075500
C	5.77769800	-1.11473900	-0.07595600
O	6.83462200	-0.56344600	-0.47624100
O	5.66637300	-2.23185700	0.48123600
H	4.01197000	1.48483900	-1.27052000

Tyr+HOBr-C3-cs-a1

Reactant:

H	0.27149400	0.24005200	2.10521900
O	2.53944300	-2.03835900	-1.45253100
H	2.04533800	-2.78323400	-1.84472000
O	2.97360200	1.19102400	2.46560400
H	2.81365900	0.22776100	2.56537000
H	2.26290400	1.54371200	1.86102000
O	4.58826800	-1.78822000	0.48579900
H	4.04671300	-2.09870700	-0.26390700
H	4.68191500	-0.81300700	0.35147800
O	2.93296700	-1.60472100	2.70169800
H	3.48707200	-1.75141400	1.89770000
H	2.05705900	-1.96467600	2.49197300
C	-0.30281900	0.53077100	1.22716200
C	-0.68661400	2.03626700	-0.62688700
C	-2.27229200	0.23527900	-0.17853400
C	-1.84776600	1.34257500	-0.93437200
H	-0.37697200	2.88720900	-1.22891900
H	-2.44596700	1.65851000	-1.78805400
H	-1.78731800	-0.99880900	1.51455200

O	1.23116500	2.30527300	0.76510400
C	0.12514900	1.65870600	0.47398300
C	-1.48684900	-0.14571200	0.90787500
O	3.73779100	0.06601100	-2.94451100
H	3.39143800	-0.75814200	-2.55453900
H	3.37277900	0.79017000	-2.39527100
O	2.87470400	2.18061100	-1.31921400
H	3.22366600	3.07264500	-1.47416600
H	2.23407200	2.26302400	-0.55235500
O	4.76622100	0.95439600	0.38342400
H	4.20409100	1.33430700	-0.32604000
H	4.21640200	1.07475600	1.19559600
C	-3.55665300	-0.48783100	-0.50437900
H	-3.85726700	-0.27424700	-1.53792900
H	-3.42707200	-1.57037800	-0.41418100
C	-4.71203500	-0.10271800	0.42717600
H	-4.47308300	-0.35923200	1.46208100
N	-4.90620300	1.37796300	0.38808600
H	-5.09515200	1.69040700	-0.57235100
H	-5.70866500	1.66039600	0.96113400
C	-6.01994200	-0.79366400	0.00926100
O	-6.93337200	-0.06567000	-0.45600800
O	-6.04194600	-2.04106000	0.15573300
H	-4.07000700	1.86846900	0.72728000
Br	1.32812900	-1.01433300	-0.45674400

TS:

H	0.34402300	-0.33045100	1.87645200
O	2.75927700	-1.68967200	-1.86587400
H	2.31263600	-2.45476500	-2.26215800
O	3.01558900	0.64939600	2.68486300
H	2.89409300	-0.32271300	2.59664000
H	2.29733500	1.07452600	2.16267600
O	4.55689500	-1.84634400	0.10900400
H	3.91655900	-1.89874700	-0.65061500
H	4.71508700	-0.88102200	0.22497400
O	3.04277300	-2.12010900	2.37688300
H	3.54432000	-2.09142200	1.52229500
H	2.16861300	-2.47965100	2.15946100
C	-0.10592800	0.04860700	0.95980900
C	-0.72877000	2.11344700	-0.25415300
C	-2.25076200	0.17501700	-0.22805300
C	-1.87696700	1.49843600	-0.65863300
H	-0.48545300	3.12454900	-0.56741800

H	**-2.55323500**	**2.02760800**	**-1.32900300**
H	**-1.63563100**	**-1.50677100**	**0.92588500**
O	**1.17122000**	**2.04705500**	**1.15483500**
C	**0.16531300**	**1.45513800**	**0.66763500**
C	**-1.39146900**	**-0.50345100**	**0.58200100**
O	**3.16605800**	**0.68067700**	**-3.12002100**
H	**2.99488600**	**-0.21862200**	**-2.74394200**
H	**3.04809300**	**1.29430700**	**-2.36849900**
O	**3.01683800**	**2.44000100**	**-0.89521600**
H	**3.34350700**	**3.35371600**	**-0.91831700**
H	**2.34297700**	**2.41440200**	**-0.17965500**
O	**4.84515100**	**0.88781300**	**0.60655200**
H	**4.29459400**	**1.38552600**	**-0.03493800**
H	**4.27706300**	**0.84065100**	**1.41071600**
C	**-3.58581800**	**-0.40110000**	**-0.63553900**
H	**-3.91760000**	**0.04360900**	**-1.58212500**
H	**-3.50369800**	**-1.48030000**	**-0.78626900**
C	**-4.67721400**	**-0.18586800**	**0.41764900**
H	**-4.39373300**	**-0.66320700**	**1.35950800**
N	**-4.83183900**	**1.27188700**	**0.71289700**
H	**-4.97309200**	**1.80760000**	**-0.15274500**
H	**-5.65997600**	**1.43071400**	**1.29796000**
C	**-6.03664300**	**-0.74568100**	**-0.04080700**
O	**-6.99358400**	**0.06531900**	**-0.12241500**
O	**-6.05807300**	**-1.97553000**	**-0.29129300**
H	**-4.01081300**	**1.65322500**	**1.19744800**
Br	**1.29184900**	**-0.82463100**	**-0.51733100**

Product

H	**0.15899600**	**0.20698500**	**1.86090700**
O	**3.39830000**	**-2.59228800**	**-1.53635800**
H	**2.53400800**	**-3.00430800**	**-1.39346000**
O	**3.02105300**	**1.38591600**	**2.43829400**
H	**2.94350000**	**0.41475900**	**2.58480000**
H	**2.24883500**	**1.65578200**	**1.90248600**
O	**4.61030000**	**-1.61612600**	**0.51279300**
H	**4.07864200**	**-2.02852200**	**-0.26052900**
H	**4.66086400**	**-0.65585100**	**0.31290800**
O	**3.17649300**	**-1.36036600**	**2.78709600**
H	**3.65226500**	**-1.53240500**	**1.92871500**
H	**2.32831100**	**-1.82513300**	**2.71819800**
C	**-0.11524200**	**0.24405800**	**0.80369600**
C	**-0.88525200**	**2.10721000**	**-0.73964000**
C	**-2.30608200**	**0.11409900**	**-0.33256600**

C	**-1.99484200**	**1.38031600**	**-0.99913400**
H	**-0.68340300**	**3.05432900**	**-1.22981000**
H	**-2.70856700**	**1.74537100**	**-1.73575300**
H	**-1.60374300**	**-1.36838200**	**1.01608900**
O	**1.00467400**	**2.34217600**	**0.65351500**
C	**0.05880300**	**1.65057700**	**0.26547800**
C	**-1.41319500**	**-0.41860000**	**0.52172300**
O	**3.45327600**	**-0.35776000**	**-2.89168300**
H	**3.35603700**	**-1.20781200**	**-2.34923800**
H	**3.09523700**	**0.37116300**	**-2.35448500**
O	**2.76455700**	**2.15603300**	**-1.62579700**
H	**3.18275500**	**2.92120300**	**-2.05317300**
H	**2.19122800**	**2.52924900**	**-0.93048900**
O	**4.69874000**	**1.18897300**	**0.21599800**
H	**4.08418600**	**1.46602800**	**-0.49554000**
H	**4.18095500**	**1.31687300**	**1.04339000**
C	**-3.63083200**	**-0.55390800**	**-0.61259400**
H	**-3.97019700**	**-0.30831400**	**-1.62630500**
H	**-3.51754500**	**-1.63814200**	**-0.54980900**
C	**-4.72146800**	**-0.16735000**	**0.38694300**
H	**-4.40811400**	**-0.42586000**	**1.40258700**
N	**-4.94983000**	**1.31090500**	**0.38198500**
H	**-5.04326200**	**1.66698000**	**-0.57786100**
H	**-5.83311700**	**1.52069200**	**0.86336700**
C	**-6.06453600**	**-0.87125500**	**0.09964200**
O	**-7.08930200**	**-0.14428800**	**0.05898100**
O	**-6.00718100**	**-2.11538300**	**-0.04607300**
H	**-4.18733400**	**1.82203300**	**0.84174600**
Br	**1.31705300**	**-0.79654400**	**-0.12823000**