

## Supplementary Information

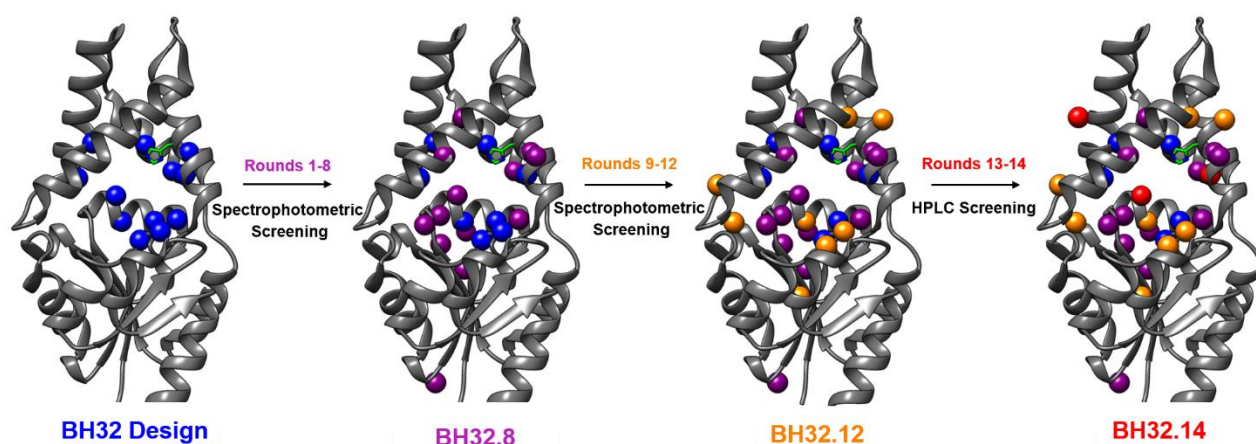
### Engineering an Efficient and Enantioselective Enzyme for the Morita-Baylis-Hillman Reaction

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## 1. Supplementary Figures 1-13

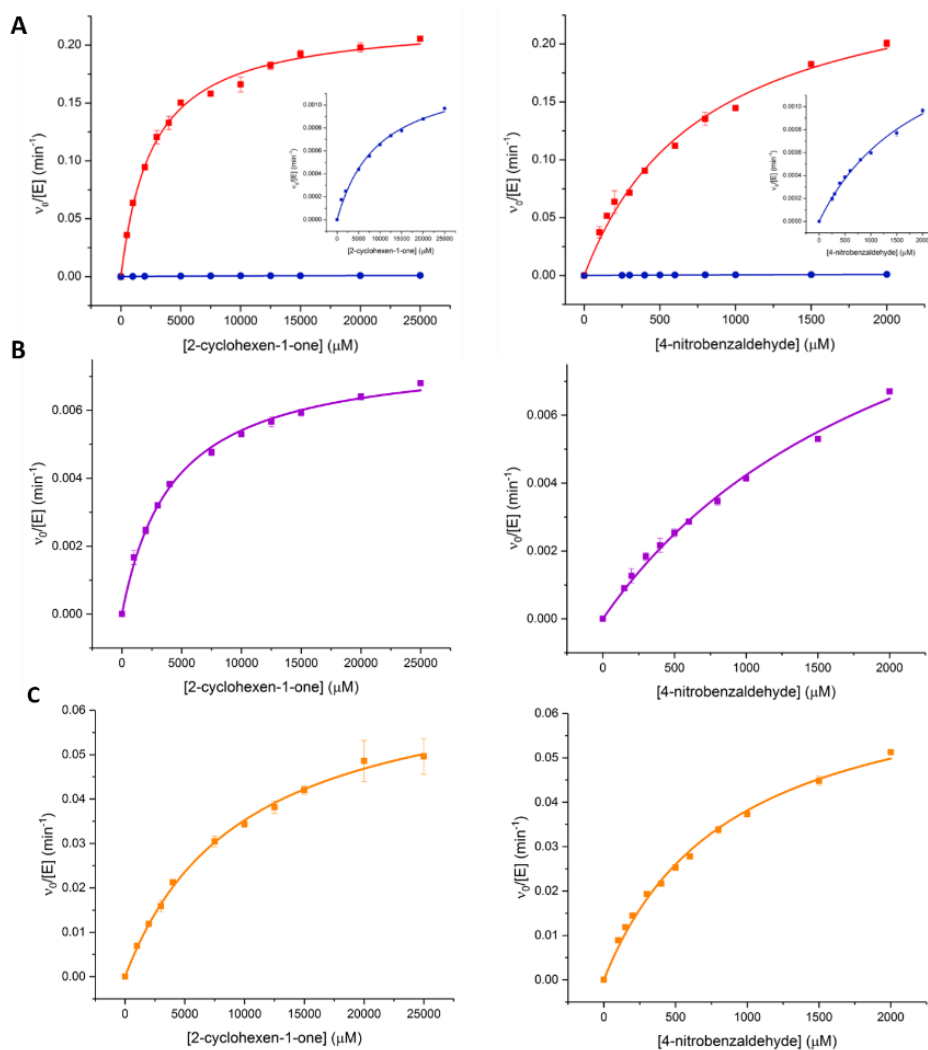


Round	Description	Clones Screened	Beneficial mutations	Best Variant <sup>[1]</sup>
1	Random mutagenesis of the entire gene	1800	T49A, A52V, F87L, Q96R, M120L, K167I, V226G	<b>BH32.1</b> = <i>BH32</i> <sup>[2]</sup> + T49A
2	Saturation mutagenesis of 'hotspots': Y45/T49 and F87/F88 (two sites simultaneously randomized), T49, R50	1980	T49A, T49M, F87L, F87T	<b>BH32.2</b> = <i>BH32</i> + T49A_F87L
3	Random mutagenesis of the entire gene	1800	N14Y, M130K, E174G	<b>BH32.3</b> = <i>BH32.2</i> + N14Y
4	Saturation mutagenesis of 'hotspots': N14, M130, E174	270	N14I, M130T, E174G	<b>BH32.4</b> = <i>BH32.2</i> + N14I_M130T
5	Saturation mutagenesis of active site positions and flexible loop regions: L10, A19, P38, L42, Y45, E46, P60, P63, F81, S91, Q96, S124, D125, Q128, M130, L133, F154, K167, E174, K202	1800	P63C, S124R, D125Q, Q128P, E174K	<b>BH32.5</b> = <i>BH32.4</i> + S124R_Q128P_E174K
6	Saturation mutagenesis of active site positions and flexible loop regions: V16, E17, G32, Y34, L36, Y61, L64, L68, M120, T122, D123, D125, T126, Q128, E149, G152, L199, E204, K205, E207	1800	D123N, P128L, E204G	<b>BH32.6</b> = <i>BH32.5</i> + D123N
7	Saturation mutagenesis of positions: S22/S95 and M120/T122 (two sites simultaneously randomized)	2700	S22V_S95A, M120V_T122L	<b>BH32.7</b> = <i>BH32.6</i> + S22V_S95A_M120V_T122L
8	Saturation mutagenesis of active site positions and flexible loop regions: L10, A20, L24, M27, L42, T45, P63, L64, S91, L92, Q96, D125, E127, A129, I145, T147	1440	A20Y, A129G	<b>BH32.8</b> = <i>BH32.7</i> + A20Y
9	Saturation mutagenesis of active site positions and flexible loop regions: L10, L24, L42, E46, A129	450	L10W, L24F, L42V, A129S	<b>BH32.9</b> = <i>BH32.8</i> + L10W_L24F_A129S
10	Random mutagenesis of the entire gene	1800	F154S	
11	Saturation mutagenesis of F154	90	F154S	<b>BH32.11</b> = <i>BH32.9</i> + F154S
12	Saturation mutagenesis of active site positions and flexible loop regions: Y20, V30, K47, Y56, I67, E70, F87, S91, R97, F153, K155, F161, L165, K171, V176, Y177, D180, S196, D210, L219, I223	1890	K47E, Y56N, Y177C, D180P, D210G,	<b>BH32.12</b> = <i>BH32.11</i> + Y56N_Y177C_D180P
13	Random mutagenesis of the entire gene	1800	V16A, A19T, E70R, P128L, S154A	<b>BH32.13</b> = <i>BH32.12</i> + A19T
14	Saturation mutagenesis of 'hotspots': V16, A19, E70, M72, E89, P128, S154	630	V16P/G, A19T, E70R, P128L/M, S154G/A	<b>BH32.14</b> = <i>BH32.12</i> + A19T_E70R_P128L

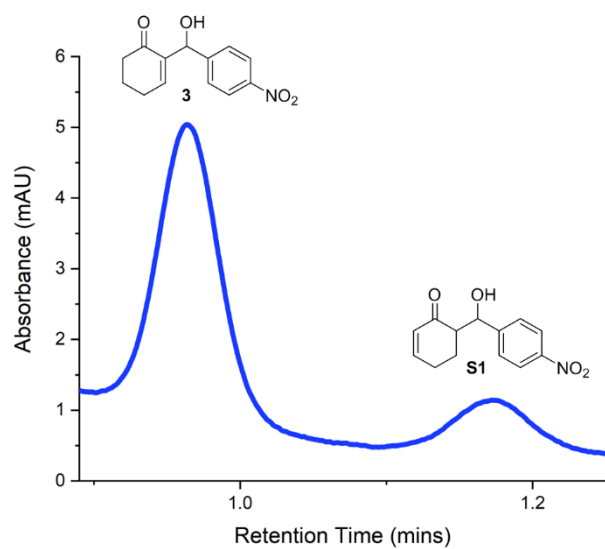
<sup>[1]</sup> The gene sequence used as the template for each round of evolution is shown in italics.

<sup>[2]</sup> BH32 = haloacid dehalogenase from *Pyrococcus horikoshii* + F9S, V10L, L14N, E19A, T22S, I64L, E68L H91S, H95S, Y128Q, L129A, H132F mutations

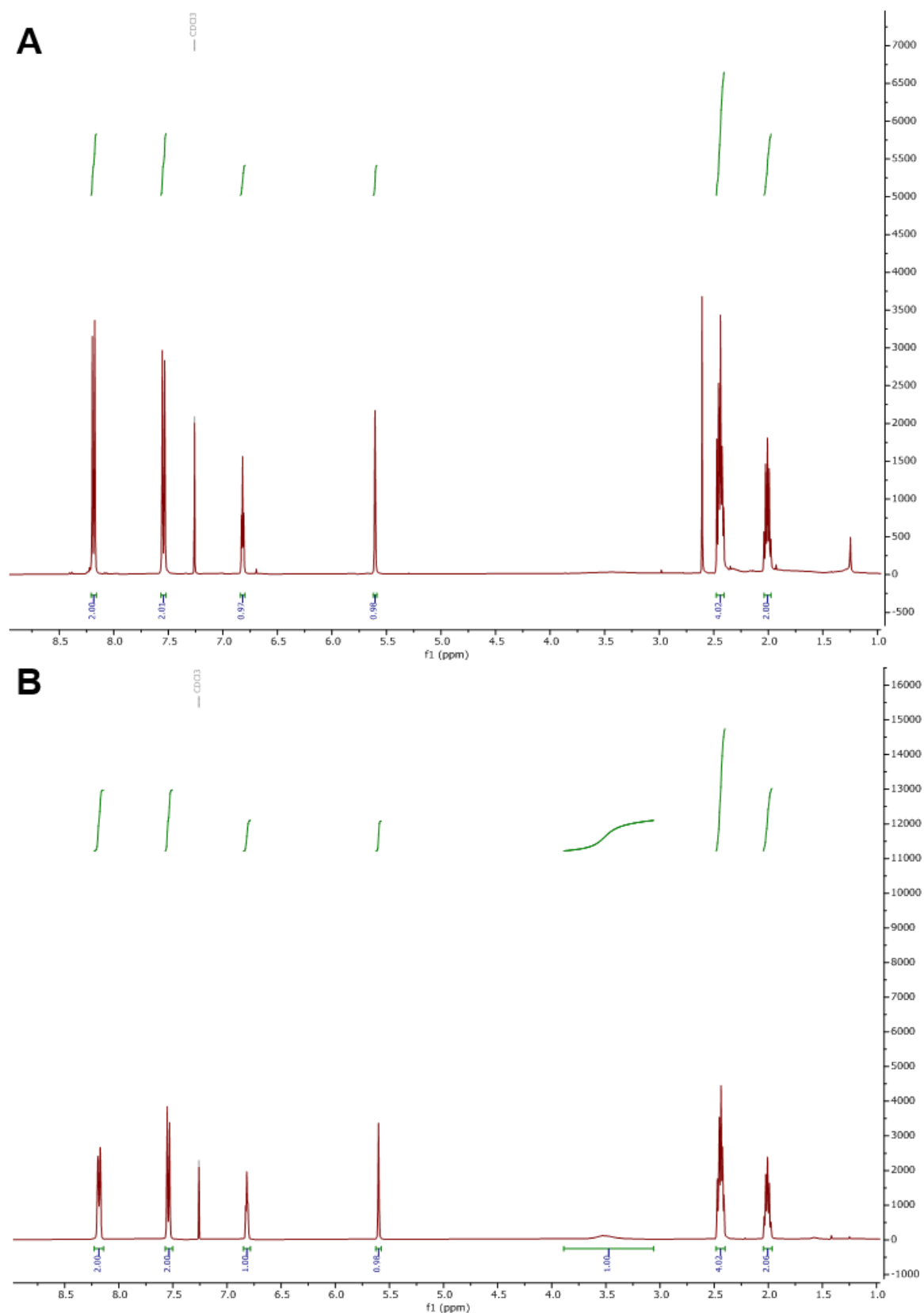
**Figure 1: Directed evolution of BH32.14.** Structures showing the amino acid positions mutated throughout evolution (represented as spheres). The original design contains twelve active site mutations (shown in blue) built into the cap domain of a haloacid dehalogenase from *Pyrococcus horikoshii*.<sup>20</sup> Fifteen mutations (shown in purple) were introduced during the first eight rounds of evolution, which exploited a spectrophotometric assay. Rounds 9-14 exploited a HPLC assay and led to the accumulation of a further nine mutations (mutations from round 9-12 are shown in orange, and from rounds 13-14 in red). The final variant BH32.14 contains 29 mutations, 5 that remain from the initial computational design and 24 that were installed during evolution. The table describes the method of library generation used, the number of clones evaluated and the sequence of the most improved variant for each round.



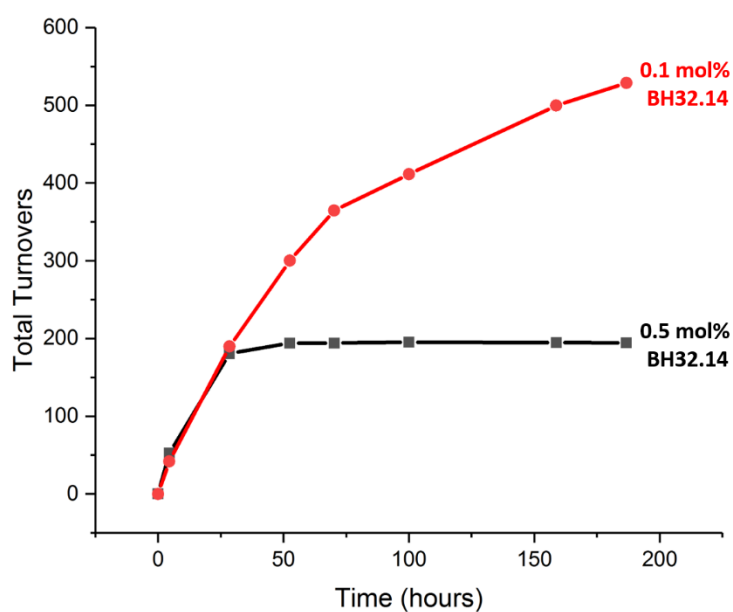
**Figure 2: Kinetic characterization of BH32, BH32.8, BH32.12 and BH32.14.** Michaelis-Menten plots for the MBH reaction with **1** and **2** catalysed by **A**) BH32 (blue) and BH32.14 (red) **B**) BH32.8 and **C**) BH32.12. Kinetic assays were performed at either a fixed concentration of **1** (25 mM) and various concentrations of **2**, or using a fixed concentration of **2** (2 mM) and various concentrations of **1**. The plots show the averaged initial rates which were fitted to the Michaelis–Menten equation using Origin software. Data are mean  $\pm$  s.d. of measurements made in triplicate



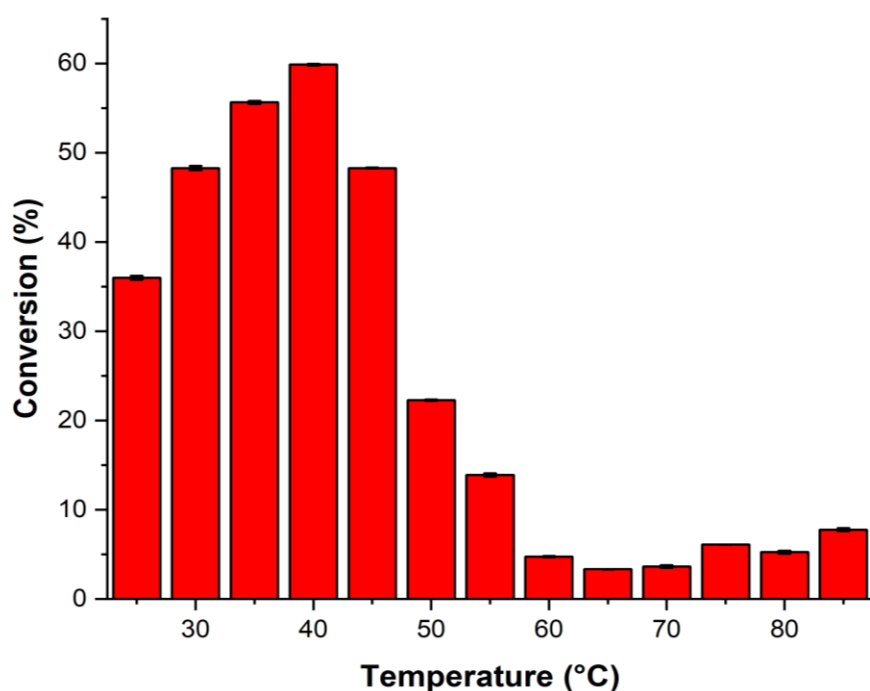
**Figure 3: HPLC analysis of the BH32 catalysed MBH reaction.** HPLC trace showing product **3** and aldol by-product **S1** (5:1 ratio of **3**:**S1**), formed during the BH32 (3 mol%) catalysed reaction of **1** (3 mM) and **2** (0.6 mM) following 22 hours incubation.



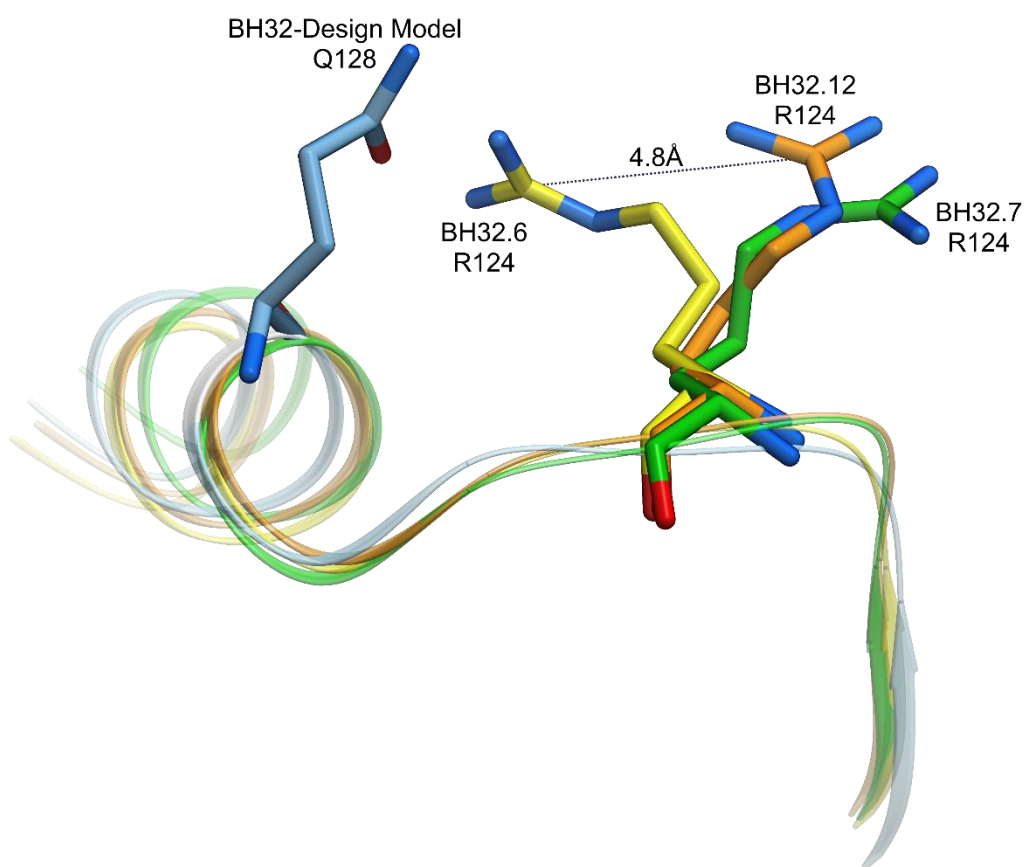
**Figure 4: Characterization of product 3 produced from a preparative scale biotransformation.** NMR traces (400 MHz; CDCl<sub>3</sub>) showing **A**) crude product extracted from the BH32.14 (50 μM) catalysed MBH reaction of **1** (50 mM) and **2** (10 mM) in PBS (pH 7.4) with 20% DMSO as a cosolvent and **B**) product isolated following purification by flash column chromatography.



**Figure 5: Total turnover numbers achieved by BH32.14.** Time-course for the conversion of **1** (50 mM) and **2** (10 mM) in PBS (pH 7.4) with 20 % DMSO cosolvent using 0.5 mol% (black) and 0.1 mol% (red) of BH32.14 as a biocatalyst.

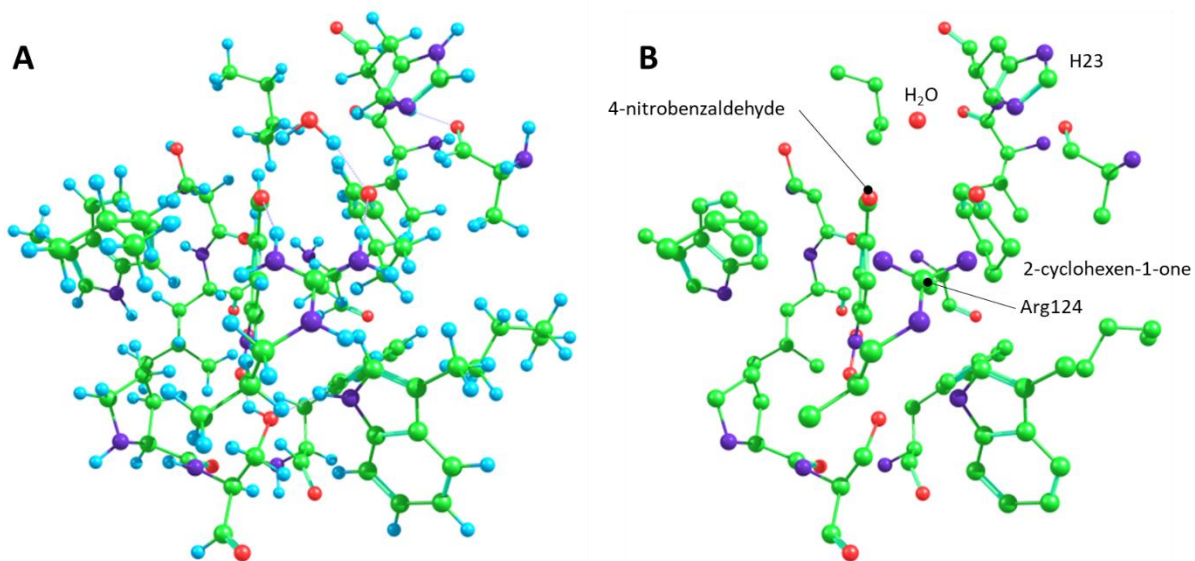


**Figure 6: Activity of BH32.14 at varying temperatures.** Reaction conversions of BH32.14 mediated biotransformations at temperatures ranging from 25 °C to 85 °C. Biotransformations performed using **1** (50mM), **2** (10mM) and BH32.14 (50  $\mu$ M) in PBS (pH 7.4) with 20% DMSO as a cosolvent, for 4 hours. The error bars represent the standard deviation of measurements made in triplicate.

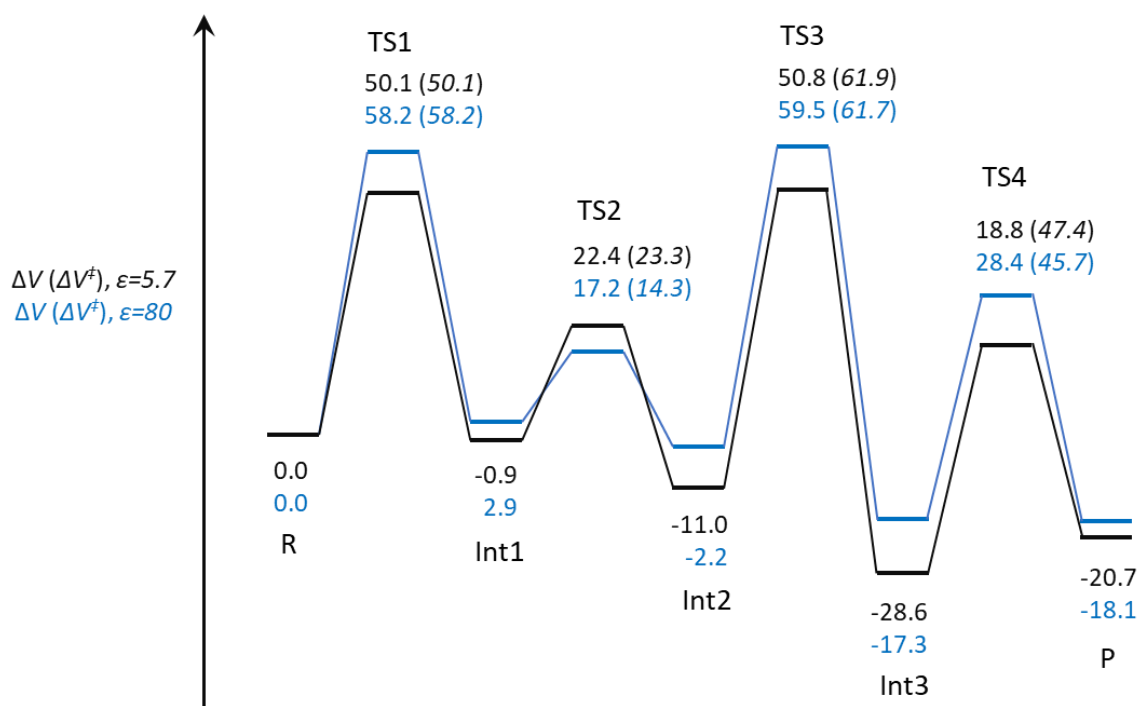


**Figure 7: Structural characterization of residues responsible for oxyanion intermediate stabilization in BH32, BH32.6, BH32.7 and BH32.12.** Four superimposed structures are displayed, the BH32 design model in blue, BH32.6 in yellow, BH32.7 in green and BH32.12 in orange. Backbone atoms are displayed in cartoon ribbon representation whilst residues are shown as all atom coloured stick models. The catalytic Arg124 in BH32.6 adopts an orientation that places the guanidinium motif in close proximity to the amide side chain of Gln128 designed to interact with the oxyanion of *Int1*. During the evolution process, Arg124 reorientates to adopt a pose ideal to support charge transfer during catalysis (BH32.12 orange).

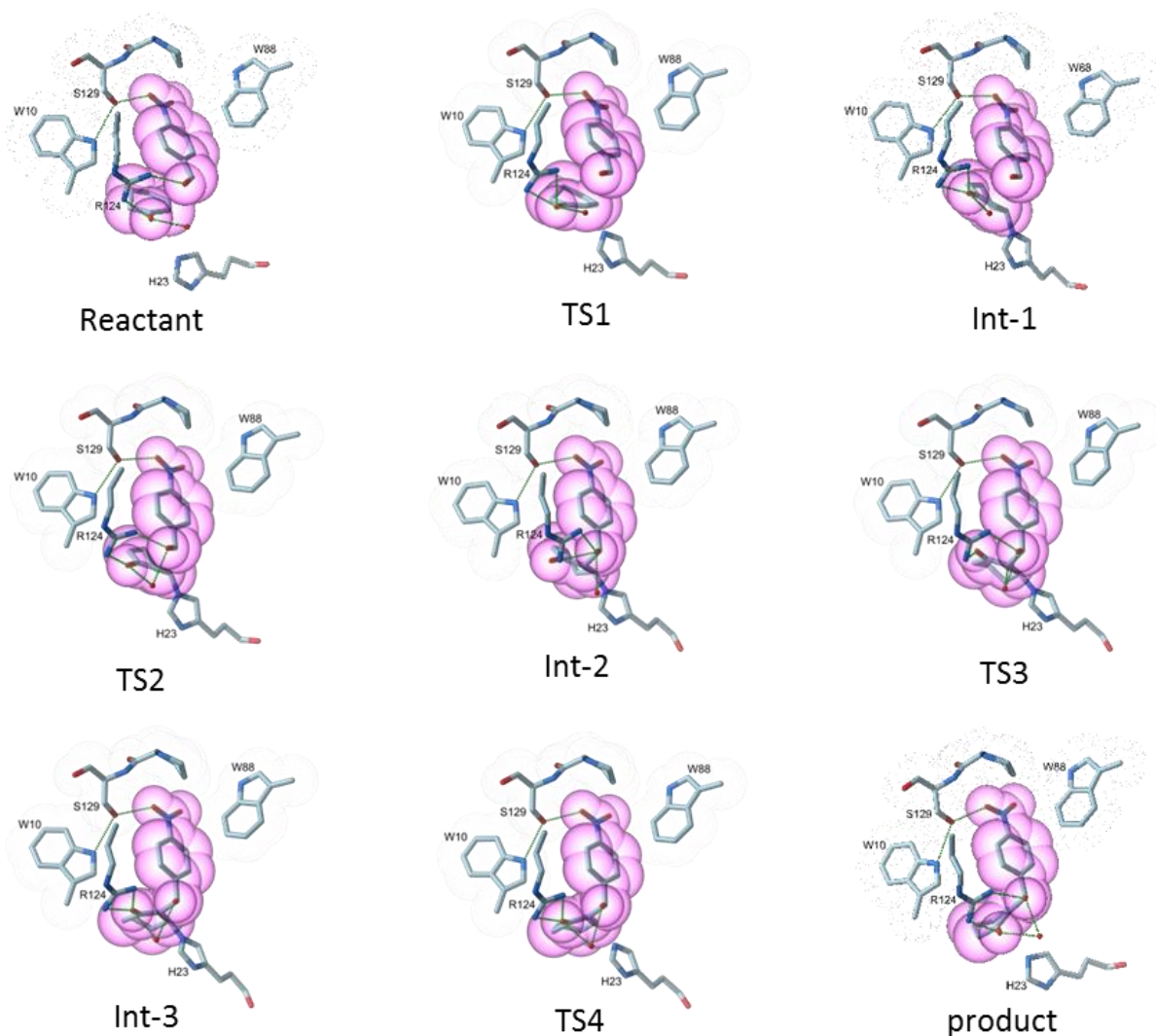




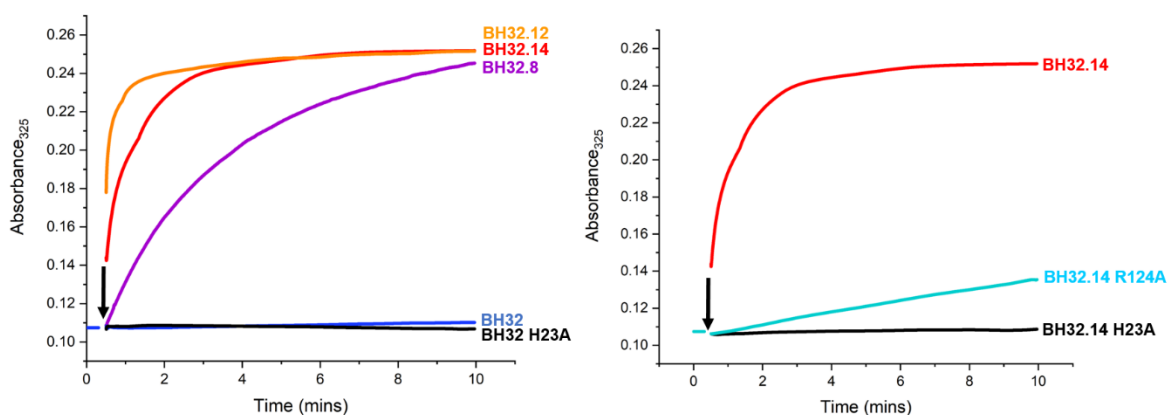
**Figure 8.** Cluster model used for DFT modelling. Models are shown with **(A)** and without **(B)** hydrogen atoms.



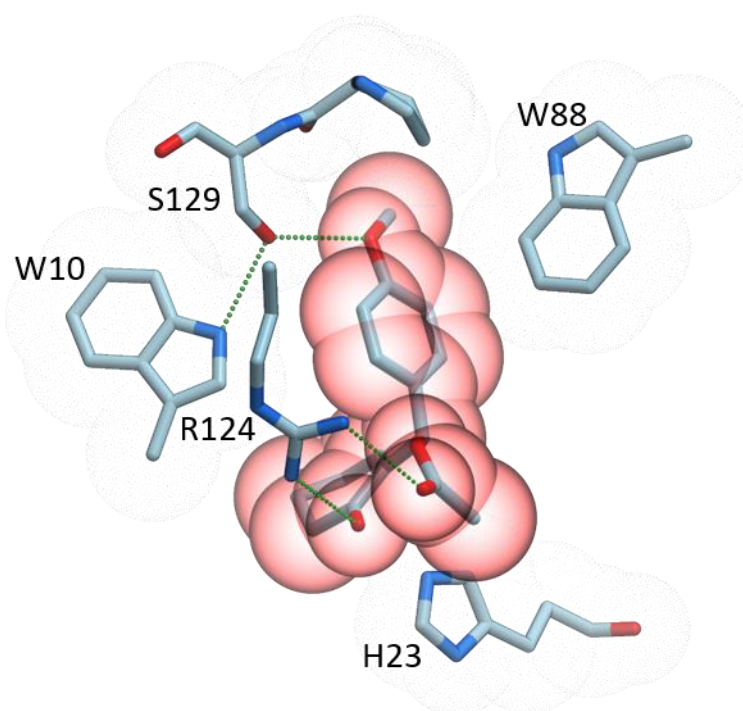
**Figure 9: Computed reaction profile for the complete MBH mechanism.** The potential energy relative to the reactant ( $\Delta V$  in  $\text{kJ mol}^{-1}$ ) is shown for each state, and the barrier energy ( $\Delta V^\ddagger$  in  $\text{kJ mol}^{-1}$ ) for each transition state is shown in parentheses. Geometry optimization was performed using a dielectric,  $\epsilon = 5.7$  (black). Single point calculations using  $\epsilon = 80$  (blue) show only modest changes in energy of each species, with no change in rate limiting step.



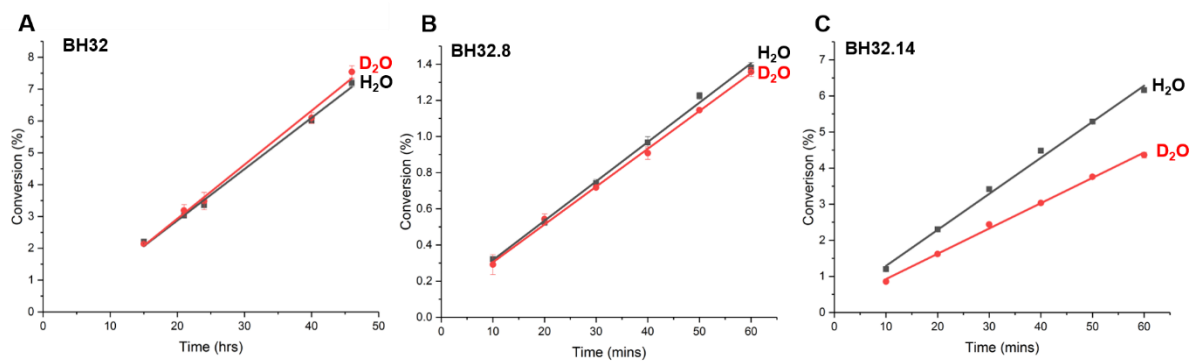
**Figure 10: DFT states showing reactants, transition states and intermediates formed along the reaction coordinate.** Stick representations of the complete DFT progression from reactant through to products are presented in all atom colours. For clarity a subset of atoms that form close packing interactions with the substrates are shown along with atoms derived from the His23 nucleophile and catalytic Arg124. Atoms derived from residues that provide close packing contacts (Trp10, Trp88 & Ser129) are shown with additional dot surfaces (blue) whilst substrate derived heavy atoms are shown with semi-transparent CPK spheres (magenta). Hydrogen bonds are shown as green dashed lines.



**Figure 11: Time course for the inhibition of BH32 and variants.** Formation of the covalently modified protein was monitored spectrophotometrically at 325 nm. **A)** Comparison of BH32, BH32 H23A, BH32.8, BH32.12 and BH32.14; **B)** Comparison of BH32.14, BH32.14 R124A and BH32.14 H23A. Reactions were performed using enzyme (10  $\mu$ M) and inhibitor **4** (25  $\mu$ M) in PBS pH 7.4 with 3% (v/v) acetonitrile at room temperature.



**Figure 12: DFT state showing inhibitor 4 bound in the active site of an engineered MBHase.** The DFT model is shown in all atom coloured stick representation. For clarity, only a subset of atoms that form close packing interactions with the inhibitor are shown along with atoms derived from the His23 nucleophile and catalytic Arg124. Atoms derived from residues that provide close packing contacts (Trp10, Trp88 & Ser129) are shown with additional dot surfaces (blue) whilst inhibitor derived heavy atoms are shown with semi-transparent CPK spheres (red). Hydrogen bonds are shown as green dashed lines.



**Figure 13: Solvent kinetic isotope effects.** Biotransformations were performed using **1** (25 mM), **2** (2 mM) and the relevant biocatalyst (50  $\mu$ M BH32, 30  $\mu$ M BH32.8, 10  $\mu$ M BH32.14) in PBS (pH/pD 7.4) with 3% acetonitrile as a cosolvent. Linear fits of reaction conversion vs time are shown in black (H<sub>2</sub>O) and red (D<sub>2</sub>O). Error bars represent the standard deviation of measurements made in triplicate.

## 2. Supplementary Tables 1-9

**Table 1: Experimental and calculated masses of apo and inhibited enzymes.** Mass spectrometry data for BH32 and variants. Enzymes were inhibited with mechanistic inhibitor **4**.

Variant	Expected Mass	Observed Mass
BH32	27788	27788
BH32 inhibited (60 minutes incubation)	28003 (80% single modification)	28002
BH32 H23A	27721	27722
BH32 H23A inhibited (60 minutes incubation)	27721 (no modification)	27722
BH32.14	27806	27806
BH32.14 H23A	27740	27739
BH32.14 W10A	27691	27690
BH32.14 R124A	27721	27720

**Table 2: Conversion and enantiomeric excess achieved by selected variants along the evolutionary trajectory.** Biotransformations were performed using **1** (3 mM), **2** (0.6 mM) and enzyme (18  $\mu$ M) in PBS (pH 7.4) with 3% MeCN as a cosolvent. To ensure that errors don't arise from determining low conversions achieved by BH32 after 4.5 hours, reactions were monitored over longer timeframes and were shown to be linear throughout this period. All variants preferentially produced the (*R*)-enantiomer. The error bars represent the standard deviation of measurements made in triplicate.

Variant	Time (hours)	Conversion (%)	Relative Conversion	<i>ee</i>
BH32	4.5	0.08 $\pm$ 0.01	0.14 $\pm$ 0.01	-
BH32	22	0.39 $\pm$ 0.01	0.68 $\pm$ 0.02	20 $\pm$ 0.9
BH32	31	0.54 $\pm$ 0.02	0.94 $\pm$ 0.03	-
BH32.4	4.5	0.22 $\pm$ 0.01	0.38 $\pm$ 0.02	23 $\pm$ 0.6
BH32.6	4.5	0.71 $\pm$ 0.02	1.23 $\pm$ 0.03	9 $\pm$ 0.7
BH32.8	4.5	1.56 $\pm$ 0.04	2.71 $\pm$ 0.07	33 $\pm$ 0.5
BH32.9	4.5	3.40 $\pm$ 0.07	5.92 $\pm$ 0.12	67 $\pm$ 0.4
BH32.11	4.5	9.74 $\pm$ 0.11	16.94 $\pm$ 0.20	82 $\pm$ 0.6
BH32.12	4.5	20.30 $\pm$ 0.21	35.33 $\pm$ 0.36	86 $\pm$ 0.8
BH32.14	4.5	57.54 $\pm$ 0.85	100 $\pm$ 1.48	93 $\pm$ 0.9

**Table 3: Kinetic characterization of BH32, BH32.8, BH32.12 and BH32.14.** Kinetic constants derived from global fitting of the combined  $V_0$  vs [1] and  $V_0$  vs [2] steady state kinetic data (Figure S2) using ordered and/or random order binding models. Fitting did not allow reliable determination of  $K_{SA}$  and it was not possible to determine the order of binding. The contribution of  $K_{SA}$  on the apparent  $k_{cat}$  and  $K_m$  values in the ordered binding equation (Eq. 2) was examined by varying  $K_{SA}K_{mB}$  over a range of  $0.1 \times K_{mA}K_{mB}$  to  $10 \times K_{mA}K_{mB}$ . The goodness of fit was not significantly different using ordered or random order binding equations across this range of values. While the apparent  $K_m$  are sensitive to the value of  $K_{SA}$ , the  $k_{cat}$  values vary by only ~25% for BH32 and 7% for BH32.14

#### BH32

Model	$k_{cat}$ (hr <sup>-1</sup> )	$K_{mA}$ (μM)	$K_{mB}$ (μM)	$K_{SA}K_{mB}$
Random	0.134 ± 0.012	7998 ± 987	1767 ± 249	-
Ordered	0.170 ± 0.023	16744 ± 3057	2766 ± 517	0.1 × $K_{mA}K_{mB}$
Ordered	0.134 ± 0.012	7998 ± 987	1767 ± 249	$K_{mA} \times K_{mB}$
Ordered	0.110 ± 0.008	1929 ± 293	1074 ± 178	10 × $K_{mA}K_{mB}$

#### BH32.8

Model	$k_{cat}$ (min <sup>-1</sup> )	$K_{mA}$ (μM)	$K_{mB}$ (μM)	$K_{SA}K_{mB}$
Random	0.0168 ± 0.001	4173 ± 254	2381 ± 224	-

#### BH32.12

Model	$k_{cat}$ (min <sup>-1</sup> )	$K_{mA}$ (μM)	$K_{mB}$ (μM)	$K_{SA}K_{mB}$
Random	0.100 ± 0.004	9719 ± 640	893 ± 53	-

#### BH32.14

Model	$k_{cat}$ (min <sup>-1</sup> )	$K_{mA}$ (μM)	$K_{mB}$ (μM)	$K_{SA}K_{mB}$
Random	0.349 ± 0.034	2556 ± 444	1137 ± 226	-
Ordered	0.368 ± 0.041	4134 ± 851	1304 ± 280	0.1 × $K_{mA}K_{mB}$
Ordered	0.349 ± 0.034	2556 ± 444	1137 ± 226	$K_{mA} \times K_{mB}$
Ordered	0.325 ± 0.029	697 ± 128	914 ± 193	10 × $K_{mA}K_{mB}$

A = 2-cyclohexen-1-one, B = 4-nitrobenzaldehyde

**Table 4: Effect of cosolvent on BH32.14 activity.** MBH reactions were performed using **1** (50mM), **2** (10mM) and BH32.14 (0.5 mol%) in PBS buffer (pH 7.4) with the stated concentration of MeCN or DMSO as a cosolvent. The percentage conversion was determined after 5 hours by HPLC analysis.

Cosolvent	Conversion (%)
20 % MeCN	2
30 % MeCN	0.3
40 % MeCN	0
20 % DMSO	50
30 % DMSO	43
40 % SMSO	16

**Table 5: Reaction conditions for the synthesis of 3 & 5a-w.** All reactions were performed using PBS buffer pH 7.4 and 20% DMSO

Product	Enone Conc. (mM) <sup>[1]</sup>	Enzyme	Catalyst loading (mol%)	Reaction time (h)	Mean % Conv. ( $\pm$ s.d.)	Wavelength (nm)	extinction coefficient (mM <sup>-1</sup> cm <sup>-1</sup> )	
							aldehyde	product
<b>3</b>	50	BH32.14	0.5	18	94 $\pm$ 0.2	280	600	600
<b>5a</b>	50	BH32.14	1.5	18	97 $\pm$ 0.2	220	240	700
<b>5b</b>	50	BH32.14	2.5	48	82 $\pm$ 0.3	220	240	480
<b>5c</b>	50	BH32.14	2.5	1.5	97 $\pm$ 0.1	220	240	400
<b>5d</b>	50	BH32.14	5	48	70 $\pm$ 0.5	220	240	589
<b>5e</b>	100	BH32.14	2.5	18	67 $\pm$ 0.3	220	130	740
<b>5f</b>	50	BH32.14	2.5	48	56 $\pm$ 0.9	220	105	800
<b>5g</b>	50	BH32.14	1.5	18	92 $\pm$ 0.2	254	1000	310
<b>5h</b>	50	BH32.14	5	48	33 $\pm$ 0.4	254	65	190
<b>5i</b>	50	BH32.14	5	48	58 $\pm$ 0.4	220	213	629
<b>5j</b>	50	BH32.14	5	48	1.2 $\pm$ 0.003	220	583	639
<b>5k</b>	50	BH32.14	1.5	18	92 $\pm$ 1.0	220	140	660
<b>5l</b>	50	BH32.14	1.5	18	99 $\pm$ 0.2	220	55	670
<b>5m</b>	50	BH32.14	1.5	48	71 $\pm$ 1.2	220	75	710
<b>5n</b>	50	BH32.14	5	18	90 $\pm$ 0.2	220	80	610
<b>5o</b> <sup>[2]</sup>	50	BH32.8	1.5	0.5	98 $\pm$ 0.1	220	390	80
<b>5p</b>	50	BH32.8	5	48	91 $\pm$ 0.07	220	1000	760
<b>5q</b>	50	BH32.8	5	48	81 $\pm$ 0.2	220	900	590
<b>5r</b>	50	BH32.8	5	48	76 $\pm$ 0.5	220	490	620
<b>5s</b>	50	BH32.14	1.5	18	97 $\pm$ 0.3	220	130	435
<b>5t</b>	50	BH32.14	1.5	18	92 $\pm$ 0.3	254	60	360
<b>5u</b>	50	BH32.14	2.5	48	99 $\pm$ 0.3	220	240	345
<b>5v+5w</b>	50	BH32.14	5	24	89 $\pm$ 0.1	220	300	<b>5v</b> 1000 <b>5w</b> 250

<sup>[1]</sup> 10 mM acceptor was used in each reaction

<sup>[2]</sup> Reaction was performed in PBS pH 7.0



**Table 6: SFC analytical methods for MBH adducts 5a-w**

	Column	Flow (mL.min <sup>-1</sup> )	Mobile Phase (% MeOH in CO <sub>2</sub> )	Run Time (min)
<b>5a</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm	1	5-10% (3min) 10% (7min)	10
<b>5b</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm	1	25%	2
<b>5c</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	2	20%	2
<b>5d</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm	1	10%	2
<b>5e</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm, 3 μm	1	35%	1
<b>5f</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	5%	5
<b>5g</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	1	20%	3
<b>5h</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	1	5%	4
<b>5i</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	10%	3
<b>5j</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	10	3.4
<b>5k</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm, 3 μm	1.2	3%	7
<b>5l</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	1	20%	2.2
<b>5m</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm, 3 μm	1.2	3%	6
<b>5n</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	1	20%	2.2
<b>5o</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm, 3 μm	1	10%	5
<b>5p</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	10%	5
<b>5q</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	20%	2
<b>5r</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	1	15%	2
<b>5s</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	2.5	3%	10
<b>5t</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IG-3, 3 mm, 50 mm, 3 μm	1.2	20%	5
<b>5u</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IA-3, 3 mm, 50 mm, 3 μm	1.5	5%	5
<b>5v+</b> <b>5w</b>	Daicel 80S82 CHIRALPAK <sup>®</sup> IC-3, 3 mm, 50 mm, 3 μm	2	5%	8

**Table 7: Data collection and refinement statistics.** Entries in parentheses refer to the statistics in the highest resolution bin.

	<b>BH32.6</b>	<b>BH32.7</b>	<b>BH32.12</b>
Wavelength	0.976	0.9763	0.9795
Resolution range	55.26 - 1.48 (1.533 - 1.48)	37.87 - 1.8 (1.864 - 1.8)	42.71 - 2.29 (2.372 - 2.29)
Space group	P 31 2 1	P 1 21 1	P 31 2 1
Unit cell	71.689 71.689 121.272 90 90 120	36.56 69.63 45.72 90 99.29 90	70.9666 70.9666 118.768 90 90 120
Total reflections	578916 (56870)	64699 (6531)	158031 (15120)
Unique reflections	60772 (5941)	20789 (2043)	16121 (1571)
Multiplicity	9.5 (9.6)	3.1 (3.2)	9.8 (9.6)
Completeness (%)	99.90 (99.13)	99.00 (98.55)	99.55 (98.66)
Mean I/sigma(I)	14.64 (1.19)	17.67 (4.27)	10.51 (1.21)
Wilson B-factor	26.4	34.48	65.35
R-merge	0.05985 (1.411)	0.03661 (0.2531)	0.0806 (1.617)
R-meas	0.0634 (1.491)	0.0443 (0.3045)	0.08509 (1.708)
R-pim	0.02062 (0.4776)	0.02464 (0.1674)	0.02701 (0.5474)
CC1/2	0.997 (0.679)	0.998 (0.919)	0.999 (0.603)
CC*	0.999 (0.899)	0.999 (0.979)	1 (0.867)
Reflections used in refinement	60762 (5939)	20802 (2043)	16120 (1551)
Reflections used for R-free	3039 (305)	1067 (117)	824 (95)
R-work	0.1572 (0.2272)	0.2039 (0.3121)	0.2226 (0.3236)
R-free	0.1771 (0.2647)	0.2546 (0.3733)	0.2616 (0.4293)
CC(work)	0.964 (0.872)	0.955 (0.823)	0.946 (0.681)
CC(free)	0.966 (0.831)	0.937 (0.760)	0.925 (0.403)
Number of non-hydrogen atoms	2210	1977	1890
macromolecules	1950	1829	1838
ligands	18	0	9
solvent	242	148	43
Protein residues	448	227	226
RMS(bonds)	0.009	0.004	0.006
RMS(angles)	1.12	0.54	1.08
Ramachandran favored (%)	98.69	99.10	97.75
Ramachandran allowed (%)	1.31	0.90	1.35
Ramachandran outliers (%)	0	0	0.9
Rotamer outliers (%)	1.43	2.05	2.02
Clash score	2.76	3.52	8.59
Average B-factor	35.89	44.94	75.73
macromolecules	34.02	44.77	75.73
ligands	60.92		80.84
solvent	49.14	47.07	74.73
Number of TLS groups	0	1	1

**Table 8: Mother liquor composition used for protein crystallization of BH32.6, BH32.7 and BH32.12**

Variant	Crystallization conditions (200+200nl drops incubated at 4°C)
BH32.6	0.06 M Divalents [0.3M Magnesium chloride hexahydrate; 0.3M calcium chloride dihydrate] 0.1 M BS1 pH 6.5 [Imidazole; MES monohydrate (acid)] 30% Precipitant mix 2 [40% v/v Ethylene glycol; 20% w/v PEG 8K] Morpheus screen condition A2 (Molecular Dimensions)
BH32.7	0.12 M Monosaccharides [0.2M D-Glucose; 0.2M D-Mannose; 0.2M D-Galactose; 0.2M L-Fucose; 0.2M D-Xylose; 0.2M N-Acetyl-D-Glucosamine] 0.1 M BS2 pH 7.5 [Sodium HEPES; MOPS (acid)] 30 % Precipitant mix 1 [40% v/v PEG 500* MME; 20 % w/v PEG 20000] Morpheus screen condition F5 (Molecular Dimensions)
BH32.12	0.1M SPG pH 9.0, 25% w/v PEG 1500 PACT premier Eco condition A6 (Molecular Dimensions)

**Table 9: Primer sequences used to generate DNA libraries**

Flanking Primers	
XHO_R	ATGCATGCctcgagagagccct
NDE_F	CATGCATGcatatgattcgtgcgta
Round 2	
Y45x_T49x_F_1	ACCCTGCTGGACGAANDTGAGAACTGNDTCGCGAAGCGTTCTCT
Y45x_T49x_F_2	ACCCTGCTGGACGAAVHGGAGAACTGVHGC GCGAAGCGTTCTCT
Y45x_T49x_F_3	ACCCTGCTGGACGAANDTGAGAACTGVHGC GCGAAGCGTTCTCT
Y45x_T49x_F_4	ACCCTGCTGGACGAAVHGGAGAACTGNDTCGCGAAGCGTTCTCT
Y45x_T49x_F_5	ACCCTGCTGGACGAANDTGAGAACTGTGGCGCGAAGCGTTCTCT
Y45x_T49x_F_6	ACCCTGCTGGACGAATGGGAGAACTGNDTCGCGAAGCGTTCTCT
Y45x_T49x_F_7	ACCCTGCTGGACGAAVHGGAGAACTGTGGCGCGAAGCGTTCTCT
Y45x_T49x_F_8	ACCCTGCTGGACGAATGGGAGAACTGVHGC GCGAAGCGTTCTCT
Y45x_T49x_F_9	ACCCTGCTGGACGAATGGGAGAACTGTGGCGCGAAGCGTTCTCT
Y45x_T49x_R	TTC GTCCAGCAGGGT
F87x_W88x_F_1	AAATACCCTGAAAACNDTNDTGAAATCTCCCTGCGT
F87x_W88x_F_2	AAATACCCTGAAAACVHGVHGGAAATCTCCCTGCGT
F87x_W88x_F_3	AAATACCCTGAAAACNDTVHGGAAATCTCCCTGCGT
F87x_W88x_F_4	AAATACCCTGAAAACVHGNDTGAAATCTCCCTGCGT
F87x_W88x_F_5	AAATACCCTGAAAACNDTTGGGAAATCTCCCTGCGT
F87x_W88x_F_6	AAATACCCTGAAAACVHGNDTGAAATCTCCCTGCGT
F87x_W88x_F_7	AAATACCCTGAAAACVHGTGGGAAATCTCCCTGCGT
F87x_W88x_F_8	AAATACCCTGAAAACVHGVHGGAAATCTCCCTGCGT
F87x_W88x_F_9	AAATACCCTGAAAACVHGTGGGAAATCTCCCTGCGT
F87x_W88x_R	GTTTTCAGGGTATTTGAAACC
T49x_F	GAATACGAGAACTGNNKCGCGAAGCGTTCTCT
T49x_R	CAGTTTCTCGTATTTCGTC
R50x_F	GAATACGAGAACTGACCNKGAAGCGTTCTCTAAC
R50x_R	GGTCAGTTTCTCGTATTTC
Round 4	
N14x_F	TTGATAGCCTGGGTA CTCTGNNKAGCGTTGAAGGCG

N14x_R	CAGAGTACCCAGGCT
M130x_F	GATACCGAGCAGGCC <b>NNK</b> GCAATTCCTGGACGCA
M130x_R	GGCCTGCTCGGTATC
E174x_F	GGCGTTAAAGGCGAG <b>NNK</b> GCAAGTGTACGTTGGT
E174x_R	CTCGCCTTTAACGCC
<b>Round 5</b>	
L10x_F	GCGGTATTCTTTGATAGC <b>NNK</b> GGTACTCTGATTAGC
A19x_F	CTGATTAGCGTTGAAGGC <b>NNK</b> GCTAAATCCCATCTG
P38x_F	GGTGACTATCCGCTGAAC <b>NNK</b> AAAACCCTGCTGGAC
L42x_F	AACCCGAAAACCCTG <b>NNK</b> GACGAATACGAGAAA
Y45x_F	ACCCTGCTGGACGA <b>NNK</b> GAGAACTGGCTCGC
E46x_F	ACCCTGCTGGACGAATAC <b>NNK</b> AAACTGGCTCGCGAA
P60x_F	AACTATGCGGGCAA <b>NNK</b> TATCGTCCGCTGCGT
P63x_F	GGCAAACCGTATCGT <b>NNK</b> CTGCGTGATATCCTG
F81x_F	GCGGAAAAGTACGGT <b>NNK</b> AAATACCCTGAAAAC
S91x_F	CCTGAAAACCTGTGGGAAATC <b>NNK</b> CTGCGTATGTCTCAA
Q96x_F	TCCCTGCGTATGTCT <b>NNK</b> CGCTACGGCGAGCTG
S124x_F	GGCATGATCACCGAT <b>NNK</b> GATACCGAGCAGGCC
D125x_F	GGCATGATCACCGATTCT <b>NNK</b> ACCGAGCAGGCCACG
Q128x_F	ACCGATTCTGATACCGAG <b>NNK</b> GCCACGGCATTCTG
M130x_F	GATACCGAGCAGGCC <b>NNK</b> GCAATTCCTGGACGCA
L133x_F	CAGGCCACGGCATT <b>NNK</b> GACGCACTGGGCATC
F154x_F	TCTGAAGAAGCTGGTTTC <b>NNK</b> AAACCGCACCCACGC
K167x_F	TTCGAACTGGCTCTGAAG <b>NNK</b> GCCGGCGTTAAAGGC
E174x_F	GGCGTTAAAGGCGAG <b>NNK</b> GCAAGTGTACGTTGGT
K202x_F	ATCCTGCTGGATCGT <b>NNK</b> GGTGAGAAACGTGAA
L10x_R	GCTATCAAAGAATACCGC
A19x_R	GCCTTCAACGCTAAT
P38x_R	CGGGTTCAGCGGATA
L42x_R	CAGGGTTTTCGGGTT
Y45x_R	TTCGTCCAGCAGGGT
E46x_R	GTATTCGTCCAGCAG
P60x_R	TTTGCCCGCATAGTT
P63x_R	ACGATACGGTTTGCC
F81x_R	ACCGTACTTTTCCGC
S91x_R	GATTTCCACAAGTTTTC
Q96x_R	AGACATACGCAGGGA
S124x_R	ATCGGTGATCATGCC
D125x_R	AGAATCGGTGATCATGCC
Q128x_R	CTCGGTATCAGAATCGGT
M130x_R	GGCCTGCTCGGTATC
L133x_R	GAATGCCGTGGCCTG
F154x_R	GAAACCAGCTTCTTCAGA
K167x_R	CTTCAGAGCCAGTTC

E174x_R	CTCGCCTTTAACGCC
K202x_R	ACGATCCAGCAGGAT
<b>Round 6</b>	
V16x_F	GGTACTCTGATTAGC <b>NNK</b> GAAGGCGCTGCTAAA
E17x_F	ACTCTGATTAGCGTT <b>NNK</b> GGCGCTGCTAAATCC
G32x_F	ATGGAGGAAGTGCTG <b>NNK</b> GACTATCCGCTGAACC
Y34x_F	GAAGTGCTGGGTGAC <b>NNK</b> CCGCTGAACCCGAAA
L36x_F	CTGGGTGACTATCCG <b>NNK</b> AACCCGAAAACCCTG
Y61x_F	TATGCGGGCAAACCG <b>NNK</b> CGTCCGCTGCGTGAT
L64x_F	AAACCGTATCGTCCG <b>NNK</b> CGTGATATCCTGGAAGAA
L68x_F	CCGCTGCGTGATATC <b>NNK</b> GAAGAAGTAATGCGTAAACT
M120x_F	AAATATCACGTTGGC <b>NNK</b> KATCACCGATAGGGATACC
T122x_F	CACGTTGGCATGATC <b>NNK</b> GATAGGGATACCGAGC
D123x_F	GTTGGCATGATCAC <b>NNK</b> KAGGGATACCGAGCCG
D125x_F	ATGATCACCGATAG <b>NNK</b> KACCGAGCCGGCC
T126x_F	ATCACCGATAGGGAT <b>NNK</b> GAGCCGGCCACG
Q128x_F	GATAGGGATACCGAG <b>NNK</b> GCCACGGCATTCTG
E149x_F	TCCATCACACGTCT <b>NNK</b> GAAGCTGGTTTCTTTAAACC
G152x_F	ACGTCTGAAGAAGCT <b>NNK</b> TTCTTTAAACCGCACCCA
L199x_F	ATGACTAGCATCCTG <b>NNK</b> GATCGTAAAGGTGAGAAAC
E204x_F	CTGGATCGTAAAGGT <b>NNK</b> AAACGTGAATTCTGGGAT
K205x_F	GATCGTAAAGGTGAG <b>NNK</b> CGTGAATTCTGGGATAAG
E207x_F	AAAGGTGAGAAACGT <b>NNK</b> TTCTGGGATAAGGCCG
V16x_R	GCTAATCAGAGTACCCAG
E17x_R	AACGCTAATCAGAGTACC
G32x_R	CAGCACTTCCTCCAT
Y34x_R	GTCACCCAGCACTTC
L36x_R	CGGATAGTCACCCAG
Y61x_R	CGGTTTGCCCGCATA
L64x_R	CGGACGATACGGTTT
L68x_R	GATATCACGCAGCGG
M120x_R	GCCAACGTGATATTTACC
T122x_R	GATCATGCCAACGTG
D123x_R	GGTGATCATGCCAAC
D125x_R	CCTATCGGTGATCATGCC
T126x_R	ATCCCTATCGGTGATCAT
Q128x_R	CTCGGTATCCCTATCG
E149x_R	AGACGTGGTGATGGA
G152x_R	AGCTTCTTCAGACGT
D199x_R	CAGGATGCTAGTCATACC
E204x_R	ACCTTTACGATCCAGCAG
K205x_R	CTCACCTTTACGATCCAG
E207x_R	ACGTTTCTCACCTTTACG
<b>Round 7</b>	

S95x_F1	ATCTCCCTGCGTATG <b>NDT</b> CAACGCTACGGCGAG
S95x_F2	ATCTCCCTGCGTATG <b>VHG</b> CAACGCTACGGCGAG
S95x_F3	ATCTCCCTGCGTATG <b>TGG</b> CAACGCTACGGCGAG
S95x_R	Catacgcaggagat
S22x_F1	GAAGGCGCTGCTAA <b>NDT</b> CATCTGAAAATTATGGAGGA
S22x_F2	GAAGGCGCTGCTAA <b>VHG</b> CATCTGAAAATTATGGAGGA
S22x_F3	GAAGGCGCTGCTAA <b>TGG</b> CATCTGAAAATTATGGAGGA
S22x_R	Tttagcagccttc
M120x_T122x_F1	AAATATCACGTTGGC <b>NDT</b> ATC <b>NDT</b> AATAGGGATACCGAG
M120x_T122x_F2	AAATATCACGTTGGC <b>VHG</b> ATC <b>VHG</b> AATAGGGATACCGAG
M120x_T122x_F3	AAATATCACGTTGGC <b>NDT</b> ATC <b>VHG</b> AATAGGGATACCGAG
M120x_T122x_F4	AAATATCACGTTGGC <b>VHG</b> ATC <b>NDT</b> AATAGGGATACCGAG
M120x_T122x_F5	AAATATCACGTTGGC <b>NDT</b> ATC <b>TGG</b> AATAGGGATACCGAG
M120x_T122x_F6	AAATATCACGTTGGC <b>TGG</b> ATC <b>NDT</b> AATAGGGATACCGAG
M120x_T122x_F7	AAATATCACGTTGGC <b>VHG</b> ATC <b>TGG</b> AATAGGGATACCGAG
M120x_T122x_F8	AAATATCACGTTGGC <b>TGG</b> ATC <b>VHG</b> AATAGGGATACCGAG
M120x_T122x_F9	AAATATCACGTTGGC <b>TGG</b> ATC <b>TGG</b> AATAGGGATACCGAG
M120x_T122x_R	GCCAACGTGATATTTAC
<b>Round 8</b>	
L10_F	GTATTCTTTGATAGC <b>NNK</b> GGTACTCTGATTAGCGTT
A20_F	AGCGTTGAAGGCGCT <b>NNK</b> AAAGTGCATCTGAAAATTATG
L24_F	GCTGCTAAAGTGCAT <b>NNK</b> AAAATTATGGAGGAAGTGCT
M27_F	GTGCATCTGAAAATT <b>NNK</b> GAGGAAGTGCTGGGT
L42_F	AACCCGAAAACCTG <b>NNK</b> GACGAATACGAGAAACTG
T45_F	ACCCTGCTGGACGA <b>NNK</b> GAGAAACTGGCTCGC
P63_F	GGCAAACCGTATCGT <b>NNK</b> CTGCGTGATATCCTG
L64_F	AAACCGTATCGTCCG <b>NNK</b> CGTGATATCCTGGAAGAA
S91_F	AACTTGTGGGAAATC <b>NNK</b> CTGCGTATGGCGCAA
L92_F	TTGTGGGAAATCTCC <b>NNK</b> CGTATGGCGCAACG
Q96_F	TCCCTGCGTATGGCG <b>NNK</b> CGCTACGGCGAGC
D125_F	GTGATCCTGAATAGG <b>NNK</b> KACCGAGCCGGC
E127_F	CTGAATAGGGATACC <b>NNK</b> KCCGGCCACGGC
A129_F	AGGGATACCGAGCCG <b>NNK</b> KACGGCATTCTGGAC
I145_F	GACCTGTTTCGATTCC <b>NNK</b> KACCAGTCTGAAGAA
T147_F	TTCGATTCCATCACC <b>NNK</b> TCTGAAGAAGCTGGT
L10_R	GCTATCAAAGAATACCGC
A20_R	AGCGCCTTCAACGCT
L24_R	ATGCACTTTAGCAGC
M27_R	AATTTTCAGATGCACTTTAG
L42_R	CAGGGTTTTTCGGGTT
T45_R	TTCGTCCAGCAGGGT
P63_R	ACGATACGGTTTGCC
L64_R	CGGACGATACGGTTT
S91_R	GATTTCCACAAGTTTTT

L92_R	GGAGATTTCCACAA
Q96_R	CGCCATACGCAGGGA
D125_R	CCTATTCAGGATCACGC
E127_R	GGTATCCCTATTCAGGA
A129_R	CGGCTCGGTATCCCT
I145_R	GGAATCGAACAGGTC
T147_R	GGTGATGGAATCGAA
<b>Round 9</b>	
L10_F	GTATTCTTTGATAGC <b>NNK</b> GGTACTCTGATTAGCGTT
L24_F	GCTTATAAAGTGCAT <b>NNK</b> AAAATTATGGAGGAAGTGCT
L42_F	AACCCGAAAACCTG <b>NNK</b> GACGAATACGAGAAACTG
E46_F	CTGCTGGACGAATAC <b>NNK</b> AAACTGGCTCGCGAA
A129_F	AGGGATACCGAGCCG <b>NNK</b> ACGGCATTCTGGAC
L10_R	GCTATCAAAGAATACCGC
L24_R	ATGCACTTTATAAGC
L42_R	CAGGGTTTTCGGGTT
E46_R	GTATTCGTCCAGCAGGGT
A129_R	CGGCTCGGTATCCCT
<b>Round 11</b>	
F154_F	TCTGAAGAAGCTGGTTTC <b>NNK</b> AAACCGCACCCACGC
F154_R	GAAACCAGCTTCTTCAGA
<b>Round 12</b>	
Y20x_F	AGCGTTGAAGGCGCT <b>NNK</b> AAAGTGCATTTTAAAATTATGGA
V30x_F	AAAATTATGGAGGA <b>NNK</b> CTGGGTGACTATCCG
K47x_F	CTGGACGAATACGAG <b>NNK</b> CTGGCTCGCGAAGCG
Y46x_F	GAAGCGTTCTCTAAC <b>NNK</b> GCGGGCAAACCGTAT
I67x_F	CGTCCGCTGCGTGAT <b>NNK</b> CTGGAAGAAGTAATGCG
E70x_F	CGTGATATCCTGGA <b>NNK</b> GTAATGCGTAAACTGGC
F87x_F	AAATACCCTGAAAAC <b>NNK</b> TGGGAAATCTCCCTG
S91x_F	AACTTGTTGGGAAATC <b>NNK</b> CTGCGTATGGCGCAA
R97x_F	CTGCGTATGGCGCA <b>NNK</b> TACGGCGAGCTGTAC
F153x_F	TCTGAAGAAGCTGGT <b>NNK</b> TCTAAACCGCACCCA
K155x_F	GAAGCTGGTTTCTCT <b>NNK</b> CCGCACCCACGCATC
F161x_F	CCGCACCCACGCATC <b>NNK</b> GAACTGGCTCTGAAG
L165x_F	ATCTTCGAACTGGCT <b>NNK</b> AAGAAAGCCGGCGTT
K171x_F	AAGAAAGCCGGCGTT <b>NNK</b> GGCGAGAAAGCAGTG
V176x_F	AAAGGCGAGAAAGC <b>NNK</b> TACGTTGGTGACAAC
Y177x_F	GGCGAGAAAGCAGTG <b>NNK</b> GTTGGTGACAACCCG
D180x_F	GCAGTGACGTTGGT <b>NNK</b> AACCCGGTCAAAGAC
S196x_F	AACCTGGGTATGACT <b>NNK</b> KATCCTGCTGGATCGT
D210x_F	AAACGTGAATTCTGG <b>NNK</b> AAGGCGGACTTTATC
L219x_F	TTTATCGTCTCCGAC <b>NNK</b> CGCGAAGTTATTAAGATTG
I223x_F	GACCTGCGCGAAGTT <b>NNK</b> AAGATTGTTGACGAACTG
Y20x_R	AGCGCCTTCAACGCT

V30x_R	TTCCTCCATAATTTTAAAATGCA
K47x_R	CTCGTATTCGTCCAG
Y56x_R	GTTAGAGAACGCTTCGC
I67x_R	ATCACGCAGCGGACG
E70x_R	TTCCAGGATATCACGCAG
F87x_R	GTTTTCAGGGTATTTGAAA
S91x_R	GATTTCCACAAGTTTTT
R97x_R	TTGCGCCATACGCAG
F153x_R	ACCAGCTTCTTCAGA
K155x_R	AGAGAAACCAGCTTC
F161x_R	GATGCGTGGGTGCGG
L165x_R	AGCCAGTTCGAAGAT
K171x_R	AACGCCGGCTTTCTT
V176x_R	TGCTTTCTCGCCTTT
Y177x_R	CACTGCTTTCTCGCC
D180x_R	ACCAACGTACACTGC
S196x_R	AGTCATACCCAGGTT
D210x_R	CCAGAATTCACGTTTCT
L219x_R	GTCGGAGACGATAAAGT
I223x_R	AACTTCGCGCAGGTC
<b>Round 14</b>	
V16x_F	GGTACTCTGATTAGC <b>NNK</b> GAAGGCACTTATAAAGTG
A19x_F	AATAGCGTTGAAGGC <b>NNK</b> TATAAAGTGCATTTT
E70x_F	CGTGATATCCTGGA <b>NNK</b> GTAAATGCGTAAA
M72x_F	ATCCTGGAACGTGT <b>NNK</b> CGTAAACTGGCGGAA
E89x_F	CCTGAAAACCTGTGG <b>NNK</b> ATCTCCCTGCGTATG
P128x_F	AATAGGGATACCGAG <b>NNK</b> TCTACGGCATTCTCG
S154x_F	GAAGAAGCTGGTTTC <b>NNK</b> AAACCGCACCCACG
V16x_R	GCTAATCAGAGTACCC
A19x_R	GCCTTCAACGCTAAT
E70x_R	TTCCAGGATATCACG
M72x_R	TACACGTTCCAGGAT
E89x_R	CCACAAGTTTTTCAGG
P128x_R	CTCGGTATCCCTATT
S154x_R	GAAACCAGCTTCTTC



### 3. DNA and protein sequence for the most active variant BH32.14

**Mutations from the BH32 Design:** L10W, N14I, A19T, A20Y, S22V, L24F, T49A, Y56N, E70R, F87L, S95A, M120V, T122L, D123N, S124R, P128L, A129S, M130T, F154S, E174K, Y177C, D180P, C186A, C212A

ATGATTCGTGCGGTATTCTTTGATAGCTGGGGTACTCTGATTAGCGTTGA  
AGGCACCTTATAAAGTGCATTTTAAAATTATGGAGGAAGTCTGGGTGACT  
ATCCGCTGAACCCGAAAACCCCTGCTGGACGAATACGAGAACTGGCTCGC  
GAAGCGTTCTCTAACAATGCGGGCAAACCGTATCGTCCGCTGCGTGATAT  
CCTGGAACGTGTAATGCGTAAACTGGCGGAAAAGTACGGTTTCAAATACC  
CTGAAAACCTTGTGGGAAATCTCCCTGCGTATGGCGCAACGCTACGGCGAG  
CTGTACCCGGAAGTGGTGGAAAGTACTGAAATCTCTGAAAGGTAAATATCA  
CGTTGGCGTGATCCTGAATAGGGATACCGAGCTGTCTACGGCATTCTG  
ACGCACTGGGCATCAAAGACCTGTTGACTCCATCACCACGTCTGAAGAA  
GCTGGTTTTCTCTAAACCGCACCCACGCATCTTCGAACTGGCTCTGAAGAA  
AGCCGGCGTTAAAGGCGAGAAAGCAGTGTGTGTTGGTCCTAACCCGGTCA  
AAGACGCGGGTGGTTCTAAGAACCTGGGTATGACTAGCATCCTGCTGGAT  
CGTAAAGGTGAGAAACGTGAATTCTGGGATAAGGCGGACTTTATCGTCTC  
CGACCTGCGCGAAGTTATTAAGATTGTTGACGAACTGAACGGTCAGGGCT  
CTCTCGAGTGGAGTCACCCACAGTTTGAGAAA

MIRAVFFDS**W**GT**L**ISVEG**T**Y**K**V**H**FKIMEEVLGDYPLNPKTLLDEYEK**L**AR  
EAFS**N**NAGKPYRPLRDIL**R**VMRKLAEKYGFYPEN**L**WEISLR**M**AQRYGE  
LYPEVVEVLKSLKGKYHVG**V**IL**N**RDTE**L**STAFLDALGIKDLFDSITTSEE  
AGF**S**KPHPRIFELALKKAGVK**G**E**K**AV**C**VG**P**NPVK**D**AGGSKNLGMTSILLD  
RKGEKREFWD**K**ADFIIVSDLREVIKIVDELNGQGSLEWSHPQFEK

#### 4. Cartesian coordinates for energy minimised cluster models.

	R				TS1		
C	2.442144000	-2.750087000	2.346668000	C	1.584125000	-3.435423000	2.735771000
C	1.957197000	-3.759099000	1.338583000	C	1.443880000	-3.976175000	1.329330000
C	1.331559000	-3.085362000	0.114040000	C	1.345721000	-2.845705000	0.299598000
C	2.274618000	-2.049440000	-0.506396000	C	2.523699000	-1.871168000	0.426472000
C	2.943909000	-1.195277000	0.525568000	C	2.780245000	-1.469457000	1.868352000
C	3.009865000	-1.510133000	1.835146000	C	2.206567000	-2.193951000	2.921562000
O	2.379015000	-2.977103000	3.561909000	O	1.108129000	-4.102083000	3.710920000
C	1.063902000	0.507394000	3.232256000	C	0.408984000	-0.030331000	3.867067000
C	0.152415000	0.556049000	2.077198000	C	-0.227147000	0.240390000	2.561683000
C	-1.029743000	-0.203150000	2.055836000	C	-1.474436000	-0.330308000	2.271253000
C	-1.908648000	-0.087838000	0.989465000	C	-2.116820000	-0.022096000	1.083991000
C	-1.576842000	0.787941000	-0.048789000	C	-1.488556000	0.850396000	0.191080000
C	-0.396916000	1.527893000	-0.071695000	C	-0.230988000	1.406954000	0.431390000
C	0.470026000	1.405751000	1.009367000	C	0.394538000	1.093609000	1.637573000
O	0.879888000	-0.173071000	4.228089000	O	-0.110472000	-0.700965000	4.741506000
C	-0.933169000	-7.122602000	1.692388000	C	-1.423394000	-7.022153000	1.348518000
C	-1.855809000	-6.127738000	1.068480000	C	-2.198669000	-5.920714000	0.702112000
C	-1.922815000	-4.767148000	1.273477000	C	-2.264662000	-4.590634000	1.058561000
C	-2.850943000	-6.438153000	0.075028000	C	-3.065746000	-6.079955000	-0.437052000
N	-2.897066000	-4.212728000	0.459174000	N	-3.124545000	-3.917030000	0.207737000
C	-3.483090000	-5.215481000	-0.284662000	C	-3.628665000	-4.803821000	-0.718869000
C	-3.248826000	-7.629982000	-0.555425000	C	-3.415012000	-7.177001000	-1.244588000
C	-4.494428000	-5.161207000	-1.249853000	C	-4.520130000	-4.605267000	-1.777588000
C	-4.254249000	-7.580083000	-1.514376000	C	-4.296877000	-6.981223000	-2.301290000
C	-4.868853000	-6.356046000	-1.855681000	C	-4.843033000	-5.705954000	-2.563022000
C	2.267450000	-7.890944000	-2.331172000	C	1.828570000	-7.906774000	-2.609568000
C	1.553171000	-6.798818000	-1.521476000	C	0.718168000	-6.955504000	-2.135923000
C	2.412936000	-7.555282000	-3.818664000	C	2.647046000	-7.359461000	-3.783999000
C	0.080527000	-6.619399000	-1.896485000	C	-0.377818000	-6.701230000	-3.174828000
N	6.591785000	-5.591382000	0.323696000	N	6.635494000	-6.337701000	-0.210879000
C	6.535803000	-4.675733000	-0.827170000	C	6.282975000	-5.080822000	-0.881072000
C	6.648051000	-3.258942000	-0.325184000	C	6.797818000	-3.908440000	-0.079562000
O	7.599906000	-2.526882000	-0.563478000	O	7.580428000	-3.069116000	-0.499658000
C	5.229035000	-4.879120000	-1.595642000	C	4.763776000	-4.975867000	-1.041430000
N	8.072287000	-0.848451000	-3.048634000	N	8.152090000	-1.322500000	-2.963521000
C	7.056421000	0.157088000	-2.709135000	C	7.227032000	-0.245149000	-2.581464000
C	7.551557000	1.002060000	-1.535568000	C	7.800219000	0.527311000	-1.388024000
O	7.719707000	2.226258000	-1.626102000	O	8.012678000	1.744466000	-1.416859000
C	5.617137000	-0.361719000	-2.430467000	C	5.764724000	-0.681323000	-2.275741000
C	4.667714000	0.807643000	-2.140921000	C	4.884769000	0.522941000	-1.918342000
C	5.103567000	-1.217673000	-3.591361000	C	5.163535000	-1.467026000	-3.444885000
N	7.781708000	0.344209000	-0.377143000	N	8.009937000	-0.193360000	-0.257351000
C	8.151816000	1.086050000	0.810153000	C	8.284139000	0.483660000	0.995797000
C	9.252875000	2.090071000	0.489705000	C	9.619435000	1.217146000	0.941128000
O	9.429317000	3.104899000	1.131724000	O	9.888709000	2.143374000	1.676083000
C	8.709463000	0.136208000	1.888962000	C	8.266454000	-0.523809000	2.154227000
C	7.746532000	-0.934582000	2.296520000	C	6.911603000	-1.143672000	2.274240000
N	8.165738000	-2.162566000	2.769047000	N	6.609127000	-2.185475000	3.133141000
C	6.371458000	-0.996324000	2.337416000	C	5.731842000	-0.857939000	1.628874000
C	7.060104000	-2.898423000	3.074087000	C	5.293557000	-2.490567000	3.003326000
N	5.952527000	-2.221589000	2.823379000	N	4.753996000	-1.706981000	2.087032000
C	6.644487000	4.981941000	0.593782000	C	7.086142000	4.489304000	0.871315000
C	5.491462000	4.352848000	-0.200959000	C	5.886437000	3.933128000	0.092642000
C	6.281655000	6.246487000	1.379492000	C	6.797477000	5.752418000	1.689440000
C	4.456653000	3.626193000	0.665304000	C	4.791448000	3.323446000	0.973977000
C	-3.640458000	2.490302000	7.456810000	C	-3.666159000	2.436240000	7.335334000
C	-2.380798000	1.620952000	7.370065000	C	-2.368320000	1.621606000	7.279122000
C	-2.719302000	0.139633000	7.584983000	C	-2.653589000	0.165916000	6.880520000
C	-1.668005000	1.818729000	6.023650000	C	-1.359732000	2.265346000	6.317192000
C	-2.867980000	9.260412000	2.170184000	C	-2.114854000	9.437861000	2.331388000
C	-2.839791000	7.853618000	1.648277000	C	-2.159003000	8.055742000	1.754265000
C	-3.531951000	7.360032000	0.569313000	C	-2.829681000	7.648107000	0.626841000
C	-2.093809000	6.740908000	2.191105000	C	-1.513816000	6.879399000	2.287939000
N	-3.261078000	6.010055000	0.404284000	N	-2.639820000	6.289736000	0.424689000
C	-2.384966000	5.599181000	1.386332000	C	-1.837495000	5.789298000	1.427449000
C	-1.221991000	6.593684000	3.284383000	C	-0.707402000	6.639116000	3.414438000
C	-1.838732000	4.338571000	1.651980000	C	-1.381655000	4.488904000	1.667299000

C	-0.682113000	5.340483000	3.555864000	C	-0.258563000	5.345986000	3.660290000
C	-0.990350000	4.225169000	2.749182000	C	-0.594885000	4.282995000	2.796158000
N	2.009279000	7.219702000	-1.076264000	N	2.761436000	7.097765000	-0.951541000
C	1.931036000	5.789217000	-0.801410000	C	2.491952000	5.702560000	-0.624239000
C	0.990272000	4.923606000	-1.612657000	C	1.437855000	4.936805000	-1.401446000
O	1.100937000	3.687508000	-1.593190000	O	1.336169000	3.708108000	-1.276284000
C	1.574793000	5.638195000	0.692563000	C	2.125734000	5.648944000	0.873742000
O	2.514645000	6.330978000	1.494346000	O	3.142485000	6.255134000	1.652020000
N	0.013285000	5.570499000	-2.270612000	N	0.613868000	5.680198000	-2.165140000
C	-1.031772000	4.871696000	-2.992421000	C	-0.465449000	5.087293000	-2.925447000
C	-0.479801000	4.567306000	-4.392350000	C	0.094726000	4.712702000	-4.301544000
O	-1.002955000	4.933101000	-5.426886000	O	-0.415027000	5.027477000	-5.359835000
C	-2.344488000	5.660395000	-3.013333000	C	-1.717242000	5.967525000	-2.990639000
C	-3.611401000	4.783897000	-2.987158000	C	-3.041993000	5.180448000	-2.937205000
C	-4.858536000	5.676991000	-2.965736000	C	-4.224349000	6.156146000	-2.980882000
C	-3.694191000	3.786527000	-4.149657000	C	-3.176281000	4.122926000	-4.040671000
N	2.213380000	2.406020000	-4.398265000	N	2.637650000	2.416916000	-4.291817000
C	1.904096000	0.978717000	-4.485538000	C	2.208309000	1.028599000	-4.469594000
C	1.187153000	0.710877000	-5.796294000	C	1.454356000	0.907681000	-5.780798000
O	1.344277000	-0.278531000	-6.483973000	O	1.492294000	-0.060284000	-6.514338000
C	0.947727000	0.590413000	-3.345135000	C	1.232732000	0.644289000	-3.341981000
C	-5.618704000	-2.579417000	4.849235000	C	-5.840607000	-2.233290000	4.528793000
C	-4.262483000	-3.120608000	4.389497000	C	-4.837702000	-3.355262000	4.267082000
C	-3.449775000	-3.639837000	5.581337000	C	-4.141723000	-3.776593000	5.564325000
N	-2.166874000	-4.241706000	5.209374000	N	-3.114176000	-4.801225000	5.366166000
C	-1.044048000	-3.573410000	4.922891000	C	-1.916864000	-4.568183000	4.823569000
N	0.038124000	-4.243177000	4.516773000	N	-1.099483000	-5.572181000	4.501852000
N	-1.001183000	-2.242734000	5.044140000	N	-1.513495000	-3.312097000	4.569783000
N	-7.598589000	2.030436000	0.914829000	N	-7.382459000	2.640454000	0.690902000
C	-7.286066000	2.006759000	-0.528084000	C	-6.991124000	2.637152000	-0.732685000
C	-7.079900000	0.574235000	-1.044579000	C	-6.847277000	1.207687000	-1.279120000
O	-6.894025000	0.327457000	-2.239828000	O	-6.595651000	0.977923000	-2.465671000
C	-5.982451000	2.831035000	-0.684258000	C	-5.628164000	3.373466000	-0.790200000
C	-5.365464000	2.773202000	0.719936000	C	-5.092976000	3.222119000	0.640435000
C	-6.599020000	2.860447000	1.620163000	C	-6.364071000	3.368406000	1.478787000
N	-7.101710000	-0.354075000	-0.062053000	N	-6.999235000	0.254384000	-0.332544000
C	-6.995951000	-1.779788000	-0.261845000	C	-6.998988000	-1.166956000	-0.587870000
C	-8.319405000	-2.457682000	0.076475000	C	-8.370796000	-1.751631000	-0.267282000
O	-8.408284000	-3.552248000	0.591170000	O	-8.541440000	-2.843773000	0.231152000
C	-5.841051000	-2.372097000	0.545376000	C	-5.891386000	-1.882246000	0.178168000
O	-4.578374000	-1.948907000	0.038930000	O	-4.607216000	-1.533467000	-0.331568000
H	3.499417000	-0.866278000	2.555300000	H	2.327537000	-1.838060000	3.937530000
H	2.839024000	-4.343993000	1.037862000	H	2.320797000	-4.605867000	1.122646000
H	1.264412000	-4.451741000	1.820935000	H	0.568066000	-4.628058000	1.286539000
H	0.402278000	-2.587829000	0.413067000	H	0.403710000	-2.306111000	0.452856000
H	1.065183000	-3.846400000	-0.620207000	H	1.316635000	-3.254268000	-0.714186000
H	3.061358000	-2.544412000	-1.096022000	H	3.427947000	-2.331571000	0.018657000
H	1.735329000	-1.414020000	-1.216481000	H	2.337760000	-0.971203000	-0.167412000
H	3.405582000	-0.271105000	0.186935000	H	2.958437000	-0.412953000	2.039059000
H	1.949628000	1.158219000	3.165999000	H	1.386702000	0.449987000	4.030621000
H	-1.260196000	-0.870011000	2.876595000	H	-1.934042000	-1.004538000	2.983169000
H	-0.163545000	2.202714000	-0.885146000	H	0.222657000	2.091240000	-0.278393000
H	1.387837000	1.984087000	1.024437000	H	1.359337000	1.534679000	1.867658000
H	-0.347767000	-7.651762000	0.931428000	H	-0.910961000	-7.639110000	0.603143000
H	-0.224712000	-6.645113000	2.375661000	H	-0.662301000	-6.632160000	2.028487000
H	-1.342599000	-4.140801000	1.935960000	H	-1.771891000	-4.061619000	1.861375000
H	-3.209366000	-3.247496000	0.449506000	H	-3.358750000	-2.931325000	0.231877000
H	-2.774460000	-8.572830000	-0.297988000	H	-2.995945000	-8.159783000	-1.048045000
H	-4.963264000	-4.229587000	-1.534793000	H	-4.945826000	-3.635202000	-1.985479000
H	-4.571277000	-8.492266000	-2.011335000	H	-4.570372000	-7.818486000	-2.936609000
H	-5.646463000	-6.339758000	-2.613672000	H	-5.526549000	-5.571953000	-3.396001000
H	3.264603000	-8.057169000	-1.903634000	H	2.502410000	-8.113178000	-1.768430000
H	2.089887000	-5.848125000	-1.653023000	H	1.169523000	-5.998672000	-1.834944000
H	1.623923000	-7.039724000	-0.452998000	H	0.257907000	-7.370282000	-1.231375000
H	2.962329000	-8.338537000	-4.350920000	H	3.465066000	-8.037012000	-4.049263000
H	2.959304000	-6.613962000	-3.952150000	H	3.086752000	-6.386825000	-3.532979000
H	1.439539000	-7.444843000	-4.306875000	H	2.030286000	-7.220471000	-4.677503000
H	-0.040702000	-6.297624000	-2.934892000	H	0.017490000	-6.216169000	-4.072624000
H	-0.406121000	-5.876735000	-1.260291000	H	-1.162521000	-6.058315000	-2.768431000
H	-0.471520000	-7.557212000	-1.771829000	H	-0.847094000	-7.643152000	-3.481574000
H	5.803667000	-5.427824000	0.948273000	H	6.191426000	-6.391000000	0.704352000

H	7.438384000	-5.434859000	0.866209000	H	7.639917000	-6.396441000	-0.058895000
H	7.396657000	-4.873740000	-1.473308000	H	6.768953000	-5.055500000	-1.861668000
H	5.833755000	-2.916821000	0.340576000	H	6.447356000	-3.870362000	0.970074000
H	5.143096000	-5.924795000	-1.902219000	H	4.392214000	-5.865592000	-1.556130000
H	5.187324000	-4.242974000	-2.483929000	H	4.486154000	-4.089875000	-1.619033000
H	4.366397000	-4.640216000	-0.963971000	H	4.274184000	-4.917749000	-0.063208000
H	8.049745000	-1.617576000	-2.381996000	H	8.027367000	-2.124128000	-2.346321000
H	7.850248000	-1.249072000	-3.955732000	H	7.911900000	-1.644878000	-3.896872000
H	6.999406000	0.856610000	-3.549820000	H	7.205316000	0.479688000	-3.401688000
H	5.657794000	-0.993470000	-1.535543000	H	5.798072000	-1.349579000	-1.406112000
H	4.637121000	1.509127000	-2.981857000	H	4.810343000	1.219736000	-2.760229000
H	4.966578000	1.368704000	-1.251159000	H	5.273723000	1.085735000	-1.065292000
H	3.648408000	0.445781000	-1.981532000	H	3.872638000	0.193375000	-1.665582000
H	5.742971000	-2.088059000	-3.764350000	H	5.730214000	-2.378562000	-3.654163000
H	5.065456000	-0.636640000	-4.520713000	H	5.148089000	-0.860143000	-4.358295000
H	4.093236000	-1.584226000	-3.383208000	H	4.132927000	-1.760283000	-3.219430000
H	7.637854000	-0.663126000	-0.308368000	H	7.851995000	-1.197435000	-0.245663000
H	7.298260000	1.645830000	1.213261000	H	7.524864000	1.253185000	1.180804000
H	9.953628000	1.765776000	-0.305194000	H	10.341750000	0.821063000	0.198499000
H	8.993671000	0.749586000	2.751591000	H	8.531284000	0.006370000	3.075096000
H	9.629772000	-0.325872000	1.511821000	H	9.028155000	-1.296327000	1.994348000
H	9.125349000	-2.464903000	2.862842000	H	7.254826000	-2.637135000	3.767204000
H	5.668535000	-0.235465000	2.031471000	H	5.527007000	-0.121104000	0.870393000
H	7.120278000	-3.902144000	3.468723000	H	4.776152000	-3.244275000	3.576894000
H	7.064811000	4.230707000	1.273676000	H	7.483929000	3.705964000	1.531325000
H	5.916807000	3.644823000	-0.918794000	H	6.254890000	3.176633000	-0.606963000
H	4.996569000	5.137649000	-0.790218000	H	5.459693000	4.741004000	-0.517855000
H	5.946707000	7.042360000	0.703449000	H	6.451662000	6.565233000	1.039825000
H	7.142040000	6.624292000	1.941692000	H	7.694813000	6.098708000	2.212723000
H	5.468185000	6.064946000	2.089709000	H	6.015880000	5.583487000	2.436673000
H	3.655413000	3.203520000	0.048065000	H	3.968468000	2.931423000	0.365244000
H	3.993821000	4.303117000	1.388352000	H	4.370905000	4.066771000	1.656098000
H	4.925764000	2.800886000	1.215770000	H	5.188677000	2.493340000	1.571573000
H	-3.400210000	3.551263000	7.329502000	H	-3.475627000	3.468845000	7.647268000
H	-4.354449000	2.212972000	6.671442000	H	-4.143231000	2.468341000	6.347920000
H	-1.693379000	1.931663000	8.169105000	H	-1.923907000	1.617370000	8.284430000
H	-3.408220000	-0.210122000	6.804220000	H	-3.098007000	0.124782000	5.877555000
H	-3.206728000	-0.028644000	8.550967000	H	-3.354730000	-0.307753000	7.576598000
H	-1.816922000	-0.481852000	7.553243000	H	-1.733989000	-0.427803000	6.860662000
H	-0.748960000	1.225305000	5.967567000	H	-0.413299000	1.715234000	6.308496000
H	-1.405179000	2.868892000	5.855155000	H	-1.148118000	3.303473000	6.595439000
H	-2.316824000	1.505191000	5.195471000	H	-1.751429000	2.271408000	5.292287000
H	-3.525119000	9.889869000	1.564171000	H	-2.697292000	10.136659000	1.724726000
H	-3.227583000	9.297099000	3.205434000	H	-2.518862000	9.460907000	3.350682000
H	-4.207923000	7.867560000	-0.104032000	H	-3.438134000	8.222701000	-0.056941000
H	-3.662439000	5.420676000	-0.306641000	H	-3.032483000	5.755026000	-0.332685000
H	-0.979282000	7.446796000	3.911411000	H	-0.444061000	7.452443000	4.084575000
H	-2.069844000	3.481097000	1.029863000	H	-1.634729000	3.674268000	0.998579000
H	-0.011034000	5.214283000	4.400085000	H	0.361162000	5.146058000	4.529130000
H	-0.554543000	3.260914000	2.985884000	H	-0.227054000	3.286689000	3.012479000
H	2.357627000	7.428995000	-2.005685000	H	3.156316000	7.222159000	-1.877579000
H	1.126383000	7.702388000	-0.930573000	H	1.945420000	7.695417000	-0.848821000
H	2.928478000	5.368569000	-0.949883000	H	3.423530000	5.146501000	-0.759086000
H	0.553964000	6.016132000	0.856842000	H	1.156305000	6.150362000	1.022835000
H	1.588730000	4.585466000	0.976835000	H	2.014540000	4.612099000	1.192975000
H	2.732682000	7.128478000	0.981437000	H	3.462872000	6.991688000	1.102665000
H	0.050890000	6.577946000	-2.329893000	H	0.824730000	6.658922000	-2.297273000
H	-1.162494000	3.906162000	-2.489838000	H	-0.686280000	4.136504000	-2.423179000
H	0.467586000	3.994261000	-4.397262000	H	1.030050000	4.120339000	-4.267881000
H	-2.362993000	6.296163000	-3.905642000	H	-1.690334000	6.562104000	-3.910654000
H	-2.360777000	6.322491000	-2.141844000	H	-1.690760000	6.667864000	-2.149795000
H	-3.582029000	4.190393000	-2.059853000	H	-3.063462000	4.635344000	-1.979842000
H	-4.912534000	6.276145000	-3.881699000	H	-4.224447000	6.709435000	-3.926868000
H	-4.854090000	6.374707000	-2.120941000	H	-4.179727000	6.893465000	-2.171594000
H	-5.772084000	5.078539000	-2.903978000	H	-5.178717000	5.627278000	-2.904219000
H	-3.696932000	4.310954000	-5.110170000	H	-3.108415000	4.583877000	-5.030523000
H	-4.613975000	3.196536000	-4.075827000	H	-4.143513000	3.614925000	-3.962171000
H	-2.857841000	3.084433000	-4.149403000	H	-2.401043000	3.356587000	-3.967512000
H	3.098988000	2.621123000	-4.845824000	H	3.521742000	2.592226000	-4.760369000
H	2.264420000	2.708276000	-3.428431000	H	2.760792000	2.629391000	-3.305349000
H	2.786003000	0.326277000	-4.449754000	H	3.033212000	0.304045000	-4.489038000

H	0.464010000	1.508464000	-6.075907000	H	0.819803000	1.791794000	-6.010983000
H	0.011128000	1.151211000	-3.408380000	H	0.328883000	1.258325000	-3.376203000
H	1.414115000	0.831078000	-2.385592000	H	1.712374000	0.812662000	-2.372806000
H	0.718044000	-0.475251000	-3.373637000	H	0.944534000	-0.404959000	-3.417999000
H	-5.495834000	-1.746382000	5.549503000	H	-5.339514000	-1.338367000	4.914644000
H	-6.203040000	-2.216610000	3.999030000	H	-6.363762000	-1.953124000	3.609994000
H	-3.700703000	-2.337890000	3.865844000	H	-4.088745000	-3.029329000	3.536782000
H	-4.399065000	-3.938450000	3.673161000	H	-5.340583000	-4.228342000	3.836676000
H	-3.274141000	-2.847584000	6.317086000	H	-3.694392000	-2.912338000	6.067217000
H	-4.008739000	-4.417514000	6.105903000	H	-4.862831000	-4.194839000	6.269265000
H	-2.164319000	-5.235221000	5.034122000	H	-3.389862000	-5.764979000	5.480941000
H	0.016202000	-5.249252000	4.474728000	H	-1.415251000	-6.527896000	4.525338000
H	0.915868000	-3.782112000	4.264714000	H	-0.186724000	-5.339827000	4.101929000
H	-0.183850000	-1.689992000	4.804500000	H	-0.545157000	-3.203840000	4.288822000
H	-1.810081000	-1.735446000	5.361458000	H	-1.915154000	-2.536329000	5.071747000
H	-8.546637000	2.343957000	1.087348000	H	-8.312195000	3.020926000	0.822959000
H	-8.090542000	2.431261000	-1.137251000	H	-7.731103000	3.129469000	-1.371607000
H	-5.336239000	2.432918000	-1.468162000	H	-4.968711000	2.958847000	-1.554233000
H	-6.238530000	3.863278000	-0.938323000	H	-5.798196000	4.429938000	-1.015664000
H	-4.655379000	3.578630000	0.917323000	H	-4.336541000	3.964769000	0.902953000
H	-4.848332000	1.820223000	0.870662000	H	-4.655241000	2.228231000	0.780077000
H	-6.421129000	2.475129000	2.628968000	H	-6.269332000	2.934672000	2.479087000
H	-6.923903000	3.906899000	1.709748000	H	-6.617927000	4.431878000	1.593149000
H	-7.322722000	0.046458000	0.852283000	H	-7.246749000	0.642216000	0.580600000
H	-6.834670000	-1.959544000	-1.330977000	H	-6.857276000	-1.305730000	-1.666402000
H	-9.215715000	-1.863036000	-0.196214000	H	-9.219075000	-1.087086000	-0.531325000
H	-5.864993000	-3.459206000	0.475783000	H	-5.999143000	-2.960683000	0.062266000
H	-5.949949000	-2.093939000	1.601567000	H	-5.963757000	-1.641704000	1.246144000
H	-4.576847000	-0.986896000	-0.085067000	H	-4.542883000	-0.570739000	-0.440639000
H	-4.142628000	2.370062000	8.422738000	H	-4.382748000	1.997052000	8.037849000
H	-6.203674000	-3.357660000	5.350168000	H	-6.595586000	-2.537498000	5.261556000
H	-1.869193000	9.713045000	2.163951000	H	-1.087918000	9.818460000	2.388282000
H	7.456499000	5.224476000	-0.103388000	H	7.891525000	4.707628000	0.158289000
H	1.721662000	-8.837178000	-2.216457000	H	1.382224000	-8.870373000	-2.890455000
H	-1.480392000	-7.884544000	2.260409000	H	-2.072047000	-7.695700000	1.923808000
N	-5.732712000	-0.564133000	-5.008653000	N	-5.483400000	0.135172000	-5.203514000
C	-4.694788000	-1.519037000	-4.556770000	C	-4.557261000	-0.948053000	-4.806673000
C	-5.233439000	-2.142150000	-3.293296000	C	-5.221970000	-1.693536000	-3.675720000
O	-5.922014000	-3.149980000	-3.257854000	O	-6.008440000	-2.615573000	-3.822411000
C	-3.384964000	-0.751176000	-4.325143000	C	-3.216005000	-0.320414000	-4.387753000
C	-2.219112000	-1.635703000	-3.952932000	C	-2.134641000	-1.318961000	-4.040000000
C	-1.196329000	-1.885334000	-4.876204000	C	-1.133016000	-1.627901000	-4.969684000
C	-2.140245000	-2.242536000	-2.689729000	C	-2.101382000	-1.955642000	-2.789343000
C	-0.116964000	-2.708524000	-4.549467000	C	-0.121156000	-2.538925000	-4.661042000
C	-1.075543000	-3.082846000	-2.367074000	C	-1.099252000	-2.877155000	-2.480633000
C	-0.054130000	-3.312547000	-3.292601000	C	-0.101163000	-3.167214000	-3.413976000
H	-5.987097000	0.044497000	-4.227797000	H	-5.739290000	0.674035000	-4.373650000
H	-6.579991000	-1.081843000	-5.235817000	H	-6.350699000	-0.280380000	-5.539077000
H	-5.060894000	-1.545701000	-2.382137000	H	-5.026610000	-1.276064000	-2.673398000
H	-3.560544000	-0.005607000	-3.541060000	H	-3.400630000	0.340533000	-3.532934000
H	-1.231484000	-1.412494000	-5.853072000	H	-1.128833000	-1.131098000	-5.935426000
H	-2.909819000	-2.062090000	-1.946538000	H	-2.858554000	-1.730104000	-2.046609000
H	-1.054432000	-3.553773000	-1.391492000	H	-1.102070000	-3.364355000	-1.511348000
H	0.782820000	-3.954985000	-3.038779000	H	0.683719000	-3.876894000	-3.172538000
H	0.679600000	-2.858193000	-5.271183000	H	0.660093000	-2.737494000	-5.387948000
H	-4.568626000	-2.290450000	-5.322480000	H	-4.423162000	-1.624401000	-5.657144000
H	-3.162357000	-0.198058000	-5.241672000	H	-2.886050000	0.315615000	-5.213996000
H	-2.822982000	-0.663072000	0.964761000	H	-3.077452000	-0.457796000	0.859164000
N	-2.521118000	0.974162000	-1.151687000	N	-2.198180000	1.229857000	-1.032837000
O	-3.639193000	0.451151000	-1.068702000	O	-3.374581000	0.865988000	-1.169584000
O	-2.171512000	1.654116000	-2.112794000	O	-1.605873000	1.907838000	-1.866916000
O	3.105195000	-1.234800000	5.650869000	O	1.325573000	-2.787357000	6.216627000
H	2.400956000	-0.596492000	5.462784000	H	0.883753000	-1.967269000	5.943620000
H	2.989177000	-1.869510000	4.920211000	H	1.349692000	-3.317158000	5.394181000

Int1

C	1.110688000	-2.837864000	2.366025000
C	0.736255000	-3.025572000	0.907583000
C	1.518045000	-2.130432000	-0.059790000

TS2

C	1.455925000	-3.154544000	2.151346000
C	1.021808000	-3.285549000	0.705717000
C	1.661776000	-2.262317000	-0.238077000

C	2.990479000	-2.068327000	0.338810000	C	3.131272000	-2.055998000	0.126236000
C	3.121031000	-1.450746000	1.737072000	C	3.240030000	-1.441801000	1.530990000
C	2.172604000	-2.047496000	2.720527000	C	2.326249000	-2.090290000	2.547522000
O	0.361589000	-3.431486000	3.244145000	O	0.997796000	-3.953794000	2.999362000
C	0.618724000	-0.010829000	3.710291000	C	1.085405000	-0.719908000	3.386128000
C	-0.040492000	0.272665000	2.416596000	C	0.239323000	-0.218905000	2.254238000
C	-1.312800000	-0.261958000	2.160749000	C	-1.027844000	-0.782623000	2.033310000
C	-1.982559000	0.061713000	0.993261000	C	-1.853460000	-0.300608000	1.031113000
C	-1.363947000	0.924381000	0.082352000	C	-1.400063000	0.755601000	0.234284000
C	-0.089407000	1.456478000	0.294997000	C	-0.142135000	1.337655000	0.416949000
C	0.565808000	1.123037000	1.478347000	C	0.663740000	0.847449000	1.442066000
O	0.043592000	-0.554753000	4.643075000	O	0.511685000	-1.270982000	4.390853000
C	-1.816191000	-6.956180000	1.415531000	C	-1.404354000	-6.985466000	1.495114000
C	-2.622234000	-5.857484000	0.799776000	C	-2.246940000	-5.948045000	0.831151000
C	-2.565226000	-4.507000000	1.065292000	C	-2.384738000	-4.622631000	1.177808000
C	-3.596716000	-6.025028000	-0.247725000	C	-3.099205000	-6.160838000	-0.310146000
N	-3.438585000	-3.824726000	0.235939000	N	-3.273888000	-3.999030000	0.321306000
C	-4.078450000	-4.728402000	-0.585829000	C	-3.725417000	-4.915674000	-0.602799000
C	-4.083547000	-7.142043000	-0.948864000	C	-3.385212000	-7.277994000	-1.114952000
C	-5.015147000	-4.528621000	-1.606281000	C	-4.613406000	-4.767592000	-1.673371000
C	-5.018564000	-6.947824000	-1.959328000	C	-4.265648000	-7.131390000	-2.181662000
C	-5.476322000	-5.652561000	-2.283860000	C	-4.871578000	-5.886174000	-2.457276000
C	1.418570000	-8.068209000	-2.499468000	C	1.837689000	-7.890719000	-2.467888000
C	0.738691000	-6.945361000	-1.701217000	C	0.356699000	-7.586940000	-2.187175000
C	1.731814000	-7.687587000	-3.949907000	C	2.654837000	-6.645569000	-2.832730000
C	-0.667921000	-6.601226000	-2.196239000	C	-0.427158000	-7.103440000	-3.411474000
N	6.311025000	-6.785103000	-0.144107000	N	7.252270000	-5.947722000	-1.394400000
C	6.011069000	-5.485078000	-0.752297000	C	6.283048000	-5.024472000	-0.783501000
C	6.458122000	-4.367955000	0.156373000	C	7.047715000	-4.070897000	0.099073000
O	7.226503000	-3.475515000	-0.167153000	O	7.237202000	-2.893147000	-0.165360000
C	4.510384000	-5.370210000	-1.042306000	C	5.234987000	-5.810174000	0.002885000
N	8.063553000	-1.921387000	-2.774248000	N	8.051700000	-1.361821000	-2.820441000
C	7.249056000	-0.730004000	-2.490796000	C	7.194604000	-0.200498000	-2.533622000
C	7.852562000	0.019887000	-1.298685000	C	7.775980000	0.589639000	-1.354667000
O	8.202126000	1.203435000	-1.350962000	O	8.005285000	1.802203000	-1.405346000
C	5.736511000	-0.989026000	-2.243636000	C	5.703009000	-0.535616000	-2.260472000
C	4.990324000	0.325720000	-1.989095000	C	4.893123000	0.727656000	-1.949581000
C	5.104752000	-1.766113000	-3.402020000	C	5.087224000	-1.309368000	-3.430048000
N	7.935840000	-0.685848000	-0.141662000	N	7.969669000	-0.115567000	-0.210326000
C	8.310905000	-0.025503000	1.089951000	C	8.261547000	0.568153000	1.032334000
C	9.740455000	0.507242000	1.021312000	C	9.638404000	1.225627000	0.997742000
O	10.135935000	1.402936000	1.735475000	O	9.935931000	2.154483000	1.717175000
C	8.145655000	-0.977268000	2.281558000	C	8.159442000	-0.406011000	2.215707000
C	6.716555000	-1.389422000	2.404636000	C	6.789693000	-0.998867000	2.273852000
N	6.278953000	-2.454262000	3.171994000	N	6.498687000	-2.209691000	2.874041000
C	5.595120000	-0.877425000	1.812724000	C	5.610466000	-0.565245000	1.732907000
C	4.948707000	-2.588259000	3.056318000	C	5.204393000	-2.511022000	2.704368000
N	4.517981000	-1.634212000	2.229192000	N	4.645649000	-1.513826000	2.011801000
C	7.347068000	4.040892000	0.912966000	C	7.041558000	4.565998000	0.874281000
C	6.120917000	3.532508000	0.145116000	C	5.842584000	3.991137000	0.109922000
C	7.123597000	5.327111000	1.715354000	C	6.749296000	5.835350000	1.681476000
C	4.981695000	3.031965000	1.039463000	C	4.746956000	3.407675000	1.007890000
C	-3.553036000	2.520561000	7.792771000	C	-3.764714000	2.289587000	7.620434000
C	-2.320076000	1.789732000	7.249283000	C	-2.372503000	1.709330000	7.346163000
C	-2.671910000	0.354939000	6.825823000	C	-2.474764000	0.290539000	6.763989000
C	-1.693442000	2.559479000	6.077646000	C	-1.570205000	2.620851000	6.406760000
C	-1.567427000	9.525774000	2.226872000	C	-2.180178000	9.479126000	3.231290000
C	-1.697321000	8.138576000	1.673239000	C	-2.245266000	8.117540000	1.696081000
C	-2.389187000	7.757776000	0.549228000	C	-2.924829000	7.773205000	0.552823000
C	-1.131198000	6.930511000	2.227384000	C	-1.615136000	6.905467000	2.170581000
N	-2.287656000	6.386966000	0.368502000	N	-2.749400000	6.426135000	0.280540000
C	-1.522735000	5.850745000	1.381983000	C	-1.950759000	5.865638000	1.253363000
C	-0.344870000	6.653656000	3.359736000	C	-0.816921000	6.588729000	3.284687000
C	-1.153985000	4.526637000	1.641696000	C	-1.504351000	4.549042000	1.413958000
C	0.017725000	5.337310000	3.625519000	C	-0.387959000	5.276531000	3.459746000
C	-0.384951000	4.285448000	2.775911000	C	-0.726414000	4.267579000	2.532782000
N	3.173193000	6.889694000	-0.943884000	N	2.702382000	7.133987000	-0.954805000
C	2.845517000	5.500669000	-0.642867000	C	2.435189000	5.740458000	-0.614781000
C	1.795932000	4.781988000	-1.468340000	C	1.381768000	4.969681000	-1.386709000
O	1.670757000	3.550661000	-1.391192000	O	1.300599000	3.738430000	-1.275763000
C	2.418010000	5.448292000	0.839072000	C	2.067746000	5.702325000	0.882231000

O	3.426047000	6.009080000	1.661635000	O	3.082375000	6.320014000	1.655105000
N	0.993274000	5.566695000	-2.210525000	N	0.530157000	5.707488000	-2.127441000
C	-0.119443000	5.032265000	-2.968825000	C	-0.527698000	5.087347000	-2.898501000
C	0.417143000	4.655020000	-4.355162000	C	0.075833000	4.656311000	-4.239704000
O	-0.046010000	5.063150000	-5.402998000	O	-0.420300000	4.889781000	-5.325272000
C	-1.316942000	5.985544000	-3.017274000	C	-1.776340000	5.962490000	-3.044063000
C	-2.687383000	5.279885000	-3.001300000	C	-3.102123000	5.175906000	-2.987571000
C	-3.806858000	6.327589000	-3.040626000	C	-4.286143000	6.143610000	-3.106215000
C	-2.870068000	4.260025000	-4.132722000	C	-3.208051000	4.066467000	-4.042199000
N	2.779718000	2.193013000	-4.277574000	N	2.654434000	2.401868000	-4.295865000
C	2.331125000	0.810401000	-4.444182000	C	2.161833000	1.028425000	-4.414174000
C	1.596449000	0.679447000	-5.765760000	C	1.363157000	0.905049000	-5.698713000
O	1.623127000	-0.305094000	-6.477475000	O	1.337130000	-0.081796000	-6.407585000
C	1.329749000	0.455643000	-3.329240000	C	1.201309000	0.726347000	-3.247392000
C	-5.981315000	-1.887832000	4.501144000	C	-5.834598000	-2.190193000	4.646347000
C	-5.132894000	-3.139191000	4.301083000	C	-4.825134000	-3.291415000	4.339682000
C	-4.483882000	-3.583970000	5.618062000	C	-4.186701000	-3.822093000	5.629704000
N	-3.403564000	-4.552535000	5.418511000	N	-3.036853000	-4.691222000	5.385224000
C	-2.252891000	-4.224438000	4.815843000	C	-1.850123000	-4.247113000	4.948199000
N	-1.423584000	-5.172822000	4.359605000	N	-0.895439000	-5.128013000	4.611537000
N	-1.903055000	-2.945532000	4.668505000	N	-1.603032000	-2.940436000	4.877819000
N	-7.187732000	3.020940000	0.602939000	N	-7.404130000	2.656571000	0.771385000
C	-6.796946000	2.984955000	-0.820457000	C	-7.031610000	2.623479000	-0.656888000
C	-6.745270000	1.546817000	-1.360369000	C	-6.910917000	1.186289000	-1.176613000
O	-6.502990000	1.296520000	-2.544838000	O	-6.726405000	0.941548000	-2.372142000
C	-5.389265000	3.630715000	-0.881444000	C	-5.663304000	3.352514000	-0.745647000
C	-4.862349000	3.445690000	0.548136000	C	-5.135126000	3.286799000	0.694282000
C	-6.119106000	3.673585000	1.390274000	C	-6.412011000	3.457460000	1.517501000
N	-6.964916000	0.613209000	-0.408864000	N	-7.006950000	0.242472000	-0.213887000
C	-7.025482000	-0.810657000	-0.637816000	C	-7.018251000	-1.179061000	-0.475932000
C	-8.432246000	-1.323591000	-0.344827000	C	-8.397649000	-1.757127000	-0.174490000
O	-8.669969000	-2.401474000	0.157330000	O	-8.581862000	-2.865014000	0.282760000
C	-5.975773000	-1.555654000	0.180516000	C	-5.919271000	-1.911042000	0.282642000
O	-4.663669000	-1.313383000	-0.317764000	O	-4.636991000	-1.608410000	-0.254069000
H	2.404763000	-1.936276000	3.773362000	H	2.778007000	-2.251898000	3.519846000
H	0.883464000	-4.085539000	0.659394000	H	1.282319000	-4.306335000	0.398020000
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H	1.097873000	-1.119279000	-0.059113000	H	1.130894000	-1.307038000	-0.187693000
H	1.423258000	-2.503418000	-1.082968000	H	1.579761000	-2.605428000	-1.271372000
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H	3.572878000	-1.491399000	-0.382032000	H	3.628365000	-1.410153000	-0.598119000
H	3.019720000	-0.359712000	1.657877000	H	3.047445000	-0.367105000	1.456156000
H	1.634194000	0.395902000	3.827233000	H	1.949038000	-0.065756000	3.578844000
H	-1.771112000	-0.921346000	2.886688000	H	-1.369986000	-1.589109000	2.668566000
H	0.363045000	2.130284000	-0.424825000	H	0.185442000	2.162841000	-0.206616000
H	1.543622000	1.547600000	1.682585000	H	1.621282000	1.323346000	1.628465000
H	-1.446802000	-7.644060000	0.647122000	H	-0.867576000	-7.590466000	0.755824000
H	-0.942223000	-6.564028000	1.942771000	H	-0.655147000	-6.528848000	2.147364000
H	-1.952416000	-3.973196000	1.776462000	H	-1.909593000	-4.070962000	1.975095000
H	-3.589084000	-2.822313000	0.203179000	H	-3.532533000	-3.017777000	0.316990000
H	-3.728451000	-8.140004000	-0.707518000	H	-2.919612000	-8.237651000	-0.909252000
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H	2.351729000	-8.350275000	-1.994891000	H	2.280002000	-8.360776000	-1.580406000
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H	0.683693000	-7.240036000	-0.645427000	H	-0.125097000	-8.489806000	-1.790442000
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H	0.822109000	-7.464692000	-4.516274000	H	2.295730000	-6.181475000	-3.757020000
H	-0.659482000	-6.234775000	-3.227031000	H	-0.039339000	-6.155640000	-3.796253000
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H	5.790568000	-6.904312000	0.723207000	H	7.720203000	-6.502928000	-0.679767000
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H	6.071132000	-4.425121000	1.193223000	H	7.511480000	-4.524381000	0.998300000
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H	4.279982000	-4.440045000	-1.568489000	H	4.442076000	-5.156616000	0.376285000
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H	7.831029000	-2.266805000	-3.701195000	H	7.864162000	-1.683750000	-3.765776000
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H	5.392481000	0.869684000	-1.130689000	H	5.282653000	1.267077000	-1.083256000
H	3.929524000	0.142872000	-1.798036000	H	3.848514000	0.479393000	-1.741955000
H	5.582876000	-2.739293000	-3.543554000	H	5.619046000	-2.245482000	-3.620479000
H	5.187315000	-1.207073000	-4.341678000	H	5.110530000	-0.712612000	-4.349613000
H	4.041784000	-1.944278000	-3.209071000	H	4.042956000	-1.560182000	-3.217383000
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H	10.396523000	-0.003095000	0.287378000	H	10.354047000	0.775800000	0.279827000
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H	6.449442000	2.730351000	-0.522945000	H	6.214148000	3.218491000	-0.569837000
H	5.751154000	4.339348000	-0.502609000	H	5.415829000	4.781219000	-0.523341000
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H	-1.785593000	-0.170846000	6.454437000	H	-1.481915000	-0.136675000	6.582894000
H	-0.797968000	2.052052000	5.703554000	H	-0.563585000	2.224320000	6.232281000
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H	-0.030111000	7.457266000	4.019356000	H	-0.544554000	7.358123000	4.001590000
H	-1.458714000	3.720039000	0.984653000	H	-1.753024000	3.783327000	0.687679000
H	0.621281000	5.110557000	4.499156000	H	0.223841000	5.021028000	4.319721000
H	-0.084170000	3.269739000	3.007035000	H	-0.364356000	3.256090000	2.686902000
H	3.591816000	7.011586000	-1.859759000	H	3.087850000	7.249440000	-1.885985000
H	2.376615000	7.514666000	-0.851435000	H	1.884591000	7.729522000	-0.853327000
H	3.762094000	4.914347000	-0.746403000	H	3.367156000	5.184441000	-0.745124000
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H	-6.482713000	-1.599318000	3.572716000	H	-6.323238000	-1.837481000	3.733509000
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H	-5.215293000	-4.055604000	6.276478000	H	-4.908045000	-4.405799000	6.204425000
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H	-1.777230000	-6.102026000	4.196513000	H	-1.160881000	-6.096762000	4.519692000
H	-0.621873000	-4.847612000	3.811439000	H	-0.144289000	-4.800032000	4.001502000
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H	-2.329446000	-2.221361000	5.221931000	H	-2.307812000	-2.286545000	5.175051000
H	-8.086915000	3.469395000	0.733244000	H	-8.350017000	2.995393000	0.904503000
H	-7.503245000	3.522217000	-1.461391000	H	-7.773282000	3.110462000	-1.298585000
H	-4.759296000	3.171960000	-1.645178000	H	-4.995231000	2.890918000	-1.474084000
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H	-4.060639000	4.139214000	0.810314000	H	-4.390285000	4.053381000	0.917716000
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H	-9.239637000	-0.620902000	-0.636882000	H	-9.237807000	-1.073704000	-0.414818000
H	-6.150059000	-2.629089000	0.112314000	H	-6.061321000	-2.987420000	0.182341000
H	-6.052316000	-1.261822000	1.234943000	H	-5.968646000	-1.657795000	1.349097000
H	-4.516171000	-0.360038000	-0.428347000	H	-4.499034000	-0.646894000	-0.290966000
H	-3.989059000	1.987767000	8.644783000	H	-4.332720000	1.654555000	8.308862000
H	-6.755683000	-2.045531000	5.259797000	H	-6.617542000	-2.544516000	5.325488000
H	-0.518627000	9.841429000	2.281956000	H	-1.149347000	9.849411000	2.377909000
H	8.160653000	4.208067000	0.195608000	H	7.841188000	4.781644000	0.154024000
H	0.777559000	-8.960004000	-2.481265000	H	1.908729000	-8.629615000	-3.277321000
H	-2.399728000	-7.559328000	2.123690000	H	-2.001403000	-7.679237000	2.100750000
N	-5.394724000	0.345886000	-5.260968000	N	-5.604918000	0.047253000	-4.976101000
C	-4.533422000	-0.777189000	-4.832599000	C	-4.594360000	-0.987456000	-4.705613000
C	-5.222261000	-1.426108000	-3.656437000	C	-5.223554000	-2.055742000	-3.840674000
O	-6.032093000	-2.335969000	-3.739026000	O	-5.688991000	-3.101479000	-4.258451000
C	-3.147764000	-0.224487000	-4.453108000	C	-3.369163000	-0.346967000	-4.029680000
C	-2.141657000	-1.282197000	-4.056694000	C	-2.252668000	-1.333855000	-3.771517000
C	-1.148486000	-1.686312000	-4.958077000	C	-1.241017000	-1.528654000	-4.721115000
C	-2.173718000	-1.883330000	-2.787696000	C	-2.222589000	-2.099631000	-2.596320000
C	-0.206954000	-2.655201000	-4.605127000	C	-0.222858000	-2.458964000	-4.504258000
C	-1.242760000	-2.861475000	-2.434966000	C	-1.216422000	-3.043956000	-2.382121000
C	-0.251338000	-3.247104000	-3.341210000	C	-0.209906000	-3.223217000	-3.334436000
H	-5.611923000	0.927147000	-4.448880000	H	-5.952717000	0.431526000	-4.096053000
H	-6.288573000	-0.026447000	-5.576941000	H	-6.403044000	-0.371455000	-5.449276000
H	-5.021922000	-0.939253000	-2.687681000	H	-5.307384000	-1.780813000	-2.769843000
H	-3.279764000	0.489115000	-3.631249000	H	-3.690941000	0.116027000	-3.090735000
H	-1.094180000	-1.219456000	-5.937144000	H	-1.235452000	-0.932306000	-5.628836000
H	-2.925245000	-1.585787000	-2.064838000	H	-2.991914000	-1.957831000	-1.846057000
H	-1.294260000	-3.318611000	-1.452170000	H	-1.222491000	-3.636484000	-1.472959000
H	0.479118000	-4.000029000	-3.063133000	H	0.580892000	-3.947266000	-3.163089000
H	0.570482000	-2.928806000	-5.311553000	H	0.568112000	-2.565441000	-5.239732000
H	-4.457005000	-1.496793000	-5.653786000	H	-4.300888000	-1.450582000	-5.654214000
H	-2.777462000	0.344050000	-5.310876000	H	-3.024393000	0.461751000	-4.681429000
H	-2.959291000	-0.351918000	0.795135000	H	-2.831159000	-0.730842000	0.875369000
N	-2.093720000	1.314772000	-1.118232000	N	-2.281687000	1.293569000	-0.786613000
O	-3.284186000	0.980980000	-1.224766000	O	-3.434622000	0.841693000	-0.881818000
O	-1.509321000	1.972340000	-1.976827000	O	-1.865191000	2.191533000	-1.518918000
O	1.219159000	-2.933753000	5.840660000	O	1.949243000	-3.245195000	5.643811000
H	0.905779000	-2.015705000	5.827405000	H	1.503214000	-2.405692000	5.401726000
H	0.994925000	-3.223586000	4.928169000	H	1.779912000	-3.760358000	4.836110000

### Int2

C	1.358708000	-2.987511000	1.705510000
C	1.033357000	-3.106646000	0.230884000
C	1.983251000	-2.326244000	-0.688370000
C	3.383596000	-2.259708000	-0.067287000
C	3.291488000	-1.379646000	1.181930000
C	2.273171000	-1.891549000	2.211805000
O	0.895373000	-3.783639000	2.506014000
C	1.476427000	-0.687075000	2.895692000
C	0.407126000	-0.172751000	1.942235000
C	-0.861729000	-0.775705000	1.934337000

### TS3

C	1.354032000	-3.054400000	1.758730000
C	1.694377000	-3.867216000	0.525110000
C	2.558835000	-3.107057000	-0.475139000
C	3.765263000	-2.540792000	0.262632000
C	3.320393000	-1.491678000	1.286247000
C	2.195295000	-1.948176000	2.205112000
O	0.388101000	-3.424624000	2.444564000
C	1.466345000	-0.728431000	2.857277000
C	0.380440000	-0.183186000	1.955182000
C	-0.905816000	-0.750675000	1.933977000

C	-1.842502000	-0.362453000	1.045192000	C	-1.862399000	-0.309332000	1.033077000
C	-1.545625000	0.670401000	0.148318000	C	-1.531824000	0.715833000	0.141704000
C	-0.302135000	1.307700000	0.138045000	C	-0.272499000	1.321648000	0.147161000
C	0.661636000	0.879328000	1.048734000	C	0.671539000	0.864574000	1.064457000
O	0.996755000	-1.049820000	4.123470000	O	0.957100000	-1.019824000	4.156280000
C	-0.867541000	-7.013866000	1.914729000	C	-0.928038000	-7.061866000	1.630401000
C	-1.785757000	-6.122786000	1.144447000	C	-1.844721000	-6.170457000	0.856417000
C	-2.026208000	-4.784993000	1.360491000	C	-2.065138000	-4.825710000	1.054774000
C	-2.615326000	-6.510994000	0.031967000	C	-2.693809000	-6.565106000	-0.237954000
N	-2.959655000	-4.318036000	0.454049000	N	-3.002763000	-4.360241000	0.151824000
C	-3.339952000	-5.352448000	-0.373740000	C	-3.405819000	-5.401840000	-0.655454000
C	-2.812123000	-7.717688000	-0.662448000	C	-2.917277000	-7.780965000	-0.907799000
C	-4.240701000	-5.378155000	-1.443792000	C	-4.323394000	-5.433620000	-1.710267000
C	-3.702153000	-7.743434000	-1.731626000	C	-3.823107000	-7.813028000	-1.962880000
C	-4.407770000	-6.583232000	-2.117600000	C	-4.518453000	-6.649895000	-2.357780000
C	2.413603000	-7.849988000	-2.032157000	C	2.371101000	-7.783742000	-2.324020000
C	0.901745000	-7.740822000	-1.773970000	C	0.953060000	-7.415216000	-1.856267000
C	3.063964000	-6.517459000	-2.424592000	C	3.278891000	-6.567324000	-2.537329000
C	0.070798000	-7.446241000	-3.026577000	C	0.099643000	-6.723647000	-2.923686000
N	7.580780000	-5.351716000	-1.330023000	N	7.407865000	-5.209992000	-1.740618000
C	6.630682000	-4.570723000	-0.523195000	C	6.600792000	-4.587533000	-0.678322000
C	7.415364000	-3.546015000	0.263577000	C	7.476778000	-3.591330000	0.044957000
O	7.475500000	-2.360538000	-0.028688000	O	7.390730000	-2.380140000	-0.094975000
C	5.836193000	-5.502243000	0.388619000	C	6.061758000	-5.662278000	0.261823000
N	8.113042000	-0.872704000	-2.711559000	N	8.169345000	-0.772297000	-2.770946000
C	7.152506000	0.222359000	-2.503923000	C	7.166397000	0.267373000	-2.489187000
C	7.623265000	1.130601000	-1.370051000	C	7.625612000	1.123037000	-1.311936000
O	7.613353000	2.361239000	-1.459803000	O	7.657478000	2.355903000	-1.362516000
C	5.694573000	-0.237681000	-2.238286000	C	5.727424000	-0.259503000	-2.234254000
C	4.749942000	0.945890000	-2.006526000	C	4.745989000	0.878574000	-1.930816000
C	5.183350000	-1.128677000	-3.375086000	C	5.225978000	-1.111249000	-3.404172000
N	7.981574000	0.500120000	-0.222297000	N	7.932619000	0.445466000	-0.174966000
C	8.175750000	1.237802000	1.012909000	C	8.175224000	1.153738000	1.066482000
C	9.569217000	1.863596000	1.035111000	C	9.583309000	1.750551000	1.069571000
O	10.291340000	1.874787000	2.009051000	O	10.269424000	1.854273000	2.064043000
C	7.955586000	0.352580000	2.240482000	C	7.961733000	0.273725000	2.294722000
C	6.644376000	-0.359341000	2.218988000	C	6.590455000	-0.302787000	2.377645000
N	6.404145000	-1.477899000	2.998417000	N	6.214042000	-1.149270000	3.408102000
C	5.503522000	-0.176090000	1.487621000	C	5.515427000	-0.256416000	1.537048000
C	5.181576000	-1.962759000	2.756971000	C	4.976101000	-1.616620000	3.205487000
N	4.610753000	-1.180892000	1.833595000	N	4.529443000	-1.078668000	2.063542000
C	6.646612000	5.117007000	0.680686000	C	6.673997000	5.052549000	0.859696000
C	5.502124000	4.480506000	-0.121460000	C	5.530344000	4.441011000	0.037321000
C	6.260559000	6.396427000	1.430602000	C	6.291965000	6.307899000	1.651150000
C	4.459521000	3.766047000	0.745298000	C	4.481895000	3.701810000	0.876380000
C	-3.694429000	2.779131000	7.377834000	C	-3.703312000	2.580577000	7.380401000
C	-2.479379000	1.843697000	7.364101000	C	-2.513601000	1.613168000	7.373292000
C	-2.870724000	0.433280000	7.820911000	C	-2.918789000	0.240617000	7.924135000
C	-1.830994000	1.812163000	5.972218000	C	-1.928739000	1.476481000	5.959389000
C	-2.922647000	9.360664000	1.984638000	C	-2.874462000	9.314205000	2.254298000
C	-2.868282000	8.007710000	1.339797000	C	-2.831349000	7.981443000	1.567180000
C	-3.486044000	7.638346000	0.170438000	C	-3.444521000	7.656383000	0.382128000
C	-2.173254000	6.832111000	1.817236000	C	-2.154256000	6.782925000	2.012495000
N	-3.208037000	6.312767000	-0.119178000	N	-3.181325000	6.336749000	0.053878000
C	-2.410428000	5.788013000	0.874560000	C	-2.397283000	5.771549000	1.036062000
C	-1.393256000	6.547545000	2.952820000	C	-1.386065000	6.453611000	3.144069000
C	-1.890751000	4.498269000	1.033488000	C	-1.894895000	4.470988000	1.158810000
C	-0.890308000	5.261178000	3.125048000	C	-0.899392000	5.156586000	3.279425000
C	-1.135741000	4.247101000	2.174786000	C	-1.150417000	4.175526000	2.296528000
N	2.052384000	7.283728000	-1.117652000	N	2.100119000	7.313830000	-0.878798000
C	1.954417000	5.858539000	-0.818871000	C	1.995932000	5.877555000	-0.640395000
C	1.008698000	4.993712000	-1.636598000	C	1.055242000	5.050837000	-1.502477000
O	1.110441000	3.756941000	-1.619272000	O	1.162044000	3.815125000	-1.548454000
C	1.580511000	5.737666000	0.670942000	C	1.608703000	5.694978000	0.839773000
O	2.515664000	6.440608000	1.471399000	O	2.538560000	6.360468000	1.677522000
N	0.036751000	5.629171000	-2.320840000	N	0.080173000	5.715168000	-2.154297000
C	-0.960989000	4.870066000	-3.042643000	C	-0.912583000	4.986452000	-2.913790000
C	-0.313871000	4.201113000	-4.256627000	C	-0.256418000	4.366025000	-4.147934000
O	-0.754314000	3.209818000	-4.799134000	O	-0.700845000	3.405259000	-4.739671000
C	-2.170413000	5.751277000	-3.439103000	C	-2.118153000	5.884284000	-3.284404000
C	-3.539552000	5.048928000	-3.323051000	C	-3.489128000	5.181222000	-3.201431000

C	-4.666049000	6.082789000	-3.451345000	C	-4.612475000	6.221696000	-3.301737000
C	-3.749307000	3.905742000	-4.322222000	C	-3.695771000	4.073165000	-4.239910000
N	2.424819000	2.377354000	-4.371073000	N	2.497837000	2.510808000	-4.344572000
C	2.029074000	0.965936000	-4.392854000	C	2.059471000	1.110837000	-4.380833000
C	1.313198000	0.685385000	-5.702033000	C	1.320194000	0.878131000	-5.686503000
O	1.441658000	-0.332207000	-6.358757000	O	1.463281000	-0.097327000	-6.401434000
C	1.052723000	0.667551000	-3.240959000	C	1.098493000	0.826228000	-3.213603000
C	-5.641243000	-2.435631000	4.880665000	C	-5.688819000	-2.556109000	4.725164000
C	-4.255427000	-3.053192000	4.696738000	C	-4.442094000	-3.429433000	4.634348000
C	-3.551157000	-3.234892000	6.046465000	C	-3.720920000	-3.524412000	5.984783000
N	-2.175229000	-3.715758000	5.925259000	N	-2.410902000	-4.169025000	5.870171000
C	-1.155045000	-2.972171000	5.476515000	C	-1.365601000	-3.588953000	5.267030000
N	0.041934000	-3.545728000	5.240162000	N	-0.274706000	-4.312487000	4.944246000
N	-1.260202000	-1.659864000	5.294797000	N	-1.365074000	-2.285211000	4.999565000
N	-7.497251000	2.106667000	0.821048000	N	-7.500267000	2.134234000	0.812463000
C	-7.240003000	2.015839000	-0.629322000	C	-7.224855000	2.093789000	-0.636792000
C	-7.037488000	0.567338000	-1.081810000	C	-7.031599000	0.659453000	-1.138960000
O	-6.960564000	0.270550000	-2.277485000	O	-6.943094000	0.401321000	-2.342657000
C	-5.971657000	2.880718000	-0.883075000	C	-5.941055000	2.948633000	-0.840920000
C	-5.379616000	3.075446000	0.520779000	C	-5.356573000	3.064112000	0.574562000
C	-6.626667000	3.146906000	1.400423000	C	-6.610138000	3.125763000	1.445867000
N	-6.959816000	-0.328111000	-0.071387000	N	-6.974230000	-0.270445000	-0.158346000
C	-6.929509000	-1.761093000	-0.271462000	C	-6.941664000	-1.695293000	-0.407890000
C	-8.248838000	-2.375025000	0.186436000	C	-8.278501000	-2.322825000	-0.026722000
O	-8.340477000	-3.451495000	0.737320000	O	-8.392663000	-3.420833000	0.475371000
C	-5.735221000	-2.417058000	0.411440000	C	-5.775028000	-2.378297000	0.296275000
O	-4.512404000	-2.075434000	-0.231104000	O	-4.529610000	-2.003532000	-0.279292000
H	2.790998000	-2.341519000	3.054782000	H	2.597975000	-2.518268000	3.308261000
H	1.053128000	-4.177007000	0.002720000	H	2.229270000	-4.763059000	0.871925000
H	-0.006148000	-2.792765000	0.095943000	H	0.748795000	-4.221946000	0.105526000
H	1.607966000	-1.307727000	-0.850484000	H	1.985886000	-2.296023000	-0.940046000
H	2.021984000	-2.800125000	-1.670641000	H	2.884433000	-3.768285000	-1.282426000
H	3.731324000	-3.264968000	0.197740000	H	4.283784000	-3.346005000	0.793302000
H	4.103937000	-1.836394000	-0.767183000	H	4.482672000	-2.092485000	-0.425873000
H	3.005329000	-0.379583000	0.849995000	H	3.028507000	-0.585802000	0.743382000
H	2.244430000	0.105508000	2.975605000	H	2.232211000	0.050557000	2.958467000
H	-1.075967000	-1.572531000	2.634828000	H	-1.150163000	-1.556351000	2.609014000
H	-0.093129000	2.116862000	-0.552821000	H	-0.035968000	2.129888000	-0.536054000
H	1.620777000	1.387499000	1.069578000	H	1.646424000	1.341381000	1.089832000
H	-0.134042000	-7.499487000	1.259237000	H	-0.228187000	-7.590380000	0.972321000
H	-0.315602000	-6.445965000	2.668790000	H	-0.337305000	-6.484236000	2.347681000
H	-1.578193000	-4.125660000	2.088787000	H	-1.586942000	-4.159642000	1.756729000
H	-3.301400000	-3.365583000	0.367337000	H	-3.345823000	-3.406218000	0.083925000
H	-2.270488000	-8.613531000	-0.371931000	H	-2.384269000	-8.679135000	-0.608068000
H	-4.783216000	-4.494146000	-1.750005000	H	-4.859522000	-4.549720000	-2.029438000
H	-3.857442000	-8.667803000	-2.280258000	H	-3.999790000	-8.744446000	-2.493072000
H	-5.090589000	-6.622137000	-2.960564000	H	-5.217191000	-6.698001000	-3.187611000
H	2.903456000	-8.230534000	-1.126873000	H	2.833171000	-8.443763000	-1.579137000
H	0.719967000	-6.958017000	-1.023988000	H	1.024866000	-6.768788000	-0.970618000
H	0.546326000	-8.677210000	-1.325251000	H	0.435090000	-8.324265000	-1.525497000
H	4.146822000	-6.621147000	-2.552448000	H	4.287296000	-6.863180000	-2.844955000
H	2.891702000	-5.757945000	-1.651663000	H	3.372546000	-5.992465000	-1.608913000
H	2.658927000	-6.129243000	-3.364960000	H	2.884411000	-5.893440000	-3.305034000
H	0.338527000	-6.487047000	-3.478891000	H	0.556743000	-5.793974000	-3.273311000
H	-0.995761000	-7.410567000	-2.786546000	H	-0.891631000	-6.479405000	-2.532091000
H	0.222597000	-8.223307000	-3.785180000	H	-0.032917000	-7.374679000	-3.795918000
H	8.230635000	-5.857501000	-0.730594000	H	8.207225000	-5.703981000	-1.347382000
H	8.133481000	-4.744022000	-1.930236000	H	7.770693000	-4.507924000	-2.381132000
H	5.965295000	-4.030339000	-1.204490000	H	5.784187000	-4.037699000	-1.153904000
H	8.017678000	-3.945282000	1.104844000	H	8.282678000	-4.028576000	0.668798000
H	5.311349000	-6.245112000	-0.216756000	H	5.479096000	-6.386238000	-0.312189000
H	5.102361000	-4.951618000	0.983339000	H	5.423017000	-5.232440000	1.038324000
H	6.503179000	-6.029042000	1.079961000	H	6.882504000	-6.193802000	0.755588000
H	7.884877000	-1.647457000	-2.090804000	H	8.013349000	-1.571083000	-2.159082000
H	8.007460000	-1.231520000	-3.655952000	H	8.030600000	-1.118292000	-3.716289000
H	7.163502000	0.854822000	-3.397271000	H	7.145074000	0.949963000	-3.344564000
H	5.737361000	-0.845236000	-1.325874000	H	5.800198000	-0.913204000	-1.357812000
H	4.677027000	1.569606000	-2.902606000	H	4.609642000	1.521607000	-2.806050000
H	5.080009000	1.595742000	-1.192893000	H	5.084665000	1.523383000	-1.115552000
H	3.741640000	0.594877000	-1.769502000	H	3.763279000	0.479591000	-1.660945000
H	5.804083000	-2.019358000	-3.502596000	H	5.871821000	-1.975282000	-3.582523000

H	5.174737000	-0.580860000	-4.324628000	H	5.181478000	-0.521799000	-4.327386000
H	4.160753000	-1.463776000	-3.173808000	H	4.218660000	-1.488036000	-3.198654000
H	8.011071000	-0.512703000	-0.180395000	H	7.938895000	-0.569566000	-0.157994000
H	7.472609000	2.082543000	1.010101000	H	7.493277000	2.015763000	1.095307000
H	9.872775000	2.313777000	0.071243000	H	9.932110000	2.092598000	0.077057000
H	8.043282000	0.973237000	3.136937000	H	8.186455000	0.870683000	3.182826000
H	8.759282000	-0.389192000	2.301800000	H	8.687489000	-0.548885000	2.285790000
H	7.051055000	-1.878675000	3.666048000	H	6.777437000	-1.374678000	4.218031000
H	5.253505000	0.566161000	0.751090000	H	5.377626000	0.259916000	0.605981000
H	4.737996000	-2.804338000	3.259337000	H	4.411859000	-2.272776000	3.868427000
H	7.037017000	4.377784000	1.394854000	H	7.064672000	4.291260000	1.550084000
H	5.931439000	3.768193000	-0.830269000	H	5.961600000	3.747332000	-0.688856000
H	5.013406000	5.263174000	-0.718139000	H	5.046559000	5.241463000	-0.539441000
H	5.949493000	7.176858000	0.726189000	H	5.977906000	7.110634000	0.973577000
H	7.100688000	6.786927000	2.014261000	H	7.135314000	6.678942000	2.242760000
H	5.422903000	6.227106000	2.114660000	H	5.457607000	6.117504000	2.333811000
H	3.675947000	3.313966000	0.126415000	H	3.693900000	3.284297000	0.238954000
H	3.974044000	4.457219000	1.438694000	H	4.002821000	4.368806000	1.597490000
H	4.926798000	2.965659000	1.332708000	H	4.940164000	2.870530000	1.426641000
H	-3.416107000	3.796063000	7.081429000	H	-3.412142000	3.571357000	7.015383000
H	-4.461321000	2.425148000	6.677780000	H	-4.506395000	2.208256000	6.732368000
H	-1.737892000	2.236242000	8.073811000	H	-1.732635000	2.026061000	8.026585000
H	-3.620406000	0.008406000	7.139928000	H	-3.699167000	-0.204790000	7.294289000
H	-3.312115000	0.443048000	8.822892000	H	-3.316498000	0.314632000	8.941789000
H	-2.004087000	-0.236336000	7.843373000	H	-2.066837000	-0.448546000	7.945212000
H	-0.925841000	1.195073000	5.965780000	H	-1.044278000	0.829734000	5.953193000
H	-1.553905000	2.817070000	5.635287000	H	-1.638580000	2.449134000	5.546197000
H	-2.528107000	1.401107000	5.229843000	H	-2.671018000	1.039688000	5.277956000
H	-3.541118000	10.047075000	1.400157000	H	-3.480275000	10.026088000	1.687286000
H	-3.342812000	9.308131000	2.996348000	H	-3.302822000	9.234879000	3.260738000
H	-4.110402000	8.223275000	-0.489877000	H	-4.056756000	8.269065000	-0.264235000
H	-3.604350000	5.791370000	-0.883331000	H	-3.571111000	5.846196000	-0.733723000
H	-1.192562000	7.320764000	3.688951000	H	-1.181438000	7.201184000	3.905219000
H	-2.072584000	3.729177000	0.291561000	H	-2.080504000	3.727044000	0.392538000
H	-0.289774000	5.032063000	4.000340000	H	-0.308007000	4.893047000	4.151261000
H	-0.718978000	3.256553000	2.328613000	H	-0.746313000	3.175742000	2.421706000
H	2.398611000	7.469113000	-2.053058000	H	2.454014000	7.535726000	-1.803373000
H	1.172318000	7.775495000	-0.984558000	H	1.219460000	7.801447000	-0.734633000
H	2.946306000	5.421299000	-0.955116000	H	2.987481000	5.442865000	-0.786931000
H	0.562028000	6.127253000	0.814667000	H	0.590100000	6.081267000	0.991053000
H	1.581850000	4.689980000	0.974601000	H	1.604555000	4.635274000	1.098857000
H	2.752168000	7.221606000	0.941544000	H	2.782816000	7.161745000	1.182617000
H	0.035159000	6.637404000	-2.366407000	H	0.074096000	6.724397000	-2.150963000
H	-1.303756000	4.061011000	-2.390082000	H	-1.261478000	4.152639000	-2.297432000
H	0.605674000	4.699080000	-4.624042000	H	0.672365000	4.870668000	-4.482391000
H	-2.044731000	6.151858000	-4.452606000	H	-1.985790000	6.321870000	-4.281602000
H	-2.173388000	6.614432000	-2.764216000	H	-2.123833000	6.722130000	-2.578374000
H	-3.586917000	4.591506000	-2.323064000	H	-3.544354000	4.690899000	-2.217601000
H	-4.661163000	6.531065000	-4.451218000	H	-4.599951000	6.703944000	-4.285620000
H	-4.565342000	6.899393000	-2.727956000	H	-4.514712000	7.012793000	-2.550111000
H	-5.643253000	5.614290000	-3.299484000	H	-5.591761000	5.750746000	-3.172382000
H	-3.687710000	4.276986000	-5.352012000	H	-3.628475000	4.479099000	-5.256150000
H	-4.741319000	3.464129000	-4.181256000	H	-4.689523000	3.629524000	-4.118675000
H	-3.001034000	3.122159000	-4.203458000	H	-2.949863000	3.284156000	-4.144396000
H	3.380486000	2.494492000	-4.690514000	H	3.460072000	2.601872000	-4.652477000
H	2.350702000	2.761876000	-3.432834000	H	2.424295000	2.888528000	-3.403737000
H	2.877354000	0.273365000	-4.324748000	H	2.890396000	0.395091000	-4.341398000
H	0.629500000	1.501908000	-6.011436000	H	0.612151000	1.692858000	-5.939842000
H	0.142581000	1.265136000	-3.335568000	H	0.208418000	1.456601000	-3.278561000
H	1.525761000	0.927097000	-2.289688000	H	1.603581000	1.056395000	-2.271779000
H	0.780637000	-0.388575000	-3.225967000	H	0.792078000	-0.219838000	-3.204133000
H	-5.572803000	-1.440144000	5.332306000	H	-5.428925000	-1.527754000	5.000577000
H	-6.156065000	-2.332891000	3.920863000	H	-6.214873000	-2.523896000	3.766810000
H	-3.646370000	-2.416321000	4.044912000	H	-3.757441000	-3.019852000	3.882650000
H	-4.328711000	-4.027669000	4.201070000	H	-4.700843000	-4.440954000	4.302259000
H	-3.553321000	-2.300444000	6.618158000	H	-3.594337000	-2.536230000	6.437586000
H	-4.084872000	-3.964591000	6.658663000	H	-4.301759000	-4.110897000	6.698982000
H	-2.015166000	-4.706924000	6.019181000	H	-2.394223000	-5.176404000	5.930789000
H	0.048949000	-4.531225000	5.023452000	H	-0.367565000	-5.317641000	4.973545000
H	0.671781000	-2.980904000	4.667206000	H	0.227811000	-3.956854000	4.123276000
H	-0.457145000	-1.186402000	4.805879000	H	-0.522069000	-1.821076000	4.627978000

H	-2.109221000	-1.169316000	5.515864000	H	-2.127855000	-1.701407000	5.298177000
H	-8.477890000	2.275869000	1.016180000	H	-8.478817000	2.320833000	1.001745000
H	-8.076466000	2.388396000	-1.231496000	H	-8.048091000	2.499125000	-1.235776000
H	-5.278970000	2.405032000	-1.578276000	H	-5.251687000	2.496220000	-1.554734000
H	-6.270712000	3.845351000	-1.303829000	H	-6.221499000	3.937877000	-1.215039000
H	-4.757236000	3.968024000	0.604803000	H	-4.713100000	3.936051000	0.704702000
H	-4.775449000	2.207130000	0.800462000	H	-4.776057000	2.168973000	0.818104000
H	-6.424309000	2.934023000	2.454730000	H	-6.423020000	2.860739000	2.491138000
H	-7.076701000	4.149224000	1.336876000	H	-7.035413000	4.140494000	1.423841000
H	-7.105403000	0.090187000	0.848487000	H	-7.134230000	0.116698000	0.772793000
H	-6.870982000	-1.916942000	-1.356720000	H	-6.840307000	-1.812661000	-1.495096000
H	-9.138476000	-1.747473000	-0.027069000	H	-9.158386000	-1.683912000	-0.247084000
H	-5.833673000	-3.501466000	0.350388000	H	-5.864368000	-3.459320000	0.181783000
H	-5.712829000	-2.137919000	1.472817000	H	-5.797297000	-2.147137000	1.369003000
H	-4.410356000	-1.109324000	-0.280634000	H	-4.432578000	-1.035960000	-0.297063000
H	-4.148229000	2.828215000	8.373430000	H	-4.115335000	2.698146000	8.388434000
H	-6.268809000	-3.055611000	5.529814000	H	-6.389677000	-2.936200000	5.476002000
H	-1.924367000	9.805097000	2.078403000	H	-1.871664000	9.743143000	2.369119000
H	7.476409000	5.341038000	-0.001279000	H	7.503931000	5.296999000	0.184775000
H	2.594514000	-8.595504000	-2.817991000	H	2.306008000	-8.365553000	-3.253296000
H	-1.413008000	-7.816487000	2.426841000	H	-1.478618000	-7.829130000	2.189404000
N	-5.634847000	-0.620824000	-4.778254000	N	-5.694207000	-0.514050000	-4.900231000
C	-4.549922000	-1.580753000	-4.529589000	C	-4.535387000	-1.384427000	-4.643461000
C	-5.099655000	-2.720764000	-3.700566000	C	-4.982017000	-2.514695000	-3.742850000
O	-5.399114000	-3.818574000	-4.135925000	O	-5.351685000	-3.603391000	-4.149965000
C	-3.376050000	-0.873972000	-3.829987000	C	-3.397653000	-0.555040000	-4.025600000
C	-2.182576000	-1.783819000	-3.653881000	C	-2.157995000	-1.374590000	-3.747019000
C	-1.145491000	-1.792143000	-4.594982000	C	-1.189299000	-1.566835000	-4.740931000
C	-2.117960000	-2.681684000	-2.578601000	C	-1.966185000	-1.987815000	-2.500743000
C	-0.066317000	-2.668561000	-4.465160000	C	-0.056566000	-2.344546000	-4.496251000
C	-1.056664000	-3.580630000	-2.459135000	C	-0.838623000	-2.772604000	-2.252264000
C	-0.022967000	-3.570515000	-3.399362000	C	0.123728000	-2.948160000	-3.249161000
H	-6.014318000	-0.274910000	-3.895025000	H	-6.059727000	-0.146233000	-4.020130000
H	-6.399259000	-1.085660000	-5.263749000	H	-6.442737000	-1.058759000	-5.323488000
H	-5.290146000	-2.454628000	-2.640788000	H	-5.027157000	-2.264816000	-2.663738000
H	-3.722876000	-0.498171000	-2.861416000	H	-3.762133000	-0.094804000	-3.100915000
H	-1.171763000	-1.095640000	-5.427967000	H	-1.310137000	-1.085642000	-5.707393000
H	-2.904278000	-2.675830000	-1.833010000	H	-2.707103000	-1.855869000	-1.722225000
H	-1.042029000	-4.284852000	-1.633989000	H	-0.724025000	-3.246500000	-1.282679000
H	0.812444000	-4.256112000	-3.298022000	H	1.012222000	-3.539179000	-3.054230000
H	0.743536000	-2.625471000	-5.186231000	H	0.699343000	-2.444411000	-5.267970000
H	-4.216274000	-1.993258000	-5.488230000	H	-4.207685000	-1.822379000	-5.592868000
H	-3.112750000	-0.000650000	-4.434517000	H	-3.171923000	0.260377000	-4.719701000
H	-2.812906000	-0.836661000	1.039884000	H	-2.841521000	-0.764912000	1.015309000
N	-2.566465000	1.108174000	-0.785313000	N	-2.531870000	1.172488000	-0.803556000
O	-3.676247000	0.549630000	-0.765299000	O	-3.639057000	0.607502000	-0.824350000
O	-2.310051000	2.026421000	-1.565921000	O	-2.261507000	2.108952000	-1.556790000
O	3.153431000	-2.108679000	5.245028000	O	2.759807000	-2.771149000	4.610217000
H	3.214265000	-1.963036000	6.197375000	H	2.416038000	-3.656356000	4.791723000
H	2.320833000	-1.639714000	4.953910000	H	1.615968000	-1.672208000	4.557579000

TS4

C	1.665950000	-3.181607000	2.110894000
C	2.168866000	-4.204363000	1.108976000
C	2.445554000	-3.610904000	-0.268424000
C	3.371706000	-2.400974000	-0.142633000
C	2.850663000	-1.425495000	0.895907000
C	1.928491000	-1.822871000	1.896635000
O	1.024600000	-3.645802000	3.114869000
C	1.344087000	-0.650567000	2.701030000
C	0.240103000	-0.051546000	1.858177000
C	-1.039794000	-0.627797000	1.869238000
C	-2.016272000	-0.189983000	0.991440000
C	-1.699715000	0.828228000	0.084352000
C	-0.447697000	1.446918000	0.069758000
C	0.511493000	1.004964000	0.975712000
O	0.826827000	-0.958727000	3.986526000
C	-0.842639000	-7.113312000	1.457491000
C	-1.703661000	-6.093557000	0.792538000

P

C	2.643969000	-2.602341000	2.464843000
C	3.065423000	-3.825158000	1.683479000
C	2.806847000	-3.759994000	0.182517000
C	3.254508000	-2.402572000	-0.361716000
C	2.636544000	-1.298463000	0.430763000
C	2.299895000	-1.376941000	1.739426000
O	2.632818000	-2.686445000	3.702477000
C	1.610579000	-0.156762000	2.392314000
C	0.389497000	0.183576000	1.563787000
C	-0.746791000	-0.633727000	1.670492000
C	-1.859774000	-0.401020000	0.882600000
C	-1.816626000	0.650897000	-0.037796000
C	-0.705562000	1.482703000	-0.164812000
C	0.395349000	1.245706000	0.655413000
O	1.166970000	-0.345190000	3.730983000
C	-0.019792000	-7.189111000	1.685935000
C	-0.984715000	-6.247654000	1.045159000

C	-1.833182000	-4.753650000	1.086758000	C	-1.352158000	-4.989598000	1.469228000
C	-2.605093000	-6.363616000	-0.296073000	C	-1.752550000	-6.517031000	-0.143234000
N	-2.767810000	-4.176703000	0.243700000	N	-2.310321000	-4.464853000	0.619321000
C	-3.257359000	-5.138991000	-0.612583000	C	-2.576806000	-5.380377000	-0.374303000
C	-2.911191000	-7.519099000	-1.036809000	C	-1.823128000	-7.605162000	-1.031629000
C	-4.198074000	-5.051510000	-1.643735000	C	-3.462975000	-5.315511000	-1.452988000
C	-3.841838000	-7.431333000	-2.065963000	C	-2.695159000	-7.537015000	-2.113287000
C	-4.478228000	-6.207216000	-2.364281000	C	-3.509220000	-6.401545000	-2.319045000
C	2.468109000	-7.710288000	-2.507734000	C	3.261318000	-7.486195000	-2.337688000
C	1.136551000	-7.172337000	-1.958824000	C	1.790704000	-7.111548000	-2.091234000
C	3.338002000	-6.644701000	-3.183171000	C	4.105357000	-6.337915000	-2.903906000
C	0.164822000	-6.675419000	-3.033209000	C	1.011262000	-6.750130000	-3.358994000
N	7.653258000	-5.252880000	-1.589012000	N	7.828253000	-4.423093000	-1.854702000
C	6.668432000	-4.520193000	-0.777220000	C	7.064399000	-3.750777000	-0.789647000
C	7.421231000	-3.535100000	0.088211000	C	7.969199000	-2.723822000	-0.141167000
O	7.491748000	-2.338203000	-0.145277000	O	7.973447000	-1.536634000	-0.426978000
C	5.847954000	-5.499971000	0.056368000	C	6.554411000	-4.778461000	0.212812000
N	8.173023000	-0.684274000	-2.741898000	N	8.063753000	0.251254000	-2.996134000
C	7.195784000	0.382263000	-2.467546000	C	6.943286000	1.127980000	-2.620671000
C	7.652471000	1.216423000	-1.273330000	C	7.368883000	2.034208000	-1.460429000
O	7.655004000	2.451394000	-1.293261000	O	7.324191000	3.268430000	-1.525797000
C	5.737626000	-0.114610000	-2.253394000	C	5.615452000	0.397719000	-2.269577000
C	4.773424000	1.040471000	-1.959642000	C	4.522597000	1.389171000	-1.852282000
C	5.255410000	-0.926729000	-3.460429000	C	5.148462000	-0.474408000	-3.439109000
N	7.996060000	0.518940000	-0.161152000	N	7.759073000	1.406060000	-0.324360000
C	8.191971000	1.189463000	1.110398000	C	7.901358000	2.156443000	0.910685000
C	9.583511000	1.817311000	1.167868000	C	8.969623000	3.230500000	0.770560000
O	10.238112000	1.921605000	2.183603000	O	8.999413000	4.227216000	1.461639000
C	7.960929000	0.249845000	2.294074000	C	8.274037000	1.207624000	2.066103000
C	6.576206000	-0.304567000	2.317085000	C	7.329809000	0.049145000	2.207352000
N	6.134180000	-1.188645000	3.286194000	N	7.722054000	-1.127793000	2.813621000
C	5.517857000	-0.163905000	1.453823000	C	6.028861000	-0.184510000	1.806508000
C	4.863647000	-1.562455000	3.003495000	C	6.680336000	-2.004419000	2.755896000
N	4.480038000	-0.948890000	1.895365000	N	5.635634000	-1.464438000	2.150463000
C	6.658452000	5.079547000	0.996737000	C	5.892980000	5.821286000	0.729554000
C	5.524242000	4.491418000	0.144396000	C	4.833331000	5.043482000	-0.062435000
C	6.264695000	6.311884000	1.818113000	C	5.364935000	7.018604000	1.526918000
C	4.473558000	3.721680000	0.952499000	C	3.907282000	4.184760000	0.805068000
C	-3.983321000	1.713088000	7.696370000	C	-4.087694000	0.964432000	7.795494000
C	-2.509418000	1.404787000	7.408712000	C	-2.617915000	1.226166000	7.446510000
C	-2.348260000	-0.014578000	6.841085000	C	-2.001757000	0.011204000	6.740571000
C	-1.905673000	2.441179000	6.450485000	C	-2.469383000	2.484670000	6.580448000
C	-2.927505000	9.225691000	2.479295000	C	-4.104015000	8.787977000	2.322943000
C	-2.881501000	7.916540000	1.750890000	C	-3.924546000	7.483660000	1.606799000
C	-3.475725000	7.630334000	0.546373000	C	-4.502707000	7.117566000	0.416111000
C	-2.219752000	6.702332000	2.173503000	C	-3.125793000	6.355832000	2.031624000
N	-3.212660000	6.319525000	0.183583000	N	-4.101278000	5.839441000	0.062766000
C	-2.452083000	5.721150000	1.164947000	C	-3.264338000	5.341985000	1.038491000
C	-1.475312000	6.336702000	3.309752000	C	-2.328776000	6.088953000	3.159602000
C	-1.963284000	4.413915000	1.262333000	C	-2.632798000	4.098332000	1.143374000
C	-1.002713000	5.032195000	3.419433000	C	-1.715040000	4.845249000	3.277574000
C	-1.244080000	4.080440000	2.405762000	C	-1.865356000	3.859408000	2.279052000
N	2.068991000	7.343930000	-0.693891000	N	0.996326000	7.454416000	-0.863450000
C	1.975807000	5.901821000	-0.490436000	C	1.116165000	6.012776000	-0.670320000
C	1.050697000	5.086544000	-1.379976000	C	0.308190000	5.080790000	-1.557477000
O	1.162185000	3.851955000	-1.446126000	O	0.612781000	3.880801000	-1.658564000
C	1.571202000	5.679808000	0.980554000	C	0.757035000	5.726932000	0.801970000
O	2.481818000	6.337576000	1.845109000	O	1.566977000	6.506697000	1.664544000
N	0.080070000	5.758362000	-2.028867000	N	-0.778741000	5.595758000	-2.160523000
C	-0.921916000	5.042719000	-2.789658000	C	-1.696478000	4.734166000	-2.878599000
C	-0.276613000	4.419927000	-4.027127000	C	-0.989609000	4.140941000	-4.095185000
O	-0.718102000	3.448532000	-4.604124000	O	-1.310272000	3.095329000	-4.620183000
C	-2.107808000	5.968353000	-3.157503000	C	-2.973900000	5.513976000	-3.277914000
C	-3.493053000	5.289464000	-3.129646000	C	-4.279219000	4.693185000	-3.237115000
C	-4.593275000	6.357060000	-3.200380000	C	-5.484263000	5.637796000	-3.341967000
C	-3.702471000	4.237475000	-4.224376000	C	-4.367516000	3.596860000	-4.304513000
N	2.482289000	2.639435000	-4.280704000	N	1.978059000	2.723797000	-4.355785000
C	2.084889000	1.229080000	-4.346525000	C	1.730993000	1.279319000	-4.402905000
C	1.362143000	0.997541000	-5.661238000	C	1.004187000	0.937075000	-5.691574000
O	1.529212000	0.033162000	-6.385730000	O	1.202102000	-0.068127000	-6.349798000
C	1.117240000	0.894241000	-3.197309000	C	0.842148000	0.832955000	-3.228608000

C	-5.645748000	-2.724671000	4.653760000	C	-5.268595000	-3.338885000	4.874914000
C	-4.495188000	-3.704710000	4.444485000	C	-3.862717000	-3.791993000	4.467228000
C	-3.722837000	-3.936123000	5.747220000	C	-2.924402000	-3.815157000	5.679515000
N	-2.552308000	-4.797463000	5.567991000	N	-1.598160000	-4.373427000	5.401160000
C	-1.446450000	-4.419993000	4.912397000	C	-0.528606000	-3.703693000	4.956641000
N	-0.548628000	-5.337263000	4.526873000	N	0.613302000	-4.363610000	4.729303000
N	-1.203848000	-3.131663000	4.664355000	N	-0.588460000	-2.391805000	4.718053000
N	-7.514933000	2.037129000	0.850395000	N	-7.823994000	1.020738000	0.984386000
C	-7.212916000	2.042275000	-0.595056000	C	-7.520237000	1.042000000	-0.460677000
C	-6.974291000	0.627471000	-1.132838000	C	-7.091846000	-0.339241000	-0.975411000
O	-6.823600000	0.409084000	-2.337947000	O	-6.885000000	-0.559406000	-2.171962000
C	-5.964614000	2.952024000	-0.758777000	C	-6.401447000	2.102392000	-0.639645000
C	-5.393718000	3.034542000	0.664512000	C	-5.823378000	2.247696000	0.775364000
C	-6.655147000	3.027800000	1.526942000	C	-7.063659000	2.094817000	1.655661000
N	-6.964105000	-0.331183000	-0.179180000	N	-6.982139000	-1.270433000	-0.000030000
C	-6.898236000	-1.748812000	-0.458401000	C	-6.732635000	-2.675256000	-0.231374000
C	-8.231464000	-2.411948000	-0.129054000	C	-7.982741000	-3.488497000	0.086776000
O	-8.335599000	-3.525801000	0.339149000	O	-7.962560000	-4.581948000	0.611115000
C	-5.736625000	-2.416579000	0.270025000	C	-5.528810000	-3.162922000	0.572758000
O	-4.487178000	-1.987750000	-0.257789000	O	-4.333932000	-2.516317000	0.149987000
H	2.090289000	-3.296885000	4.505996000	H	4.139804000	-3.913904000	1.883477000
H	3.076038000	-4.662519000	1.527570000	H	2.586307000	-4.692165000	2.149363000
H	1.414262000	-4.994891000	1.059537000	H	1.736263000	-3.890689000	-0.013683000
H	1.499967000	-3.301330000	-0.723333000	H	3.329279000	-4.575552000	-0.323232000
H	2.893485000	-4.357222000	-0.930610000	H	4.347469000	-2.301629000	-0.290739000
H	4.373130000	-2.731853000	0.144032000	H	2.993464000	-2.286314000	-1.417480000
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H	2.768797000	-0.400026000	0.549655000	H	2.310180000	0.684755000	2.362953000
H	2.142413000	0.096326000	2.804148000	H	-0.755558000	-1.463680000	2.364702000
H	-1.262504000	-1.431545000	2.558996000	H	-0.676842000	2.288205000	-0.886002000
H	-0.221463000	2.247610000	-0.624467000	H	1.263782000	1.890888000	0.566960000
H	1.483963000	1.486432000	0.985723000	H	0.788575000	-7.469047000	0.999234000
H	-0.316447000	-7.730000000	0.720653000	H	0.439121000	-6.743838000	2.573969000
H	-0.082380000	-6.647495000	2.089812000	H	-1.000516000	-4.423767000	2.318994000
H	-1.319523000	-4.160124000	1.829486000	H	-2.788417000	-3.575151000	0.703889000
H	-3.104507000	-3.219979000	0.262788000	H	-1.202651000	-8.483082000	-0.876069000
H	-2.421152000	-8.462185000	-0.811462000	H	-4.088732000	-4.450803000	-1.606766000
H	-4.683693000	-4.118435000	-1.884520000	H	-2.754436000	-8.368222000	-2.809720000
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H	-5.193241000	-6.152425000	-3.178735000	H	3.703199000	-7.822213000	-1.390934000
H	3.034311000	-8.162749000	-1.683657000	H	1.745446000	-6.270830000	-1.385459000
H	1.340993000	-6.360175000	-1.247746000	H	1.288328000	-7.949950000	-1.592855000
H	0.646904000	-7.965672000	-1.380225000	H	5.161757000	-6.615442000	-2.980377000
H	4.288341000	-7.066365000	-3.526506000	H	4.044350000	-5.451350000	-2.261716000
H	3.570892000	-5.829994000	-2.487571000	H	3.767943000	-6.040546000	-3.901803000
H	2.839345000	-6.202588000	-4.051525000	H	1.420461000	-5.861615000	-3.849270000
H	0.583424000	-5.845247000	-3.609130000	H	-0.037966000	-6.547438000	-3.125738000
H	-0.769640000	-6.328696000	-2.583218000	H	1.042098000	-7.573218000	-4.083021000
H	-0.079881000	-7.479075000	-3.737871000	H	8.630469000	-4.912830000	-1.461184000
H	8.288956000	-5.778958000	-0.991528000	H	8.190611000	-3.740954000	-2.517433000
H	8.219344000	-4.608899000	-2.136935000	H	6.232654000	-3.214943000	-1.258807000
H	6.025118000	-3.948449000	-1.454455000	H	8.722771000	-3.130095000	0.564285000
H	7.992678000	-3.976463000	0.930041000	H	5.931569000	-5.517044000	-0.297620000
H	5.341112000	-6.209026000	-0.602817000	H	5.968561000	-4.295485000	0.996697000
H	5.097821000	-4.978250000	0.655627000	H	7.389603000	-5.303070000	0.689932000
H	6.492857000	-6.063483000	0.739343000	H	8.093945000	-0.546284000	-2.362344000
H	7.961703000	-1.493532000	-2.159837000	H	7.883433000	-0.133055000	-3.919660000
H	8.058758000	-0.996540000	-3.701918000	H	6.755442000	1.808776000	-3.457181000
H	7.205944000	1.073720000	-3.316126000	H	5.827167000	-0.263474000	-1.418944000
H	5.761394000	-0.787722000	-1.387206000	H	4.304133000	2.101385000	-2.655865000
H	4.687381000	1.708390000	-2.822517000	H	4.802376000	1.963635000	-0.965295000
H	5.091540000	1.653696000	-1.113312000	H	3.592403000	0.860685000	-1.625467000
H	3.772639000	0.657647000	-1.738682000	H	5.883420000	-1.244706000	-3.689248000
H	5.881309000	-1.806091000	-3.634183000	H	4.974486000	0.133088000	-4.335505000
H	5.264780000	-0.316177000	-4.371264000	H	4.210319000	-0.980707000	-3.190690000
H	4.229956000	-1.277385000	-3.304913000	H	7.774783000	0.393222000	-0.278782000
H	7.984404000	-0.495232000	-0.163801000	H	6.961817000	2.669326000	1.152223000
H	7.489557000	2.034678000	1.156081000	H	9.756076000	3.006883000	0.020985000
H	9.953134000	2.187219000	0.192153000	H	8.308919000	1.804577000	2.984018000
H	8.179963000	0.802640000	3.212179000	H	9.287181000	0.819755000	1.902782000
H	8.684622000	-0.573928000	2.250148000	H	8.629788000	-1.311614000	3.217850000

H	6.667704000	-1.501491000	4.086142000	H	5.365523000	0.481511000	1.273476000
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H	4.261566000	-2.220607000	3.614841000	H	6.418589000	5.131463000	1.402863000
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H	5.964093000	3.823766000	-0.600798000	H	4.236634000	5.755967000	-0.649239000
H	5.041577000	5.308634000	-0.409724000	H	4.910231000	7.760302000	0.859357000
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H	7.098564000	6.665543000	2.433378000	H	4.596620000	6.719914000	2.247939000
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H	3.692487000	3.318301000	0.297715000	H	3.349653000	4.793534000	1.521543000
H	3.985253000	4.364185000	1.689630000	H	4.483504000	3.435087000	1.361780000
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H	-1.991952000	3.456054000	6.853442000	H	-2.994477000	2.363242000	5.624867000
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H	-3.603708000	5.850161000	-0.616472000	H	-2.202298000	6.841278000	3.932960000
H	-1.279925000	7.061584000	4.094911000	H	-2.744553000	3.354771000	0.364300000
H	-2.143268000	3.694222000	0.472816000	H	-1.105227000	4.627198000	4.149196000
H	-0.433914000	4.738258000	4.296509000	H	-1.368396000	2.901286000	2.392859000
H	-0.854310000	3.073260000	2.512846000	H	1.306322000	7.756085000	-1.781254000
H	2.436569000	7.590634000	-1.606758000	H	0.051641000	7.795516000	-0.704228000
H	1.181507000	7.820061000	-0.553768000	H	2.162615000	5.739720000	-0.824524000
H	2.973306000	5.480371000	-0.633761000	H	-0.310883000	5.941733000	0.955759000
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H	1.578064000	4.614298000	1.214830000	H	1.679923000	7.351751000	1.195448000
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H	-1.289074000	4.213868000	-2.177339000	H	-0.154193000	4.752152000	-4.489922000
H	0.640302000	4.932622000	-4.380182000	H	-2.853069000	5.971929000	-4.267646000
H	-1.944646000	6.437937000	-4.135606000	H	-3.075650000	6.341441000	-2.566619000
H	-2.116079000	6.781490000	-2.423025000	H	-4.315624000	4.180011000	-2.264475000
H	-3.577412000	4.754705000	-2.171654000	H	-5.493396000	6.140967000	-4.315468000
H	-4.554909000	6.883166000	-4.160935000	H	-5.468066000	6.417378000	-2.572248000
H	-4.492067000	7.111160000	-2.412115000	H	-6.422235000	5.083006000	-3.242483000
H	-5.583707000	5.900993000	-3.107565000	H	-4.301151000	4.031046000	-5.309291000
H	-3.597115000	4.688711000	-5.218180000	H	-5.327364000	3.075609000	-4.225758000
H	-4.711155000	3.817735000	-4.149923000	H	-3.566902000	2.865080000	-4.199641000
H	-2.981740000	3.423815000	-4.145626000	H	2.932113000	2.936580000	-4.627036000
H	3.433940000	2.765911000	-4.608989000	H	1.823429000	3.088434000	-3.419244000
H	2.423659000	2.987045000	-3.327302000	H	2.654460000	0.686805000	-4.382644000
H	2.934046000	0.535349000	-4.309337000	H	0.239050000	1.687389000	-5.977584000
H	0.638061000	1.800150000	-5.909462000	H	-0.130845000	1.328488000	-3.266971000
H	0.200788000	1.484142000	-3.275656000	H	1.324357000	1.110592000	-2.287882000
H	1.591737000	1.139578000	-2.243321000	H	0.689368000	-0.247184000	-3.244127000
H	0.858150000	-0.164912000	-3.201658000	H	-5.252048000	-2.326666000	5.293112000
H	-5.274705000	-1.744468000	4.972667000	H	-5.942590000	-3.334198000	4.013786000
H	-6.213641000	-2.582977000	3.729644000	H	-3.457994000	-3.129447000	3.692868000
H	-3.813664000	-3.323609000	3.675372000	H	-3.899316000	-4.797044000	4.032180000
H	-4.870714000	-4.668718000	4.083274000	H	-2.808674000	-2.815876000	6.109662000
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H	-2.692481000	-5.790193000	5.683311000	H	0.701271000	-5.332561000	4.989074000
H	-0.820360000	-6.306858000	4.496981000	H	1.452746000	-3.862565000	4.440301000
H	0.202620000	-5.019538000	3.908492000	H	0.212090000	-1.840302000	4.399094000
H	-0.360420000	-2.864626000	4.151983000	H	-1.440806000	-1.885044000	4.887022000
H	-1.783649000	-2.409860000	5.057264000	H	-8.818856000	1.100332000	1.152047000
H	-8.499657000	2.203919000	1.025438000	H	-8.394996000	1.308814000	-1.064573000
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H	-6.282284000	3.944573000	-1.092610000	H	-5.310661000	3.197633000	0.936158000
H	-4.777102000	3.919540000	0.831103000	H	-5.116819000	1.437662000	0.982461000
H	-4.790491000	2.148450000	0.884348000	H	-6.827364000	1.811865000	2.686180000



H	-6.467273000	2.729115000	2.562977000	H	-7.624452000	3.040530000	1.683800000
H	-7.108723000	4.030136000	1.539570000	H	-7.241219000	-0.911418000	0.921258000
H	-7.152040000	0.031947000	0.756786000	H	-6.553660000	-2.802904000	-1.304514000
H	-6.764312000	-1.842302000	-1.543992000	H	-8.932521000	-2.995040000	-0.205810000
H	-9.118299000	-1.785557000	-0.357117000	H	-5.388709000	-4.233196000	0.418907000
H	-5.789929000	-3.496988000	0.134085000	H	-5.707287000	-2.992173000	1.642249000
H	-5.801315000	-2.204191000	1.345051000	H	-4.492798000	-1.562259000	0.060527000
H	-4.468704000	-1.018123000	-0.333201000	H	-4.194525000	0.079506000	8.432126000
H	-4.412269000	0.990012000	8.398469000	H	-5.693850000	-4.008812000	5.629447000
H	-6.341332000	-3.084993000	5.419288000	H	-3.150874000	9.315865000	2.448464000
H	-1.924030000	9.643495000	2.625591000	H	6.657251000	6.180434000	0.028213000
H	7.496183000	5.343831000	0.339145000	H	3.306259000	-8.345116000	-3.020732000
H	2.261716000	-8.520373000	-3.220249000	H	-0.510274000	-8.120264000	1.994779000
H	-1.427107000	-7.798301000	2.085142000	N	-5.597436000	-1.107290000	-4.875749000
N	-5.625861000	-0.417038000	-4.948798000	C	-4.466186000	-1.954306000	-4.445969000
C	-4.488395000	-1.314017000	-4.681160000	C	-4.959455000	-2.841188000	-3.310800000
C	-4.977863000	-2.429387000	-3.788717000	O	-5.587877000	-3.874242000	-3.470753000
O	-5.373070000	-3.508771000	-4.194626000	C	-3.300122000	-1.046729000	-4.017013000
C	-3.341098000	-0.509871000	-4.048687000	C	-2.035832000	-1.779564000	-3.621294000
C	-2.111925000	-1.346005000	-3.773811000	C	-1.042394000	-2.043046000	-4.575340000
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C	0.006578000	-2.285656000	-4.515885000	C	-0.643786000	-2.870409000	-1.944918000
C	-0.831047000	-2.813707000	-2.313343000	C	0.337057000	-3.124501000	-2.905239000
C	0.154788000	-2.946962000	-3.294113000	H	-5.985076000	-0.636537000	-4.055660000
H	-6.000781000	-0.060538000	-4.067648000	H	-6.342570000	-1.709905000	-5.220973000
H	-6.375115000	-0.943418000	-5.393657000	H	-4.786546000	-2.435883000	-2.297542000
H	-5.038417000	-2.166385000	-2.713706000	H	-3.650683000	-0.424610000	-3.186732000
H	-3.707945000	-0.055896000	-3.122555000	H	-1.177711000	-1.699115000	-5.596742000
H	-1.217886000	-0.972213000	-5.698590000	H	-2.572953000	-2.018088000	-1.547436000
H	-2.709444000	-1.914037000	-1.783450000	H	-0.506171000	-3.193844000	-0.918073000
H	-0.739235000	-3.333318000	-1.364529000	H	1.250425000	-3.643074000	-2.631289000
H	1.034185000	-3.554661000	-3.106547000	H	0.897607000	-2.879977000	-4.975187000
H	0.779577000	-2.353835000	-5.274169000	H	-4.170113000	-2.592356000	-5.285606000
H	-4.160599000	-1.757781000	-5.627811000	H	-3.094431000	-0.371554000	-4.852795000
H	-3.102209000	0.310044000	-4.732995000	H	-2.732405000	-1.030406000	0.970080000
H	-2.996427000	-0.641836000	0.999030000	N	-2.958691000	0.871467000	-0.901752000
N	-2.700732000	1.253367000	-0.868681000	O	-3.909760000	0.077465000	-0.848927000
O	-3.777868000	0.635389000	-0.921367000	O	-2.948029000	1.833320000	-1.673204000
O	-2.461775000	2.212803000	-1.605042000	H	1.946629000	-0.290870000	4.331671000
O	2.640653000	-2.715709000	5.076092000	O	3.386991000	-0.539281000	5.212024000
H	1.521148000	-1.430657000	4.489822000	H	3.225608000	-0.623166000	6.161736000
H	2.513389000	-3.026680000	5.982057000	H	3.327337000	-1.446776000	4.852282000

