

Supporting Information

Computational Study on the Reaction Mechanism of LigW-Catalyzed Carboxylation of Monohydroxybenzoic Acids

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1. Selected residues in the computational model

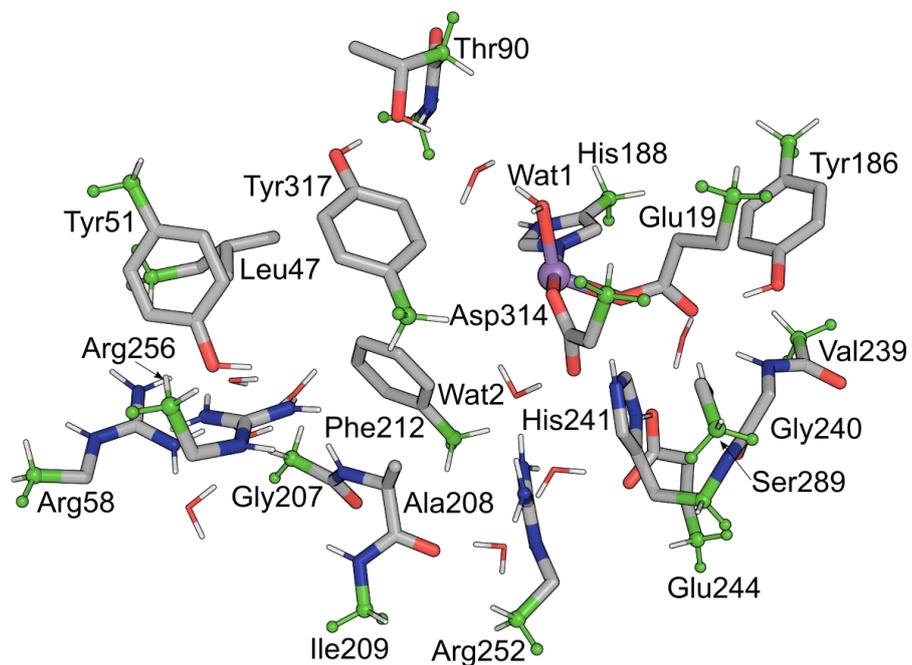


Figure S1. The designed active site model of LigW used in the present mechanistic study (without the binding of the substrate and CO₂). For clarity, only polar hydrogen atoms and hydrogen atoms on the truncated carbons are shown. Atoms fixed during the geometry optimization are shown in green.

2. Pathway starting from E:4-HBA':CO₂

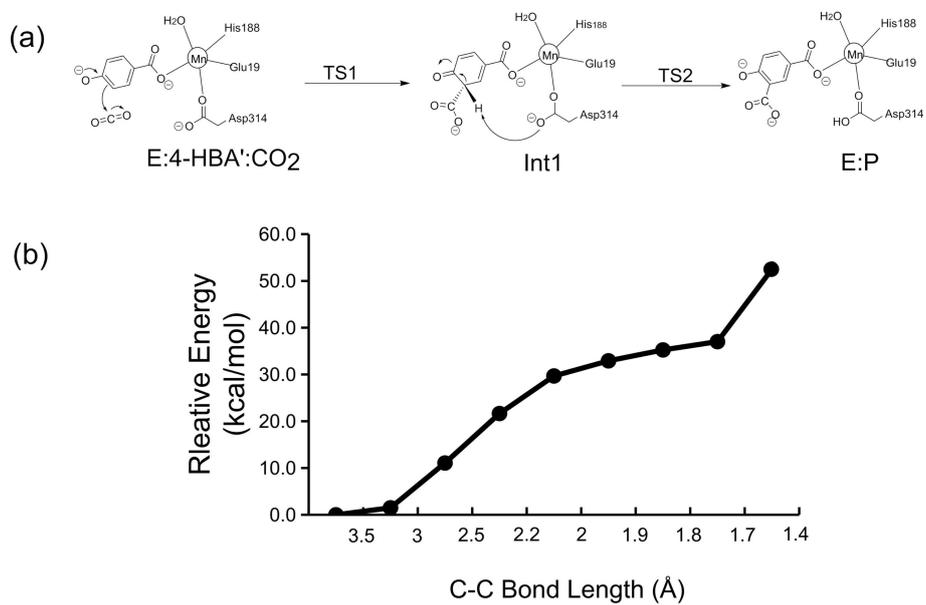


Figure S2. (a) Considered mechanism proceeding from E:4-HBA':CO₂, and (b) the energy profile for the scan of the distance between the C3 atom of 4-HBA and the C atom of CO₂ using the quantum chemical calculations.

3. Optimized structures for the carboxylation reaction of 4-HBA

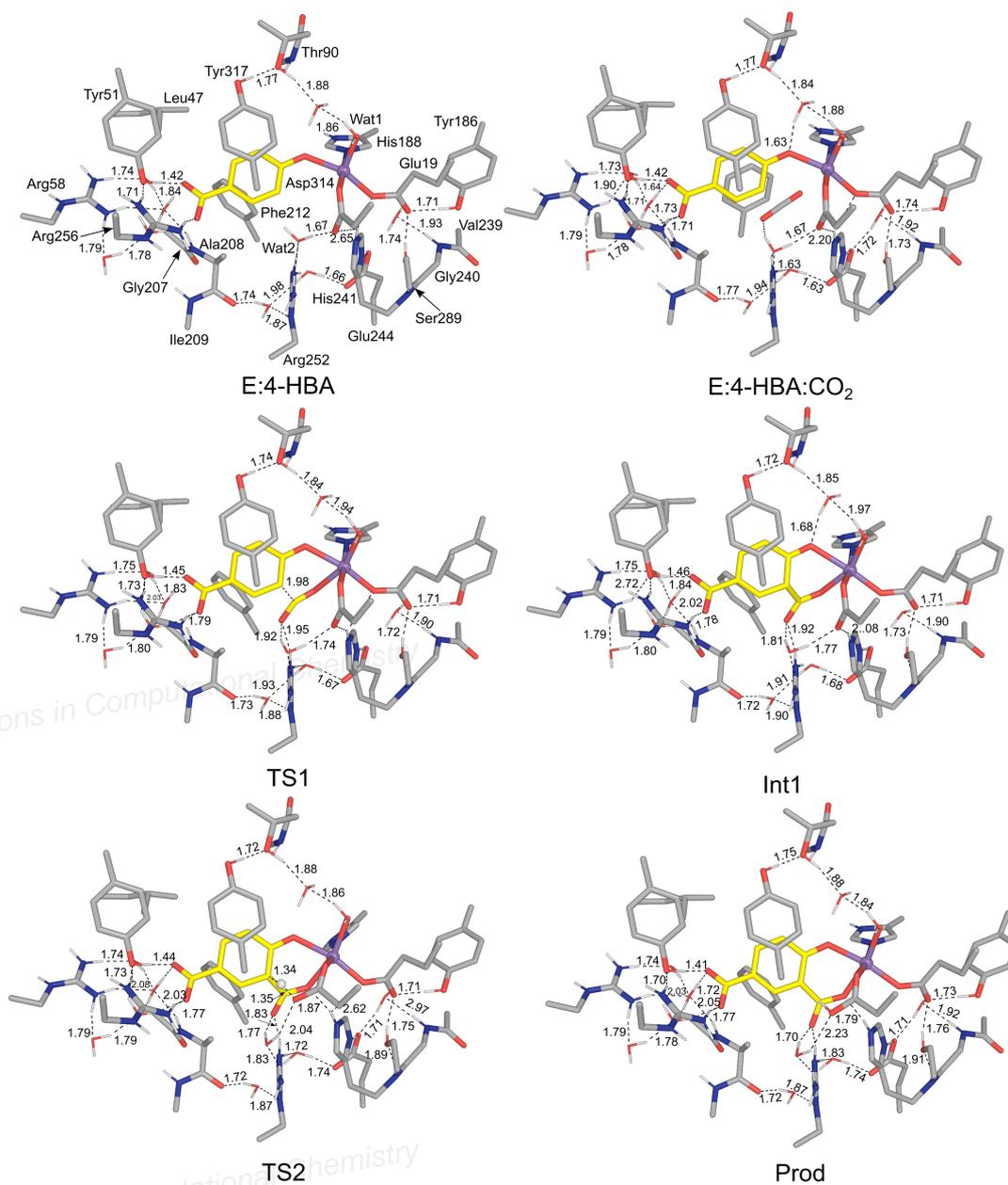


Figure S3. Optimized structures of the species involved in the LigW-catalyzed carboxylation of 4-HBA. Selected distances are given in Å. For clarity, most of the hydrogen atoms are omitted.

4. Optimized structures of the E:3-HBA complexes

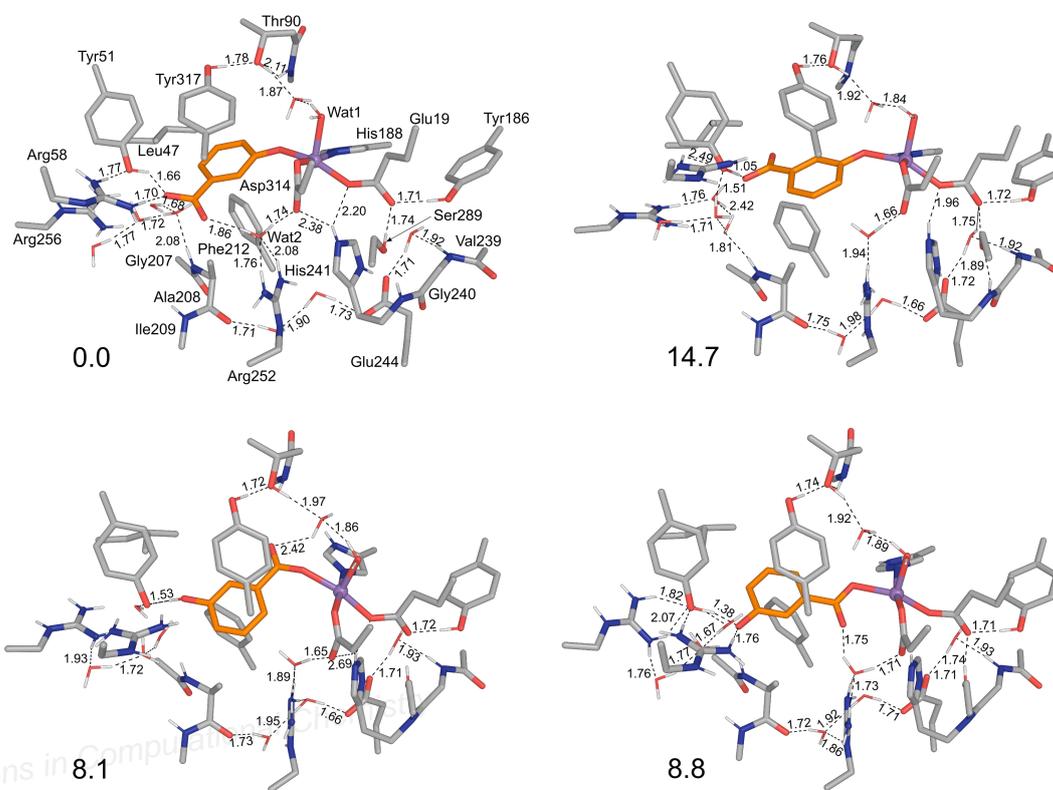


Figure S4. Four considered binding modes of 3-HBA for its carboxylation reaction catalyzed by LigW. The energies, provided in parentheses in kcal/mol, are all referenced relative to the lowest energy one. Selected distances are given in Å. For clarity, most of the hydrogen atoms are omitted.

5. Results on the carboxylation reaction of 3-HBA

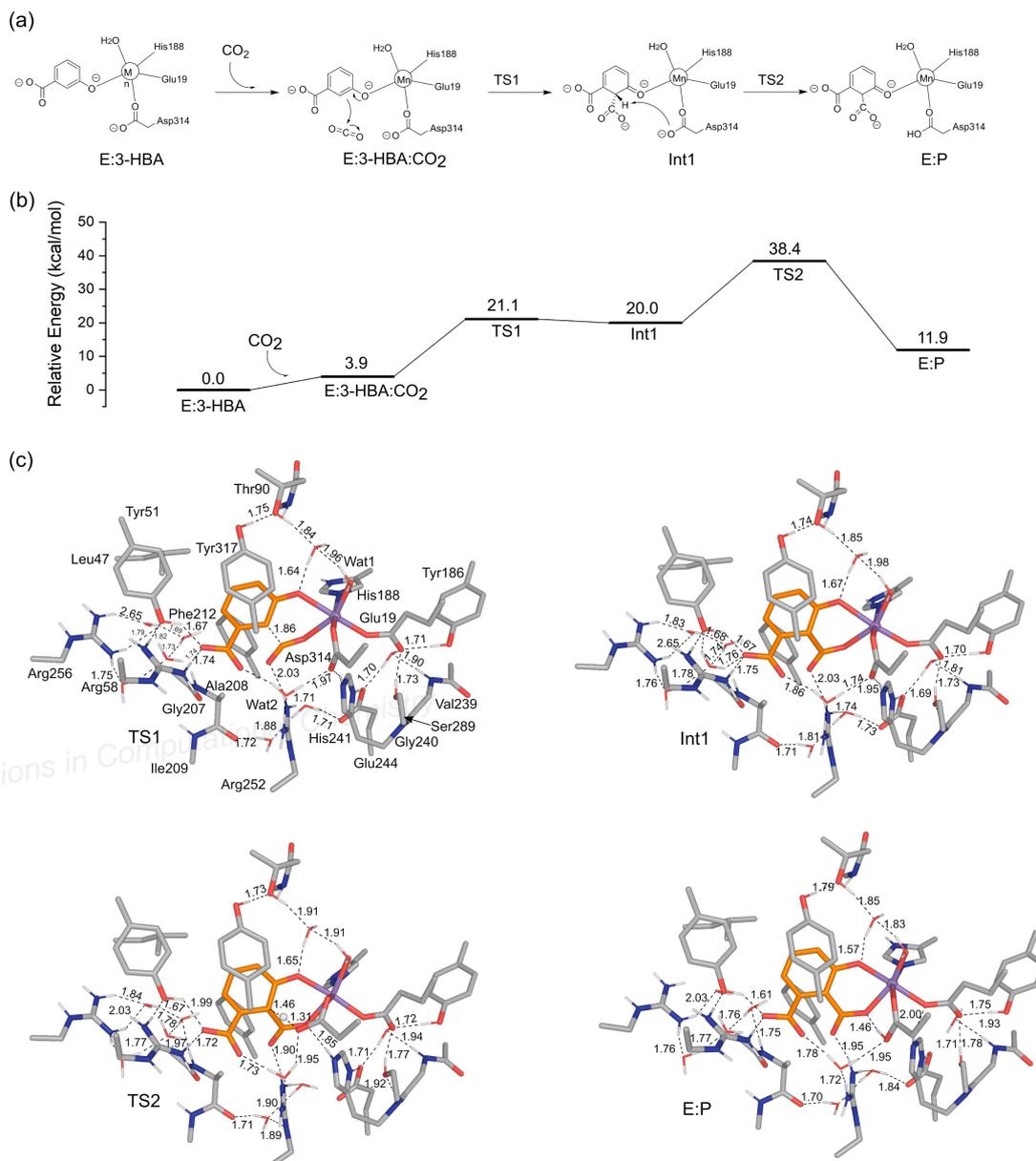


Figure S5. (a) The reaction mechanism of carboxylation of 3-HBA catalyzed by LigW, (b) calculated energy profile, and (c) optimized structures of the stationary points along the proposed reaction pathway. Selected distances are given in Å. For clarity, most of the hydrogen atoms are omitted.

6. Absolute energies and energy corrections

Table S1. Calculated absolute energies and energy corrections.

	E_{BS1}	E_{BS2}	E_{solvation}	E_{ZPE}	E_{total}	ΔE_{total}
	(au)	(au)	(au)	(au)	(au)	(kcal/mol)
The carboxylation of 4-hydroxybenzoate (4-HBA)						
E:4-HBA	-6649.933676	-6652.021914	-6650.060554	2.218479	-6649.930314	0.0
E:4-HBA:CO2	-6838.52466	-6840.680994	-6838.654045	2.230623	-6838.579756	5.4
TS1	-6838.510948	-6840.663356	-6838.640698	2.231473	-6838.561632	16.8
Int1	-6838.517064	-6840.668911	-6838.650481	2.233715	-6838.568613	12.4
TS2	-6838.51103	-6840.659155	-6838.6387	2.229076	-6838.557749	19.2
Prod	-6838.537403	-6840.690819	-6838.667122	2.233557	-6838.586981	0.9
The carboxylation of 3-hydroxybenzoate (3-HBA)						
3HBA-ModeA1	-6649.926178	-6652.014154	-6650.060381	2.217558	-6649.930799	0.0
3HBA-ModeA2	-6649.909714	-6651.994545	-6650.039304	2.216793	-6649.907342	14.7
3HBA-ModeB1	-6649.912761	-6651.997361	-6650.051239	2.218068	-6649.917771	8.1
3HBA-ModeB2	-6649.916003	-6652.003243	-6650.047467	2.217963	-6649.916744	8.8

BS1=LAN2DZ for Mn and 6-31G(d,p) for other elements

BS2=LAN2TZ for Mn and 6-311+G(2d,2p) for other elements

7. Cartesian coordinates

E:4-HBA

C 6.76042300	5.12386800	3.62275600	C -9.33672200	0.41978500	7.13523100
C 6.63124900	3.65825000	3.17700900	C -8.74207800	-0.97395800	6.94752500
C 5.70860500	3.52926400	1.94216000	N -7.40341100	-0.94266600	6.34294000
C 5.38839600	2.08455800	1.57817100	C -7.13824800	-0.69406500	5.04162100
O 6.32462000	1.28000500	1.35852700	N -8.12507500	-0.73970500	4.13915800
O 4.15724700	1.71677500	1.51756600	N -5.89525400	-0.42880100	4.64491500
H 7.09880400	5.74959200	2.78858100	H -9.37557000	0.95481300	6.18122000
H 7.60644000	3.22894100	2.93443600	H -8.72085900	1.00900000	7.82055000
H 6.21259300	3.06459200	3.99964500	H -8.63558100	-1.48986300	7.90442800
H 4.77317500	4.07612100	2.10028400	H -9.39057900	-1.61533700	6.34037900
H 6.22274200	3.98383600	1.08464800	H -6.61755500	-0.90833300	6.97476700
C -8.93716200	1.19437600	-4.86061500	H -9.05673300	-0.98452300	4.42694300
C -7.44508800	1.40772800	-5.13774700	H -7.98457500	-0.44214200	3.16296900
C -6.73470500	2.26219200	-4.06718600	H -5.16907100	-0.30376900	5.33302100
C -6.86257300	1.69416800	-2.64552500	H -5.61666100	-0.47697200	3.62502800
C -5.25964500	2.45721900	-4.43714400	C -0.58332900	8.42441400	-2.18784600
H -9.05523200	0.50515900	-4.01510600	C -0.52239400	7.92611500	-3.62160500
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H -6.36353700	2.34944200	-1.92437300	H 0.21313000	7.90415700	-1.63453200
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H -4.74326000	3.08306300	-3.70180300	H -1.18085000	6.37244100	-0.81907700
H -5.15022400	2.92979000	-5.41878900	H -3.23701600	8.09534400	-3.10065000
H -4.74011700	1.49194400	-4.47746000	H -3.10351700	9.68644100	-2.32961900
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C -9.17226600	3.72860000	0.22847000	N -0.62647800	6.56331800	-3.72064400
C -9.90769500	2.54435400	0.07795300	C -0.73524100	5.93582400	-5.02503200
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C -7.35260600	2.40546100	1.16579000	C 10.39287300	5.45852700	-2.93892700
C -8.11867000	1.24498600	1.02536700	C 10.00559600	4.48501300	-1.84847100
O -7.67356100	0.01593700	1.46256400	C 8.92328000	3.60349000	-1.98121500
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C	2.33051800	1.45763900	5.46697200	H	3.01009900	-7.15213900	2.36025200
C	2.13760600	1.27917700	3.95584500	H	1.94542500	-6.15205100	0.52206000
O	1.74789300	2.28719600	3.26909300	H	0.81052900	-4.32330300	3.34667800
O	2.36754600	0.13540200	3.48598600	H	0.98135100	-2.79778200	2.51978200
H	2.92828200	3.51251300	5.10417600	H	2.26757300	-3.99895400	-0.45595700
H	3.12201600	0.76077300	5.75496400	H	1.53115600	-2.68460200	0.47699900
H	1.41797400	1.07093500	5.93969900	C	-12.70207500	-3.72045500	-0.55808400
C	-2.59835600	2.06487400	4.43297900	C	-11.21045000	-3.90458000	-0.80518300
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C	-4.28227400	3.48053600	3.19615100	C	-9.62006200	-2.81465500	-2.41546200
C	-1.97618400	3.69430200	2.58964300	N	-8.54049000	-3.28993300	-1.80550300
C	-4.63176500	4.42822900	2.24227700	N	-9.45949900	-2.06758100	-3.52465300
C	-2.31189300	4.64244600	1.62255900	H	-13.28029700	-4.09151300	-1.41203200
C	-3.65007100	5.00581200	1.42291500	H	-12.93050300	-2.65603800	-0.43584900
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H	-1.51531000	1.94592900	4.52768000	H	-10.96500700	-4.95476600	-1.00339800
H	-3.01449700	1.08095900	4.18941200	H	-11.62204800	-2.78747600	-2.56137800
H	-5.06145300	3.04301900	3.81788700	H	-8.56389100	-3.85662100	-0.94472600
H	-0.93506100	3.40950900	2.72464400	H	-7.64902200	-2.99749500	-2.19840500
H	-5.65922500	4.75123300	2.12736300	H	-10.22630800	-1.51603100	-3.87523100
H	-1.53567300	5.10151800	1.02518900	H	-8.51238300	-1.73516800	-3.71681500
H	-3.31008700	6.17669100	-0.08732900	H	-9.48534200	0.76000300	-5.70370400
Mn	2.23994800	2.40683300	1.21175200	H	-0.25583600	9.46988100	-2.18992200
C	-4.23550900	-0.07377100	1.52988200	H	5.76679600	5.47644700	3.91895400
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C	-4.28426900	0.85174100	0.46344500	H	11.81656800	-0.18555800	-2.23451400
C	-1.87595900	1.13333200	0.56644000	H	10.71586300	-1.48972300	-2.89713200
O	0.48184200	1.42225100	0.54851700	H	7.11516500	-1.53572100	5.40207300
O	-0.78700000	2.82528000	-0.67370600	H	5.38098000	-2.03216400	5.36476800
O	-5.35821100	-0.60261700	2.04851300	H	8.68125500	-6.81178400	-1.84247200
C	-0.64832100	1.85170200	0.11218900	H	7.48228000	-5.20372600	1.95086200
C	-1.82239600	0.17223600	1.58536400	H	8.17127500	-8.20841500	-2.84512000
C	-3.11959700	1.46072200	0.00979700	H	-2.38546400	-8.63706600	-0.53526600
H	-0.86935800	-0.09761900	2.01968200	H	-4.00603600	-8.54194100	0.22616200
H	-3.15658500	2.21664300	-0.76631800	H	-5.22249300	-5.18189800	-4.21531300
C	1.01008400	-7.48129600	3.09682600	H	1.78389800	3.38576600	6.44264700
C	2.13724900	-6.54335100	2.61791200	H	3.50227500	2.89526400	6.67226200
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TS1

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