Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Deamidation reaction network mapping of pharmacologic and related proteins: Identification of the impact of solvation dielectric on the degradation energetics of Asparagine dipeptides

Supporting Information

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Table of Contents

Reaction Path Degeneracies

Table S1.A. Reaction path degeneracies and symmetry numbers of the Asn-X Direct Hydrolysis Reaction (Implicit Solvation). This is a bimolecular elimination reaction in both the forward and reverse directions, and as such, Δn is equal to -1 for all reactions and V_m has units of $L.mol^{-1}.s^{-1}$.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala DH	2	C_{1V} (1)	2
Asn-Arg	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg DH	2	C_{1V} (1)	2
Asn-Asn	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn DH	2	C_{1V} (1)	2
Asn-Asp	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp DH	2	C_{1V} (1)	2
Asn-Cys	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys DH	2	C_{1V} (1)	2
Asn-Gln	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln DH	2	C_{1V} (1)	2
Asn-Glu	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	2

						Glu DH		(1)	
Asn-Gly	1	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly DH	1	C_{1V} (1)	2
Asn-His	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His DH	2	C_{1V} (1)	2
Asn-Ile	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile DH	2	C_{1V} (1)	2
Asn-Leu	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu DH	2	C_{1V} (1)	2
Asn-Lys	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys DH	2	C_{1V} (1)	2
Asn-Met	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met DH	2	C_{1V} (1)	2
Asn-Phe	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe DH	2	C_{1V} (1)	2
Asn-Pro	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Pro DH	2	C_{1V} (1)	2

Asn-Ser	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser DH	2	C_{1V} (1)	2
Asn-Thr	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr DH	2	C_{1V} (1)	2
Asn-Trp	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp DH	2	C_{1V} (1)	2
Asn-Tyr	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr DH	2	C_{1V} (1)	2
Asn-Val	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val DH	2	C_{1V} (1)	2
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asp-Ala	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala DH	2	C_{1V} (1)	3
Asp-Arg	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg DH	2	C_{1V} (1)	3
Asp-Asn	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn	2	C_{1V} (1)	3

						DH			
Asp-Asp	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp DH	2	C_{1V} (1)	3
Asp-Cys	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys DH	2	C_{1V} (1)	3
Asp-Gln	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln DH	2	C_{1V} (1)	3
Asp-Glu	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu DH	2	C_{1V} (1)	3
Asp-Gly	1	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly DH	1	C_{1V} (1)	3
Asp-His	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His DH	2	C_{1V} (1)	3
Asp-Ile	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile DH	2	C_{1V} (1)	3
Asp-Leu	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu DH	2	C_{1V} (1)	3
Asp-Lys	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-	2	C_{1V}	3

						Lys DH		(1)	
Asp-Met	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met DH	2	C_{1V} (1)	3
Asp-Phe	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe DH	2	C_{1V} (1)	3
Asp-Pro	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Pro DH	2	C_{1V} (1)	3
Asp-Ser	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ser DH	2	C_{1V} (1)	3
Asp-Thr	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr DH	2	C_{1V} (1)	3
Asp-Trp	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp DH	2	C_{1V} (1)	3
Asp-Tyr	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr DH	2	C_{1V} (1)	3
Asp-Val	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Val	2	C_{1V} (1)	3

						DH			

Table S1.B. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Formation Reaction (Implicit Solvation). This is a unimolecular addition reaction in the forward direction and a bimolecular elimination reaction in the reverse direction. As such, in the forward direction: Δn is 0 and the units of $V_{m\ are}$ s^{-1}; in the reverse direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$.

Forward Direction									
R1	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**R2**	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**TS**	$n_{chiral}^{\neq}$	$\sigma^{\neq}$	**rpd^F**
Asn-Ala	2	C_{1V} (1)	-	-	-	Asn-Ala SF	2	C_{1V} (1)	1
Asn-Arg	2	C_{1V} (1)	-	-	-	Asn-Arg SF	2	C_{1V} (1)	1
Asn-Asn	2	C_{1V} (1)	-	-	-	Asn-Asn SF	2	C_{1V} (1)	1
Asn-Asp	2	C_{1V} (1)	-	-	-	Asn-Asp SF	2	C_{1V} (1)	1
Asn-Cys	2	C_{1V} (1)	-	-	-	Asn-Cys SF	2	C_{1V} (1)	1
Asn-Gln	2	C_{1V} (1)	-	-	-	Asn-Gln	2	C_{1V} (1)	1

						SF			
Asn-Glu	2	C_{1V} (1)	-	-	-	Asn-Glu SF	2	C_{1V} (1)	1
Asn-Gly	1	C_{1V} (1)	-	-	-	Asn-Gly SF	1	C_{1V} (1)	1
Asn-His	2	C_{1V} (1)	-	-	-	Asn-His SF	2	C_{1V} (1)	1
Asn-Ile	2	C_{1V} (1)	-	-	-	Asn-Ile SF	2	C_{1V} (1)	1
Asn-Leu	2	C_{1V} (1)	-	-	-	Asn-Leu SF	2	C_{1V} (1)	1
Asn-Lys	2	C_{1V} (1)	-	-	-	Asn-Lys SF	2	C_{1V} (1)	1
Asn-Met	2	C_{1V} (1)	-	-	-	Asn-Met SF	2	C_{1V} (1)	1
Asn-Phe	2	C_{1V} (1)	-	-	-	Asn-Phe SF	2	C_{1V} (1)	1
Asn-Ser	2	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	1

						Ser SF		(1)	
Asn-Thr	2	C_{1V} (1)	-	-	-	Asn-Thr SF	2	C_{1V} (1)	1
Asn-Trp	2	C_{1V} (1)	-	-	-	Asn-Trp SF	2	C_{1V} (1)	1
Asn-Tyr	2	C_{1V} (1)	-	-	-	Asn-Tyr SF	2	C_{1V} (1)	1
Asn-Val	2	C_{1V} (1)	-	-	-	Asn-Val SF	2	C_{1V} (1)	1
Reverse Direction									
P1	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**P2**	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**TS**	**$n_{chiral}^{\neq}$**	**$\sigma^{\neq}$**	**rpd^{R}**
Asn-Ala Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala SF	2	C_{1V} (1)	3
Asn-Arg Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg SF	2	C_{1V} (1)	3
Asn-Asn Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn SF	2	C_{1V} (1)	3

Asn-Asp Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp SF	2	C_{1V} (1)	3
Asn-Cys Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys SF	2	C_{1V} (1)	3
Asn-Gln Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln SF	2	C_{1V} (1)	3
Asn-Glu Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu SF	2	C_{1V} (1)	3
Asn-Gly Succinimide	1	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly SF	1	C_{1V} (1)	3
Asn-His Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His SF	2	C_{1V} (1)	3
Asn-Ile Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile SF	2	C_{1V} (1)	3
Asn-Leu Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu SF	2	C_{1V} (1)	3
Asn-Lys Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Lys	2	C_{1V} (1)	3

						SF			
Asn-Met Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met SF	2	C_{1V} (1)	3
Asn-Phe Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe SF	2	C_{1V} (1)	3
Asn-Ser Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ser SF	2	C_{1V} (1)	3
Asn-Thr Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr SF	2	C_{1V} (1)	3
Asn-Trp Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp SF	2	C_{1V} (1)	3
Asn-Tyr Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr SF	2	C_{1V} (1)	3
Asn-Val Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Val SF	2	C_{1V} (1)	3

Table S1.C. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Hydrolysis into Asp-X Reaction (Implicit Solvation). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}.

Forward Direction									
R1	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**R2**	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**TS**	$n_{chiral}^{\neq}$	$\sigma^{\neq}$	**rpd^F**
Asn-Ala Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala SHD	2	C_{1V} (1)	2
Asn-Arg Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg SHD	2	C_{1V} (1)	2
Asn-Asn Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn SHD	2	C_{1V} (1)	2
Asn-Asp Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp SHD	2	C_{1V} (1)	2
Asn-Cys Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys SHD	2	C_{1V} (1)	2
Asn-Gln Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln SHD	2	C_{1V} (1)	2
Asn-Glu Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Glu	2	C_{1V} (1)	2

						SHD			
Asn-Gly Succinimide	1	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly SHD	1	C_{1V} (1)	2
Asn-His Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His SHD	2	C_{1V} (1)	2
Asn-Ile Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile SHD	2	C_{1V} (1)	2
Asn-Leu Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu SHD	2	C_{1V} (1)	2
Asn-Lys Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys SHD	2	C_{1V} (1)	2
Asn-Met Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met SHD	2	C_{1V} (1)	2
Asn-Phe Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe SHD	2	C_{1V} (1)	2
Asn-Ser Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser SHD	2	C_{1V} (1)	2

Asn-Thr Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr SHD	2	C_{1V} (1)	2
Asn-Trp Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp SHD	2	C_{1V} (1)	2
Asn-Tyr Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr SHD	2	C_{1V} (1)	2
Asn-Val Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val SHD	2	C_{1V} (1)	2
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asp-Ala	2	C_{1V} (1)	-	-	-	Asn-Ala SHD	2	C_{1V} (1)	1
Asp-Arg	2	C_{1V} (1)	-	-	-	Asn-Arg SHD	2	C_{1V} (1)	1
Asp-Asn	2	C_{1V} (1)	-	-	-	Asn-Asn SHD	2	C_{1V} (1)	1
Asp-Asp	2	C_{1V} (1)	-	-	-	Asn-Asp	2	C_{1V} (1)	1

						SHD			
Asp-Cys	2	C_{1V} (1)	-	-	-	Asn-Cys SHD	2	C_{1V} (1)	1
Asp-Gln	2	C_{1V} (1)	-	-	-	Asn-Gln SHD	2	C_{1V} (1)	1
Asp-Glu	2	C_{1V} (1)	-	-	-	Asn-Glu SHD	2	C_{1V} (1)	1
Asp-Gly	1	C_{1V} (1)	-	-	-	Asn-Gly SHD	1	C_{1V} (1)	1
Asp-His	2	C_{1V} (1)	-	-	-	Asn-His SHD	2	C_{1V} (1)	1
Asp-Ile	2	C_{1V} (1)	-	-	-	Asn-Ile SHD	2	C_{1V} (1)	1
Asp-Leu	2	C_{1V} (1)	-	-	-	Asn-Leu SHD	2	C_{1V} (1)	1
Asp-Lys	2	C_{1V} (1)	-	-	-	Asn-Lys SHD	2	C_{1V} (1)	1

Asp-Met	2	C_{1V} (1)	-	-	-	Asn-Met SHD	2	C_{1V} (1)	1
Asp-Phe	2	C_{1V} (1)	-	-	-	Asn-Phe SHD	2	C_{1V} (1)	1
Asp-Ser	2	C_{1V} (1)	-	-	-	Asn-Ser SHD	2	C_{1V} (1)	1
Asp-Thr	2	C_{1V} (1)	-	-	-	Asn-Thr SHD	2	C_{1V} (1)	1
Asp-Trp	2	C_{1V} (1)	-	-	-	Asn-Trp SHD	2	C_{1V} (1)	1
Asp-Tyr	2	C_{1V} (1)	-	-	-	Asn-Tyr SHD	2	C_{1V} (1)	1
Asp-Val	2	C_{1V} (1)	-	-	-	Asn-Val SHD	2	C_{1V} (1)	1

Table S1.D. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction (Implicit Solvation). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala SHD	2	C_{1V} (1)	2
Asn-Arg Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg SHD	2	C_{1V} (1)	2
Asn-Asn Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn SHD	2	C_{1V} (1)	2
Asn-Asp Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp SHD	2	C_{1V} (1)	2
Asn-Cys Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys SHD	2	C_{1V} (1)	2
Asn-Gln Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln SHD	2	C_{1V} (1)	2
Asn-Glu Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Glu SHD	2	C_{1V} (1)	2
Asn-Gly Succinimide	1	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly	1	C_{1V} (1)	2

						SHD			
Asn-His Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His SHD	2	C_{1V} (1)	2
Asn-Ile Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile SHD	2	C_{1V} (1)	2
Asn-Leu Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu SHD	2	C_{1V} (1)	2
Asn-Lys Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys SHD	2	C_{1V} (1)	2
Asn-Met Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met SHD	2	C_{1V} (1)	2
Asn-Phe Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe SHD	2	C_{1V} (1)	2
Asn-Ser Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser SHD	2	C_{1V} (1)	2
Asn-Thr Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr SHD	2	C_{1V} (1)	2

Asn-Trp Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp SHD	2	C_{1V} (1)	2
Asn-Tyr Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr SHD	2	C_{1V} (1)	2
Asn-Val Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val SHD	2	C_{1V} (1)	2
Reverse Direction									
P1	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**P2**	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**TS**	**$n_{chiral}^{\neq}$**	**$\sigma^{\neq}$**	**rpd^{R}**
Iso-Asp-Ala	2	C_{1V} (1)	-	-	-	Asn-Ala SHI	2	C_{1V} (1)	1
Iso-Asp-Arg	2	C_{1V} (1)	-	-	-	Asn-Arg SHI	2	C_{1V} (1)	1
Iso-Asp-Asn	2	C_{1V} (1)	-	-	-	Asn-Asn SHI	2	C_{1V} (1)	1
Iso-Asp-Asp	2	C_{1V} (1)	-	-	-	Asn-Asp SHI	2	C_{1V} (1)	1
Iso-Asp-Cys	2	C_{1V} (1)	-	-	-	Asn-Cys	2	C_{1V} (1)	1

						SHI			
Iso-Asp-Gln	2	C_{1V} (1)	-	-	-	Asn-Gln SHI	2	C_{1V} (1)	1
Iso-Asp-Glu	2	C_{1V} (1)	-	-	-	Asn-Glu SHI	2	C_{1V} (1)	1
Iso-Asp-Gly	1	C_{1V} (1)	-	-	-	Asn-Gly SHI	1	C_{1V} (1)	1
Iso-Asp-His	2	C_{1V} (1)	-	-	-	Asn-His SHI	2	C_{1V} (1)	1
Iso-Asp-Ile	2	C_{1V} (1)	-	-	-	Asn-Ile SHI	2	C_{1V} (1)	1
Iso-Asp-Leu	2	C_{1V} (1)	-	-	-	Asn-Leu SHI	2	C_{1V} (1)	1
Iso-Asp-Lys	2	C_{1V} (1)	-	-	-	Asn-Lys SHI	2	C_{1V} (1)	1
Iso-Asp-Met	2	C_{1V} (1)	-	-	-	Asn-Met SHI	2	C_{1V} (1)	1

Iso-Asp-Phe	2	C_{1V} (1)	-	-	-	Asn-Phe SHI	2	C_{1V} (1)	1
Iso-Asp-Ser	2	C_{1V} (1)	-	-	-	Asn-Ser SHI	2	C_{1V} (1)	1
Iso-Asp-Thr	2	C_{1V} (1)	-	-	-	Asn-Thr SHI	2	C_{1V} (1)	1
Iso-Asp-Trp	2	C_{1V} (1)	-	-	-	Asn-Trp SHI	2	C_{1V} (1)	1
Iso-Asp-Tyr	2	C_{1V} (1)	-	-	-	Asn-Tyr SHI	2	C_{1V} (1)	1
Iso-Asp-Val	2	C_{1V} (1)	-	-	-	Asn-Val SHI	2	C_{1V} (1)	1

Table S1.E. Reaction path degeneracies and symmetry numbers of the Asn-X Isoimide Formation Reaction (Implicit Solvation). This is a unimolecular addition reaction in the forward direction and a bimolecular elimination reaction in the reverse direction. As such, in the forward direction: Δn is 0 and the units of V_m are s^{-1}; in the reverse direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala	2	C_{1V} (1)	-	-	-	Asn-Ala IF	2	C_{1V} (1)	1

Asn-Arg	2	C_{1V} (1)	-	-	-	Asn-Arg IF	2	C_{1V} (1)	1
Asn-Asn	2	C_{1V} (1)	-	-	-	Asn-Asn IF	2	C_{1V} (1)	1
Asn-Asp	2	C_{1V} (1)	-	-	-	Asn-Asp IF	2	C_{1V} (1)	1
Asn-Cys	2	C_{1V} (1)	-	-	-	Asn-Cys IF	2	C_{1V} (1)	1
Asn-Gln	2	C_{1V} (1)	-	-	-	Asn-Gln IF	2	C_{1V} (1)	1
Asn-Glu	2	C_{1V} (1)	-	-	-	Asn-Glu IF	2	C_{1V} (1)	1
Asn-Gly	1	C_{1V} (1)	-	-	-	Asn-Gly IF	1	C_{1V} (1)	1
Asn-His	2	C_{1V} (1)	-	-	-	Asn-His IF	2	C_{1V} (1)	1
Asn-Ile	2	C_{1V} (1)	-	-	-	Asn-Ile IF	2	C_{1V} (1)	1
Asn-Leu	2	C_{1V} (1)	-	-	-	Asn-Leu IF	2	C_{1V} (1)	1
Asn-Lys	2	C_{1V} (1)	-	-	-	Asn-Lys IF	2	C_{1V} (1)	1
Asn-Met	2	C_{1V} (1)	-	-	-	Asn-Met IF	2	C_{1V} (1)	1
Asn-Phe	2	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	1

						Phe IF		(1)	
Asn-Ser	2	C_{1V} (1)	-	-	-	Asn-Ser IF	2	C_{1V} (1)	1
Asn-Thr	2	C_{1V} (1)	-	-	-	Asn-Thr IF	2	C_{1V} (1)	1
Asn-Trp	2	C_{1V} (1)	-	-	-	Asn-Trp IF	2	C_{1V} (1)	1
Asn-Tyr	2	C_{1V} (1)	-	-	-	Asn-Tyr IF	2	C_{1V} (1)	1
Asn-Val	2	C_{1V} (1)	-	-	-	Asn-Val IF	2	C_{1V} (1)	1
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asn-Ala Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala IF	2	C_{1V} (1)	3
Asn-Arg Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg IF	2	C_{1V} (1)	3
Asn-Asn Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn IF	2	C_{1V} (1)	3
Asn-Asp Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp IF	2	C_{1V} (1)	3
Asn-Cys Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys IF	2	C_{1V} (1)	3
Asn-Gln Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln IF	2	C_{1V} (1)	3

Asn-Glu Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu IF	2	C_{1V} (1)	3
Asn-Gly Isoimide	1	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly IF	1	C_{1V} (1)	3
Asn-His Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His IF	2	C_{1V} (1)	3
Asn-Ile Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile IF	2	C_{1V} (1)	3
Asn-Leu Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu IF	2	C_{1V} (1)	3
Asn-Lys Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Lys IF	2	C_{1V} (1)	3
Asn-Met Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met IF	2	C_{1V} (1)	3
Asn-Phe Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe IF	2	C_{1V} (1)	3
Asn-Ser Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ser IF	2	C_{1V} (1)	3
Asn-Thr Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr IF	2	C_{1V} (1)	3
Asn-Trp Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp IF	2	C_{1V} (1)	3
Asn-Tyr Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr IF	2	C_{1V} (1)	3
Asn-Val	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-	2	C_{1V}	3

Isoimide						Val IF		(1)	

Table S1.F. Reaction path degeneracies and symmetry numbers of the Asn-X Isoimide Hydrolysis into Asp-X Reaction (Implicit Solvation). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}.

Forward Direction									
R1	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**R2**	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**TS**	$n_{chiral}^{\neq}$	$\sigma^{\neq}$	rpd^{F}
Asn-Ala Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala IHD	2	C_{1V} (1)	2
Asn-Arg Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg IHD	2	C_{1V} (1)	2
Asn-Asn Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn IHD	2	C_{1V} (1)	2
Asn-Asp Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp IHD	2	C_{1V} (1)	2
Asn-Cys Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys IHD	2	C_{1V} (1)	2
Asn-Gln Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln IHD	2	C_{1V} (1)	2
Asn-Glu	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	2

Isoimide						Glu IHD		(1)	
Asn-Gly Isoimide	1	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly IHD	1	C_{1V} (1)	2
Asn-His Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His IHD	2	C_{1V} (1)	2
Asn-Ile Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile IHD	2	C_{1V} (1)	2
Asn-Leu Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu IHD	2	C_{1V} (1)	2
Asn-Lys Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys IHD	2	C_{1V} (1)	2
Asn-Met Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met IHD	2	C_{1V} (1)	2
Asn-Phe Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe IHD	2	C_{1V} (1)	2
Asn-Ser Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser	2	C_{1V} (1)	2

						IHD			
Asn-Thr Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr IHD	2	C_{1V} (1)	2
Asn-Trp Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp IHD	2	C_{1V} (1)	2
Asn-Tyr Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr IHD	2	C_{1V} (1)	2
Asn-Val Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val IHD	2	C_{1V} (1)	2
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asp-Ala	2	C_{1V} (1)	-	-	-	Asn-Ala IHD	2	C_{1V} (1)	1
Asp-Arg	2	C_{1V} (1)	-	-	-	Asn-Arg IHD	2	C_{1V} (1)	1
Asp-Asn	2	C_{1V} (1)	-	-	-	Asn-Asn IHD	2	C_{1V} (1)	1
Asp-Asp	2	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	1

						Asp IHD		(1)	
Asp-Cys	2	C_{1V} (1)	-	-	-	Asn-Cys IHD	2	C_{1V} (1)	1
Asp-Gln	2	C_{1V} (1)	-	-	-	Asn-Gln IHD	2	C_{1V} (1)	1
Asp-Glu	2	C_{1V} (1)	-	-	-	Asn-Glu IHD	2	C_{1V} (1)	1
Asp-Gly	1	C_{1V} (1)	-	-	-	Asn-Gly IHD	1	C_{1V} (1)	1
Asp-His	2	C_{1V} (1)	-	-	-	Asn-His IHD	2	C_{1V} (1)	1
Asp-Ile	2	C_{1V} (1)	-	-	-	Asn-Ile IHD	2	C_{1V} (1)	1
Asp-Leu	2	C_{1V} (1)	-	-	-	Asn-Leu IHD	2	C_{1V} (1)	1
Asp-Lys	2	C_{1V} (1)	-	-	-	Asn-Lys	2	C_{1V} (1)	1

						IHD			
Asp-Met	2	C_{1V} (1)	-	-	-	Asn-Met IHD	2	C_{1V} (1)	1
Asp-Phe	2	C_{1V} (1)	-	-	-	Asn-Phe IHD	2	C_{1V} (1)	1
Asp-Ser	2	C_{1V} (1)	-	-	-	Asn-Ser IHD	2	C_{1V} (1)	1
Asp-Thr	2	C_{1V} (1)	-	-	-	Asn-Thr IHD	2	C_{1V} (1)	1
Asp-Trp	2	C_{1V} (1)	-	-	-	Asn-Trp IHD	2	C_{1V} (1)	1
Asp-Tyr	2	C_{1V} (1)	-	-	-	Asn-Tyr IHD	2	C_{1V} (1)	1
Asp-Val	2	C_{1V} (1)	-	-	-	Asn-Val IHD	2	C_{1V} (1)	1

Table S1.G. Reaction path degeneracies and symmetry numbers of the Asn-X Direct Hydrolysis Reaction (Implicit Solvation + 1 H_2O). This is a bimolecular elimination reaction in both the forward and reverse directions, and as such, Δn is equal to -1 for all reactions and V_m has units of $L.mol^{-1}.s^{-1}$. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala DH	2	C_{1V} (1)	2
Asn-Arg	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg DH	2	C_{1V} (1)	2
Asn-Asn	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn DH	2	C_{1V} (1)	2
Asn-Asp	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp DH	2	C_{1V} (1)	2
Asn-Cys	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys DH	2	C_{1V} (1)	2
Asn-Gln	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln DH	2	C_{1V} (1)	2
Asn-Glu	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	2

						Glu DH		(1)	
Asn-Gly	1	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly DH	1	C_{1V} (1)	2
Asn-His	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His DH	2	C_{1V} (1)	2
Asn-Ile	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile DH	2	C_{1V} (1)	2
Asn-Leu	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu DH	2	C_{1V} (1)	2
Asn-Lys	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys DH	2	C_{1V} (1)	2
Asn-Met	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met DH	2	C_{1V} (1)	2
Asn-Phe	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe DH	2	C_{1V} (1)	2
Asn-Pro	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Pro DH	2	C_{1V} (1)	2

Asn-Ser	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser DH	2	C_{1V} (1)	2
Asn-Thr	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr DH	2	C_{1V} (1)	2
Asn-Trp	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp DH	2	C_{1V} (1)	2
Asn-Tyr	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr DH	2	C_{1V} (1)	2
Asn-Val	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val DH	2	C_{1V} (1)	2
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asp-Ala	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala DH	2	C_{1V} (1)	6
Asp-Arg	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg DH	2	C_{1V} (1)	6
Asp-Asn	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn	2	C_{1V} (1)	6

						DH			
Asp-Asp	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp DH	2	C_{1V} (1)	6
Asp-Cys	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys DH	2	C_{1V} (1)	6
Asp-Gln	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln DH	2	C_{1V} (1)	6
Asp-Glu	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu DH	2	C_{1V} (1)	6
Asp-Gly	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly DH	1	C_{1V} (1)	6
Asp-His	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His DH	2	C_{1V} (1)	6
Asp-Ile	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile DH	2	C_{1V} (1)	6
Asp-Leu	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu DH	2	C_{1V} (1)	6
Asp-Lys	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-	2	C_{1V}	6

						Lys DH		(1)	
Asp-Met	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met DH	2	C_{1V} (1)	6
Asp-Phe	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe DH	2	C_{1V} (1)	6
Asp-Pro	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Pro DH	2	C_{1V} (1)	6
Asp-Ser	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ser DH	2	C_{1V} (1)	6
Asp-Thr	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr DH	2	C_{1V} (1)	6
Asp-Trp	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp DH	2	C_{1V} (1)	6
Asp-Tyr	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr DH	2	C_{1V} (1)	6
Asp-Val	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Val	2	C_{1V} (1)	6

						DH			

Table S1.H. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Formation Reaction (Implicit Solvation + 1 H_2O). This is a unimolecular addition reaction in the forward direction and a bimolecular elimination reaction in the reverse direction. As such, in the forward direction: Δn is 0 and the units of V_m are s^{-1}; in the reverse direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala	4	C_{1V} (1)	-	-	-	Asn-Ala SF	2	C_{1V} (1)	2
Asn-Arg	4	C_{1V} (1)	-	-	-	Asn-Arg SF	2	C_{1V} (1)	2
Asn-Asn	4	C_{1V} (1)	-	-	-	Asn-Asn SF	2	C_{1V} (1)	2
Asn-Asp	4	C_{1V} (1)	-	-	-	Asn-Asp SF	2	C_{1V} (1)	2
Asn-Cys	4	C_{1V} (1)	-	-	-	Asn-Cys SF	2	C_{1V} (1)	2
Asn-Gln	4	C_{1V} (1)	-	-	-	Asn-Gln	2	C_{1V} (1)	2

						SF			
Asn-Glu	4	C_{1V} (1)	-	-	-	Asn-Glu SF	2	C_{1V} (1)	2
Asn-Gly	2	C_{1V} (1)	-	-	-	Asn-Gly SF	1	C_{1V} (1)	2
Asn-His	4	C_{1V} (1)	-	-	-	Asn-His SF	2	C_{1V} (1)	2
Asn-Ile	4	C_{1V} (1)	-	-	-	Asn-Ile SF	2	C_{1V} (1)	2
Asn-Leu	4	C_{1V} (1)	-	-	-	Asn-Leu SF	2	C_{1V} (1)	2
Asn-Lys	4	C_{1V} (1)	-	-	-	Asn-Lys SF	2	C_{1V} (1)	2
Asn-Met	4	C_{1V} (1)	-	-	-	Asn-Met SF	2	C_{1V} (1)	2
Asn-Phe	4	C_{1V} (1)	-	-	-	Asn-Phe SF	2	C_{1V} (1)	2
Asn-Ser	4	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	2

						Ser SF		(1)	
Asn-Thr	4	C_{1V} (1)	-	-	-	Asn-Thr SF	2	C_{1V} (1)	2
Asn-Trp	4	C_{1V} (1)	-	-	-	Asn-Trp SF	2	C_{1V} (1)	2
Asn-Tyr	4	C_{1V} (1)	-	-	-	Asn-Tyr SF	2	C_{1V} (1)	2
Asn-Val	4	C_{1V} (1)	-	-	-	Asn-Val SF	2	C_{1V} (1)	2
Reverse Direction									
P1	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**P2**	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**TS**	**$n_{chiral}^{\neq}$**	**$\sigma^{\neq}$**	**rpd^{R}**
Asn-Ala Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala SF	2	C_{1V} (1)	6
Asn-Arg Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg SF	2	C_{1V} (1)	6
Asn-Asn Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn SF	2	C_{1V} (1)	6

Asn-Asp Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp SF	2	C_{1V} (1)	6
Asn-Cys Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys SF	2	C_{1V} (1)	6
Asn-Gln Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln SF	2	C_{1V} (1)	6
Asn-Glu Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu SF	2	C_{1V} (1)	6
Asn-Gly Succinimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly SF	1	C_{1V} (1)	6
Asn-His Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His SF	2	C_{1V} (1)	6
Asn-Ile Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile SF	2	C_{1V} (1)	6
Asn-Leu Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu SF	2	C_{1V} (1)	6
Asn-Lys Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Lys	2	C_{1V} (1)	6

						SF			
Asn-Met Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met SF	2	C_{1V} (1)	6
Asn-Phe Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe SF	2	C_{1V} (1)	6
Asn-Ser Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ser SF	2	C_{1V} (1)	6
Asn-Thr Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr SF	2	C_{1V} (1)	6
Asn-Trp Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp SF	2	C_{1V} (1)	6
Asn-Tyr Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr SF	2	C_{1V} (1)	6
Asn-Val Succinimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Val SF	2	C_{1V} (1)	6

Table S1.I. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Hydrolysis into Asp-X Reaction (Implicit Solvation + 1 H_2O). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**R2**	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**TS**	$n_{chiral}^{\neq}$	$\sigma^{\neq}$	rpd^{F}
Asn-Ala Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala SHD	2	C_{1V} (1)	4
Asn-Arg Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg SHD	2	C_{1V} (1)	4
Asn-Asn Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn SHD	2	C_{1V} (1)	4
Asn-Asp Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp SHD	2	C_{1V} (1)	4
Asn-Cys Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys SHD	2	C_{1V} (1)	4
Asn-Gln Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln SHD	2	C_{1V} (1)	4
Asn-Glu	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	4

Succinimide						Glu SHD		(1)	
Asn-Gly Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly SHD	1	C_{1V} (1)	4
Asn-His Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His SHD	2	C_{1V} (1)	4
Asn-Ile Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile SHD	2	C_{1V} (1)	4
Asn-Leu Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu SHD	2	C_{1V} (1)	4
Asn-Lys Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys SHD	2	C_{1V} (1)	4
Asn-Met Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met SHD	2	C_{1V} (1)	4
Asn-Phe Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe SHD	2	C_{1V} (1)	4
Asn-Ser Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser	2	C_{1V} (1)	4

						SHD			
Asn-Thr Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr SHD	2	C_{1V} (1)	4
Asn-Trp Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp SHD	2	C_{1V} (1)	4
Asn-Tyr Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr SHD	2	C_{1V} (1)	4
Asn-Val Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val SHD	2	C_{1V} (1)	4
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Asp-Ala	4	C_{1V} (1)	-	-	-	Asn-Ala SHD	2	C_{1V} (1)	2
Asp-Arg	4	C_{1V} (1)	-	-	-	Asn-Arg SHD	2	C_{1V} (1)	2
Asp-Asn	4	C_{1V} (1)	-	-	-	Asn-Asn SHD	2	C_{1V} (1)	2
Asp-Asp	4	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	2

						Asp SHD		(1)	
Asp-Cys	4	C_{1V} (1)	-	-	-	Asn-Cys SHD	2	C_{1V} (1)	2
Asp-Gln	4	C_{1V} (1)	-	-	-	Asn-Gln SHD	2	C_{1V} (1)	2
Asp-Glu	4	C_{1V} (1)	-	-	-	Asn-Glu SHD	2	C_{1V} (1)	2
Asp-Gly	2	C_{1V} (1)	-	-	-	Asn-Gly SHD	1	C_{1V} (1)	2
Asp-His	4	C_{1V} (1)	-	-	-	Asn-His SHD	2	C_{1V} (1)	2
Asp-Ile	4	C_{1V} (1)	-	-	-	Asn-Ile SHD	2	C_{1V} (1)	2
Asp-Leu	4	C_{1V} (1)	-	-	-	Asn-Leu SHD	2	C_{1V} (1)	2
Asp-Lys	4	C_{1V} (1)	-	-	-	Asn-Lys	2	C_{1V} (1)	2

						SHD			
Asp-Met	4	C_{1V} (1)	-	-	-	Asn-Met SHD	2	C_{1V} (1)	2
Asp-Phe	4	C_{1V} (1)	-	-	-	Asn-Phe SHD	2	C_{1V} (1)	2
Asp-Ser	4	C_{1V} (1)	-	-	-	Asn-Ser SHD	2	C_{1V} (1)	2
Asp-Thr	4	C_{1V} (1)	-	-	-	Asn-Thr SHD	2	C_{1V} (1)	2
Asp-Trp	4	C_{1V} (1)	-	-	-	Asn-Trp SHD	2	C_{1V} (1)	2
Asp-Tyr	4	C_{1V} (1)	-	-	-	Asn-Tyr SHD	2	C_{1V} (1)	2
Asp-Val	4	C_{1V} (1)	-	-	-	Asn-Val SHD	2	C_{1V} (1)	2

Table S1.J. Reaction path degeneracies and symmetry numbers of the Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction (Implicit Solvation + 1 H_2O). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**R2**	$n_{chiral}^{react,j}$	$\sigma_{sym}^{react,j}$	**TS**	$n_{chiral}^{\neq}$	$\sigma^{\neq}$	**rpd^F**
Asn-Ala Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala SHI	2	C_{1V} (1)	4
Asn-Arg Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg SHI	2	C_{1V} (1)	4
Asn-Asn Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn SHI	2	C_{1V} (1)	4
Asn-Asp Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp SHI	2	C_{1V} (1)	4
Asn-Cys Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys SHI	2	C_{1V} (1)	4
Asn-Gln Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln SHI	2	C_{1V} (1)	4
Asn-Glu	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	4

Succinimide						Glu SHI		(1)	
Asn-Gly Succinimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly SHI	1	C_{1V} (1)	4
Asn-His Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His SHI	2	C_{1V} (1)	4
Asn-Ile Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile SHI	2	C_{1V} (1)	4
Asn-Leu Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu SHI	2	C_{1V} (1)	4
Asn-Lys Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Lys SHI	2	C_{1V} (1)	4
Asn-Met Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met SHI	2	C_{1V} (1)	4
Asn-Phe Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe SHI	2	C_{1V} (1)	4
Asn-Ser Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser	2	C_{1V} (1)	4

						SHI			
Asn-Thr Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr SHI	2	C_{1V} (1)	4
Asn-Trp Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp SHI	2	C_{1V} (1)	4
Asn-Tyr Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr SHI	2	C_{1V} (1)	4
Asn-Val Succinimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val SHI	2	C_{1V} (1)	4
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$
Iso-Asp-Ala	4	C_{1V} (1)	-	-	-	Asn-Ala SHI	2	C_{1V} (1)	2
Iso-Asp-Arg	4	C_{1V} (1)	-	-	-	Asn-Arg SHI	2	C_{1V} (1)	2
Iso-Asp-Asn	4	C_{1V} (1)	-	-	-	Asn-Asn SHI	2	C_{1V} (1)	2
Iso-Asp-	4	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	2

Asp						Asp SHI		(1)	
Iso-Asp-Cys	4	C_{1V} (1)	-	-	-	Asn-Cys SHI	2	C_{1V} (1)	2
Iso-Asp-Gln	4	C_{1V} (1)	-	-	-	Asn-Gln SHI	2	C_{1V} (1)	2
Iso-Asp-Glu	4	C_{1V} (1)	-	-	-	Asn-Glu SHI	2	C_{1V} (1)	2
Iso-Asp-Gly	2	C_{1V} (1)	-	-	-	Asn-Gly SHI	1	C_{1V} (1)	2
Iso-Asp-His	4	C_{1V} (1)	-	-	-	Asn-His SHI	2	C_{1V} (1)	2
Iso-Asp-Ile	4	C_{1V} (1)	-	-	-	Asn-Ile SHI	2	C_{1V} (1)	2
Iso-Asp-Leu	4	C_{1V} (1)	-	-	-	Asn-Leu SHI	2	C_{1V} (1)	2
Iso-Asp-Lys	4	C_{1V} (1)	-	-	-	Asn-Lys	2	C_{1V} (1)	2

						SHI			
Iso-Asp-Met	4	C_{1V} (1)	-	-	-	Asn-Met SHI	2	C_{1V} (1)	2
Iso-Asp-Phe	4	C_{1V} (1)	-	-	-	Asn-Phe SHI	2	C_{1V} (1)	2
Iso-Asp-Ser	4	C_{1V} (1)	-	-	-	Asn-Ser SHI	2	C_{1V} (1)	2
Iso-Asp-Thr	4	C_{1V} (1)	-	-	-	Asn-Thr SHI	2	C_{1V} (1)	2
Iso-Asp-Trp	4	C_{1V} (1)	-	-	-	Asn-Trp SHI	2	C_{1V} (1)	2
Iso-Asp-Tyr	4	C_{1V} (1)	-	-	-	Asn-Tyr SHI	2	C_{1V} (1)	2
Iso-Asp-Val	4	C_{1V} (1)	-	-	-	Asn-Val SHI	2	C_{1V} (1)	2

Table S1.K. Reaction path degeneracies and symmetry numbers of the Asn-X Isoimide Formation Reaction (Implicit Solvation + 1 H_2O). This is a unimolecular addition reaction in the forward direction and a bimolecular elimination reaction in the reverse direction. As such, in the forward direction: Δn is 0 and the units of V_m are s^{-1}; in the reverse direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{F}}$
Asn-Ala	4	C_{1V} (1)	-	-	-	Asn-Ala IF	2	C_{1V} (1)	2
Asn-Arg	4	C_{1V} (1)	-	-	-	Asn-Arg IF	2	C_{1V} (1)	2
Asn-Asn	4	C_{1V} (1)	-	-	-	Asn-Asn IF	2	C_{1V} (1)	2
Asn-Asp	4	C_{1V} (1)	-	-	-	Asn-Asp IF	2	C_{1V} (1)	2
Asn-Cys	4	C_{1V} (1)	-	-	-	Asn-Cys IF	2	C_{1V} (1)	2
Asn-Gln	4	C_{1V} (1)	-	-	-	Asn-Gln IF	2	C_{1V} (1)	2
Asn-Glu	4	C_{1V} (1)	-	-	-	Asn-Glu IF	2	C_{1V} (1)	2
Asn-Gly	2	C_{1V} (1)	-	-	-	Asn-Gly IF	1	C_{1V} (1)	2
Asn-His	4	C_{1V} (1)	-	-	-	Asn-His IF	2	C_{1V} (1)	2
Asn-Ile	4	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	2

						Ile IF		(1)	
Asn-Leu	4	C_{1V} (1)	-	-	-	Asn-Leu IF	2	C_{1V} (1)	2
Asn-Lys	4	C_{1V} (1)	-	-	-	Asn-Lys IF	2	C_{1V} (1)	2
Asn-Met	4	C_{1V} (1)	-	-	-	Asn-Met IF	2	C_{1V} (1)	2
Asn-Phe	4	C_{1V} (1)	-	-	-	Asn-Phe IF	2	C_{1V} (1)	2
Asn-Ser	4	C_{1V} (1)	-	-	-	Asn-Ser IF	2	C_{1V} (1)	2
Asn-Thr	4	C_{1V} (1)	-	-	-	Asn-Thr IF	2	C_{1V} (1)	2
Asn-Trp	4	C_{1V} (1)	-	-	-	Asn-Trp IF	2	C_{1V} (1)	2
Asn-Tyr	4	C_{1V} (1)	-	-	-	Asn-Tyr IF	2	C_{1V} (1)	2
Asn-Val	4	C_{1V} (1)	-	-	-	Asn-Val IF	2	C_{1V} (1)	2
Reverse Direction									
P1	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**P2**	**$n_{chiral}^{prod,j}$**	**$\sigma_{sym}^{prod,j}$**	**TS**	**$n_{chiral}^{\neq}$**	**$\sigma^{\neq}$**	**rpd^{R}**
Asn-Ala Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ala IF	2	C_{1V} (1)	6
Asn-Arg Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Arg IF	2	C_{1V} (1)	6

Asn-Asn Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asn IF	2	C_{1V} (1)	6
Asn-Asp Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Asp IF	2	C_{1V} (1)	6
Asn-Cys Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Cys IF	2	C_{1V} (1)	6
Asn-Gln Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gln IF	2	C_{1V} (1)	6
Asn-Glu Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Glu IF	2	C_{1V} (1)	6
Asn-Gly Isoimide	2	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Gly IF	1	C_{1V} (1)	6
Asn-His Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-His IF	2	C_{1V} (1)	6
Asn-Ile Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Ile IF	2	C_{1V} (1)	6
Asn-Leu Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Leu IF	2	C_{1V} (1)	6
Asn-Lys Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Lys IF	2	C_{1V} (1)	6
Asn-Met Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Met IF	2	C_{1V} (1)	6
Asn-Phe Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Phe IF	2	C_{1V} (1)	6
Asn-Ser	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-	2	C_{1V}	6

Isoimide						Ser IF		(1)	
Asn-Thr Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Thr IF	2	C_{1V} (1)	6
Asn-Trp Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Trp IF	2	C_{1V} (1)	6
Asn-Tyr Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Tyr IF	2	C_{1V} (1)	6
Asn-Val Isoimide	4	C_{1V} (1)	NH_3	1	C_{3V} (3)	Asn-Val IF	2	C_{1V} (1)	6

Table S1.L. Reaction path degeneracies and symmetry numbers of the Asn-X Isoimide Hydrolysis into Asp-X Reaction (Implicit Solvation + 1 H_2O). This is a bimolecular elimination reaction in the forward direction and a unimolecular addition reaction in the reverse direction. As such, in the forward direction: Δn is -1 and the units of V_m are $L.mol^{-1}.s^{-1}$; in the reverse direction: Δn is 0 and the units of V_m are s^{-1}. The addition of the explicit H_2O in our solvation methodology is accounted for by doubling the reaction path degeneracy in both the forward and reverse directions.

Forward Direction									
R1	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**R2**	$\mathbf{n_{chiral}^{react,j}}$	$\mathbf{\sigma_{sym}^{react,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^F}$
Asn-Ala Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ala IHD	2	C_{1V} (1)	4
Asn-Arg Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Arg IHD	2	C_{1V} (1)	4
Asn-Asn Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asn IHD	2	C_{1V} (1)	4

Asn-Asp Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Asp IHD	2	C_{1V} (1)	4
Asn-Cys Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Cys IHD	2	C_{1V} (1)	4
Asn-Gln Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gln IHD	2	C_{1V} (1)	4
Asn-Glu Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Glu IHD	2	C_{1V} (1)	4
Asn-Gly Isoimide	2	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Gly IHD	1	C_{1V} (1)	4
Asn-His Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-His IHD	2	C_{1V} (1)	4
Asn-Ile Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ile IHD	2	C_{1V} (1)	4
Asn-Leu Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Leu IHD	2	C_{1V} (1)	4
Asn-Lys	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-	2	C_{1V}	4

Isoimide						Lys IHD		(1)	
Asn-Met Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Met IHD	2	C_{1V} (1)	4
Asn-Phe Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Phe IHD	2	C_{1V} (1)	4
Asn-Ser Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Ser IHD	2	C_{1V} (1)	4
Asn-Thr Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Thr IHD	2	C_{1V} (1)	4
Asn-Trp Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Trp IHD	2	C_{1V} (1)	4
Asn-Tyr Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Tyr IHD	2	C_{1V} (1)	4
Asn-Val Isoimide	4	C_{1V} (1)	H_2O	1	C_{2V} (2)	Asn-Val IHD	2	C_{1V} (1)	4
Reverse Direction									
P1	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**P2**	$\mathbf{n_{chiral}^{prod,j}}$	$\mathbf{\sigma_{sym}^{prod,j}}$	**TS**	$\mathbf{n_{chiral}^{\neq}}$	$\mathbf{\sigma^{\neq}}$	$\mathbf{rpd^{R}}$

Asp-Ala	4	C_{1V} (1)	-	-	-	Asn-Ala IHD	2	C_{1V} (1)	2
Asp-Arg	4	C_{1V} (1)	-	-	-	Asn-Arg IHD	2	C_{1V} (1)	2
Asp-Asn	4	C_{1V} (1)	-	-	-	Asn-Asn IHD	2	C_{1V} (1)	2
Asp-Asp	4	C_{1V} (1)	-	-	-	Asn-Asp IHD	2	C_{1V} (1)	2
Asp-Cys	4	C_{1V} (1)	-	-	-	Asn-Cys IHD	2	C_{1V} (1)	2
Asp-Gln	4	C_{1V} (1)	-	-	-	Asn-Gln IHD	2	C_{1V} (1)	2
Asp-Glu	4	C_{1V} (1)	-	-	-	Asn-Glu SIHD	2	C_{1V} (1)	2
Asp-Gly	2	C_{1V} (1)	-	-	-	Asn-Gly IHD	1	C_{1V} (1)	2
Asp-His	4	C_{1V} (1)	-	-	-	Asn-	2	C_{1V}	2

						His IHD		(1)	
Asp-Ile	4	C_{1V} (1)	-	-	-	Asn-Ile IHD	2	C_{1V} (1)	2
Asp-Leu	4	C_{1V} (1)	-	-	-	Asn-Leu IHD	2	C_{1V} (1)	2
Asp-Lys	4	C_{1V} (1)	-	-	-	Asn-Lys IHD	2	C_{1V} (1)	2
Asp-Met	4	C_{1V} (1)	-	-	-	Asn-Met IHD	2	C_{1V} (1)	2
Asp-Phe	4	C_{1V} (1)	-	-	-	Asn-Phe IHD	2	C_{1V} (1)	2
Asp-Ser	4	C_{1V} (1)	-	-	-	Asn-Ser IHD	2	C_{1V} (1)	2
Asp-Thr	4	C_{1V} (1)	-	-	-	Asn-Thr IHD	2	C_{1V} (1)	2
Asp-Trp	4	C_{1V} (1)	-	-	-	Asn-Trp	2	C_{1V} (1)	2

						IHD			
Asp-Tyr	4	C_{1V} (1)	-	-	-	Asn-Tyr IHD	2	C_{1V} (1)	2
Asp-Val	4	C_{1V} (1)	-	-	-	Asn-Val IHD	2	C_{1V} (1)	2

Thermochemistry and Arrhenius Parameters (Implicit Solvation)

Table S2.A. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	4.083	3.878	-0.689
Asn-Arg	1	1	4.528	3.873	-2.196
Asn-Asn	0	1	4.140	3.926	-0.719
Asn-Asp	-1	1	4.037	3.837	-0.670
Asn-Cys	0	1	1.894	1.408	-1.629
Asn-Gln	0	1	6.158	5.571	-1.970
Asn-Glu	-1	1	4.614	5.987	4.604
Asn-Gly	0	1	3.271	2.515	-2.534
Asn-His	0	1	3.927	4.204	0.929
Asn-Ile	0	1	6.821	7.166	1.159
Asn-Leu	0	1	3.714	2.743	-3.255
Asn-Lys	1	1	6.887	6.847	-0.134
Asn-Met	0	1	3.759	2.958	-2.687
Asn-Phe	0	1	6.820	5.993	-2.775
Asn-Pro	0	1	6.755	7.377	2.085
Asn-Ser	0	1	0.345	0.254	-0.303
Asn-Thr	0	1	6.982	6.687	-0.988
Asn-Trp	0	1	6.770	6.319	-1.510
Asn-Tyr	0	1	4.256	4.160	-0.322
Asn-Val	0	1	3.383	3.922	1.808
Average			**4.657**	**4.481**	**-0.590**

Table S2.B. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.17	42.58	6.080
Asn-Arg	1	1	45.73	45.01	5.870
Asn-Asn	0	1	41.13	41.63	6.450
Asn-Asp	-1	1	35.53	36.15	6.990
Asn-Cys	0	1	35.83	36.12	6.660
Asn-Gln	0	1	41.92	42.43	6.530
Asn-Glu	-1	1	45.66	46.61	7.710
Asn-Gly	0	1	39.80	40.59	6.830
Asn-His	0	1	42.81	43.38	6.530
Asn-Ile	0	1	42.84	41.87	5.910
Asn-Leu	0	1	43.08	42.16	6.020
Asn-Lys	1	1	41.12	41.71	6.350

Asn-Met	0	1	42.50	43.08	6.730
Asn-Phe	0	1	43.37	44.08	7.190
Asn-Pro	0	1	12.09	14.48	10.38
Asn-Ser	0	1	41.74	42.56	8.190
Asn-Thr	0	1	46.03	45.54	6.610
Asn-Trp	0	1	41.14	41.57	6.210
Asn-Tyr	0	1	43.27	43.80	6.310
Asn-Val	0	1	36.56	36.99	6.820
Average			**40.22**	**40.62**	**6.819**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	37.71	38.69	6.600
Asn-Arg	1	1	41.04	41.04	6.740
Asn-Asn	0	1	36.67	37.69	6.960
Asn-Asp	-1	1	31.37	32.40	7.470
Asn-Cys	0	1	33.49	34.57	7.410
Asn-Gln	0	1	35.75	36.81	7.310
Asn-Glu	-1	1	39.63	40.77	6.990
Asn-Gly	0	1	36.40	37.94	7.770
Asn-His	0	1	38.12	39.20	6.680
Asn-Ile	0	1	35.29	34.75	5.990
Asn-Leu	0	1	39.60	39.35	7.110
Asn-Lys	1	1	33.92	34.89	6.690
Asn-Met	0	1	38.85	40.07	7.690
Asn-Phe	0	1	36.69	38.02	8.150
Asn-Pro	0	1	4.620	7.210	10.20
Asn-Ser	0	1	40.53	42.33	8.770
Asn-Thr	0	1	38.81	38.84	7.180
Asn-Trp	0	1	34.23	35.22	6.900
Asn-Tyr	0	1	38.57	39.64	6.740
Asn-Val	0	1	32.19	33.10	6.770
Average			**35.17**	**36.13**	**7.306**

Table S2.C. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	4.571	4.758	0.629
Asn-Arg	1	1	4.983	4.103	-2.951
Asn-Asn	0	1	4.774	4.740	-0.112
Asn-Asp	-1	1	4.544	4.756	0.711
Asn-Cys	0	1	2.073	1.918	-0.519
Asn-Gln	0	1	6.123	6.072	-0.171
Asn-Glu	-1	1	3.415	3.256	-0.531
Asn-Gly	0	1	3.625	3.124	-1.678
Asn-His	0	1	4.794	4.958	0.551
Asn-Ile	0	1	6.952	7.374	1.418

Asn-Leu	0	1	4.387	3.722	-2.231
Asn-Lys	1	1	6.816	6.613	-0.678
Asn-Met	0	1	4.477	4.024	-1.522
Asn-Phe	0	1	7.196	6.273	-3.096
Asn-Pro	0	1	6.388	6.132	-0.860
Asn-Ser	0	1	0.250	0.176	-0.248
Asn-Thr	0	1	7.110	6.806	-1.019
Asn-Trp	0	1	6.492	6.553	0.206
Asn-Tyr	0	1	5.031	4.847	-0.616
Asn-Val	0	1	4.337	4.777	1.474
Average			**4.917**	**4.749**	**-0.562**

Table S2.D. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	41.47	42.05	6.670
Asn-Arg	1	1	45.74	44.88	5.540
Asn-Asn	0	1	41.34	41.95	6.550
Asn-Asp	-1	1	36.52	37.06	7.080
Asn-Cys	0	1	36.13	36.56	6.960
Asn-Gln	0	1	41.38	42.03	7.050
Asn-Glu	-1	1	41.92	42.61	6.860
Asn-Gly	0	1	39.43	40.34	7.140
Asn-His	0	1	42.41	43.07	6.710
Asn-Ile	0	1	42.91	41.91	5.840
Asn-Leu	0	1	42.83	41.86	5.970
Asn-Lys	1	1	40.77	41.52	6.680
Asn-Met	0	1	41.87	42.53	7.080
Asn-Phe	0	1	42.76	43.58	7.310
Asn-Pro	0	1	11.82	13.78	9.230
Asn-Ser	0	1	41.51	42.43	8.130
Asn-Thr	0	1	46.29	45.81	6.820
Asn-Trp	0	1	40.74	41.32	6.530
Asn-Tyr	0	1	42.21	42.8	6.100
Asn-Val	0	1	36.97	37.51	6.930
Average			**39.85**	**40.28**	**6.859**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	36.24	37.32	6.880
Asn-Arg	1	1	40.85	40.68	6.560
Asn-Asn	0	1	36.14	37.23	6.920
Asn-Asp	-1	1	31.26	32.32	7.280
Asn-Cys	0	1	33.34	34.51	7.460
Asn-Gln	0	1	34.79	35.96	7.440
Asn-Glu	-1	1	37.94	39.29	7.350

Asn-Gly	0	1	35.50	37.11	7.880
Asn-His	0	1	36.98	38.13	6.940
Asn-Ile	0	1	35.22	34.62	5.860
Asn-Leu	0	1	38.47	38.10	6.820
Asn-Lys	1	1	33.82	34.93	7.130
Asn-Met	0	1	37.24	38.49	7.780
Asn-Phe	0	1	35.80	37.24	8.340
Asn-Pro	0	1	5.080	7.610	9.770
Asn-Ser	0	1	40.35	42.27	8.700
Asn-Thr	0	1	38.91	38.99	7.400
Asn-Trp	0	1	33.71	34.79	6.840
Asn-Tyr	0	1	36.84	37.96	6.590
Asn-Val	0	1	31.75	32.77	6.960
Average			**34.51**	**35.52**	**7.345**

Table S2.E. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	4.663	4.876	0.714
Asn-Arg	1	1	5.367	4.118	-4.190
Asn-Asn	0	1	4.689	4.856	0.561
Asn-Asp	-1	1	4.840	4.840	0.000
Asn-Cys	0	1	2.088	1.989	-0.335
Asn-Gln	0	1	6.099	6.159	0.202
Asn-Glu	-1	1	3.566	3.401	-0.551
Asn-Gly	0	1	3.648	3.204	-1.489
Asn-His	0	1	4.960	5.061	0.339
Asn-Ile	0	1	7.087	7.399	1.049
Asn-Leu	0	1	4.489	3.852	-2.135
Asn-Lys	1	1	6.642	6.581	-0.205
Asn-Met	0	1	4.564	4.171	-1.317
Asn-Phe	0	1	7.245	6.303	-3.159
Asn-Pro	0	1	6.412	6.128	-0.951
Asn-Ser	0	1	0.275	0.166	-0.368
Asn-Thr	0	1	7.162	6.825	-1.130
Asn-Trp	0	1	6.553	6.581	0.093
Asn-Tyr	0	1	4.980	4.944	-0.119
Asn-Val	0	1	4.518	4.890	1.248
Average			**4.992**	**4.817**	**-0.587**

Table S2.F. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 40)

Forward

Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	41.36	41.96	6.710
Asn-Arg	1	1	45.75	44.85	5.020
Asn-Asn	0	1	41.21	41.84	6.610
Asn-Asp	-1	1	36.78	37.31	6.940
Asn-Cys	0	1	36.68	37.24	7.400
Asn-Gln	0	1	41.44	42.03	6.660
Asn-Glu	-1	1	41.81	42.53	7.010
Asn-Gly	0	1	39.38	40.28	7.070
Asn-His	0	1	42.26	42.93	6.740
Asn-Ile	0	1	42.91	41.91	5.850
Asn-Leu	0	1	42.79	41.81	5.950
Asn-Lys	1	1	40.71	41.47	6.730
Asn-Met	0	1	41.77	42.43	7.060
Asn-Phe	0	1	42.63	43.48	7.340
Asn-Pro	0	1	11.88	13.83	9.200
Asn-Ser	0	1	41.38	41.43	6.480
Asn-Thr	0	1	46.34	45.85	6.800
Asn-Trp	0	1	40.67	41.27	6.560
Asn-Tyr	0	1	42.03	42.64	6.110
Asn-Val	0	1	37.02	37.56	6.920
Average			**39.84**	**40.23**	**6.758**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	36.02	37.11	6.910
Asn-Arg	1	1	40.78	40.60	6.320
Asn-Asn	0	1	35.94	37.02	6.830
Asn-Asp	-1	1	31.39	32.46	7.300
Asn-Cys	0	1	33.82	35.13	7.860
Asn-Gln	0	1	34.80	35.89	6.970
Asn-Glu	-1	1	37.69	39.06	7.500
Asn-Gly	0	1	35.38	36.97	7.770
Asn-His	0	1	36.73	37.89	7.020
Asn-Ile	0	1	35.19	34.59	5.950
Asn-Leu	0	1	38.31	37.93	6.780
Asn-Lys	1	1	33.82	34.92	7.070
Asn-Met	0	1	37.01	38.25	7.720
Asn-Phe	0	1	35.65	37.11	8.400
Asn-Pro	0	1	5.140	7.660	9.770
Asn-Ser	0	1	40.23	41.27	7.080
Asn-Thr	0	1	38.93	39.01	7.410
Asn-Trp	0	1	33.61	34.72	6.900
Asn-Tyr	0	1	36.60	37.71	6.490
Asn-Val	0	1	31.67	32.71	7.000
Average			**34.44**	**35.40**	**7.253**

Table S2.G. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	4.705	4.935	0.771
Asn-Arg	1	1	5.385	4.115	-4.260
Asn-Asn	0	1	4.654	4.913	0.869
Asn-Asp	-1	1	4.754	4.896	0.474
Asn-Cys	0	1	2.117	2.017	-0.335
Asn-Gln	0	1	6.076	6.203	0.424
Asn-Glu	-1	1	3.897	3.473	-1.422
Asn-Gly	0	1	3.668	3.241	-1.433
Asn-His	0	1	5.041	5.110	0.233
Asn-Ile	0	1	7.157	7.410	0.850
Asn-Leu	0	1	4.538	3.916	-2.085
Asn-Lys	1	1	6.502	6.568	0.222
Asn-Met	0	1	4.644	4.237	-1.367
Asn-Phe	0	1	7.254	6.318	-3.138
Asn-Pro	0	1	6.373	6.130	-0.816
Asn-Ser	0	1	0.309	0.166	-0.480
Asn-Thr	0	1	7.143	6.843	-1.006
Asn-Trp	0	1	6.544	6.592	0.162
Asn-Tyr	0	1	4.853	4.995	0.477
Asn-Val	0	1	4.606	4.945	1.136
Average			**5.011**	**4.851**	**-0.536**

Table S2.H. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	41.30	41.91	6.740
Asn-Arg	1	1	45.61	44.77	4.980
Asn-Asn	0	1	41.15	41.79	6.650
Asn-Asp	-1	1	36.87	37.42	7.060
Asn-Cys	0	1	36.65	37.21	7.180
Asn-Gln	0	1	41.30	41.96	6.940
Asn-Glu	-1	1	41.78	42.50	6.820
Asn-Gly	0	1	39.34	40.25	7.070
Asn-His	0	1	42.17	42.86	6.760
Asn-Ile	0	1	42.91	41.91	5.860
Asn-Leu	0	1	42.77	41.79	5.950
Asn-Lys	1	1	40.66	41.44	6.800
Asn-Met	0	1	41.72	42.38	7.040
Asn-Phe	0	1	42.56	43.42	7.360
Asn-Pro	0	1	11.90	13.86	9.230

Asn-Ser	0	1	36.47	36.73	6.580
Asn-Thr	0	1	46.37	45.88	6.830
Asn-Trp	0	1	40.65	41.25	6.570
Asn-Tyr	0	1	41.91	42.55	6.230
Asn-Val	0	1	37.05	37.59	6.920
Average			**39.56**	**39.97**	**6.779**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	35.91	37.01	6.930
Asn-Arg	1	1	40.75	40.56	6.270
Asn-Asn	0	1	35.83	36.92	6.800
Asn-Asp	-1	1	31.45	32.53	7.310
Asn-Cys	0	1	33.77	35.07	7.640
Asn-Gln	0	1	34.62	35.78	7.190
Asn-Glu	-1	1	37.56	38.94	7.510
Asn-Gly	0	1	35.31	36.90	7.760
Asn-His	0	1	36.58	37.76	7.060
Asn-Ile	0	1	35.17	34.57	6.010
Asn-Leu	0	1	38.23	37.84	6.760
Asn-Lys	1	1	33.8	34.91	7.040
Asn-Met	0	1	36.89	38.14	7.710
Asn-Phe	0	1	35.57	37.04	8.410
Asn-Pro	0	1	5.160	7.690	9.760
Asn-Ser	0	1	35.3	36.57	7.210
Asn-Thr	0	1	38.94	39.02	7.420
Asn-Trp	0	1	33.58	34.69	6.890
Asn-Tyr	0	1	36.46	37.58	6.470
Asn-Val	0	1	31.64	32.67	7.030
Average			**34.13**	**35.11**	**7.259**

Table S3.A. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-2.044	7.265	31.22
Asn-Arg	1	1	-2.767	6.890	32.39
Asn-Asn	0	1	-3.025	6.511	31.99
Asn-Asp	-1	1	-3.308	6.515	32.94
Asn-Cys	0	1	-3.840	4.799	28.97
Asn-Gln	0	1	-2.259	7.465	32.62
Asn-Glu	-1	1	0.467	11.05	35.50
Asn-Gly	0	1	-3.861	5.590	31.70
Asn-His	0	1	-2.626	6.469	30.50
Asn-Ile	0	1	0.986	10.41	31.60
Asn-Leu	0	1	-2.359	7.172	31.97
Asn-Lys	1	1	-2.543	7.322	33.09
Asn-Met	0	1	-2.054	6.997	30.36

Asn-Phe	0	1	-1.431	8.309	32.67
Asn-Ser	0	1	-1.607	9.095	35.89
Asn-Thr	0	1	2.526	12.06	31.97
Asn-Trp	0	1	-1.688	7.635	31.27
Asn-Tyr	0	1	-2.778	6.993	32.77
Asn-Val	0	1	0.751	10.54	32.83
Average			**-1.761**	**7.846**	**32.22**

Table S3.B. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	48.99	47.32	9.970
Asn-Arg	1	1	31.21	30.49	10.30
Asn-Asn	0	1	40.94	40.79	11.29
Asn-Asp	-1	1	45.33	45.01	10.47
Asn-Cys	0	1	46.28	44.76	9.920
Asn-Gln	0	1	48.65	47.26	10.29
Asn-Glu	-1	1	45.34	44.83	10.70
Asn-Gly	0	1	48.02	46.72	10.93
Asn-His	0	1	48.13	46.73	10.10
Asn-Ile	0	1	43.10	42.93	11.31
Asn-Leu	0	1	48.47	46.88	9.930
Asn-Lys	1	1	17.44	16.69	9.770
Asn-Met	0	1	48.39	48.23	11.53
Asn-Phe	0	1	47.35	46.97	10.87
Asn-Ser	0	1	53.09	51.54	10.36
Asn-Thr	0	1	43.40	41.20	9.520
Asn-Trp	0	1	39.57	39.15	10.65
Asn-Tyr	0	1	45.49	43.87	9.780
Asn-Val	0	1	47.00	46.74	11.05
Average			**44.01**	**43.06**	**10.46**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.07	41.68	6.280
Asn-Arg	1	1	24.66	25.20	6.350
Asn-Asn	0	1	34.92	35.94	7.410
Asn-Asp	-1	1	39.52	40.20	6.350
Asn-Cys	0	1	41.60	41.44	6.710
Asn-Gln	0	1	41.68	41.44	6.270
Asn-Glu	-1	1	35.32	35.58	5.960
Asn-Gly	0	1	42.76	42.74	7.140
Asn-His	0	1	42.06	41.89	6.550
Asn-Ile	0	1	33.06	34.13	7.520
Asn-Leu	0	1	41.80	41.35	6.040
Asn-Lys	1	1	10.71	11.06	5.640

Asn-Met	0	1	41.75	42.83	8.020
Asn-Phe	0	1	39.47	40.30	6.850
Asn-Ser	0	1	44.78	44.22	5.600
Asn-Thr	0	1	31.71	30.76	5.660
Asn-Trp	0	1	32.35	33.14	6.940
Asn-Tyr	0	1	38.98	38.53	5.730
Asn-Val	0	1	36.95	37.86	6.990
Average			**36.64**	**36.86**	**6.527**

Table S3.C. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation, ε =20)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-2.763	6.929	32.51
Asn-Arg	1	1	-2.381	6.437	29.57
Asn-Asn	0	1	-3.312	6.339	32.37
Asn-Asp	-1	1	-4.128	5.715	33.01
Asn-Cys	0	1	-4.477	4.418	29.83
Asn-Gln	0	1	-2.654	7.272	33.29
Asn-Glu	-1	1	-2.440	6.543	30.13
Asn-Gly	0	1	-4.470	5.327	32.86
Asn-His	0	1	-3.045	6.058	30.53
Asn-Ile	0	1	0.591	10.12	31.97
Asn-Leu	0	1	-2.820	6.747	32.09
Asn-Lys	1	1	-3.084	6.618	32.54
Asn-Met	0	1	-2.662	6.616	31.12
Asn-Phe	0	1	-1.934	7.953	33.16
Asn-Ser	0	1	-3.043	8.287	38.00
Asn-Thr	0	1	1.675	11.24	32.07
Asn-Trp	0	1	-2.112	7.291	31.54
Asn-Tyr	0	1	-2.811	6.430	30.99
Asn-Val	0	1	0.489	10.25	32.75
Average			**-2.388**	**7.189**	**32.12**

Table S3.D. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε =20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	48.57	46.91	10.26
Asn-Arg	1	1	30.09	29.26	9.620
Asn-Asn	0	1	40.30	39.73	10.78
Asn-Asp	-1	1	42.56	42.27	11.10
Asn-Cys	0	1	46.12	44.58	10.13
Asn-Gln	0	1	48.12	46.67	10.17

Asn-Glu	-1	1	39.82	38.91	9.740
Asn-Gly	0	1	47.21	45.86	10.90
Asn-His	0	1	47.26	45.82	10.08
Asn-Ile	0	1	41.99	41.82	11.32
Asn-Leu	0	1	48.11	46.49	10.01
Asn-Lys	1	1	17.54	16.72	9.330
Asn-Met	0	1	45.67	45.55	11.64
Asn-Phe	0	1	44.93	44.62	11.16
Asn-Ser	0	1	47.90	46.34	10.49
Asn-Thr	0	1	50.22	48.78	10.51
Asn-Trp	0	1	36.69	36.30	10.78
Asn-Tyr	0	1	47.78	46.13	9.660
Asn-Val	0	1	43.22	42.79	10.76
Average			**42.85**	**41.87**	**10.44**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.03	41.63	6.290
Asn-Arg	1	1	23.86	24.35	6.280
Asn-Asn	0	1	34.47	35.06	6.820
Asn-Asp	-1	1	37.31	38.22	7.010
Asn-Cys	0	1	41.84	41.65	6.740
Asn-Gln	0	1	41.33	41.05	6.010
Asn-Glu	-1	1	33.57	33.94	6.280
Asn-Gly	0	1	42.28	42.18	6.850
Asn-His	0	1	41.60	41.39	6.530
Asn-Ile	0	1	32.28	33.33	7.460
Asn-Leu	0	1	41.82	41.38	6.110
Asn-Lys	1	1	11.53	11.80	5.310
Asn-Met	0	1	39.43	40.55	7.960
Asn-Phe	0	1	37.43	38.32	7.040
Asn-Ser	0	1	40.49	39.87	5.270
Asn-Thr	0	1	39.28	39.14	6.630
Asn-Trp	0	1	29.83	30.65	7.020
Asn-Tyr	0	1	41.73	41.32	6.010
Asn-Val	0	1	33.45	34.20	6.730
Average			**36.08**	**36.32**	**6.545**

Table S3.E. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation, ε =40)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-2.831	6.890	32.60
Asn-Arg	1	1	-1.937	6.365	27.85
Asn-Asn	0	1	-3.470	6.329	32.87
Asn-Asp	-1	1	-3.927	5.736	32.41
Asn-Cys	0	1	-4.578	4.375	30.03
Asn-Gln	0	1	-2.690	7.278	33.43

Asn-Glu	-1	1	-2.431	6.445	29.77
Asn-Gly	0	1	-4.590	5.304	33.18
Asn-His	0	1	-3.072	6.015	30.48
Asn-Ile	0	1	0.546	10.09	32.02
Asn-Leu	0	1	-2.856	6.696	32.04
Asn-Lys	1	1	-3.266	6.528	32.85
Asn-Met	0	1	-2.731	6.573	31.20
Asn-Phe	0	1	-1.987	7.909	33.19
Asn-Ser	0	1	-2.663	8.208	36.46
Asn-Thr	0	1	1.625	11.14	31.92
Asn-Trp	0	1	-2.162	7.251	31.57
Asn-Tyr	0	1	-2.957	6.361	31.25
Asn-Val	0	1	0.470	10.22	32.70
Average			**-2.395**	**7.143**	**31.99**

Table S3.F. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε =40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	48.51	46.86	10.28
Asn-Arg	1	1	29.98	29.10	9.280
Asn-Asn	0	1	40.09	39.52	10.80
Asn-Asp	-1	1	42.14	41.87	11.08
Asn-Cys	0	1	46.09	44.56	10.18
Asn-Gln	0	1	48.03	46.57	10.16
Asn-Glu	-1	1	39.36	38.51	9.880
Asn-Gly	0	1	47.09	45.74	10.90
Asn-His	0	1	47.16	45.70	10.06
Asn-Ile	0	1	41.82	41.65	11.34
Asn-Leu	0	1	48.06	46.44	10.01
Asn-Lys	1	1	17.52	16.71	9.400
Asn-Met	0	1	45.25	45.14	11.73
Asn-Phe	0	1	44.57	44.26	11.21
Asn-Ser	0	1	47.85	46.29	10.43
Asn-Thr	0	1	50.32	48.88	10.47
Asn-Trp	0	1	36.32	35.91	10.77
Asn-Tyr	0	1	47.81	46.18	9.710
Asn-Val	0	1	42.69	42.28	10.88
Average			**42.67**	**41.69**	**10.45**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.02	41.62	6.300
Asn-Arg	1	1	23.71	24.21	6.320
Asn-Asn	0	1	34.30	34.87	6.730
Asn-Asp	-1	1	36.84	37.78	7.130
Asn-Cys	0	1	41.87	41.68	6.740

Asn-Gln	0	1	41.24	40.95	5.970
Asn-Glu	-1	1	33.18	33.63	6.500
Asn-Gly	0	1	42.20	42.09	6.790
Asn-His	0	1	41.54	41.31	6.520
Asn-Ile	0	1	32.14	33.19	7.460
Asn-Leu	0	1	41.81	41.37	6.120
Asn-Lys	1	1	11.61	11.88	5.320
Asn-Met	0	1	39.05	40.18	8.040
Asn-Phe	0	1	37.11	38.01	7.080
Asn-Ser	0	1	40.46	39.87	5.560
Asn-Thr	0	1	39.47	39.33	6.630
Asn-Trp	0	1	29.48	30.30	6.990
Asn-Tyr	0	1	41.85	41.44	5.990
Asn-Val	0	1	32.94	33.72	6.860
Average			**35.94**	**36.18**	**6.582**

Table S3.G. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation, ε =80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-2.865	6.870	32.65
Asn-Arg	1	1	-1.902	6.321	27.58
Asn-Asn	0	1	-3.548	6.328	33.13
Asn-Asp	-1	1	-4.051	5.760	32.90
Asn-Cys	0	1	-4.618	4.352	30.08
Asn-Gln	0	1	-2.689	7.282	33.44
Asn-Glu	-1	1	-2.172	6.418	28.81
Asn-Gly	0	1	-4.643	5.292	33.32
Asn-His	0	1	-3.077	5.993	30.42
Asn-Ile	0	1	0.521	10.08	32.05
Asn-Leu	0	1	-2.874	6.672	32.02
Asn-Lys	1	1	-3.380	6.486	33.09
Asn-Met	0	1	-2.767	6.551	31.25
Asn-Phe	0	1	-2.009	7.887	33.19
Asn-Ser	0	1	-2.525	8.176	35.89
Asn-Thr	0	1	1.564	11.10	31.99
Asn-Trp	0	1	-2.171	7.231	31.53
Asn-Tyr	0	1	-3.109	6.329	31.65
Asn-Val	0	1	0.460	10.20	32.68
Average			**-2.413**	**7.123**	**31.98**

Table S3.H. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε =80)

Forward

Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	48.49	46.83	10.3
Asn-Arg	1	1	29.77	28.95	9.23
Asn-Asn	0	1	39.97	39.40	10.82
Asn-Asp	-1	1	41.9	41.65	11.25
Asn-Cys	0	1	46.08	44.55	10.19
Asn-Gln	0	1	47.98	46.52	10.16
Asn-Glu	-1	1	39.25	38.35	9.310
Asn-Gly	0	1	47.03	45.68	10.92
Asn-His	0	1	47.11	45.64	10.04
Asn-Ile	0	1	41.73	41.56	11.36
Asn-Leu	0	1	48.04	46.41	10.01
Asn-Lys	1	1	17.51	16.71	9.45
Asn-Met	0	1	45.03	44.93	11.91
Asn-Phe	0	1	44.38	44.08	11.24
Asn-Ser	0	1	47.84	46.27	10.40
Asn-Thr	0	1	50.38	48.93	10.49
Asn-Trp	0	1	36.13	35.72	10.74
Asn-Tyr	0	1	47.82	46.20	9.800
Asn-Val	0	1	42.41	42.03	10.95
Average			**42.57**	**41.60**	**10.45**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.01	41.61	6.310
Asn-Arg	1	1	23.64	24.14	6.320
Asn-Asn	0	1	34.19	34.76	6.690
Asn-Asp	-1	1	36.59	37.55	7.190
Asn-Cys	0	1	41.89	41.69	6.740
Asn-Gln	0	1	41.19	40.89	5.960
Asn-Glu	-1	1	33.07	33.48	6.140
Asn-Gly	0	1	42.16	42.04	6.770
Asn-His	0	1	41.51	41.27	6.510
Asn-Ile	0	1	32.07	33.12	7.470
Asn-Leu	0	1	41.81	41.37	6.130
Asn-Lys	1	1	11.65	11.93	5.320
Asn-Met	0	1	38.85	40.00	8.200
Asn-Phe	0	1	36.94	37.86	7.110
Asn-Ser	0	1	40.44	39.86	5.650
Asn-Thr	0	1	39.56	39.43	6.640
Asn-Trp	0	1	29.31	30.13	6.980
Asn-Tyr	0	1	41.91	41.50	6.000
Asn-Val	0	1	32.68	33.48	6.930
Average			**35.87**	**36.11**	**6.582**

Table S4.A. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	12.37	0.828	-38.70
Asn-Arg	1	1	6.889	-2.494	-31.47
Asn-Asn	0	1	8.481	-1.184	-32.42
Asn-Asp	-1	1	9.951	-0.415	-34.77
Asn-Cys	0	1	8.884	0.147	-29.30
Asn-Gln	0	1	8.082	-1.903	-33.49
Asn-Glu	-1	1	15.12	4.313	-36.26
Asn-Gly	0	1	14.18	3.607	-35.45
Asn-His	0	1	9.720	0.426	-31.17
Asn-Ile	0	1	6.142	-4.464	-35.57
Asn-Leu	0	1	8.579	-1.640	-34.27
Asn-Lys	1	1	7.655	-1.647	-31.20
Asn-Met	0	1	7.602	-2.280	-33.14
Asn-Phe	0	1	10.80	0.729	-33.77
Asn-Ser	0	1	12.31	3.378	-29.96
Asn-Thr	0	1	8.078	-2.193	-34.45
Asn-Trp	0	1	11.05	1.411	-32.31
Asn-Tyr	0	1	4.399	-6.916	-37.95
Asn-Val	0	1	8.591	-1.220	-32.90
Average			**9.414**	**-0.606**	**-33.609**

Table S4.B. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	10.26	10.53	6.300
Asn-Arg	1	1	14.81	14.62	4.970
Asn-Asn	0	1	13.99	14.70	7.050
Asn-Asp	-1	1	10.66	10.62	5.640
Asn-Cys	0	1	14.07	14.28	6.390
Asn-Gln	0	1	14.16	14.40	5.450
Asn-Glu	-1	1	12.69	12.71	5.740
Asn-Gly	0	1	14.21	14.58	6.190
Asn-His	0	1	13.57	14.16	6.750
Asn-Ile	0	1	14.36	14.94	6.690
Asn-Leu	0	1	12.46	12.62	5.920
Asn-Lys	1	1	14.58	14.97	6.160
Asn-Met	0	1	11.06	11.52	6.790
Asn-Phe	0	1	14.76	14.92	5.620
Asn-Ser	0	1	17.11	17.60	6.230
Asn-Thr	0	1	14.77	15.51	6.860
Asn-Trp	0	1	13.44	13.66	5.890
Asn-Tyr	0	1	16.84	16.84	5.710
Asn-Val	0	1	11.78	11.64	5.530

Average			13.66	13.94	6.099
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	7.740	7.870	12.11
Asn-Arg	1	1	16.29	15.46	9.090
Asn-Asn	0	1	14.12	14.24	11.38
Asn-Asp	-1	1	9.950	9.340	10.49
Asn-Cys	0	1	13.10	12.61	10.05
Asn-Gln	0	1	15.02	14.63	10.01
Asn-Glu	-1	1	7.080	6.660	10.95
Asn-Gly	0	1	9.310	9.170	11.17
Asn-His	0	1	12.21	12.09	10.78
Asn-Ile	0	1	17.70	17.69	11.71
Asn-Leu	0	1	12.93	12.55	10.66
Asn-Lys	1	1	15.35	15.05	10.23
Asn-Met	0	1	12.34	12.17	11.29
Asn-Phe	0	1	12.94	12.46	10.22
Asn-Ser	0	1	13.15	12.66	9.930
Asn-Thr	0	1	15.67	15.92	11.64
Asn-Trp	0	1	10.95	10.53	10.17
Asn-Tyr	0	1	22.14	21.97	11.36
Asn-Val	0	1	12.01	11.22	9.970
Average			**13.16**	**12.86**	**10.70**

Table S4.C. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 20)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	12.18	0.564	-38.96
Asn-Arg	1	1	8.028	-1.229	-31.05
Asn-Asn	0	1	9.231	-0.274	-31.88
Asn-Asp	-1	1	10.35	0.372	-33.45
Asn-Cys	0	1	9.595	0.691	-29.86
Asn-Gln	0	1	9.034	-1.208	-34.35
Asn-Glu	-1	1	16.78	7.920	-29.72
Asn-Gly	0	1	14.71	3.990	-35.96
Asn-His	0	1	9.836	1.079	-29.37
Asn-Ile	0	1	6.698	-3.714	-34.92
Asn-Leu	0	1	9.364	-0.855	-34.28
Asn-Lys	1	1	7.633	-1.816	-31.69
Asn-Met	0	1	8.437	-1.115	-32.03
Asn-Phe	0	1	11.93	1.326	-35.56
Asn-Ser	0	1	10.95	0.308	-35.71
Asn-Thr	0	1	8.735	-1.523	-34.41
Asn-Trp	0	1	12.40	2.182	-34.28
Asn-Tyr	0	1	5.132	-5.711	-36.37
Asn-Val	0	1	8.217	-1.467	-32.48

Average			**9.960**	**-0.025**	**-33.49**

Table S4.D. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.49	11.76	6.290
Asn-Arg	1	1	15.47	15.26	5.200
Asn-Asn	0	1	14.36	15.05	6.820
Asn-Asp	-1	1	12.03	11.90	5.120
Asn-Cys	0	1	15.21	15.43	6.410
Asn-Gln	0	1	14.34	14.56	5.420
Asn-Glu	-1	1	13.63	13.70	5.870
Asn-Gly	0	1	14.43	14.76	6.100
Asn-His	0	1	13.70	14.28	6.760
Asn-Ile	0	1	15.03	15.62	6.660
Asn-Leu	0	1	13.31	13.50	6.000
Asn-Lys	1	1	14.59	6.960	15.16
Asn-Met	0	1	12.46	12.99	6.940
Asn-Phe	0	1	15.18	15.33	5.560
Asn-Ser	0	1	15.40	15.55	5.080
Asn-Thr	0	1	12.11	12.55	6.380
Asn-Trp	0	1	14.72	14.90	5.570
Asn-Tyr	0	1	17.22	17.23	5.590
Asn-Val	0	1	12.89	12.77	5.580
Average			**14.08**	**13.90**	**6.448**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	9.220	9.360	12.16
Asn-Arg	1	1	15.70	14.85	9.230
Asn-Asn	0	1	13.70	13.71	11.03
Asn-Asp	-1	1	10.62	9.860	9.670
Asn-Cys	0	1	13.67	13.18	10.19
Asn-Gln	0	1	14.54	14.11	10.16
Asn-Glu	-1	1	4.980	4.220	9.570
Asn-Gly	0	1	9.140	8.940	11.18
Asn-His	0	1	11.75	11.59	10.40
Asn-Ile	0	1	17.69	17.65	11.53
Asn-Leu	0	1	13.08	12.67	10.73
Asn-Lys	1	1	15.54	15.40	11.12
Asn-Met	0	1	12.69	12.52	11.18
Asn-Phe	0	1	12.73	12.27	10.56
Asn-Ser	0	1	13.88	13.43	10.08
Asn-Thr	0	1	12.40	12.30	11.14
Asn-Trp	0	1	11.36	10.99	10.31
Asn-Tyr	0	1	21.41	21.20	10.90

Asn-Val	0	1	13.35	12.61	9.94
Average			**13.02**	**12.68**	**10.58**

Table S4.E. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	12.14	0.514	-38.98
Asn-Arg	1	1	7.848	-1.057	-29.87
Asn-Asn	0	1	9.369	-0.159	-31.96
Asn-Asp	-1	1	10.33	0.458	-33.11
Asn-Cys	0	1	9.685	0.755	-29.95
Asn-Gln	0	1	9.045	-1.120	-34.09
Asn-Glu	-1	1	17.07	7.994	-30.46
Asn-Gly	0	1	14.72	4.034	-35.84
Asn-His	0	1	9.792	1.122	-29.08
Asn-Ile	0	1	6.785	-3.626	-34.92
Asn-Leu	0	1	9.399	-0.759	-34.07
Asn-Lys	1	1	7.663	-1.848	-31.90
Asn-Met	0	1	8.485	-0.958	-31.67
Asn-Phe	0	1	11.86	1.204	-35.74
Asn-Ser	0	1	10.61	0.236	-34.80
Asn-Thr	0	1	8.799	-1.456	-34.39
Asn-Trp	0	1	12.35	2.045	-34.57
Asn-Tyr	0	1	5.075	-5.549	-35.63
Asn-Val	0	1	8.181	-1.512	-32.51
Average			**9.959**	**0.017**	**-33.34**

Table S4.F. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.65	11.92	6.290
Asn-Arg	1	1	15.57	15.34	5.140
Asn-Asn	0	1	14.39	15.08	6.820
Asn-Asp	-1	1	12.20	12.10	5.190
Asn-Cys	0	1	15.37	15.58	6.410
Asn-Gln	0	1	14.35	14.57	5.400
Asn-Glu	-1	1	13.72	13.82	5.990
Asn-Gly	0	1	14.44	14.77	6.080
Asn-His	0	1	13.74	14.3	6.590
Asn-Ile	0	1	15.12	15.70	6.660
Asn-Leu	0	1	13.42	13.61	6.010

Asn-Lys	1	1	14.62	15.17	6.550
Asn-Met	0	1	12.64	13.17	6.960
Asn-Phe	0	1	15.22	15.37	5.570
Asn-Ser	0	1	15.40	15.57	5.330
Asn-Thr	0	1	15.07	15.83	6.870
Asn-Trp	0	1	13.42	13.95	6.860
Asn-Tyr	0	1	17.26	17.28	5.550
Asn-Val	0	1	13.04	12.91	5.580
Average			**14.24**	**14.53**	**6.097**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	9.430	9.570	12.16
Asn-Arg	1	1	15.69	14.78	8.900
Asn-Asn	0	1	13.61	13.62	11.04
Asn-Asp	-1	1	10.73	9.99	9.660
Asn-Cys	0	1	13.75	13.27	10.21
Asn-Gln	0	1	14.48	14.04	10.09
Asn-Glu	-1	1	5.000	4.270	9.850
Asn-Gly	0	1	9.110	8.910	11.14
Asn-His	0	1	11.76	11.57	10.17
Asn-Ile	0	1	17.69	17.65	11.53
Asn-Leu	0	1	13.11	12.69	10.70
Asn-Lys	1	1	15.59	15.44	10.76
Asn-Met	0	1	12.74	12.56	11.13
Asn-Phe	0	1	12.87	12.43	10.60
Asn-Ser	0	1	13.97	13.53	10.14
Asn-Thr	0	1	15.31	15.51	11.62
Asn-Trp	0	1	10.17	10.17	11.67
Asn-Tyr	0	1	21.32	21.10	10.69
Asn-Val	0	1	13.53	12.80	9.950
Average			**13.15**	**12.84**	**10.63**

Table S4.G. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 80)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	12.13	0.492	-39.04
Asn-Arg	1	1	8.005	-0.987	-30.16
Asn-Asn	0	1	9.443	-0.108	-32.04
Asn-Asp	-1	1	10.31	0.498	-32.91
Asn-Cys	0	1	9.729	0.786	-30.00
Asn-Gln	0	1	9.054	-1.078	-33.98
Asn-Glu	-1	1	17.18	8.018	-30.73
Asn-Gly	0	1	14.32	4.068	-34.38
Asn-His	0	1	9.875	1.155	-29.25
Asn-Ile	0	1	6.803	-3.582	-34.83

Asn-Leu	0	1	9.405	-0.710	-33.93
Asn-Lys	1	1	7.672	-1.863	-31.98
Asn-Met	0	1	8.572	-0.886	-31.72
Asn-Phe	0	1	11.80	1.143	-35.76
Asn-Ser	0	1	10.48	0.196	-34.49
Asn-Thr	0	1	8.803	-1.423	-34.30
Asn-Trp	0	1	12.32	1.975	-34.70
Asn-Tyr	0	1	5.036	-5.465	-35.22
Asn-Val	0	1	7.995	-1.532	-31.95
Average			**9.944**	**0.037**	**-33.23**

Table S4.H. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.72	12.00	6.290
Asn-Arg	1	1	15.63	15.39	5.080
Asn-Asn	0	1	14.40	15.09	6.800
Asn-Asp	-1	1	12.28	12.20	5.240
Asn-Cys	0	1	15.45	15.66	6.400
Asn-Gln	0	1	14.36	14.57	5.390
Asn-Glu	-1	1	13.77	13.87	5.990
Asn-Gly	0	1	14.44	14.77	6.070
Asn-His	0	1	13.74	14.31	6.590
Asn-Ile	0	1	15.16	15.74	6.660
Asn-Leu	0	1	13.47	13.66	6.020
Asn-Lys	1	1	14.64	15.19	6.520
Asn-Met	0	1	12.72	13.27	6.970
Asn-Phe	0	1	15.24	15.39	5.570
Asn-Ser	0	1	15.40	15.58	5.410
Asn-Thr	0	1	15.08	15.84	6.870
Asn-Trp	0	1	14.70	14.91	5.650
Asn-Tyr	0	1	17.28	17.29	5.550
Asn-Val	0	1	13.11	12.99	5.580
Average			**14.35**	**14.62**	**6.034**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	9.530	9.660	12.17
Asn-Arg	1	1	15.67	14.75	8.910
Asn-Asn	0	1	13.57	13.57	11.04
Asn-Asp	-1	1	10.78	10.05	9.670
Asn-Cys	0	1	13.79	13.32	10.21
Asn-Gln	0	1	14.46	14.01	10.05
Asn-Glu	-1	1	5.010	4.280	9.910
Asn-Gly	0	1	9.110	8.890	10.81
Asn-His	0	1	11.72	11.54	10.20

Asn-Ile	0	1	17.69	17.65	11.51
Asn-Leu	0	1	13.12	12.70	10.68
Asn-Lys	1	1	15.62	15.47	10.74
Asn-Met	0	1	12.75	12.58	11.15
Asn-Phe	0	1	12.95	12.51	10.61
Asn-Ser	0	1	14.02	13.59	10.15
Asn-Thr	0	1	15.30	15.50	11.59
Asn-Trp	0	1	11.51	11.20	10.48
Asn-Tyr	0	1	21.26	21.04	10.60
Asn-Val	0	1	13.63	12.90	9.820
Average			**13.24**	**12.91**	**10.54**

Table S5.A. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	13.68	3.250	-34.99
Asn-Arg	1	1	11.21	1.525	-32.49
Asn-Asn	0	1	9.491	-0.164	-32.38
Asn-Asp	-1	1	5.274	-7.265	-42.06
Asn-Cys	0	1	9.072	-0.595	-32.42
Asn-Gln	0	1	11.00	0.736	-34.42
Asn-Glu	-1	1	4.585	-5.435	-33.61
Asn-Gly	0	1	10.75	0.392	-34.73
Asn-His	0	1	12.73	3.846	-29.79
Asn-Ile	0	1	14.12	4.015	-33.91
Asn-Leu	0	1	10.62	1.355	-31.08
Asn-Lys	1	1	10.69	1.113	-32.13
Asn-Met	0	1	7.163	-3.648	-36.26
Asn-Phe	0	1	11.95	1.362	-35.52
Asn-Ser	0	1	9.339	-0.191	-31.96
Asn-Thr	0	1	3.468	-7.363	-36.33
Asn-Trp	0	1	9.047	-1.017	-33.76
Asn-Tyr	0	1	11.04	1.274	-32.75
Asn-Val	0	1	10.80	0.464	-34.65
Average			**9.791**	**-0.334**	**-33.96**

Table S5.B. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.18	13.71	6.750
Asn-Arg	1	1	10.96	11.70	7.010

Asn-Asn	0	1	9.60	9.59	5.870
Asn-Asp	-1	1	2.32	2.08	5.660
Asn-Cys	0	1	9.40	9.97	6.820
Asn-Gln	0	1	10.12	10.62	6.610
Asn-Glu	-1	1	12.66	12.92	5.970
Asn-Gly	0	1	11.60	12.13	6.420
Asn-His	0	1	13.15	13.21	5.830
Asn-Ile	0	1	10.87	11.04	5.710
Asn-Leu	0	1	11.11	11.69	6.690
Asn-Lys	1	1	12.26	12.53	5.630
Asn-Met	0	1	12.91	13.19	6.030
Asn-Phe	0	1	8.750	8.750	4.830
Asn-Ser	0	1	8.910	9.320	6.500
Asn-Thr	0	1	9.270	10.000	6.890
Asn-Trp	0	1	10.64	11.07	5.820
Asn-Tyr	0	1	15.04	15.27	5.340
Asn-Val	0	1	8.670	8.610	5.290
Average			**10.60**	**10.92**	**6.087895**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.830	8.730	11.62
Asn-Arg	1	1	8.640	8.560	11.31
Asn-Asn	0	1	8.590	8.050	10.21
Asn-Asp	-1	1	7.500	7.300	12.20
Asn-Cys	0	1	8.800	8.720	11.09
Asn-Gln	0	1	8.060	8.140	11.41
Asn-Glu	-1	1	16.66	16.69	10.69
Asn-Gly	0	1	9.920	9.970	11.27
Asn-His	0	1	8.450	7.760	9.570
Asn-Ile	0	1	5.700	5.290	10.36
Asn-Leu	0	1	8.790	8.670	10.70
Asn-Lys	1	1	10.09	9.730	9.890
Asn-Met	0	1	15.10	14.97	11.21
Asn-Phe	0	1	6.090	5.610	9.850
Asn-Ser	0	1	8.090	7.870	10.72
Asn-Thr	0	1	14.68	15.50	12.25
Asn-Trp	0	1	10.32	10.30	10.46
Asn-Tyr	0	1	12.78	12.33	9.720
Asn-Val	0	1	6.890	6.390	10.14
Average			**9.683**	**9.504**	**10.77**

Table S5.C. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	14.29	3.883	-34.89

Asn-Arg	1	1	11.21	1.860	-31.35
Asn-Asn	0	1	11.27	1.104	-34.09
Asn-Asp	-1	1	8.871	-3.440	-41.29
Asn-Cys	0	1	9.726	-0.222	-33.37
Asn-Gln	0	1	11.74	1.630	-33.92
Asn-Glu	-1	1	6.973	-2.699	-32.44
Asn-Gly	0	1	11.93	1.181	-36.05
Asn-His	0	1	13.05	4.065	-30.13
Asn-Ile	0	1	15.10	4.451	-35.73
Asn-Leu	0	1	11.48	1.958	-31.95
Asn-Lys	1	1	12.39	2.048	-34.70
Asn-Met	0	1	8.812	-2.416	-37.66
Asn-Phe	0	1	12.89	2.203	-35.84
Asn-Ser	0	1	9.715	-1.565	-37.83
Asn-Thr	0	1	4.831	-6.084	-36.61
Asn-Trp	0	1	9.782	0.048	-32.65
Asn-Tyr	0	1	12.03	1.995	-33.65
Asn-Val	0	1	11.57	1.238	-34.65
Average			**10.93**	**0.592**	**-34.67**

Table S5.D. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.68	14.19	6.640
Asn-Arg	1	1	11.94	12.49	6.740
Asn-Asn	0	1	10.22	10.20	5.770
Asn-Asp	-1	1	6.010	5.880	5.920
Asn-Cys	0	1	10.42	10.99	6.840
Asn-Gln	0	1	10.97	11.53	6.670
Asn-Glu	-1	1	9.850	9.910	5.790
Asn-Gly	0	1	12.22	12.73	6.340
Asn-His	0	1	13.88	13.93	5.880
Asn-Ile	0	1	11.86	12.04	5.730
Asn-Leu	0	1	11.85	12.45	6.830
Asn-Lys	1	1	12.85	13.14	5.760
Asn-Met	0	1	13.54	13.87	6.190
Asn-Phe	0	1	10.30	10.42	5.070
Asn-Ser	0	1	7.92	8.090	5.520
Asn-Thr	0	1	12.74	13.17	6.130
Asn-Trp	0	1	11.75	12.29	6.060
Asn-Tyr	0	1	15.52	15.79	5.450
Asn-Val	0	1	9.070	9.050	5.440
Average			**11.40**	**11.69**	**6.041**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**

Asn-Ala	0	1	8.720	8.570	11.47
Asn-Arg	1	1	9.350	9.060	10.79
Asn-Asn	0	1	7.880	7.370	10.48
Asn-Asp	-1	1	7.510	7.290	12.26
Asn-Cys	0	1	9.410	9.360	11.32
Asn-Gln	0	1	8.080	8.170	11.35
Asn-Glu	-1	1	11.15	10.95	10.25
Asn-Gly	0	1	9.680	9.750	11.48
Asn-His	0	1	8.910	8.250	9.690
Asn-Ile	0	1	6.150	5.830	10.79
Asn-Leu	0	1	8.900	8.820	11.03
Asn-Lys	1	1	9.540	9.310	10.58
Asn-Met	0	1	14.46	14.40	11.67
Asn-Phe	0	1	6.770	6.430	10.16
Asn-Ser	0	1	7.860	7.750	11.06
Asn-Thr	0	1	16.90	17.40	11.54
Asn-Trp	0	1	10.45	10.48	10.45
Asn-Tyr	0	1	12.55	12.12	10.01
Asn-Val	0	1	6.510	6.070	10.29
Average			**9.515**	**9.336**	**10.88**

Table S5.E. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation, $\varepsilon = 40$)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	14.38	3.964	-34.92
Asn-Arg	1	1	11.11	1.862	-31.01
Asn-Asn	0	1	11.44	1.271	-34.09
Asn-Asp	-1	1	9.306	-2.956	-41.13
Asn-Cys	0	1	9.821	-0.185	-33.56
Asn-Gln	0	1	12.15	1.697	-35.06
Asn-Glu	-1	1	7.450	-2.336	-32.82
Asn-Gly	0	1	12.07	1.269	-36.24
Asn-His	0	1	13.10	4.073	-30.29
Asn-Ile	0	1	15.21	4.501	-35.91
Asn-Leu	0	1	11.55	2.027	-31.95
Asn-Lys	1	1	12.65	2.165	-35.16
Asn-Met	0	1	9.007	-2.254	-37.77
Asn-Phe	0	1	13.01	2.314	-35.87
Asn-Ser	0	1	9.525	-1.400	-36.64
Asn-Thr	0	1	4.944	-5.927	-36.46
Asn-Trp	0	1	9.859	0.183	-32.45
Asn-Tyr	0	1	12.18	2.089	-33.85
Asn-Val	0	1	11.42	1.333	-33.83
Average			**11.06**	**0.721**	**-34.69**

Table S5.F. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.74	14.25	6.620
Asn-Arg	1	1	11.68	12.46	7.230
Asn-Asn	0	1	10.28	10.25	5.730
Asn-Asp	-1	1	6.490	6.370	5.980
Asn-Cys	0	1	10.55	11.12	6.840
Asn-Gln	0	1	11.21	11.79	6.700
Asn-Glu	-1	1	10.94	11.35	6.010
Asn-Gly	0	1	12.30	12.80	6.320
Asn-His	0	1	13.97	14.03	5.880
Asn-Ile	0	1	11.98	12.16	5.740
Asn-Leu	0	1	11.94	12.55	6.830
Asn-Lys	1	1	12.89	13.20	5.830
Asn-Met	0	1	13.62	13.95	6.210
Asn-Phe	0	1	10.45	10.63	5.440
Asn-Ser	0	1	8.120	8.340	5.860
Asn-Thr	0	1	12.90	13.31	6.100
Asn-Trp	0	1	11.90	12.45	6.070
Asn-Tyr	0	1	15.58	15.85	5.450
Asn-Val	0	1	9.110	9.100	5.460
Average			**11.56**	**11.89**	**6.121**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.70	8.55	11.46
Asn-Arg	1	1	9.12	9.04	11.21
Asn-Asn	0	1	7.79	7.25	10.44
Asn-Asp	-1	1	7.53	7.31	12.28
Asn-Cys	0	1	9.49	9.45	11.36
Asn-Gln	0	1	8.24	8.34	11.64
Asn-Glu	-1	1	11.88	12.03	10.56
Asn-Gly	0	1	9.660	9.730	11.50
Asn-His	0	1	8.990	8.330	9.720
Asn-Ile	0	1	6.200	5.900	10.84
Asn-Leu	0	1	8.930	8.850	11.03
Asn-Lys	1	1	9.440	9.250	10.75
Asn-Met	0	1	14.37	14.32	11.71
Asn-Phe	0	1	6.820	6.530	10.54
Asn-Ser	0	1	7.940	7.840	11.14
Asn-Thr	0	1	16.91	17.39	11.48
Asn-Trp	0	1	10.48	10.51	10.41
Asn-Tyr	0	1	12.51	12.08	10.06
Asn-Val	0	1	6.470	6.030	10.13
Average			**9.551**	**9.407**	**10.96**

Table S5.G. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	14.42	4.004	-34.93
Asn-Arg	1	1	10.91	1.873	-30.32
Asn-Asn	0	1	11.53	1.351	-34.14
Asn-Asp	-1	1	9.514	-2.719	-41.03
Asn-Cys	0	1	9.871	-0.166	-33.66
Asn-Gln	0	1	12.25	1.748	-35.21
Asn-Glu	-1	1	7.653	-2.180	-32.98
Asn-Gly	0	1	12.14	1.310	-36.33
Asn-His	0	1	13.25	4.077	-30.76
Asn-Ile	0	1	15.25	4.526	-35.96
Asn-Leu	0	1	11.58	2.061	-31.94
Asn-Lys	1	1	12.74	2.223	-35.29
Asn-Met	0	1	9.100	-2.174	-37.81
Asn-Phe	0	1	13.06	2.368	-35.87
Asn-Ser	0	1	9.490	-1.319	-36.25
Asn-Thr	0	1	5.023	-5.850	-36.47
Asn-Trp	0	1	9.919	0.248	-32.44
Asn-Tyr	0	1	12.26	2.135	-33.97
Asn-Val	0	1	11.50	1.372	-33.97
Average			**11.13**	**0.784**	**-34.70**

Table S5.H. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.77	14.27	6.610
Asn-Arg	1	1	11.72	12.50	7.220
Asn-Asn	0	1	10.32	10.28	5.680
Asn-Asp	-1	1	6.720	6.610	6.020
Asn-Cys	0	1	10.61	11.19	6.840
Asn-Gln	0	1	11.24	11.81	6.680
Asn-Glu	-1	1	10.98	11.42	6.400
Asn-Gly	0	1	12.33	12.83	6.310
Asn-His	0	1	14.02	14.07	5.880
Asn-Ile	0	1	12.04	12.22	5.750
Asn-Leu	0	1	11.99	12.60	6.830
Asn-Lys	1	1	12.91	13.23	5.870
Asn-Met	0	1	13.65	13.99	6.220
Asn-Phe	0	1	10.70	10.73	4.860

Asn-Ser	0	1	8.20	8.450	6.020
Asn-Thr	0	1	12.98	13.39	6.100
Asn-Trp	0	1	11.98	12.53	6.070
Asn-Tyr	0	1	15.61	15.88	5.460
Asn-Val	0	1	9.130	9.120	5.460
Average			**11.63**	**11.95**	**6.120**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.70	8.54	11.45
Asn-Arg	1	1	9.18	9.08	11.04
Asn-Asn	0	1	7.74	7.20	10.41
Asn-Asp	-1	1	7.54	7.32	12.30
Asn-Cys	0	1	9.53	9.49	11.38
Asn-Gln	0	1	8.21	8.32	11.64
Asn-Glu	-1	1	11.75	11.94	10.99
Asn-Gly	0	1	9.650	9.720	11.51
Asn-His	0	1	9.010	8.360	9.830
Asn-Ile	0	1	6.230	5.930	10.87
Asn-Leu	0	1	8.950	8.860	11.03
Asn-Lys	1	1	9.400	9.220	10.82
Asn-Met	0	1	14.33	14.28	11.73
Asn-Phe	0	1	7.010	6.570	9.960
Asn-Ser	0	1	7.960	7.890	11.22
Asn-Thr	0	1	16.91	17.38	11.47
Asn-Trp	0	1	10.50	10.53	10.41
Asn-Tyr	0	1	12.49	12.07	10.10
Asn-Val	0	1	6.450	6.010	10.17
Average			**9.555**	**9.406**	**10.96**

Table S6.A. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	25.48	35.65	34.12
Asn-Arg	1	1	25.18	36.60	38.28
Asn-Asn	0	1	25.50	36.26	36.10
Asn-Asp	-1	1	25.01	36.04	37.02
Asn-Cys	0	1	24.12	33.78	32.40
Asn-Gln	0	1	24.60	35.50	36.57
Asn-Glu	-1	1	26.59	38.42	39.68
Asn-Gly	0	1	26.78	36.47	32.49
Asn-His	0	1	26.06	35.93	33.13
Asn-Ile	0	1	26.05	36.46	34.91
Asn-Leu	0	1	25.13	35.41	34.50
Asn-Lys	1	1	24.10	34.76	35.76
Asn-Met	0	1	25.30	35.60	34.55
Asn-Phe	0	1	25.01	35.68	35.77

Asn-Ser	0	1	24.97	36.26	37.86
Asn-Thr	0	1	26.04	36.85	36.26
Asn-Trp	0	1	25.10	35.90	36.21
Asn-Tyr	0	1	27.72	38.24	35.31
Asn-Val	0	1	25.64	36.34	35.89
Average			**25.49**	**36.11**	**35.62**

Table S6.B. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	80.04	81.19	13.86
Asn-Arg	1	1	76.71	78.12	15.35
Asn-Asn	0	1	71.21	71.75	12.64
Asn-Asp	-1	1	62.76	62.55	10.81
Asn-Cys	0	1	76.26	77.54	14.24
Asn-Gln	0	1	78.81	80.16	14.23
Asn-Glu	-1	1	49.45	49.28	10.78
Asn-Gly	0	1	78.26	79.47	13.58
Asn-His	0	1	78.02	79.05	13.37
Asn-Ile	0	1	53.66	53.22	10.72
Asn-Leu	0	1	53.86	53.17	9.730
Asn-Lys	1	1	81.05	82.16	13.82
Asn-Met	0	1	58.94	59.17	11.85
Asn-Phe	0	1	95.15	96.02	13.28
Asn-Ser	0	1	64.60	65.19	13.32
Asn-Thr	0	1	55.29	55.01	11.24
Asn-Trp	0	1	59.12	59.39	12.17
Asn-Tyr	0	1	80.20	81.63	14.54
Asn-Val	0	1	60.25	60.35	11.65
Average			**69.14**	**69.71**	**12.69**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	45.23	47.16	9.380
Asn-Arg	1	1	41.28	43.31	9.960
Asn-Asn	0	1	35.95	37.19	7.730
Asn-Asp	-1	1	27.93	28.25	5.660
Asn-Cys	0	1	43.09	45.28	10.140
Asn-Gln	0	1	44.40	46.36	9.180
Asn-Glu	-1	1	12.59	12.70	4.990
Asn-Gly	0	1	42.52	44.58	9.460
Asn-His	0	1	42.92	44.74	9.110
Asn-Ile	0	1	18.08	18.41	6.070
Asn-Leu	0	1	19.33	19.40	5.170
Asn-Lys	1	1	47.26	49.01	8.920
Asn-Met	0	1	24.23	25.23	7.280

Asn-Phe	0	1	60.43	62.02	8.440
Asn-Ser	0	1	29.44	30.67	8.010
Asn-Thr	0	1	19.46	19.84	6.270
Asn-Trp	0	1	24.21	25.19	7.230
Asn-Tyr	0	1	42.92	45.05	9.780
Asn-Val	0	1	24.86	25.68	6.780
Average			**34.01**	**35.27**	**7.872**

Table S6.C. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation, ε = 20)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	25.50	36.00	35.24
Asn-Arg	1	1	26.07	36.08	33.57
Asn-Asn	0	1	25.71	36.54	36.32
Asn-Asp	-1	1	24.84	36.10	37.75
Asn-Cys	0	1	24.05	34.14	33.82
Asn-Gln	0	1	24.93	35.97	37.03
Asn-Glu	-1	1	25.20	35.51	34.59
Asn-Gly	0	1	26.99	36.92	33.31
Asn-His	0	1	26.19	36.19	33.56
Asn-Ile	0	1	26.43	36.79	34.76
Asn-Leu	0	1	25.36	35.76	34.89
Asn-Lys	1	1	23.81	33.77	33.41
Asn-Met	0	1	25.51	35.99	35.14
Asn-Phe	0	1	25.45	35.96	35.27
Asn-Ser	0	1	25.24	36.41	37.49
Asn-Thr	0	1	26.27	37.10	36.35
Asn-Trp	0	1	25.13	36.13	36.90
Asn-Tyr	0	1	27.68	38.00	34.61
Asn-Val	0	1	25.94	36.68	36.00
Average			**25.59**	**36.11**	**35.26**

Table S6.D. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	72.81	73.63	13.80
Asn-Arg	1	1	72.65	73.55	13.78
Asn-Asn	0	1	76.87	76.90	11.41
Asn-Asp	-1	1	60.17	59.76	10.73
Asn-Cys	0	1	69.80	70.81	14.08
Asn-Gln	0	1	73.17	74.20	14.14
Asn-Glu	-1	1	65.63	65.89	11.86

Asn-Gly	0	1	70.74	71.37	12.86
Asn-His	0	1	70.82	71.52	13.03
Asn-Ile	0	1	62.70	63.12	11.98
Asn-Leu	0	1	62.32	61.78	10.27
Asn-Lys	1	1	67.68	68.51	13.47
Asn-Met	0	1	61.89	62.42	12.66
Asn-Phe	0	1	89.49	90.09	12.64
Asn-Ser	0	1	61.72	62.32	13.24
Asn-Thr	0	1	54.94	54.81	11.53
Asn-Trp	0	1	73.13	74.19	14.02
Asn-Tyr	0	1	69.74	70.00	10.83
Asn-Val	0	1	57.19	57.14	11.58
Average			**68.08**	**68.53**	**12.52**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	37.72	39.28	9.080
Asn-Arg	1	1	37.41	39.10	9.430
Asn-Asn	0	1	41.37	42.07	6.440
Asn-Asp	-1	1	25.12	25.39	5.460
Asn-Cys	0	1	36.38	38.23	9.660
Asn-Gln	0	1	38.25	39.94	9.010
Asn-Glu	-1	1	31.04	32.03	7.270
Asn-Gly	0	1	34.63	36.07	8.560
Asn-His	0	1	35.52	36.97	8.660
Asn-Ile	0	1	26.83	27.99	7.350
Asn-Leu	0	1	27.47	27.68	5.620
Asn-Lys	1	1	34.78	36.29	9.080
Asn-Met	0	1	26.84	28.11	7.960
Asn-Phe	0	1	54.47	55.80	7.910
Asn-Ser	0	1	26.41	27.65	8.010
Asn-Thr	0	1	18.85	19.37	6.540
Asn-Trp	0	1	38.06	39.78	8.930
Asn-Tyr	0	1	32.72	33.65	6.220
Asn-Val	0	1	21.48	22.14	6.680
Average			**32.91**	**34.08**	**7.783**

Table S6.E. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation, ε = 40)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	25.53	36.05	35.32
Asn-Arg	1	1	26.56	36.00	31.68
Asn-Asn	0	1	25.63	36.58	36.75
Asn-Asp	-1	1	25.05	36.23	37.49
Asn-Cys	0	1	24.03	34.19	34.09
Asn-Gln	0	1	24.95	36.05	37.24
Asn-Glu	-1	1	25.39	35.64	34.36

Asn-Gly	0	1	26.96	36.99	33.62
Asn-His	0	1	26.23	36.23	33.56
Asn-Ile	0	1	26.46	36.84	34.82
Asn-Leu	0	1	25.41	35.81	34.86
Asn-Lys	1	1	23.58	33.65	33.76
Asn-Met	0	1	25.56	36.04	35.17
Asn-Phe	0	1	25.50	36.00	35.22
Asn-Ser	0	1	25.33	36.44	37.23
Asn-Thr	0	1	26.35	37.15	36.22
Asn-Trp	0	1	25.15	36.17	36.95
Asn-Tyr	0	1	27.55	37.97	34.95
Asn-Val	0	1	26.01	36.73	35.95
Average			**25.64**	**36.15**	**35.22**

Table S6.F. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	71.77	72.53	13.54
Asn-Arg	1	1	71.9	72.81	13.36
Asn-Asn	0	1	76.82	76.86	11.50
Asn-Asp	-1	1	59.96	59.49	10.37
Asn-Cys	0	1	68.83	69.85	14.23
Asn-Gln	0	1	72.23	73.24	14.15
Asn-Glu	-1	1	65.25	65.50	11.93
Asn-Gly	0	1	71.11	71.85	13.13
Asn-His	0	1	69.81	70.44	12.78
Asn-Ile	0	1	62.14	62.56	12.00
Asn-Leu	0	1	61.89	61.35	10.26
Asn-Lys	1	1	74.35	75.04	12.72
Asn-Met	0	1	61.31	61.85	12.79
Asn-Phe	0	1	88.71	89.28	12.55
Asn-Ser	0	1	61.35	61.93	13.12
Asn-Thr	0	1	54.72	54.58	11.52
Asn-Trp	0	1	72.22	73.24	13.97
Asn-Tyr	0	1	69.00	69.500	11.62
Asn-Val	0	1	56.78	56.7	11.54
Average			**67.90**	**68.35**	**12.48**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	36.64	38.13	8.790
Asn-Arg	1	1	36.63	38.38	9.410
Asn-Asn	0	1	41.29	41.99	6.430
Asn-Asp	-1	1	24.77	24.99	5.150
Asn-Cys	0	1	35.38	37.22	9.750
Asn-Gln	0	1	37.24	38.91	8.970

Asn-Glu	-1	1	30.52	31.50	7.380
Asn-Gly	0	1	34.96	36.49	8.760
Asn-His	0	1	34.48	35.85	8.410
Asn-Ile	0	1	26.23	27.38	7.360
Asn-Leu	0	1	27.00	27.19	5.610
Asn-Lys	1	1	41.59	42.94	8.250
Asn-Met	0	1	26.21	27.49	8.080
Asn-Phe	0	1	53.66	54.96	7.830
Asn-Ser	0	1	26.01	27.23	7.940
Asn-Thr	0	1	18.58	19.10	6.560
Asn-Trp	0	1	37.13	38.79	8.860
Asn-Tyr	0	1	32.03	33.19	6.930
Asn-Val	0	1	21.02	21.65	6.650
Average			**32.70**	**33.86**	**7.743**

Table S6.G. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	25.54	36.08	35.35
Asn-Arg	1	1	26.62	35.95	31.30
Asn-Asn	0	1	25.59	36.61	36.93
Asn-Asp	-1	1	24.92	36.31	38.20
Asn-Cys	0	1	24.03	34.22	34.18
Asn-Gln	0	1	24.98	36.09	37.25
Asn-Glu	-1	1	25.79	35.70	33.23
Asn-Gly	0	1	26.96	37.02	33.73
Asn-His	0	1	26.26	36.25	33.52
Asn-Ile	0	1	26.48	36.87	34.86
Asn-Leu	0	1	25.44	35.83	34.85
Asn-Lys	1	1	23.45	33.60	34.04
Asn-Met	0	1	25.58	36.07	35.20
Asn-Phe	0	1	25.53	36.02	35.19
Asn-Ser	0	1	25.40	36.45	37.08
Asn-Thr	0	1	26.34	37.18	36.33
Asn-Trp	0	1	25.18	36.18	36.92
Asn-Tyr	0	1	27.39	37.96	35.46
Asn-Val	0	1	26.04	36.75	35.91
Average			**25.66**	**36.17**	**35.24**

Table S6.H. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**

Asn-Ala	0	1	71.25	71.98	13.41
Asn-Arg	1	1	71.40	72.38	13.31
Asn-Asn	0	1	76.79	76.83	11.54
Asn-Asp	-1	1	59.82	59.38	10.55
Asn-Cys	0	1	68.34	69.36	14.31
Asn-Gln	0	1	71.76	72.77	14.13
Asn-Glu	-1	1	88.14	88.66	11.82
Asn-Gly	0	1	70.58	71.28	13.06
Asn-His	0	1	69.33	69.91	12.58
Asn-Ile	0	1	61.85	62.28	12.04
Asn-Leu	0	1	61.67	61.12	10.27
Asn-Lys	1	1	73.90	74.58	12.74
Asn-Met	0	1	61.00	61.57	12.89
Asn-Phe	0	1	88.31	88.88	12.55
Asn-Ser	0	1	61.17	61.74	13.05
Asn-Thr	0	1	54.62	54.47	11.54
Asn-Trp	0	1	71.78	72.75	13.79
Asn-Tyr	0	1	67.93	68.16	10.94
Asn-Val	0	1	56.58	56.49	11.52
Average			**68.75**	**69.19**	**12.42**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	36.10	37.56	8.660
Asn-Arg	1	1	36.26	38.02	9.440
Asn-Asn	0	1	41.25	41.95	6.430
Asn-Asp	-1	1	24.58	24.82	5.170
Asn-Cys	0	1	34.87	36.71	9.810
Asn-Gln	0	1	36.74	38.39	8.940
Asn-Glu	-1	1	53.32	54.59	7.530
Asn-Gly	0	1	34.41	35.89	8.670
Asn-His	0	1	33.98	35.30	8.220
Asn-Ile	0	1	25.92	27.07	7.390
Asn-Leu	0	1	26.74	26.94	5.620
Asn-Lys	1	1	41.20	42.53	8.210
Asn-Met	0	1	25.88	27.17	8.170
Asn-Phe	0	1	53.24	54.53	7.830
Asn-Ser	0	1	25.8	27.01	7.910
Asn-Thr	0	1	18.45	18.97	6.550
Asn-Trp	0	1	36.67	38.29	8.690
Asn-Tyr	0	1	30.99	31.87	6.140
Asn-Val	0	1	20.79	21.41	6.640
Average			**33.54**	**34.69**	**7.685**

Table S7.A. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 4)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN}**	**ΔH_{RXN}**	**ΔS**

			(kcal.mol^{-1})	(kcal.mol^{-1})	(kcal.mol^{-1})
Asn-Ala	0	1	-23.63	-33.90	-34.44
Asn-Arg	1	1	-19.25	-28.83	-32.10
Asn-Asn	0	1	-20.36	-31.04	-35.83
Asn-Asp	-1	1	-23.19	-34.02	-36.34
Asn-Cys	0	1	-19.69	-29.03	-31.32
Asn-Gln	0	1	-23.37	-34.01	-35.69
Asn-Glu	-1	1	-19.15	-29.96	-36.25
Asn-Gly	0	1	-20.96	-30.55	-32.19
Asn-His	0	1	-22.00	-31.79	-32.84
Asn-Ile	0	1	-21.92	-32.50	-35.47
Asn-Leu	0	1	-23.18	-33.84	-35.76
Asn-Lys	1	1	-21.09	-31.15	-33.74
Asn-Met	0	1	-19.26	-29.42	-34.08
Asn-Phe	0	1	-21.43	-32.53	-37.22
Asn-Ser	0	1	-19.59	-29.76	-34.09
Asn-Thr	0	1	-22.51	-33.10	-35.52
Asn-Trp	0	1	-22.99	-33.59	-35.56
Asn-Tyr	0	1	-22.37	-33.52	-37.38
Asn-Val	0	1	-20.62	-31.15	-35.32
Average			**-21.40**	**-31.77**	**-34.80**

Table S7.B. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.19	11.93	7.480
Asn-Arg	1	1	9.93	10.41	6.850
Asn-Asn	0	1	8.820	9.140	6.140
Asn-Asp	-1	1	10.89	11.22	6.390
Asn-Cys	0	1	10.18	10.83	7.070
Asn-Gln	0	1	9.140	9.710	7.360
Asn-Glu	-1	1	2.660	2.460	5.550
Asn-Gly	0	1	11.04	11.54	7.360
Asn-His	0	1	4.830	4.920	6.320
Asn-Ile	0	1	11.84	12.25	7.060
Asn-Leu	0	1	14.31	14.51	5.540
Asn-Lys	1	1	1.880	2.210	7.330
Asn-Met	0	1	13.03	13.44	6.490
Asn-Phe	0	1	4.540	4.750	6.790
Asn-Ser	0	1	11.10	11.64	7.090
Asn-Thr	0	1	10.28	10.96	6.950
Asn-Trp	0	1	16.26	16.54	5.200
Asn-Tyr	0	1	10.85	11.24	6.300
Asn-Val	0	1	11.45	11.88	6.490
Average			**9.696**	**10.08**	**6.619**

Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	43.61	44.18	12.41
Asn-Arg	1	1	37.52	37.67	11.24
Asn-Asn	0	1	38.29	38.49	11.37
Asn-Asp	-1	1	43.35	43.56	11.73
Asn-Cys	0	1	37.97	38.33	11.31
Asn-Gln	0	1	41.56	42.04	12.57
Asn-Glu	-1	1	31.16	30.79	10.88
Asn-Gly	0	1	40.26	40.50	11.78
Asn-His	0	1	35.17	35.07	10.88
Asn-Ile	0	1	42.84	43.08	12.20
Asn-Leu	0	1	46.6	46.67	10.75
Asn-Lys	1	1	31.65	31.83	12.15
Asn-Met	0	1	41.12	41.27	11.32
Asn-Phe	0	1	35.39	35.52	12.32
Asn-Ser	0	1	39.49	39.74	11.90
Asn-Thr	0	1	41.80	42.37	12.11
Asn-Trp	0	1	48.33	48.46	10.37
Asn-Tyr	0	1	42.66	42.99	11.87
Asn-Val	0	1	41.12	41.37	11.59
Average			**39.99**	**40.21**	**11.62**

Table S7.C. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-23.31	-33.45	-34.04
Asn-Arg	1	1	-19.56	-29.31	-32.71
Asn-Asn	0	1	-20.64	-31.11	-35.09
Asn-Asp	-1	1	-22.85	-33.43	-35.48
Asn-Cys	0	1	-19.07	-29.15	-33.80
Asn-Gln	0	1	-22.76	-33.43	-35.78
Asn-Glu	-1	1	-18.75	-29.95	-37.56
Asn-Gly	0	1	-20.86	-30.71	-33.03
Asn-His	0	1	-21.98	-31.87	-33.18
Asn-Ile	0	1	-22.14	-32.60	-35.06
Asn-Leu	0	1	-22.79	-33.37	-35.48
Asn-Lys	1	1	-20.09	-29.12	-30.30
Asn-Met	0	1	-19.14	-29.48	-34.67
Asn-Phe	0	1	-21.40	-32.28	-36.52
Asn-Ser	0	1	-19.78	-30.23	-35.05
Asn-Thr	0	1	-23.47	-32.86	-31.50
Asn-Trp	0	1	-22.51	-33.15	-35.68
Asn-Tyr	0	1	-21.90	-33.65	-39.41
Asn-Val	0	1	-20.78	-31.34	-35.41

Average			**-21.25**	**-31.60**	**-34.72**

Table S7.D. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.68	12.35	7.210
Asn-Arg	1	1	11.02	11.56	7.230
Asn-Asn	0	1	9.850	10.18	6.540
Asn-Asp	-1	1	10.40	10.99	7.110
Asn-Cys	0	1	11.30	11.97	7.060
Asn-Gln	0	1	10.12	10.73	7.390
Asn-Glu	-1	1	3.070	2.850	5.540
Asn-Gly	0	1	11.61	12.13	7.570
Asn-His	0	1	4.790	4.830	6.200
Asn-Ile	0	1	12.66	13.09	7.120
Asn-Leu	0	1	15.12	15.33	5.550
Asn-Lys	1	1	27.51	27.89	7.120
Asn-Met	0	1	11.35	12.04	7.260
Asn-Phe	0	1	3.540	3.740	6.280
Asn-Ser	0	1	11.59	12.11	7.100
Asn-Thr	0	1	11.16	11.86	6.960
Asn-Trp	0	1	16.92	17.14	5.070
Asn-Tyr	0	1	12.07	12.43	6.250
Asn-Val	0	1	12.14	12.57	6.530
Average			**11.47**	**11.88**	**6.689**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	43.68	44.16	12.05
Asn-Arg	1	1	39.08	39.31	11.75
Asn-Asn	0	1	39.41	39.60	11.60
Asn-Asp	-1	1	42.32	42.760	12.26
Asn-Cys	0	1	39.00	39.500	11.85
Asn-Gln	0	1	42.02	42.49	12.61
Asn-Glu	-1	1	31.46	31.12	11.15
Asn-Gly	0	1	40.94	41.21	12.17
Asn-His	0	1	35.16	35.04	10.85
Asn-Ile	0	1	43.76	44.02	12.18
Asn-Leu	0	1	46.95	47.02	10.70
Asn-Lys	1	1	55.50	55.60	11.18
Asn-Met	0	1	39.45	39.91	12.22
Asn-Phe	0	1	34.16	34.26	11.65
Asn-Ser	0	1	40.34	40.64	12.14
Asn-Thr	0	1	42.55	43.10	11.25
Asn-Trp	0	1	48.51	48.60	10.26
Asn-Tyr	0	1	43.87	44.27	12.28

Asn-Val	0	1	42.00	42.25	11.65
Average			**41.59**	**41.83**	**11.67**

Table S7.E. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-23.25	-33.40	-34.05
Asn-Arg	1	1	-19.85	-29.38	-31.96
Asn-Asn	0	1	-21.40	-31.17	-32.77
Asn-Asp	-1	1	-22.68	-33.35	-35.79
Asn-Cys	0	1	-19.08	-29.17	-33.81
Asn-Gln	0	1	-22.65	-33.35	-35.88
Asn-Glu	-1	1	-18.74	-29.95	-37.62
Asn-Gly	0	1	-20.84	-30.73	-33.16
Asn-His	0	1	-21.98	-31.89	-33.24
Asn-Ile	0	1	-22.18	-32.62	-35.01
Asn-Leu	0	1	-22.76	-33.31	-35.41
Asn-Lys	1	1	-19.80	-28.88	-30.42
Asn-Met	0	1	-19.14	-29.49	-34.71
Asn-Phe	0	1	-21.39	-32.25	-36.44
Asn-Ser	0	1	-19.86	-30.30	-35.02
Asn-Thr	0	1	-23.21	-32.89	-32.46
Asn-Trp	0	1	-22.42	-33.09	-35.80
Asn-Tyr	0	1	-21.87	-33.67	-39.60
Asn-Val	0	1	-20.81	-31.37	-35.42
Average			**-21.26**	**-31.59**	**-34.66**

Table S7.F. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.73	12.40	7.190
Asn-Arg	1	1	11.00	11.70	7.890
Asn-Asn	0	1	10.13	10.45	6.150
Asn-Asp	-1	1	10.46	11.09	7.710
Asn-Cys	0	1	11.45	12.12	7.060
Asn-Gln	0	1	10.26	10.88	7.390
Asn-Glu	-1	1	3.220	2.990	5.410
Asn-Gly	0	1	11.71	12.21	7.490
Asn-His	0	1	4.780	4.820	6.180
Asn-Ile	0	1	12.77	13.20	7.110
Asn-Leu	0	1	15.22	15.44	5.570

Asn-Lys	1	1	27.30	27.67	7.090
Asn-Met	0	1	11.42	12.10	7.260
Asn-Phe	0	1	3.380	3.590	6.380
Asn-Ser	0	1	11.44	12.11	7.480
Asn-Thr	0	1	11.27	11.98	6.980
Asn-Trp	0	1	17.00	17.21	5.060
Asn-Tyr	0	1	13.47	13.83	6.050
Asn-Val	0	1	12.23	12.66	6.500
Average			**11.59**	**12.02**	**6.734**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	43.68	44.16	12.03
Asn-Arg	1	1	39.18	39.54	12.25
Asn-Asn	0	1	39.78	39.93	10.70
Asn-Asp	-1	1	42.29	42.78	12.93
Asn-Cys	0	1	39.16	39.66	11.85
Asn-Gln	0	1	42.07	42.55	12.64
Asn-Glu	-1	1	31.61	31.26	11.03
Asn-Gly	0	1	41.04	41.31	12.12
Asn-His	0	1	35.16	35.03	10.84
Asn-Ile	0	1	43.89	44.15	12.15
Asn-Leu	0	1	46.99	47.07	10.70
Asn-Lys	1	1	55.07	55.15	11.17
Asn-Met	0	1	39.51	39.97	12.23
Asn-Phe	0	1	33.97	34.09	11.74
Asn-Ser	0	1	40.25	40.72	12.51
Asn-Thr	0	1	42.67	43.23	11.48
Asn-Trp	0	1	48.53	48.61	10.28
Asn-Tyr	0	1	45.29	45.69	12.12
Asn-Val	0	1	42.12	42.37	11.63
Average			**41.70**	**41.96**	**11.71**

Table S7.G. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation, ε = 80)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-23.23	-33.37	-34.04
Asn-Arg	1	1	-20.00	-29.41	-31.57
Asn-Asn	0	1	-20.98	-31.18	-34.21
Asn-Asp	-1	1	-22.58	-33.31	-35.99
Asn-Cys	0	1	-19.04	-29.17	-33.99
Asn-Gln	0	1	-22.59	-33.31	-35.94
Asn-Glu	-1	1	-18.73	-29.95	-37.65
Asn-Gly	0	1	-20.84	-30.74	-33.20
Asn-His	0	1	-21.98	-31.90	-33.27
Asn-Ile	0	1	-22.20	-32.63	-35.01

Asn-Leu	0	1	-22.74	-33.28	-35.37
Asn-Lys	1	1	-19.72	-28.76	-30.29
Asn-Met	0	1	-19.12	-29.49	-34.77
Asn-Phe	0	1	-21.39	-32.24	-36.40
Asn-Ser	0	1	-19.88	-30.34	-35.06
Asn-Thr	0	1	-23.02	-32.90	-33.13
Asn-Trp	0	1	-22.37	-33.06	-35.85
Asn-Tyr	0	1	-21.85	-33.69	-39.70
Asn-Val	0	1	-20.82	-31.38	-35.43
Average			**-21.22**	**-31.59**	**-34.78**

Table S7.H. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.76	12.42	7.180
Asn-Arg	1	1	11.07	11.78	7.890
Asn-Asn	0	1	10.63	11.03	6.420
Asn-Asp	-1	1	10.53	11.14	7.270
Asn-Cys	0	1	11.52	12.19	7.050
Asn-Gln	0	1	10.33	10.95	7.410
Asn-Glu	-1	1	3.120	2.910	5.860
Asn-Gly	0	1	11.75	12.25	7.470
Asn-His	0	1	4.780	4.810	6.180
Asn-Ile	0	1	12.82	13.25	7.110
Asn-Leu	0	1	15.27	15.49	5.570
Asn-Lys	1	1	4.060	4.320	7.130
Asn-Met	0	1	11.45	12.13	7.250
Asn-Phe	0	1	3.310	3.520	6.400
Asn-Ser	0	1	11.68	12.19	7.110
Asn-Thr	0	1	11.32	12.03	6.980
Asn-Trp	0	1	17.04	17.25	5.060
Asn-Tyr	0	1	12.31	12.67	6.250
Asn-Val	0	1	12.28	12.70	6.500
Average			**10.37**	**10.79**	**6.742**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	43.68	44.16	12.02
Asn-Arg	1	1	39.30	39.66	12.17
Asn-Asn	0	1	40.25	40.52	11.29
Asn-Asp	-1	1	42.31	42.78	12.54
Asn-Cys	0	1	39.23	39.74	11.89
Asn-Gln	0	1	42.10	42.58	12.67
Asn-Glu	-1	1	31.50	31.18	11.49
Asn-Gly	0	1	41.09	41.36	12.11
Asn-His	0	1	35.16	35.03	10.84

Asn-Ile	0	1	43.96	44.22	12.15
Asn-Leu	0	1	47.02	47.09	10.70
Asn-Lys	1	1	31.72	31.69	11.18
Asn-Met	0	1	39.54	40.01	12.24
Asn-Phe	0	1	33.88	34.00	11.74
Asn-Ser	0	1	40.52	40.83	12.14
Asn-Thr	0	1	42.73	43.30	11.63
Asn-Trp	0	1	48.54	48.62	10.29
Asn-Tyr	0	1	44.13	44.54	12.34
Asn-Val	0	1	42.18	42.42	11.63
Average			**40.47**	**40.72**	**11.74**

Thermochemistry and Arrhenius Parameters (Implicit + 1 H_2O Solvation)

Table S8.A. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 4)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	2.816	2.866	0.169
Asn-Arg	1	1	3.798	4.024	0.757
Asn-Asn	0	1	3.298	3.534	0.792
Asn-Asp	-1	1	1.476	-0.104	-5.298
Asn-Cys	0	1	3.565	3.471	-0.314
Asn-Gln	0	1	7.317	8.559	4.165
Asn-Glu	-1	1	4.525	5.435	3.054
Asn-Gly	0	1	3.176	4.731	5.217
Asn-His	0	1	3.785	3.376	-1.372
Asn-Ile	0	1	7.264	4.685	-8.650
Asn-Leu	0	1	3.254	2.461	-2.659
Asn-Lys	1	1	7.656	9.205	5.198
Asn-Met	0	1	3.112	3.187	0.252
Asn-Phe	0	1	7.277	8.642	4.577
Asn-Pro	0	1	6.508	6.981	1.584
Asn-Ser	0	1	2.034	2.904	2.919
Asn-Thr	0	1	8.737	5.565	-10.638
Asn-Trp	0	1	7.365	8.827	4.902
Asn-Tyr	0	1	4.777	5.981	4.037
Asn-Val	0	1	2.701	-0.111	-9.432
Average			**4.822**	**4.808**	**-0.048**

Table S8.B. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	43.89	44.46	7.400
Asn-Arg	1	1	44.07	43.47	6.070
Asn-Asn	0	1	43.09	43.94	7.660
Asn-Asp	-1	1	37.38	38.28	7.770
Asn-Cys	0	1	37.22	38.03	8.610
Asn-Gln	0	1	42.93	43.79	8.560
Asn-Glu	-1	1	45.41	46.20	8.150
Asn-Gly	0	1	40.22	41.43	8.340
Asn-His	0	1	42.47	43.03	7.140
Asn-Ile	0	1	38.90	37.38	4.390
Asn-Leu	0	1	42.53	41.76	6.590
Asn-Lys	1	1	39.69	39.97	6.950
Asn-Met	0	1	43.45	44.52	8.560

Asn-Phe	0	1	42.59	43.37	8.190
Asn-Pro	0	1	12.27	14.63	10.21
Asn-Ser	0	1	40.60	41.74	8.550
Asn-Thr	0	1	43.04	42.01	4.920
Asn-Trp	0	1	41.26	41.67	7.390
Asn-Tyr	0	1	42.54	42.84	6.590
Asn-Val	0	1	36.08	36.20	5.970
Average			**39.78**	**40.22**	**7.401**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	40.57	41.71	7.770
Asn-Arg	1	1	39.78	39.59	6.270
Asn-Asn	0	1	39.22	40.51	7.850
Asn-Asp	-1	1	36.63	38.32	9.350
Asn-Cys	0	1	33.44	34.54	8.950
Asn-Gln	0	1	34.49	35.39	7.890
Asn-Glu	-1	1	39.51	40.78	7.830
Asn-Gly	0	1	35.45	36.82	7.460
Asn-His	0	1	38.53	39.71	7.850
Asn-Ile	0	1	32.77	32.35	6.710
Asn-Leu	0	1	39.41	39.32	7.590
Asn-Lys	1	1	31.16	31.06	5.960
Asn-Met	0	1	39.81	41.43	8.900
Asn-Phe	0	1	34.13	34.92	7.430
Asn-Pro	0	1	5.130	7.710	10.13
Asn-Ser	0	1	37.44	39.04	8.310
Asn-Thr	0	1	36.31	36.07	7.560
Asn-Trp	0	1	32.81	33.10	6.530
Asn-Tyr	0	1	36.60	37.01	5.970
Asn-Val	0	1	34.60	36.00	8.540
Average			**34.59**	**35.46**	**7.741**

Table S8.C. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	3.247	4.771	5.112
Asn-Arg	1	1	1.828	1.989	0.542
Asn-Asn	0	1	1.667	1.518	-0.499
Asn-Asp	-1	1	1.586	1.494	-0.308
Asn-Cys	0	1	1.162	1.437	0.922
Asn-Gln	0	1	5.326	5.938	2.053
Asn-Glu	-1	1	1.417	-0.351	-5.931
Asn-Gly	0	1	1.119	2.467	4.520
Asn-His	0	1	2.173	2.162	-0.037
Asn-Ile	0	1	4.626	2.960	-5.589
Asn-Leu	0	1	1.953	1.026	-3.109

Asn-Lys	1	1	4.963	8.513	11.907
Asn-Met	0	1	1.992	1.825	-0.563
Asn-Phe	0	1	4.889	6.008	3.753
Asn-Pro	0	1	4.370	4.696	1.096
Asn-Ser	0	1	3.951	4.047	0.323
Asn-Thr	0	1	5.448	3.501	-6.530
Asn-Trp	0	1	5.862	6.151	0.970
Asn-Tyr	0	1	3.028	4.177	3.854
Asn-Val	0	1	0.628	-1.012	-5.499
Average			**3.052**	**3.081**	**0.099**

Table S8.D. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	39.07	39.70	7.040
Asn-Arg	1	1	40.98	40.21	5.690
Asn-Asn	0	1	38.61	39.49	7.500
Asn-Asp	-1	1	34.97	35.85	7.710
Asn-Cys	0	1	34.50	35.39	8.310
Asn-Gln	0	1	39.42	40.33	8.150
Asn-Glu	-1	1	38.19	38.65	6.440
Asn-Gly	0	1	36.10	37.39	8.520
Asn-His	0	1	38.44	39.24	7.510
Asn-Ile	0	1	36.18	34.73	5.110
Asn-Leu	0	1	38.11	37.32	6.640
Asn-Lys	1	1	36.13	36.81	7.490
Asn-Met	0	1	39.82	40.97	8.690
Asn-Phe	0	1	38.87	39.81	8.140
Asn-Pro	0	1	9.230	11.48	9.980
Asn-Ser	0	1	39.53	40.63	8.390
Asn-Thr	0	1	39.99	39.00	5.880
Asn-Trp	0	1	37.18	37.55	6.840
Asn-Tyr	0	1	37.66	38.03	6.750
Asn-Val	0	1	33.34	33.71	6.760
Average			**36.17**	**36.66**	**7.395**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	34.46	35.11	6.160
Asn-Arg	1	1	38.72	38.37	5.940
Asn-Asn	0	1	36.66	38.06	7.980
Asn-Asp	-1	1	33.00	34.46	8.180
Asn-Cys	0	1	32.78	33.95	8.370
Asn-Gln	0	1	33.41	34.50	7.960
Asn-Glu	-1	1	37.32	38.76	8.170
Asn-Gly	0	1	33.57	35.04	7.800

Asn-His	0	1	35.91	37.21	7.910
Asn-Ile	0	1	31.87	31.48	6.770
Asn-Leu	0	1	36.40	36.31	7.730
Asn-Lys	1	1	28.82	28.87	5.040
Asn-Met	0	1	37.44	39.21	9.220
Asn-Phe	0	1	32.93	33.96	7.580
Asn-Pro	0	1	4.290	6.830	10.03
Asn-Ser	0	1	35.03	36.68	8.720
Asn-Thr	0	1	35.52	35.25	7.650
Asn-Trp	0	1	31.08	31.54	6.880
Asn-Tyr	0	1	33.58	34.03	6.160
Asn-Val	0	1	33.02	34.53	8.450
Average			**32.70**	**33.63**	**7.713**

Table S8.E. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	5.561	7.094	5.143
Asn-Arg	1	1	4.449	4.290	-0.533
Asn-Asn	0	1	4.053	3.824	-0.766
Asn-Asp	-1	1	4.329	3.902	-1.431
Asn-Cys	0	1	3.543	3.740	0.662
Asn-Gln	0	1	7.624	8.172	1.837
Asn-Glu	-1	1	3.714	2.107	-5.389
Asn-Gly	0	1	3.423	4.752	4.457
Asn-His	0	1	4.574	4.590	0.055
Asn-Ile	0	1	6.669	5.402	-4.246
Asn-Leu	0	1	4.379	3.427	-3.193
Asn-Lys	1	1	7.032	10.78	12.57
Asn-Met	0	1	4.560	4.224	-1.127
Asn-Phe	0	1	7.381	8.224	2.828
Asn-Pro	0	1	6.515	6.968	1.521
Asn-Ser	0	1	4.175	4.155	-0.065
Asn-Thr	0	1	7.611	5.843	-5.930
Asn-Trp	0	1	8.247	8.382	0.453
Asn-Tyr	0	1	5.381	6.530	3.852
Asn-Val	0	1	2.960	1.530	-4.796
Average			**5.296**	**5.307**	**0.040**

Table S8.F. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**

Asn-Ala	0	1	42.30	42.93	6.980
Asn-Arg	1	1	44.42	43.63	5.670
Asn-Asn	0	1	41.76	42.73	8.080
Asn-Asp	-1	1	38.55	39.43	7.630
Asn-Cys	0	1	38.05	38.91	8.080
Asn-Gln	0	1	42.82	43.75	8.360
Asn-Glu	-1	1	41.61	42.11	6.410
Asn-Gly	0	1	39.40	40.72	8.510
Asn-His	0	1	41.79	42.61	7.520
Asn-Ile	0	1	39.72	38.32	5.420
Asn-Leu	0	1	41.40	40.60	6.590
Asn-Lys	1	1	39.61	40.31	7.410
Asn-Met	0	1	43.22	44.37	8.670
Asn-Phe	0	1	42.25	43.20	8.080
Asn-Pro	0	1	12.70	14.95	9.990
Asn-Ser	0	1	39.36	40.45	8.340
Asn-Thr	0	1	43.48	42.51	6.060
Asn-Trp	0	1	40.51	40.89	6.890
Asn-Tyr	0	1	40.85	41.23	6.810
Asn-Val	0	1	36.90	37.32	6.840
Average			**39.39**	**39.90**	**7.440**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	35.36	36.01	6.10
Asn-Arg	1	1	39.82	39.46	6.15
Asn-Asn	0	1	37.48	38.98	8.62
Asn-Asp	-1	1	34.11	35.60	8.35
Asn-Cys	0	1	34.02	35.15	8.20
Asn-Gln	0	1	34.56	35.66	8.22
Asn-Glu	-1	1	38.31	39.77	8.01
Asn-Gly	0	1	34.59	36.07	7.81
Asn-His	0	1	36.85	38.15	7.89
Asn-Ile	0	1	33.05	32.67	6.78
Asn-Leu	0	1	37.29	37.18	7.71
Asn-Lys	1	1	30.11	30.13	4.80
Asn-Met	0	1	38.40	40.19	9.32
Asn-Phe	0	1	34.01	35.10	7.72
Asn-Pro	0	1	5.510	8.030	9.94
Asn-Ser	0	1	34.73	36.38	8.750
Asn-Thr	0	1	36.70	36.43	7.69
Asn-Trp	0	1	32.09	32.61	7.05
Asn-Tyr	0	1	34.41	34.87	6.23
Asn-Val	0	1	34.10	35.61	8.37
Average			**33.69**	**34.63**	**7.769**

Table S8.G. Asn-X Direct Hydrolysis Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	5.601	7.117	5.086
Asn-Arg	1	1	4.433	4.316	-0.391
Asn-Asn	0	1	4.075	3.835	-0.802
Asn-Asp	-1	1	6.152	7.091	3.149
Asn-Cys	0	1	3.556	3.755	0.665
Asn-Gln	0	1	7.615	8.148	1.789
Asn-Glu	-1	1	3.853	2.187	-5.588
Asn-Gly	0	1	3.435	4.756	4.433
Asn-His	0	1	4.660	4.664	0.014
Asn-Ile	0	1	6.612	5.483	-3.789
Asn-Leu	0	1	4.449	3.487	-3.227
Asn-Lys	1	1	7.082	10.81	12.50
Asn-Met	0	1	4.695	4.286	-1.373
Asn-Phe	0	1	7.401	8.199	2.677
Asn-Pro	0	1	6.512	6.963	1.510
Asn-Ser	0	1	4.211	4.210	-0.004
Asn-Thr	0	1	7.651	5.869	-5.977
Asn-Trp	0	1	8.154	8.362	0.700
Asn-Tyr	0	1	5.420	6.565	3.838
Asn-Val	0	1	2.975	1.667	-4.388
Average			**5.418**	**5.508**	**0.302**

Table S8.H. Asn-X Direct Hydrolysis Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, $\varepsilon = 80$)

Forward					
Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	42.19	42.83	6.970
Asn-Arg	1	1	44.42	43.62	5.680
Asn-Asn	0	1	41.66	42.64	7.870
Asn-Asp	-1	1	38.64	39.50	7.500
Asn-Cys	0	1	38.07	38.95	8.100
Asn-Gln	0	1	42.83	43.75	8.250
Asn-Glu	-1	1	41.61	42.13	6.290
Asn-Gly	0	1	39.37	40.67	8.460
Asn-His	0	1	41.75	42.58	7.500
Asn-Ile	0	1	39.77	38.40	5.530
Asn-Leu	0	1	41.34	40.53	6.570
Asn-Lys	1	1	39.65	40.36	7.330
Asn-Met	0	1	43.22	44.36	8.660
Asn-Phe	0	1	42.23	43.18	8.070
Asn-Pro	0	1	12.72	14.96	9.980
Asn-Ser	0	1	39.27	40.36	8.360
Asn-Thr	0	1	43.51	42.55	6.080
Asn-Trp	0	1	40.45	40.84	6.980

Asn-Tyr	0	1	40.72	41.11	6.800
Asn-Val	0	1	36.95	37.40	6.890
Average			**39.38**	**39.89**	**7.416**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	35.23	35.89	6.100
Asn-Arg	1	1	39.82	39.44	6.130
Asn-Asn	0	1	37.37	38.88	8.420
Asn-Asp	-1	1	31.60	32.55	7.060
Asn-Cys	0	1	34.03	35.18	8.210
Asn-Gln	0	1	34.59	35.69	8.120
Asn-Glu	-1	1	38.23	39.70	7.940
Asn-Gly	0	1	34.54	36.02	7.760
Asn-His	0	1	36.74	38.05	7.880
Asn-Ile	0	1	33.07	32.69	6.790
Asn-Leu	0	1	37.16	37.05	7.690
Asn-Lys	1	1	30.16	30.16	4.740
Asn-Met	0	1	38.31	40.11	9.370
Asn-Phe	0	1	33.99	35.09	7.750
Asn-Pro	0	1	5.530	8.050	9.930
Asn-Ser	0	1	34.58	36.23	8.760
Asn-Thr	0	1	36.71	36.44	7.720
Asn-Trp	0	1	32.03	32.57	7.080
Asn-Tyr	0	1	34.25	34.71	6.210
Asn-Val	0	1	34.06	35.57	8.330
Average			**33.51**	**34.43**	**7.678**

Table S9.A. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 4)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-0.179	10.53	35.92
Asn-Arg	1	1	-1.642	9.346	36.85
Asn-Asn	0	1	-1.834	8.051	33.15
Asn-Asp	-1	1	-1.047	9.898	36.71
Asn-Cys	0	1	-1.606	8.144	32.70
Asn-Gln	0	1	-0.781	10.70	38.51
Asn-Glu	-1	1	1.088	12.54	38.40
Asn-Gly	0	1	-3.103	9.942	43.75
Asn-His	0	1	-0.802	10.15	36.74
Asn-Ile	0	1	2.251	11.72	31.77
Asn-Leu	0	1	-1.062	11.74	42.94
Asn-Lys	1	1	-1.196	9.858	37.08
Asn-Met	0	1	-0.329	10.99	37.97
Asn-Phe	0	1	0.172	11.62	38.39
Asn-Ser	0	1	-2.804	10.49	44.59

Asn-Thr	0	1	-0.097	5.747	19.60
Asn-Trp	0	1	-0.510	11.22	39.33
Asn-Tyr	0	1	-3.246	9.082	41.35
Asn-Val	0	1	1.520	9.404	26.45
Average			**-0.800**	**10.06**	**36.43**

Table S9.B. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	41.45	41.39	11.89
Asn-Arg	1	1	31.01	30.65	11.20
Asn-Asn	0	1	40.06	40.12	12.17
Asn-Asp	-1	1	44.17	43.90	10.87
Asn-Cys	0	1	46.93	45.95	11.84
Asn-Gln	0	1	35.37	33.90	9.640
Asn-Glu	-1	1	47.17	47.03	11.97
Asn-Gly	0	1	46.90	45.86	12.05
Asn-His	0	1	37.34	37.63	13.11
Asn-Ile	0	1	36.25	35.16	8.720
Asn-Leu	0	1	48.40	47.33	11.71
Asn-Lys	1	1	22.54	22.87	12.80
Asn-Met	0	1	37.53	36.64	10.77
Asn-Phe	0	1	42.06	42.15	12.58
Asn-Ser	0	1	47.92	47.01	12.40
Asn-Thr	0	1	39.78	37.30	8.190
Asn-Trp	0	1	35.56	35.43	12.14
Asn-Tyr	0	1	45.36	43.65	9.680
Asn-Val	0	1	43.14	42.69	10.46
Average			**40.47**	**39.82**	**11.27**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	32.15	32.69	7.020
Asn-Arg	1	1	23.14	23.25	6.110
Asn-Asn	0	1	32.76	33.78	7.990
Asn-Asp	-1	1	35.78	35.89	5.770
Asn-Cys	0	1	39.73	39.51	7.680
Asn-Gln	0	1	26.11	25.10	4.180
Asn-Glu	-1	1	35.96	36.32	6.520
Asn-Gly	0	1	38.66	38.03	5.490
Asn-His	0	1	28.55	29.34	8.030
Asn-Ile	0	1	25.14	25.10	4.860
Asn-Leu	0	1	38.56	37.72	5.280
Asn-Lys	1	1	14.02	14.91	7.690
Asn-Met	0	1	27.96	27.54	5.430
Asn-Phe	0	1	31.89	32.44	7.140

Asn-Ser	0	1	39.26	38.62	5.610
Asn-Thr	0	1	33.18	32.69	7.130
Asn-Trp	0	1	25.92	26.20	6.500
Asn-Tyr	0	1	37.61	36.53	3.680
Asn-Val	0	1	33.96	34.73	7.740
Average			**31.60**	**31.60**	**6.308**

Table S9.C. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 20)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-1.086	9.441	35.31
Asn-Arg	1	1	-1.118	9.107	34.29
Asn-Asn	0	1	-1.960	8.070	33.64
Asn-Asp	-1	1	-2.557	8.194	36.06
Asn-Cys	0	1	-2.507	7.226	32.64
Asn-Gln	0	1	-1.493	9.785	37.83
Asn-Glu	-1	1	-1.389	6.817	27.52
Asn-Gly	0	1	-3.970	9.286	44.46
Asn-His	0	1	-1.754	9.282	37.01
Asn-Ile	0	1	0.560	11.43	36.45
Asn-Leu	0	1	-2.690	11.04	46.05
Asn-Lys	1	1	-1.896	10.04	40.04
Asn-Met	0	1	-1.164	9.902	37.12
Asn-Phe	0	1	-0.711	10.56	37.80
Asn-Ser	0	1	-3.734	9.843	45.54
Asn-Thr	0	1	-0.971	5.820	22.77
Asn-Trp	0	1	-0.786	9.943	35.98
Asn-Tyr	0	1	-4.741	8.508	44.44
Asn-Val	0	1	0.235	8.795	28.71
Average			**-1.775**	**9.110**	**36.51**

Table S9.D. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	40.16	40.08	11.81
Asn-Arg	1	1	29.67	29.43	11.43
Asn-Asn	0	1	38.90	38.97	12.14
Asn-Asp	-1	1	41.79	41.71	11.42
Asn-Cys	0	1	46.48	45.35	11.53
Asn-Gln	0	1	35.41	35.31	12.13
Asn-Glu	-1	1	40.51	39.81	9.750

Asn-Gly	0	1	46.96	46.18	13.09
Asn-His	0	1	34.77	35.17	13.70
Asn-Ile	0	1	34.86	33.87	9.590
Asn-Leu	0	1	47.55	46.39	11.61
Asn-Lys	1	1	22.13	22.71	13.30
Asn-Met	0	1	35.87	35.15	11.44
Asn-Phe	0	1	39.37	39.43	12.46
Asn-Ser	0	1	47.19	46.18	12.16
Asn-Thr	0	1	40.63	38.26	9.270
Asn-Trp	0	1	37.45	37.42	11.44
Asn-Tyr	0	1	46.10	44.54	11.04
Asn-Val	0	1	41.63	41.37	11.40
Average			**39.34**	**38.81**	**11.62**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	31.87	32.45	7.090
Asn-Arg	1	1	21.64	22.10	6.930
Asn-Asn	0	1	31.68	32.65	7.840
Asn-Asp	-1	1	34.89	35.37	6.510
Asn-Cys	0	1	40.10	39.79	7.400
Asn-Gln	0	1	26.97	27.39	6.820
Asn-Glu	-1	1	33.92	34.45	6.800
Asn-Gly	0	1	39.42	39.04	6.380
Asn-His	0	1	26.91	27.77	8.560
Asn-Ile	0	1	24.23	24.21	4.710
Asn-Leu	0	1	38.52	37.56	4.510
Asn-Lys	1	1	13.70	14.66	7.510
Asn-Met	0	1	27.25	27.10	6.310
Asn-Phe	0	1	30.15	30.73	7.170
Asn-Ser	0	1	39.17	38.44	5.180
Asn-Thr	0	1	34.02	33.62	7.530
Asn-Trp	0	1	28.75	29.35	6.580
Asn-Tyr	0	1	39.03	38.04	4.360
Asn-Val	0	1	33.15	34.06	8.180
Average			**31.34**	**31.51**	**6.651**

Table S9.E. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 40)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-1.182	9.311	35.19
Asn-Arg	1	1	-1.120	9.087	34.24
Asn-Asn	0	1	-2.023	8.091	33.92
Asn-Asp	-1	1	-2.662	7.982	35.70
Asn-Cys	0	1	-2.513	7.111	32.28
Asn-Gln	0	1	-1.528	9.675	37.58

Asn-Glu	-1	1	-1.482	6.684	27.39
Asn-Gly	0	1	-4.373	9.159	45.39
Asn-His	0	1	-1.833	9.181	36.94
Asn-Ile	0	1	0.980	11.38	34.88
Asn-Leu	0	1	-1.669	10.85	41.97
Asn-Lys	1	1	-1.404	10.57	40.17
Asn-Met	0	1	-1.151	9.766	36.62
Asn-Phe	0	1	-0.734	10.42	37.42
Asn-Ser	0	1	-1.776	11.94	46.01
Asn-Thr	0	1	-1.101	5.869	23.38
Asn-Trp	0	1	-0.962	9.822	36.17
Asn-Tyr	0	1	-4.369	8.372	42.73
Asn-Val	0	1	0.183	8.794	28.88
Average			**-1.617**	**9.162**	**36.15**

Table S9.F. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	39.98	39.89	11.80
Asn-Arg	1	1	29.49	29.26	11.47
Asn-Asn	0	1	38.73	38.79	11.99
Asn-Asp	-1	1	41.30	41.20	11.30
Asn-Cys	0	1	46.39	45.26	11.57
Asn-Gln	0	1	35.17	35.06	12.13
Asn-Glu	-1	1	40.10	39.41	9.810
Asn-Gly	0	1	46.72	45.94	13.11
Asn-His	0	1	34.46	34.84	13.52
Asn-Ile	0	1	34.69	33.74	9.790
Asn-Leu	0	1	47.44	46.27	11.63
Asn-Lys	1	1	22.15	22.73	13.21
Asn-Met	0	1	35.69	34.95	11.33
Asn-Phe	0	1	39.00	39.05	12.46
Asn-Ser	0	1	47.11	46.06	12.05
Asn-Thr	0	1	40.79	38.42	9.350
Asn-Trp	0	1	37.00	36.95	11.42
Asn-Tyr	0	1	46.09	44.53	10.99
Asn-Val	0	1	41.35	41.16	11.65
Average			**39.14**	**38.61**	**11.61**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	31.81	32.39	7.100
Asn-Arg	1	1	21.47	21.95	6.990
Asn-Asn	0	1	31.52	32.46	7.630
Asn-Asp	-1	1	34.58	35.07	6.480
Asn-Cys	0	1	40.09	39.82	7.520

Asn-Gln	0	1	26.81	27.23	6.880
Asn-Glu	-1	1	33.63	34.19	6.900
Asn-Gly	0	1	39.36	38.94	6.200
Asn-His	0	1	26.70	27.54	8.400
Asn-Ile	0	1	24.02	24.07	5.250
Asn-Leu	0	1	38.37	37.53	5.440
Asn-Lys	1	1	13.50	14.27	7.370
Asn-Met	0	1	27.16	27.02	6.310
Asn-Phe	0	1	29.86	30.48	7.260
Asn-Ser	0	1	37.26	36.34	4.950
Asn-Thr	0	1	34.16	33.75	7.480
Asn-Trp	0	1	28.41	28.99	6.520
Asn-Tyr	0	1	39.05	38.12	4.690
Asn-Val	0	1	32.89	33.86	8.390
Average			**31.09**	**31.26**	**6.724**

Table S9.G. Asn-X Succinimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-1.231	9.248	35.15
Asn-Arg	1	1	-1.149	9.084	34.32
Asn-Asn	0	1	-2.047	8.099	34.03
Asn-Asp	-1	1	-2.562	7.874	35.00
Asn-Cys	0	1	-2.535	7.056	32.17
Asn-Gln	0	1	-1.921	9.632	38.75
Asn-Glu	-1	1	-1.390	6.607	26.82
Asn-Gly	0	1	-4.138	9.059	44.26
Asn-His	0	1	-1.855	9.132	36.85
Asn-Ile	0	1	0.830	11.38	35.37
Asn-Leu	0	1	-1.733	10.77	41.93
Asn-Lys	1	1	-1.224	10.58	39.59
Asn-Met	0	1	-1.137	9.700	36.35
Asn-Phe	0	1	-0.776	10.36	37.36
Asn-Ser	0	1	-1.826	11.86	45.90
Asn-Thr	0	1	-1.085	5.890	23.40
Asn-Trp	0	1	-1.087	9.764	36.40
Asn-Tyr	0	1	-4.838	8.308	44.09
Asn-Val	0	1	0.141	8.803	29.05
Average			**-1.661**	**9.116**	**36.15**

Table S9.H. Asn-X Succinimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 80)

Forward

Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	39.89	39.80	11.81
Asn-Arg	1	1	29.40	29.18	11.51
Asn-Asn	0	1	38.64	38.70	11.97
Asn-Asp	-1	1	41.07	40.95	11.16
Asn-Cys	0	1	46.32	45.22	11.69
Asn-Gln	0	1	35.05	34.93	12.08
Asn-Glu	-1	1	39.91	39.22	9.720
Asn-Gly	0	1	46.61	45.82	13.05
Asn-His	0	1	34.30	34.68	13.50
Asn-Ile	0	1	34.62	33.67	9.850
Asn-Leu	0	1	47.38	46.21	11.65
Asn-Lys	1	1	22.04	21.58	11.40
Asn-Met	0	1	35.61	34.86	11.25
Asn-Phe	0	1	38.81	38.87	12.49
Asn-Ser	0	1	47.07	46.00	12.03
Asn-Thr	0	1	40.87	38.50	9.330
Asn-Trp	0	1	36.79	36.71	11.31
Asn-Tyr	0	1	46.06	44.52	11.10
Asn-Val	0	1	41.26	41.07	11.64
Average			**39.04**	**38.45**	**11.50**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	31.77	32.36	7.120
Asn-Arg	1	1	21.39	21.88	7.010
Asn-Asn	0	1	31.43	32.37	7.580
Asn-Asp	-1	1	34.42	34.91	6.500
Asn-Cys	0	1	40.06	39.82	7.670
Asn-Gln	0	1	26.75	27.16	6.580
Asn-Glu	-1	1	33.48	34.06	6.940
Asn-Gly	0	1	39.27	38.89	6.380
Asn-His	0	1	26.59	27.42	8.400
Asn-Ile	0	1	24.00	24.03	5.190
Asn-Leu	0	1	38.39	37.54	5.460
Asn-Lys	1	1	13.36	13.11	5.690
Asn-Met	0	1	27.12	26.98	6.290
Asn-Phe	0	1	29.73	30.36	7.310
Asn-Ser	0	1	37.28	36.36	4.950
Asn-Thr	0	1	34.23	33.81	7.450
Asn-Trp	0	1	28.25	28.82	6.360
Asn-Tyr	0	1	39.09	38.18	4.500
Asn-Val	0	1	32.82	33.77	8.340
Average			**31.02**	**31.15**	**6.617**

Table S10.A. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 4$)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	11.54	1.794	-32.67
Asn-Arg	1	1	5.845	-4.528	-34.79
Asn-Asn	0	1	6.125	-2.782	-29.87
Asn-Asp	-1	1	5.754	-6.723	-41.85
Asn-Cys	0	1	6.489	-2.471	-30.05
Asn-Gln	0	1	9.142	-0.338	-31.80
Asn-Glu	-1	1	15.85	3.794	-40.45
Asn-Gly	0	1	14.32	3.555	-36.10
Asn-His	0	1	7.059	-3.939	-36.89
Asn-Ile	0	1	6.956	-3.885	-36.36
Asn-Leu	0	1	8.893	-3.909	-42.94
Asn-Lys	1	1	5.687	-4.189	-33.13
Asn-Met	0	1	7.976	-1.605	-32.14
Asn-Phe	0	1	10.08	-0.199	-34.48
Asn-Ser	0	1	12.36	0.932	-38.33
Asn-Thr	0	1	11.68	2.247	-31.65
Asn-Trp	0	1	10.32	0.299	-33.62
Asn-Tyr	0	1	5.777	-8.442	-47.69
Asn-Val	0	1	4.528	-5.335	-33.08
Average			**8.757**	**-1.880**	**-35.68**

Table S10.B. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =4)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	10.54	10.77	7.190
Asn-Arg	1	1	15.55	15.70	6.750
Asn-Asn	0	1	13.78	14.66	8.210
Asn-Asp	-1	1	11.66	11.55	6.080
Asn-Cys	0	1	14.25	14.65	7.590
Asn-Gln	0	1	14.32	14.43	6.060
Asn-Glu	-1	1	13.44	13.73	7.160
Asn-Gly	0	1	13.85	14.38	6.420
Asn-His	0	1	10.99	11.48	7.690
Asn-Ile	0	1	13.92	14.28	5.820
Asn-Leu	0	1	11.48	11.70	6.170
Asn-Lys	1	1	13.20	13.44	6.180
Asn-Met	0	1	13.05	13.96	8.210
Asn-Phe	0	1	12.97	13.61	7.620
Asn-Ser	0	1	18.45	19.16	6.330
Asn-Thr	0	1	13.53	13.80	6.980
Asn-Trp	0	1	15.62	15.40	5.370
Asn-Tyr	0	1	14.98	15.35	6.110
Asn-Val	0	1	11.69	11.90	7.220

Average			13.54	13.89	6.798
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	7.480	7.390	11.70
Asn-Arg	1	1	18.51	18.41	11.66
Asn-Asn	0	1	15.51	15.88	12.06
Asn-Asp	-1	1	16.35	16.39	12.66
Asn-Cys	0	1	15.48	15.56	11.53
Asn-Gln	0	1	13.98	13.25	10.22
Asn-Glu	-1	1	7.850	8.060	13.37
Asn-Gly	0	1	8.990	9.010	11.54
Asn-His	0	1	13.09	13.60	13.16
Asn-Ile	0	1	16.70	16.44	10.99
Asn-Leu	0	1	13.38	13.55	12.85
Asn-Lys	1	1	15.89	15.93	10.79
Asn-Met	0	1	13.92	14.07	12.48
Asn-Phe	0	1	11.89	12.02	12.41
Asn-Ser	0	1	15.94	16.29	11.95
Asn-Thr	0	1	10.46	9.850	11.04
Asn-Trp	0	1	13.85	13.21	9.960
Asn-Tyr	0	1	20.88	21.60	13.93
Asn-Val	0	1	15.68	15.48	11.73
Average			**13.99**	**14.00**	**11.90**

Table S10.C. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	11.37	1.681	-32.49
Asn-Arg	1	1	6.116	-3.489	-32.22
Asn-Asn	0	1	8.505	-0.186	-29.15
Asn-Asp	-1	1	10.78	0.550	-34.32
Asn-Cys	0	1	7.957	-1.278	-30.97
Asn-Gln	0	1	10.12	0.445	-32.45
Asn-Glu	-1	1	18.06	7.144	-36.62
Asn-Gly	0	1	22.61	8.547	-47.15
Asn-His	0	1	7.619	-2.732	-34.72
Asn-Ile	0	1	7.783	-3.683	-38.46
Asn-Leu	0	1	10.44	-3.504	-46.76
Asn-Lys	1	1	5.837	-4.336	-34.12
Asn-Met	0	1	9.389	-0.266	-32.39
Asn-Phe	0	1	11.26	3.402	-26.37
Asn-Ser	0	1	12.38	-0.042	-41.66
Asn-Thr	0	1	11.34	1.338	-33.55
Asn-Trp	0	1	10.66	1.718	-30.00
Asn-Tyr	0	1	6.740	-7.880	-49.04

Asn-Val	0	1	9.751	1.488	-27.71
Average			**10.46**	**-0.057**	**-35.27**

Table S10.D. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.58	11.81	7.070
Asn-Arg	1	1	15.46	15.85	7.820
Asn-Asn	0	1	13.10	13.82	7.810
Asn-Asp	-1	1	13.26	13.27	6.240
Asn-Cys	0	1	14.57	14.96	7.720
Asn-Gln	0	1	14.39	14.76	6.890
Asn-Glu	-1	1	14.37	14.77	7.430
Asn-Gly	0	1	13.80	14.30	6.120
Asn-His	0	1	11.35	11.86	7.740
Asn-Ile	0	1	14.27	14.54	5.390
Asn-Leu	0	1	12.29	12.43	5.390
Asn-Lys	1	1	13.22	13.46	5.710
Asn-Met	0	1	14.48	15.51	8.540
Asn-Phe	0	1	12.98	13.56	7.390
Asn-Ser	0	1	16.38	16.81	5.650
Asn-Thr	0	1	17.55	18.76	8.370
Asn-Trp	0	1	12.84	13.06	6.200
Asn-Tyr	0	1	14.81	15.01	5.140
Asn-Val	0	1	12.91	13.13	7.320
Average			**13.87**	**14.30**	**6.839**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.640	8.550	11.55
Asn-Arg	1	1	17.66	17.62	12.15
Asn-Asn	0	1	12.56	12.44	11.38
Asn-Asp	-1	1	11.44	11.05	11.05
Asn-Cys	0	1	14.69	14.68	11.84
Asn-Gln	0	1	13.15	12.76	11.22
Asn-Glu	-1	1	5.940	5.860	12.69
Asn-Gly	0	1	2.400	3.250	13.74
Asn-His	0	1	12.47	12.84	12.70
Asn-Ile	0	1	16.70	16.42	11.02
Asn-Leu	0	1	13.56	13.78	12.92
Asn-Lys	1	1	16.18	16.12	10.51
Asn-Met	0	1	14.01	14.26	12.86
Asn-Phe	0	1	9.160	8.750	10.36
Asn-Ser	0	1	14.60	14.82	12.02
Asn-Thr	0	1	15.19	15.65	12.87
Asn-Trp	0	1	10.00	9.660	10.02

Asn-Tyr	0	1	19.94	20.63	13.27
Asn-Val	0	1	10.86	10.23	10.62
Average			**12.59**	**12.60**	**11.83**

Table S10.E. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	11.36	1.643	-32.60
Asn-Arg	1	1	6.625	-3.380	-33.56
Asn-Asn	0	1	8.377	-0.237	-28.89
Asn-Asp	-1	1	8.751	-3.581	-41.36
Asn-Cys	0	1	8.161	-1.127	-31.15
Asn-Gln	0	1	10.26	0.542	-32.59
Asn-Glu	-1	1	18.25	7.294	-36.74
Asn-Gly	0	1	15.16	3.712	-38.41
Asn-His	0	1	7.581	-2.575	-34.06
Asn-Ile	0	1	6.931	-3.548	-35.15
Asn-Leu	0	1	9.414	-3.351	-42.81
Asn-Lys	1	1	5.465	-4.825	-34.52
Asn-Met	0	1	9.521	-0.119	-32.33
Asn-Phe	0	1	11.41	3.252	-27.37
Asn-Ser	0	1	10.36	-2.364	-42.69
Asn-Thr	0	1	11.19	1.194	-33.53
Asn-Trp	0	1	10.74	1.560	-30.79
Asn-Tyr	0	1	6.453	-7.757	-47.66
Asn-Val	0	1	9.626	1.442	-27.45
Average			**9.771**	**-0.643**	**-34.93**

Table S10.F. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.65	11.80	6.700
Asn-Arg	1	1	15.49	15.87	7.650
Asn-Asn	0	1	13.01	13.70	7.720
Asn-Asp	-1	1	13.73	13.61	5.830
Asn-Cys	0	1	14.62	15.02	7.770
Asn-Gln	0	1	14.42	14.76	6.730
Asn-Glu	-1	1	14.49	14.91	7.430
Asn-Gly	0	1	13.89	14.35	5.900
Asn-His	0	1	11.43	11.95	7.810
Asn-Ile	0	1	14.21	14.58	6.060

Asn-Leu	0	1	12.28	12.53	6.250
Asn-Lys	1	1	13.03	13.10	5.630
Asn-Met	0	1	14.66	15.70	8.570
Asn-Phe	0	1	12.97	13.54	7.370
Asn-Ser	0	1	14.47	14.72	5.480
Asn-Thr	0	1	17.49	18.69	8.350
Asn-Trp	0	1	12.91	13.15	6.290
Asn-Tyr	0	1	14.73	14.97	5.420
Asn-Val	0	1	13.07	13.29	7.340
Average			**13.82**	**14.22**	**6.858**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.730	8.560	11.20
Asn-Arg	1	1	17.53	17.51	12.28
Asn-Asn	0	1	12.50	12.37	11.24
Asn-Asp	-1	1	15.37	15.33	12.29
Asn-Cys	0	1	14.60	14.59	11.92
Asn-Gln	0	1	13.07	12.65	11.08
Asn-Glu	-1	1	5.910	5.840	12.72
Asn-Gly	0	1	8.700	8.730	11.53
Asn-His	0	1	12.42	12.78	12.63
Asn-Ile	0	1	16.70	16.41	10.96
Asn-Leu	0	1	13.60	13.82	12.92
Asn-Lys	1	1	16.20	16.13	10.54
Asn-Met	0	1	14.04	14.30	12.88
Asn-Phe	0	1	9.230	8.860	10.56
Asn-Ser	0	1	14.68	14.92	12.10
Asn-Thr	0	1	15.27	15.72	12.84
Asn-Trp	0	1	10.18	9.880	10.28
Asn-Tyr	0	1	19.81	20.50	13.25
Asn-Val	0	1	11.05	10.43	10.59
Average			**13.14**	**13.12**	**11.78**

Table S10.G. Asn-X Succinimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 80$)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	11.39	1.619	-32.77
Asn-Arg	1	1	6.738	-3.320	-33.73
Asn-Asn	0	1	8.413	-0.257	-29.08
Asn-Asp	-1	1	10.92	0.686	-34.31
Asn-Cys	0	1	8.260	-1.052	-31.23
Asn-Gln	0	1	10.67	0.584	-33.81
Asn-Glu	-1	1	18.31	7.360	-36.73
Asn-Gly	0	1	14.90	3.779	-37.31
Asn-His	0	1	7.633	-2.500	-33.98

Asn-Ile	0	1	6.888	-3.498	-34.84
Asn-Leu	0	1	9.477	-3.296	-42.84
Asn-Lys	1	1	5.462	-4.810	-34.45
Asn-Met	0	1	9.587	-0.048	-32.32
Asn-Phe	0	1	11.34	3.188	-27.35
Asn-Ser	0	1	10.33	-2.388	-42.65
Asn-Thr	0	1	11.12	1.121	-33.55
Asn-Trp	0	1	10.71	1.496	-30.92
Asn-Tyr	0	1	6.942	-7.705	-49.13
Asn-Val	0	1	9.223	1.429	-26.14
Average			**9.911**	**-0.401**	**-34.59**

Table S10.H. Asn-X Succinimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.72	11.86	6.710
Asn-Arg	1	1	15.51	15.88	7.630
Asn-Asn	0	1	12.97	13.64	7.680
Asn-Asp	-1	1	13.83	13.75	5.920
Asn-Cys	0	1	14.65	15.05	7.790
Asn-Gln	0	1	14.46	14.76	6.400
Asn-Glu	-1	1	14.48	14.96	7.770
Asn-Gly	0	1	13.88	14.37	6.110
Asn-His	0	1	11.47	11.99	7.820
Asn-Ile	0	1	14.25	14.61	6.070
Asn-Leu	0	1	12.37	12.62	6.230
Asn-Lys	1	1	13.05	13.12	5.640
Asn-Met	0	1	14.75	15.8	8.600
Asn-Phe	0	1	12.96	13.53	7.370
Asn-Ser	0	1	15.55	16.00	5.810
Asn-Thr	0	1	17.45	18.65	8.350
Asn-Trp	0	1	12.94	13.19	6.290
Asn-Tyr	0	1	14.75	14.97	5.070
Asn-Val	0	1	13.15	13.37	7.340
Average			**13.90**	**14.32**	**6.874**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.800	8.640	11.25
Asn-Arg	1	1	17.49	17.46	12.29
Asn-Asn	0	1	12.47	12.32	11.24
Asn-Asp	-1	1	11.88	11.41	10.73
Asn-Cys	0	1	14.55	14.55	11.96
Asn-Gln	0	1	13.03	12.60	11.02
Asn-Glu	-1	1	5.830	5.830	13.05
Asn-Gly	0	1	8.690	8.720	11.49

Asn-His	0	1	12.39	12.76	12.63
Asn-Ile	0	1	16.71	16.41	10.90
Asn-Leu	0	1	13.62	13.85	12.91
Asn-Lys	1	1	16.22	16.14	10.54
Asn-Met	0	1	14.05	14.32	12.90
Asn-Phe	0	1	9.300	8.920	10.55
Asn-Ser	0	1	15.79	16.23	12.42
Asn-Thr	0	1	15.31	15.75	12.85
Asn-Trp	0	1	10.27	9.99	10.30
Asn-Tyr	0	1	19.75	20.44	13.23
Asn-Val	0	1	11.17	10.54	10.30
Average			**13.02**	**12.99**	**11.71**

Table S11.A. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 4$)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1			
Asn-Arg	1	1	12.90	2.819	-33.81
Asn-Asn	0	1	7.370	-4.911	-41.19
Asn-Asp	-1	1	10.08	0.380	-32.52
Asn-Cys	0	1	1.206	-12.52	-46.05
Asn-Gln	0	1	8.419	-2.453	-36.47
Asn-Glu	-1	1	10.48	-0.147	-35.64
Asn-Gly	0	1	4.484	-4.825	-31.22
Asn-His	0	1	9.542	-3.417	-43.47
Asn-Ile	0	1	11.45	0.730	-35.95
Asn-Leu	0	1	15.43	3.536	-39.90
Asn-Lys	1	1	10.71	0.323	-34.85
Asn-Met	0	1	8.706	-1.750	-35.07
Asn-Phe	0	1	4.030	-8.275	-41.27
Asn-Ser	0	1	11.25	0.796	-35.07
Asn-Thr	0	1	8.095	-3.731	-39.66
Asn-Trp	0	1	7.324	-3.108	-34.99
Asn-Tyr	0	1	7.102	-4.638	-39.38
Asn-Val	0	1	9.799	-2.316	-40.63
Average			10.69	0.210	-35.15

Table S11.B. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, $\varepsilon = 4$)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	12.96	13.68	8.670

Asn-Arg	1	1	9.090	9.130	5.900
Asn-Asn	0	1	9.900	10.45	8.250
Asn-Asp	-1	1	1.670	1.310	5.710
Asn-Cys	0	1	9.570	10.05	7.200
Asn-Gln	0	1	9.590	9.390	5.650
Asn-Glu	-1	1	9.350	9.910	6.860
Asn-Gly	0	1	8.350	8.270	5.830
Asn-His	0	1	11.79	12.13	8.070
Asn-Ile	0	1	9.900	10.04	5.220
Asn-Leu	0	1	9.140	9.170	6.120
Asn-Lys	1	1	11.11	11.59	6.810
Asn-Met	0	1	9.000	8.710	4.750
Asn-Phe	0	1	10.02	10.31	6.920
Asn-Ser	0	1	7.950	8.340	5.910
Asn-Thr	0	1	6.960	7.520	8.150
Asn-Trp	0	1	9.410	9.860	6.930
Asn-Tyr	0	1	7.930	7.900	4.530
Asn-Val	0	1	10.10	10.13	6.950
Average			**9.147**	**9.363**	**6.549**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	9.080	9.200	13.31
Asn-Arg	1	1	11.66	11.98	12.32
Asn-Asn	0	1	8.830	8.500	12.54
Asn-Asp	-1	1	11.31	11.56	13.25
Asn-Cys	0	1	10.36	10.49	12.39
Asn-Gln	0	1	8.300	7.780	10.75
Asn-Glu	-1	1	12.92	13.18	11.08
Asn-Gly	0	1	9.610	9.590	12.65
Asn-His	0	1	9.540	9.590	13.24
Asn-Ile	0	1	4.840	4.550	11.15
Asn-Leu	0	1	7.420	7.000	10.98
Asn-Lys	1	1	11.45	11.53	11.75
Asn-Met	0	1	14.90	14.89	11.18
Asn-Phe	0	1	7.840	7.740	11.87
Asn-Ser	0	1	9.870	10.15	11.92
Asn-Thr	0	1	8.570	8.890	13.14
Asn-Trp	0	1	11.80	12.39	12.89
Asn-Tyr	0	1	8.370	8.280	10.76
Asn-Val	0	1	8.150	8.050	11.97
Average			**9.727**	**9.755**	**12.06**

Table S11.C. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 20)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**

Asn-Ala	0	1	14.00	4.204	-32.85
Asn-Arg	1	1	7.960	-3.367	-37.99
Asn-Asn	0	1	11.47	1.654	-32.91
Asn-Asp	-1	1	5.839	-7.496	-44.72
Asn-Cys	0	1	9.452	-1.754	-37.59
Asn-Gln	0	1	11.69	1.159	-35.32
Asn-Glu	-1	1	6.565	-1.953	-28.57
Asn-Gly	0	1	10.98	-2.395	-44.86
Asn-His	0	1	19.34	7.281	-40.46
Asn-Ile	0	1	16.55	3.633	-43.31
Asn-Leu	0	1	12.19	1.752	-35.00
Asn-Lys	1	1	9.413	-1.086	-35.21
Asn-Met	0	1	5.542	-6.479	-40.32
Asn-Phe	0	1	12.32	2.093	-34.29
Asn-Ser	0	1	9.658	-3.089	-42.75
Asn-Thr	0	1	8.591	-0.456	-30.34
Asn-Trp	0	1	8.890	-2.948	-39.71
Asn-Tyr	0	1	10.77	-1.331	-40.60
Asn-Val	0	1	12.06	1.013	-37.06
Average			**10.70**	**-0.504**	**-37.57**

Table S11.D. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.69	14.31	8.280
Asn-Arg	1	1	10.21	10.47	6.230
Asn-Asn	0	1	9.280	9.710	8.010
Asn-Asp	-1	1	6.280	5.980	5.750
Asn-Cys	0	1	10.18	10.62	6.910
Asn-Gln	0	1	10.23	10.00	5.590
Asn-Glu	-1	1	10.78	11.51	7.370
Asn-Gly	0	1	8.240	8.090	5.640
Asn-His	0	1	11.46	11.74	7.860
Asn-Ile	0	1	10.84	10.88	4.640
Asn-Leu	0	1	9.960	9.730	4.460
Asn-Lys	1	1	10.90	11.29	6.230
Asn-Met	0	1	10.38	10.24	5.130
Asn-Phe	0	1	9.610	10.12	7.450
Asn-Ser	0	1	9.730	10.16	5.630
Asn-Thr	0	1	7.010	7.580	8.210
Asn-Trp	0	1	10.73	11.19	6.820
Asn-Tyr	0	1	9.020	8.950	4.090
Asn-Val	0	1	10.13	10.13	6.920
Average			**9.929**	**10.14**	**6.380**
Reverse					

Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	8.360	8.420	12.72
Asn-Arg	1	1	11.85	12.00	11.90
Asn-Asn	0	1	6.910	6.480	12.40
Asn-Asp	-1	1	11.05	11.24	12.97
Asn-Cys	0	1	10.21	10.32	12.35
Asn-Gln	0	1	7.580	7.070	10.63
Asn-Glu	-1	1	11.67	11.99	11.00
Asn-Gly	0	1	8.370	8.330	12.77
Asn-His	0	1	2.310	2.270	13.88
Asn-Ile	0	1	5.450	5.200	11.34
Asn-Leu	0	1	7.060	6.240	9.330
Asn-Lys	1	1	10.55	10.59	11.21
Asn-Met	0	1	14.53	14.65	11.34
Asn-Phe	0	1	6.220	6.290	12.22
Asn-Ser	0	1	10.85	11.25	12.31
Asn-Thr	0	1	6.540	6.440	12.08
Asn-Trp	0	1	11.49	12.03	12.84
Asn-Tyr	0	1	8.540	8.350	10.29
Asn-Val	0	1	7.320	7.220	12.36
Average			**8.782**	**8.757**	**11.89**

Table S11.E. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 40$)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	14.12	4.319	-32.87
Asn-Arg	1	1	8.044	-3.172	-37.62
Asn-Asn	0	1	11.64	1.827	-32.93
Asn-Asp	-1	1	6.476	-6.831	-44.63
Asn-Cys	0	1	9.512	-1.672	-37.51
Asn-Gln	0	1	11.96	1.320	-35.69
Asn-Glu	-1	1	6.938	-1.567	-28.53
Asn-Gly	0	1	11.44	-2.211	-45.80
Asn-His	0	1	11.60	2.297	-31.19
Asn-Ile	0	1	15.85	3.745	-40.60
Asn-Leu	0	1	11.23	1.822	-31.55
Asn-Lys	1	1	8.760	-1.556	-34.60
Asn-Met	0	1	5.673	-6.241	-39.96
Asn-Phe	0	1	12.20	2.021	-34.15
Asn-Ser	0	1	7.883	-5.192	-43.85
Asn-Thr	0	1	8.594	-0.382	-30.11
Asn-Trp	0	1	9.181	-2.732	-39.95
Asn-Tyr	0	1	10.64	-1.148	-39.55
Asn-Val	0	1	12.16	1.117	-37.05
Average			**10.21**	**-0.749**	**-36.74**

Table S11.F. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	13.79	14.38	8.160
Asn-Arg	1	1	10.39	10.65	6.220
Asn-Asn	0	1	9.270	9.690	8.010
Asn-Asp	-1	1	6.900	6.610	5.730
Asn-Cys	0	1	10.26	10.70	6.900
Asn-Gln	0	1	10.3	10.08	5.600
Asn-Glu	-1	1	10.96	11.70	7.440
Asn-Gly	0	1	8.210	8.080	5.710
Asn-His	0	1	11.40	11.67	7.860
Asn-Ile	0	1	10.87	11.00	5.270
Asn-Leu	0	1	9.970	9.870	5.440
Asn-Lys	1	1	10.70	10.88	6.040
Asn-Met	0	1	7.690	7.680	6.040
Asn-Phe	0	1	9.780	10.31	7.660
Asn-Ser	0	1	8.130	8.330	5.300
Asn-Thr	0	1	7.010	7.590	8.260
Asn-Trp	0	1	10.91	11.34	6.630
Asn-Tyr	0	1	9.070	9.070	4.470
Asn-Val	0	1	10.12	10.12	6.930
Average			**9.775**	**9.987**	**6.509**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.340	8.370	12.60
Asn-Arg	1	1	11.90	12.01	11.80
Asn-Asn	0	1	6.740	6.280	12.39
Asn-Asp	-1	1	11.02	11.20	12.93
Asn-Cys	0	1	10.22	10.32	12.31
Asn-Gln	0	1	7.490	6.980	10.72
Asn-Glu	-1	1	11.47	11.80	11.05
Asn-Gly	0	1	8.110	8.110	13.05
Asn-His	0	1	8.030	7.750	11.96
Asn-Ile	0	1	5.530	5.290	11.37
Asn-Leu	0	1	7.150	6.370	9.550
Asn-Lys	1	1	10.57	10.55	10.92
Asn-Met	0	1	11.63	11.86	12.18
Asn-Phe	0	1	6.470	6.550	12.40
Asn-Ser	0	1	11.03	11.40	12.25
Asn-Thr	0	1	6.50	6.39	12.08
Asn-Trp	0	1	11.45	11.96	12.70
Asn-Tyr	0	1	8.500	8.330	10.44
Asn-Val	0	1	7.210	7.110	12.36

Average			8.914	8.875	11.85

Table S11.G. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	14.18	4.376	-32.87
Asn-Arg	1	1	8.095	-3.078	-37.47
Asn-Asn	0	1	11.72	1.916	-32.87
Asn-Asp	-1	1	6.771	-6.499	-44.51
Asn-Cys	0	1	9.540	-1.632	-37.47
Asn-Gln	0	1	12.44	1.389	-37.08
Asn-Glu	-1	1	7.143	-1.380	-28.58
Asn-Gly	0	1	11.24	-2.079	-44.67
Asn-His	0	1	11.96	2.328	-32.29
Asn-Ile	0	1	15.91	3.783	-40.68
Asn-Leu	0	1	11.34	1.850	-31.82
Asn-Lys	1	1	8.437	-1.525	-33.41
Asn-Met	0	1	5.804	-6.127	-40.02
Asn-Phe	0	1	12.51	2.343	-34.11
Asn-Ser	0	1	7.641	-5.056	-42.59
Asn-Thr	0	1	8.693	-0.351	-30.33
Asn-Trp	0	1	10.28	-1.358	-39.05
Asn-Tyr	0	1	11.14	-1.060	-40.91
Asn-Val	0	1	12.22	1.166	-37.07
Average			**10.37**	**-0.579**	**-36.73**

Table S11.H. Asn-X Succinimide Hydrolysis into iso-Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =80)

Forward					
Dipeptide	Charge	Multiplicity	E_0	E_A	Log(Ã)
Asn-Ala	0	1	13.83	14.41	8.110
Asn-Arg	1	1	10.48	10.74	6.200
Asn-Asn	0	1	9.280	9.670	7.940
Asn-Asp	-1	1	7.200	6.910	5.750
Asn-Cys	0	1	10.29	10.73	6.900
Asn-Gln	0	1	10.36	10.13	5.350
Asn-Glu	-1	1	11.03	11.79	7.490
Asn-Gly	0	1	8.220	8.130	5.990
Asn-His	0	1	11.32	11.62	8.040
Asn-Ile	0	1	10.94	11.08	5.290
Asn-Leu	0	1	10.07	9.970	5.480
Asn-Lys	1	1	10.70	10.87	6.020

Asn-Met	0	1	12.04	11.58	5.750
Asn-Phe	0	1	9.890	10.40	7.520
Asn-Ser	0	1	8.270	8.480	5.280
Asn-Thr	0	1	7.000	7.590	8.300
Asn-Trp	0	1	10.97	11.41	6.720
Asn-Tyr	0	1	9.140	9.150	4.240
Asn-Val	0	1	10.06	10.08	6.980
Average			**10.06**	**10.25**	**6.492**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.330	8.350	12.55
Asn-Arg	1	1	11.92	12.01	11.75
Asn-Asn	0	1	6.660	6.190	12.31
Asn-Asp	-1	1	11.00	11.18	12.91
Asn-Cys	0	1	10.22	10.32	12.30
Asn-Gln	0	1	7.440	6.940	10.77
Asn-Glu	-1	1	11.36	11.71	11.12
Asn-Gly	0	1	8.070	8.070	13.08
Asn-His	0	1	7.870	7.650	12.38
Asn-Ile	0	1	5.560	5.330	11.40
Asn-Leu	0	1	7.190	6.430	9.650
Asn-Lys	1	1	10.61	10.54	10.63
Asn-Met	0	1	15.87	15.65	11.89
Asn-Phe	0	1	6.270	6.320	12.25
Asn-Ser	0	1	11.10	11.44	11.95
Asn-Thr	0	1	6.460	6.360	12.17
Asn-Trp	0	1	10.32	10.70	12.56
Asn-Tyr	0	1	8.460	8.310	10.51
Asn-Val	0	1	7.100	7.010	12.42
Average			**9.043**	**8.974**	**11.82**

Table S12.A. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	26.97	40.73	46.13
Asn-Arg	1	1	26.99	40.39	44.91
Asn-Asn	0	1	25.90	41.00	50.67
Asn-Asp	-1	1	27.70	39.67	40.15
Asn-Cys	0	1	26.36	38.79	41.70
Asn-Gln	0	1	26.47	41.29	49.72
Asn-Glu	-1	1	28.52	40.06	38.71
Asn-Gly	0	1	27.87	41.41	45.41
Asn-His	0	1	27.52	41.00	45.23
Asn-Ile	0	1	28.16	38.55	34.84

Asn-Leu	0	1	27.29	40.60	44.63
Asn-Lys	1	1	26.28	38.62	41.38
Asn-Met	0	1	27.01	41.13	47.37
Asn-Phe	0	1	26.42	41.63	51.02
Asn-Ser	0	1	27.25	40.23	43.52
Asn-Thr	0	1	27.37	38.12	36.06
Asn-Trp	0	1	26.80	38.90	40.58
Asn-Tyr	0	1	28.55	37.48	29.97
Asn-Val	0	1	28.35	37.61	31.04
Average			**27.25**	**39.85**	**42.26**

Table S12.B. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	85.04	87.42	17.26
Asn-Arg	1	1	80.89	83.02	17.00
Asn-Asn	0	1	78.36	78.91	13.24
Asn-Asp	-1	1	63.29	62.85	10.01
Asn-Cys	0	1	52.32	52.20	11.15
Asn-Gln	0	1	85.71	88.03	17.99
Asn-Glu	-1	1	49.11	48.24	10.63
Asn-Gly	0	1	52.08	52.18	13.05
Asn-His	0	1	77.81	79.20	14.92
Asn-Ile	0	1	51.24	49.97	8.080
Asn-Leu	0	1	54.01	54.3	12.09
Asn-Lys	1	1	71.19	71.89	13.37
Asn-Met	0	1	47.99	47.19	10.56
Asn-Phe	0	1	77.94	79.24	14.85
Asn-Ser	0	1	67.27	69.06	16.77
Asn-Thr	0	1	55.55	54.54	8.800
Asn-Trp	0	1	55.71	55.51	11.54
Asn-Tyr	0	1	54.99	55.43	12.59
Asn-Val	0	1	57.79	57.68	11.59
Average			**64.12**	**64.57**	**12.92**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	46.65	48.83	9.980
Asn-Arg	1	1	43.05	44.82	9.950
Asn-Asn	0	1	39.90	40.18	5.000
Asn-Asp	-1	1	25.60	25.10	4.030
Asn-Cys	0	1	15.55	15.40	4.860
Asn-Gln	0	1	47.11	48.99	9.890
Asn-Glu	-1	1	10.64	9.920	4.970
Asn-Gly	0	1	12.97	12.90	5.940
Asn-His	0	1	39.16	40.30	7.820

Asn-Ile	0	1	13.91	13.12	3.370
Asn-Leu	0	1	15.80	15.84	5.140
Asn-Lys	1	1	34.41	35.12	7.110
Asn-Met	0	1	9.380	8.250	3.000
Asn-Phe	0	1	39.06	39.91	6.480
Asn-Ser	0	1	29.23	30.85	10.05
Asn-Thr	0	1	18.78	18.17	3.810
Asn-Trp	0	1	18.48	18.46	5.520
Asn-Tyr	0	1	17.86	19.40	9.060
Asn-Val	0	1	20.99	21.58	7.720
Average			**26.24**	**26.69**	**6.511**

Table S12.C. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 20)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	26.91	40.26	44.76
Asn-Arg	1	1	28.02	41.27	44.43
Asn-Asn	0	1	26.53	40.87	48.10
Asn-Asp	-1	1	28.01	39.53	38.63
Asn-Cys	0	1	26.10	38.33	41.02
Asn-Gln	0	1	26.65	40.83	47.56
Asn-Glu	-1	1	27.48	36.20	29.24
Asn-Gly	0	1	28.02	40.99	43.50
Asn-His	0	1	27.06	40.65	45.57
Asn-Ile	0	1	27.19	38.47	37.86
Asn-Leu	0	1	27.33	40.12	42.92
Asn-Lys	1	1	24.07	37.79	46.03
Asn-Met	0	1	27.08	40.70	45.67
Asn-Phe	0	1	25.96	41.21	51.14
Asn-Ser	0	1	27.28	39.76	41.87
Asn-Thr	0	1	26.45	38.35	39.92
Asn-Trp	0	1	26.46	38.36	39.93
Asn-Tyr	0	1	27.14	40.51	44.83
Asn-Val	0	1	27.58	37.70	33.95
Average			**26.91**	**39.57**	**42.47**

Table S12.D. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	77.29	79.16	16.82
Asn-Arg	1	1	75.19	76.88	15.73
Asn-Asn	0	1	78.15	78.75	13.12

Asn-Asp	-1	1	63.02	62.55	10.27
Asn-Cys	0	1	51.28	51.22	11.39
Asn-Gln	0	1	76.77	78.60	16.66
Asn-Glu	-1	1	74.45	75.68	13.95
Asn-Gly	0	1	75.02	77.02	16.74
Asn-His	0	1	70.68	72.01	15.12
Asn-Ile	0	1	56.1	56.16	10.77
Asn-Leu	0	1	63.51	64.08	12.96
Asn-Lys	1	1	65.16	66.06	13.87
Asn-Met	0	1	55.83	55.69	12.04
Asn-Phe	0	1	69.23	69.99	14.06
Asn-Ser	0	1	64.43	66.17	16.15
Asn-Thr	0	1	54.90	53.98	9.610
Asn-Trp	0	1	53.76	53.40	10.73
Asn-Tyr	0	1	67.29	67.81	12.63
Asn-Val	0	1	54.32	54.07	11.49
Average			**65.60**	**66.28**	**13.37**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	39.25	40.98	9.860
Asn-Arg	1	1	36.59	37.84	8.780
Asn-Asn	0	1	39.72	40.09	5.440
Asn-Asp	-1	1	25.26	24.89	4.660
Asn-Cys	0	1	14.87	14.83	5.260
Asn-Gln	0	1	38.38	39.93	9.060
Asn-Glu	-1	1	38.92	40.92	10.48
Asn-Gly	0	1	36.19	38.10	10.06
Asn-His	0	1	32.50	33.49	7.930
Asn-Ile	0	1	18.97	19.43	5.390
Asn-Leu	0	1	25.59	26.02	6.390
Asn-Lys	1	1	29.72	30.31	6.560
Asn-Met	0	1	17.46	17.10	4.860
Asn-Phe	0	1	30.76	31.08	5.670
Asn-Ser	0	1	26.70	28.35	9.800
Asn-Thr	0	1	18.05	17.47	3.780
Asn-Trp	0	1	17.10	16.92	4.860
Asn-Tyr	0	1	28.74	29.30	5.680
Asn-Val	0	1	17.58	17.92	6.960
Average			**28.02**	**28.68**	**6.920**

Table S12.E. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 40)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	26.94	40.20	44.50
Asn-Arg	1	1	28.02	41.27	44.43
Asn-Asn	0	1	26.98	40.76	46.24

Asn-Asp	-1	1	28.14	39.52	38.19
Asn-Cys	0	1	26.17	38.28	40.62
Asn-Gln	0	1	26.92	40.77	46.46
Asn-Glu	-1	1	27.49	36.33	29.63
Asn-Gly	0	1	27.99	40.95	43.46
Asn-His	0	1	27.02	40.62	45.61
Asn-Ile	0	1	26.85	38.57	39.29
Asn-Leu	0	1	27.33	40.08	42.76
Asn-Lys	1	1	23.90	37.74	46.43
Asn-Met	0	1	27.16	40.66	45.29
Asn-Phe	0	1	25.96	41.16	50.97
Asn-Ser	0	1	27.40	39.72	41.32
Asn-Thr	0	1	26.11	38.44	41.36
Asn-Trp	0	1	26.47	38.29	39.67
Asn-Tyr	0	1	27.16	40.44	44.53
Asn-Val	0	1	27.59	37.80	34.25
Average			**26.93**	**39.56**	**42.37**

Table S12.F. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	76.01	77.81	16.57
Asn-Arg	1	1	74.49	76.09	15.51
Asn-Asn	0	1	78.10	78.72	13.16
Asn-Asp	-1	1	62.57	62.83	11.63
Asn-Cys	0	1	51.15	51.09	11.33
Asn-Gln	0	1	75.34	77.09	16.30
Asn-Glu	-1	1	73.22	74.37	13.61
Asn-Gly	0	1	73.89	75.78	16.41
Asn-His	0	1	69.72	71.02	15.10
Asn-Ile	0	1	55.86	55.89	10.89
Asn-Leu	0	1	63.59	63.89	12.30
Asn-Lys	1	1	64.27	65.23	14.09
Asn-Met	0	1	55.57	55.39	11.96
Asn-Phe	0	1	68.05	68.71	13.69
Asn-Ser	0	1	64.15	65.85	16.02
Asn-Thr	0	1	54.81	53.92	9.800
Asn-Trp	0	1	53.52	53.14	10.74
Asn-Tyr	0	1	66.06	66.53	12.50
Asn-Val	0	1	54.01	53.66	11.18
Average			**64.97**	**65.63**	**13.30**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	38.01	39.68	9.660
Asn-Arg	1	1	35.87	37.04	8.560

Asn-Asn	0	1	39.64	40.1	5.880
Asn-Asp	-1	1	24.77	25.17	6.120
Asn-Cys	0	1	14.77	14.74	5.280
Asn-Gln	0	1	36.95	38.46	8.950
Asn-Glu	-1	1	37.58	39.49	10.05
Asn-Gly	0	1	35.10	36.90	9.740
Asn-His	0	1	31.57	32.54	7.900
Asn-Ile	0	1	18.73	19.11	5.190
Asn-Leu	0	1	25.69	25.87	5.770
Asn-Lys	1	1	28.94	29.57	6.690
Asn-Met	0	1	17.22	16.84	4.860
Asn-Phe	0	1	29.60	29.83	5.340
Asn-Ser	0	1	26.43	28.07	9.790
Asn-Thr	0	1	17.94	17.35	3.660
Asn-Trp	0	1	16.88	16.71	4.930
Asn-Tyr	0	1	27.57	28.08	5.620
Asn-Val	0	1	17.21	17.43	6.590
Average			**27.39**	**28.05**	**6.873**

Table S12.G. Asn-X Isoimide Formation Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 80)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	26.94	40.18	44.43
Asn-Arg	1	1	28.18	43.31	50.75
Asn-Asn	0	1	26.93	40.73	46.29
Asn-Asp	-1	1	28.33	39.52	37.54
Asn-Cys	0	1	26.18	38.25	40.49
Asn-Gln	0	1	26.98	40.74	46.15
Asn-Glu	-1	1	27.68	36.38	29.19
Asn-Gly	0	1	28.01	40.93	43.36
Asn-His	0	1	27.03	40.60	45.51
Asn-Ile	0	1	26.78	38.61	39.68
Asn-Leu	0	1	27.34	40.06	42.64
Asn-Lys	1	1	23.98	37.70	46.01
Asn-Met	0	1	27.19	40.64	45.11
Asn-Phe	0	1	25.92	41.14	51.07
Asn-Ser	0	1	27.38	39.70	41.31
Asn-Thr	0	1	26.18	38.46	41.19
Asn-Trp	0	1	26.31	38.28	40.15
Asn-Tyr	0	1	27.07	40.41	44.75
Asn-Val	0	1	27.58	37.85	34.43
Average			**26.95**	**39.66**	**42.63**

Table S12.H. Asn-X Isoimide Formation Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε = 80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	75.34	77.14	16.68
Asn-Arg	1	1	74.09	75.68	15.49
Asn-Asn	0	1	78.08	78.71	13.18
Asn-Asp	-1	1	62.41	62.68	11.58
Asn-Cys	0	1	51.09	51.02	11.33
Asn-Gln	0	1	74.73	76.48	16.35
Asn-Glu	-1	1	72.41	73.69	14.21
Asn-Gly	0	1	73.29	75.16	16.35
Asn-His	0	1	69.21	70.52	15.12
Asn-Ile	0	1	55.66	55.73	11.06
Asn-Leu	0	1	63.77	63.30	11.26
Asn-Lys	1	1	63.87	64.83	13.93
Asn-Met	0	1	55.44	55.25	11.92
Asn-Phe	0	1	67.47	68.08	13.51
Asn-Ser	0	1	63.97	65.66	16.04
Asn-Thr	0	1	54.76	53.89	9.84
Asn-Trp	0	1	53.39	53.01	10.78
Asn-Tyr	0	1	65.45	65.90	12.44
Asn-Val	0	1	53.80	53.44	11.18
Average			**64.64**	**65.27**	**13.28**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	37.36	39.03	9.780
Asn-Arg	1	1	34.36	34.97	7.100
Asn-Asn	0	1	39.64	40.11	5.890
Asn-Asp	-1	1	24.59	25.00	6.210
Asn-Cys	0	1	14.72	14.70	5.310
Asn-Gln	0	1	36.35	37.86	9.070
Asn-Glu	-1	1	36.70	38.75	10.74
Asn-Gly	0	1	34.51	36.29	9.700
Asn-His	0	1	31.08	32.05	7.940
Asn-Ile	0	1	18.53	18.93	5.280
Asn-Leu	0	1	25.89	25.30	4.750
Asn-Lys	1	1	28.56	29.19	6.620
Asn-Met	0	1	17.09	16.71	4.860
Asn-Phe	0	1	29.04	29.22	5.140
Asn-Ser	0	1	26.26	27.90	9.810
Asn-Thr	0	1	17.87	17.29	3.740
Asn-Trp	0	1	16.79	16.61	4.870
Asn-Tyr	0	1	27.00	27.48	5.510
Asn-Val	0	1	16.97	17.17	6.540
Average			**27.02**	**27.61**	**6.782**

Table S13.A. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 4$)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-25.14	-37.60	-41.77
Asn-Arg	1	1	-19.42	-28.34	-29.94
Asn-Asn	0	1	-19.14	-32.02	-43.20
Asn-Asp	-1	1	-23.19	-33.54	-34.73
Asn-Cys	0	1	-20.23	-29.15	-29.91
Asn-Gln	0	1	-24.92	-37.72	-42.93
Asn-Glu	-1	1	-21.18	-31.96	-36.16
Asn-Gly	0	1	-26.72	-40.39	-45.86
Asn-His	0	1	-24.31	-36.05	-39.38
Asn-Ile	0	1	-23.79	-36.44	-42.40
Asn-Leu	0	1	-22.98	-33.98	-36.88
Asn-Lys	1	1	-23.77	-34.64	-36.44
Asn-Met	0	1	-20.21	-32.24	-40.36
Asn-Phe	0	1	-23.10	-36.43	-44.72
Asn-Ser	0	1	-21.21	-31.41	-34.18
Asn-Thr	0	1	-23.91	-36.71	-42.92
Asn-Trp	0	1	-24.29	-34.32	-33.64
Asn-Tyr	0	1	-23.31	-33.43	-33.94
Asn-Val	0	1	-21.68	-30.30	-28.90
Average			**-22.76**	**-34.03**	**-37.80**

Table S13.B. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, $\varepsilon = 4$)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	7.190	7.090	5.200
Asn-Arg	1	1	5.970	5.870	5.460
Asn-Asn	0	1	6.230	5.970	4.620
Asn-Asp	-1	1	9.640	10.33	7.560
Asn-Cys	0	1	7.930	8.100	6.750
Asn-Gln	0	1	9.150	9.460	6.700
Asn-Glu	-1	1	3.760	3.710	6.590
Asn-Gly	0	1	12.55	13.26	7.610
Asn-His	0	1	4.040	4.280	6.790
Asn-Ile	0	1	11.32	12.06	7.840
Asn-Leu	0	1	11.27	11.03	5.230
Asn-Lys	1	1	2.430	2.660	7.360

Asn-Met	0	1	11.14	11.54	6.740
Asn-Phe	0	1	1.680	1.320	4.790
Asn-Ser	0	1	10.95	11.64	7.690
Asn-Thr	0	1	10.59	10.93	6.170
Asn-Trp	0	1	12.20	12.61	7.120
Asn-Tyr	0	1	13.43	14.68	8.990
Asn-Val	0	1	11.69	12.21	7.170
Average			**8.587**	**8.882**	**6.652**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.35	42.77	11.87
Asn-Arg	1	1	33.08	32.75	9.440
Asn-Asn	0	1	36.13	36.04	11.47
Asn-Asp	-1	1	41.69	42.20	12.57
Asn-Cys	0	1	35.83	35.74	10.70
Asn-Gln	0	1	44.34	45.22	13.63
Asn-Glu	-1	1	33.91	34.06	12.02
Asn-Gly	0	1	49.70	51.52	15.30
Asn-His	0	1	37.56	38.38	12.95
Asn-Ile	0	1	45.20	46.52	14.65
Asn-Leu	0	1	43.45	43.26	10.72
Asn-Lys	1	1	34.93	35.61	12.92
Asn-Met	0	1	41.23	41.90	13.03
Asn-Phe	0	1	35.37	35.66	12.10
Asn-Ser	0	1	40.76	41.34	12.56
Asn-Thr	0	1	44.65	45.61	13.10
Asn-Trp	0	1	44.99	45.27	11.88
Asn-Tyr	0	1	45.53	46.41	13.72
Asn-Val	0	1	41.00	41.10	10.89
Average			**40.62**	**41.12**	**12.40**

Table S13.C. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 20$)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-24.63	-36.55	-39.97
Asn-Arg	1	1	-21.05	-30.44	-31.48
Asn-Asn	0	1	-19.82	-32.16	-41.40
Asn-Asp	-1	1	-22.91	-33.19	-34.50
Asn-Cys	0	1	-20.01	-29.15	-30.67
Asn-Gln	0	1	-24.01	-36.56	-42.11
Asn-Glu	-1	1	-21.03	-31.91	-36.49
Asn-Gly	0	1	-26.66	-39.88	-44.34
Asn-His	0	1	-23.83	-35.12	-37.88
Asn-Ile	0	1	-23.19	-35.77	-42.19
Asn-Leu	0	1	-22.53	-33.15	-35.62

Asn-Lys	1	1	-21.50	-32.33	-36.35
Asn-Met	0	1	-20.26	-31.40	-37.38
Asn-Phe	0	1	-22.63	-35.65	-43.66
Asn-Ser	0	1	-21.58	-31.06	-31.77
Asn-Thr	0	1	-23.33	-36.20	-43.16
Asn-Trp	0	1	-22.64	-33.75	-37.27
Asn-Tyr	0	1	-22.99	-37.25	-47.81
Asn-Val	0	1	-21.82	-30.75	-29.94
Average			**-22.44**	**-33.80**	**-38.11**

Table S13.D. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =20)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	8.150	8.160	5.560
Asn-Arg	1	1	10.86	11.25	7.200
Asn-Asn	0	1	9.940	10.23	6.680
Asn-Asp	-1	1	10.89	11.84	8.770
Asn-Cys	0	1	8.700	8.880	6.780
Asn-Gln	0	1	10.19	10.60	7.320
Asn-Glu	-1	1	3.350	3.470	6.820
Asn-Gly	0	1	13.34	14.10	7.740
Asn-His	0	1	3.710	3.920	6.910
Asn-Ile	0	1	12.44	13.15	7.860
Asn-Leu	0	1	12.13	12.08	5.670
Asn-Lys	1	1	4.020	4.190	6.740
Asn-Met	0	1	11.62	12.10	7.140
Asn-Phe	0	1	1.540	1.100	4.440
Asn-Ser	0	1	11.28	11.95	7.870
Asn-Thr	0	1	10.98	11.38	6.710
Asn-Trp	0	1	12.96	13.09	6.160
Asn-Tyr	0	1	12.46	12.72	6.330
Asn-Val	0	1	13.43	14.00	8.120
Average			**9.578**	**9.906**	**6.885**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	42.47	42.86	11.82
Asn-Arg	1	1	39.87	40.11	11.50
Asn-Asn	0	1	40.02	40.45	13.14
Asn-Asp	-1	1	42.63	43.42	13.72
Asn-Cys	0	1	36.51	36.49	10.90
Asn-Gln	0	1	44.39	45.26	14.05
Asn-Glu	-1	1	33.48	33.77	12.31
Asn-Gly	0	1	50.03	51.88	15.11
Asn-His	0	1	36.43	37.13	12.72
Asn-Ile	0	1	45.73	46.96	14.61

Asn-Leu	0	1	43.63	43.55	10.89
Asn-Lys	1	1	34.31	34.85	12.25
Asn-Met	0	1	41.12	41.72	12.75
Asn-Phe	0	1	34.54	34.70	11.51
Asn-Ser	0	1	40.99	41.39	12.20
Asn-Thr	0	1	44.53	45.56	13.69
Asn-Trp	0	1	44.82	45.02	11.73
Asn-Tyr	0	1	46.70	47.71	14.29
Asn-Val	0	1	43.08	43.30	12.06
Average			**41.33**	**41.90**	**12.70**

Table S13.E. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, ε = 40)

Dipeptide	Charge	Multiplicity	ΔG_{RXN} (kcal.mol^{-1})	ΔH_{RXN} (kcal.mol^{-1})	ΔS (kcal.mol^{-1})
Asn-Ala	0	1	-24.62	-36.41	-39.55
Asn-Arg	1	1	-21.23	-30.55	-31.26
Asn-Asn	0	1	-20.27	-32.08	-39.63
Asn-Asp	-1	1	-22.83	-33.12	-34.53
Asn-Cys	0	1	-20.07	-29.14	-30.44
Asn-Gln	0	1	-24.13	-36.41	-41.18
Asn-Glu	-1	1	-21.09	-31.90	-36.27
Asn-Gly	0	1	-26.61	-39.82	-44.32
Asn-His	0	1	-23.73	-35.01	-37.85
Asn-Ile	0	1	-23.14	-35.69	-42.10
Asn-Leu	0	1	-22.29	-33.08	-36.21
Asn-Lys	1	1	-21.15	-32.08	-36.67
Asn-Met	0	1	-19.78	-31.39	-38.93
Asn-Phe	0	1	-22.55	-35.55	-43.62
Asn-Ser	0	1	-21.24	-31.15	-33.23
Asn-Thr	0	1	-23.91	-36.14	-41.02
Asn-Trp	0	1	-22.51	-33.64	-37.33
Asn-Tyr	0	1	-23.06	-37.29	-47.73
Asn-Val	0	1	-22.28	-30.80	-28.59
Average			**-22.44**	**-33.75**	**-37.92**

Table S13.F. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =40)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.15	11.87	7.720
Asn-Arg	1	1	10.98	11.41	7.270
Asn-Asn	0	1	9.920	10.21	6.320

Asn-Asp	-1	1	10.98	11.93	8.780
Asn-Cys	0	1	8.840	9.000	6.720
Asn-Gln	0	1	10.54	10.79	6.350
Asn-Glu	-1	1	3.320	3.440	6.780
Asn-Gly	0	1	13.45	14.21	7.750
Asn-His	0	1	3.640	3.850	7.020
Asn-Ile	0	1	12.58	13.29	7.870
Asn-Leu	0	1	12.22	12.58	6.700
Asn-Lys	1	1	4.260	4.410	6.830
Asn-Met	0	1	11.70	12.18	7.120
Asn-Phe	0	1	1.500	1.050	4.370
Asn-Ser	0	1	11.30	11.95	7.610
Asn-Thr	0	1	11.05	11.42	6.450
Asn-Trp	0	1	13.02	13.17	6.290
Asn-Tyr	0	1	12.61	12.87	6.420
Asn-Val	0	1	11.72	12.12	6.920
Average			**9.725**	**10.09**	**6.910**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	45.37	46.45	13.89
Asn-Arg	1	1	40.17	40.42	11.53
Asn-Asn	0	1	40.07	40.43	12.39
Asn-Asp	-1	1	42.65	43.44	13.74
Asn-Cys	0	1	36.65	36.61	10.79
Asn-Gln	0	1	44.64	45.31	12.86
Asn-Glu	-1	1	33.46	33.74	12.22
Asn-Gly	0	1	50.08	51.93	15.11
Asn-His	0	1	36.25	36.95	12.83
Asn-Ile	0	1	45.81	47.02	14.60
Asn-Leu	0	1	43.60	43.96	12.05
Asn-Lys	1	1	34.30	34.81	12.41
Asn-Met	0	1	41.10	41.73	13.07
Asn-Phe	0	1	34.42	34.56	11.43
Asn-Ser	0	1	41.01	41.45	12.26
Asn-Thr	0	1	44.59	45.57	12.96
Asn-Trp	0	1	44.78	44.99	11.87
Asn-Tyr	0	1	46.88	47.90	14.36
Asn-Val	0	1	41.50	41.50	10.57
Average			**41.44**	**42.04**	**12.68**

Table S13.G. Asn-X Isoimide Hydrolysis into Asp-X Reaction Thermochemistry (Implicit Solvation + 1 H_2O, $\varepsilon = 80$)

Dipeptide	**Charge**	**Multiplicity**	**ΔG_{RXN} (kcal.mol^{-1})**	**ΔH_{RXN} (kcal.mol^{-1})**	**ΔS (kcal.mol^{-1})**
Asn-Ala	0	1	-24.61	-36.35	-39.38
Asn-Arg	1	1	-21.34	-32.66	-38.00

Asn-Asn	0	1	-20.25	-32.06	-39.61
Asn-Asp	-1	1	-22.80	-33.09	-34.52
Asn-Cys	0	1	-20.06	-29.14	-30.45
Asn-Gln	0	1	-24.14	-36.32	-40.87
Asn-Glu	-1	1	-21.11	-31.90	-36.18
Asn-Gly	0	1	-26.59	-39.79	-44.25
Asn-His	0	1	-23.70	-34.95	-37.73
Asn-Ile	0	1	-23.12	-35.64	-41.99
Asn-Leu	0	1	-22.26	-33.04	-36.15
Asn-Lys	1	1	-20.92	-31.95	-36.99
Asn-Met	0	1	-17.19	-25.89	-29.19
Asn-Phe	0	1	-22.49	-35.51	-43.69
Asn-Ser	0	1	-21.28	-31.20	-33.28
Asn-Thr	0	1	-23.73	-36.12	-41.57
Asn-Trp	0	1	-22.37	-33.59	-37.63
Asn-Tyr	0	1	-22.99	-37.32	-48.07
Asn-Val	0	1	-22.33	-30.84	-28.52
Average			**-22.28**	**-33.55**	**-37.79**

Table S13.H. Asn-X Isoimide Hydrolysis into Asp-X Reaction Forward and Reverse Arrhenius Parameters (Implicit Solvation + 1 H_2O, ε =80)

Forward					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	11.21	11.93	7.740
Asn-Arg	1	1	10.07	8.830	3.630
Asn-Asn	0	1	10.01	10.30	6.340
Asn-Asp	-1	1	11.04	11.99	8.700
Asn-Cys	0	1	8.890	9.050	6.730
Asn-Gln	0	1	10.59	10.86	6.400
Asn-Glu	-1	1	3.310	3.430	6.820
Asn-Gly	0	1	13.49	14.26	7.780
Asn-His	0	1	3.610	3.820	7.030
Asn-Ile	0	1	12.63	13.35	7.940
Asn-Leu	0	1	12.26	12.62	6.710
Asn-Lys	1	1	4.260	4.480	6.730
Asn-Met	0	1	10.60	10.98	6.610
Asn-Phe	0	1	1.480	1.020	4.330
Asn-Ser	0	1	11.34	11.97	7.590
Asn-Thr	0	1	11.06	11.44	6.510
Asn-Trp	0	1	13.08	13.21	6.280
Asn-Tyr	0	1	12.70	12.95	6.510
Asn-Val	0	1	11.61	11.00	5.600
Average			**9.644**	**9.868**	**6.631**
Reverse					
Dipeptide	**Charge**	**Multiplicity**	**E_0**	**E_A**	**Log(Ã)**
Asn-Ala	0	1	45.38	46.45	13.86

Asn-Arg	1	1	40.42	39.55	9.420
Asn-Asn	0	1	40.15	40.51	12.41
Asn-Asp	-1	1	42.67	43.47	13.66
Asn-Cys	0	1	36.70	36.65	10.81
Asn-Gln	0	1	44.64	45.3	12.85
Asn-Glu	-1	1	33.45	33.72	12.24
Asn-Gly	0	1	50.09	51.95	15.13
Asn-His	0	1	36.17	36.87	12.81
Asn-Ile	0	1	45.84	47.05	14.65
Asn-Leu	0	1	43.59	43.95	12.04
Asn-Lys	1	1	34.19	34.75	12.38
Asn-Met	0	1	36.24	35.68	10.26
Asn-Phe	0	1	34.35	34.48	11.40
Asn-Ser	0	1	41.09	41.52	12.25
Asn-Thr	0	1	44.59	45.57	13.14
Asn-Trp	0	1	44.77	44.98	11.92
Asn-Tyr	0	1	46.98	47.99	14.52
Asn-Val	0	1	41.44	40.43	9.230
Average			**41.20**	**41.62**	**12.37**

XYZ Coordinates

Table S14.A. Direct Hydrolysis XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions							
H_2O				NH_3			
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
O	-0.999631	0.482902	0	N	-1.133326	-0.563263	0.000024
H	-0.03661	0.526297	0	H	-0.744703	-1.50246	-0.000031
H	-1.280189	1.405171	0	H	-0.744689	-0.093642	0.813368
				H	-0.7447	-0.093681	-0.813362
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.89113	-2.88425	0.251026	N	-1.2015	-2.57231	1.13264
H	-0.95616	-2.90785	0.649126	H	-0.60625	-2.21433	1.874683
C	-2.47859	-1.5646	0.463042	C	-2.39599	-1.73865	1.018612
H	-3.41318	-1.50571	-0.09863	H	-2.95464	-2.05716	0.135929
C	-2.79954	-1.24379	1.946244	C	-3.33904	-1.82203	2.241922
C	-1.50184	-0.51034	-0.07178	C	-1.9375	-0.28495	0.832125
H	-3.40149	-2.06611	2.346382	H	-3.46866	-2.87408	2.519891
H	-1.87528	-1.20072	2.528218	H	-2.90455	-1.32499	3.11302
C	-3.63214	0.020374	2.107956	C	-4.72717	-1.28396	1.990161
O	-0.2821	-0.67265	-0.00889	O	-0.94145	0.147075	1.41481
O	-4.56342	0.276189	1.34013	O	-5.20983	-1.06606	0.898335
N	-3.30323	0.830859	3.134184	N	-2.70603	0.479014	0.030945
H	-3.85231	1.660376	3.303569	H	-3.56835	0.102114	-0.34157
H	-2.54518	0.619918	3.7626	C	-2.44125	1.893387	-0.16415
N	-2.06596	0.613276	-0.56173	H	-2.12408	2.326613	0.788237
H	-3.0711	0.728352	-0.52181	C	-1.33869	2.137769	-1.21236
C	-1.26848	1.74318	-1.00313	C	-3.72994	2.579243	-0.58171
H	-0.41347	1.851669	-0.33077	H	-1.6426	1.742283	-2.18448
C	-0.74877	1.561198	-2.44225	H	-1.1316	3.204597	-1.30808
C	-2.10609	3.005279	-0.89877	H	-0.43042	1.626838	-0.8911
H	-1.58414	1.477638	-3.14156	O	-4.73729	2.008692	-0.93742
H	-0.12135	2.40522	-2.73248	H	-1.45877	-3.52263	1.380237
H	-0.15711	0.646245	-2.4878	O	-3.60755	3.913154	-0.53694
O	-3.3052	3.031904	-0.73109	H	-4.43681	4.312398	-0.84629
H	-2.44132	-3.59236	0.727048	O	-5.40678	-1.09766	3.135034
O	-1.35179	4.103353	-1.04704	H	-6.30151	-0.78999	2.915424
H	-1.92824	4.883985	-1.01301				
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.77355	-3.90117	-0.30998	N	-2.36592	-2.90823	2.234816
H	-1.92857	-4.25082	0.13375	H	-2.44889	-2.3758	3.096597

C	-3.10055	-2.58521	0.229565	C	-2.61264	-2.03515	1.091706
H	-3.92286	-2.16501	-0.35352	H	-2.39108	-2.59063	0.177527
C	-3.53822	-2.60008	1.71833	C	-4.06919	-1.51534	1.001758
C	-1.86956	-1.68267	0.085495	C	-1.66911	-0.83107	1.193472
H	-4.35269	-3.32406	1.822226	H	-4.75339	-2.35773	1.152511
H	-2.71173	-2.94193	2.346497	H	-4.283	-0.79925	1.799314
C	-4.08704	-1.25824	2.182489	C	-4.44247	-0.90829	-0.32957
O	-0.72548	-2.13054	0.169856	O	-1.34265	-0.35637	2.280051
O	-4.85073	-0.59915	1.471981	O	-3.80425	-1.01325	-1.35793
N	-3.69921	-0.83862	3.403629	N	-1.26441	-0.29916	0.01691
H	-4.06492	0.0289	3.76687	H	-1.73375	-0.61934	-0.82107
H	-3.07642	-1.37756	3.983016	C	-0.59956	0.988332	-0.02386
N	-2.1308	-0.36865	-0.08207	H	0.284384	0.954504	0.615639
H	-3.08999	-0.04567	-0.10087	C	-0.18065	1.29727	-1.47347
C	-1.07728	0.629542	-0.11448	C	-1.52934	2.075786	0.523102
H	-0.2829	0.323254	0.569179	H	0.391251	0.434131	-1.82747
C	-0.48875	0.763664	-1.54044	H	-1.07937	1.367428	-2.09594
C	-1.65723	1.948554	0.370655	C	0.662799	2.565663	-1.62268
H	-0.20852	-0.24916	-1.84229	O	-2.73448	2.061887	0.42771
H	-1.28338	1.095538	-2.21615	H	0.089702	3.444204	-1.31306
C	0.72584	1.688894	-1.64423	H	1.542007	2.505996	-0.97321
O	-2.82505	2.255799	0.282517	C	1.115755	2.74671	-3.07002
H	0.436799	2.719935	-1.42174	H	1.716777	1.88729	-3.38212
H	1.483158	1.399227	-0.90857	H	0.242868	2.815078	-3.72844
C	1.334451	1.626898	-3.04395	N	1.926592	3.961137	-3.19114
H	1.697669	0.61461	-3.24413	H	1.925154	4.603548	-2.41236
H	0.575965	1.876632	-3.7939	C	2.609276	4.31459	-4.27946
N	2.45757	2.562883	-3.1447	N	2.538389	3.57408	-5.38936
H	2.538929	3.270964	-2.42989	N	3.37603	5.41214	-4.26164
C	3.310098	2.626566	-4.16668	H	1.839678	2.85785	-5.49692
N	3.172364	1.811448	-5.216	H	3.070455	3.820957	-6.20813
N	4.324355	3.498987	-4.1365	H	3.59394	5.878367	-3.39578
H	2.351923	1.241691	-5.33625	H	3.888672	5.698439	-5.07984
H	3.841137	1.821956	-5.969	O	-0.83853	3.074539	1.095181
H	4.50134	4.065217	-3.32292	H	-1.46349	3.760916	1.381116
H	4.925069	3.627231	-4.93418	H	-3.05856	-3.64967	2.26699
H	-3.51885	-4.55876	-0.10301	O	-5.61085	-0.25096	-0.267
O	-0.71284	2.749963	0.880646	H	-5.82017	0.091013	-1.15168
H	-1.12063	3.597466	1.124567				

Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.02276	-3.63904	-0.1579	N	0.047978	-2.560659	1.409286
H	-0.15911	-3.60238	0.376757	H	1.014698	-2.728841	1.674301
C	-1.8483	-2.47909	0.165658	C	-0.432879	-1.342728	2.05703
H	-2.69882	-2.45616	-0.51876	H	-1.421897	-1.107782	1.657714
C	-2.40763	-2.48163	1.612055	C	-0.548022	-1.453505	3.595591
C	-1.00549	-1.21526	-0.04078	C	0.538833	-0.208417	1.702669
H	-2.89898	-3.44545	1.781146	H	-1.04598	-2.396788	3.846559

H	-1.58869	-2.40241	2.331983	H	0.437859	-1.491112	4.065952
C	-3.46701	-1.41175	1.839413	C	-1.374313	-0.362931	4.234007
O	0.209617	-1.20723	0.15903	O	1.74958	-0.411392	1.604114
O	-4.30176	-1.14101	0.972054	O	-2.134113	0.378761	3.646434
N	-3.4479	-0.79245	3.036788	N	-0.010267	1.012538	1.537882
H	-4.15907	-0.10928	3.250767	H	-0.993234	1.151427	1.735595
H	-2.77194	-1.02064	3.747448	C	0.804164	2.186512	1.296149
N	-1.68803	-0.10987	-0.41077	H	1.695313	2.152433	1.928661
H	-2.69692	-0.14321	-0.49212	C	1.278393	2.259042	-0.175543
C	-1.03705	1.177687	-0.53865	C	-0.002442	3.419361	1.672903
H	-0.30742	1.299241	0.265828	H	1.608768	1.254292	-0.449688
C	-0.27774	1.300052	-1.88323	H	0.448805	2.529188	-0.832183
C	-2.08765	2.268695	-0.40433	C	2.486299	3.168905	-0.36041
H	0.277524	0.368305	-2.01383	O	-1.171344	3.410578	1.986927
H	-0.98308	1.388936	-2.7119	O	3.445035	3.12093	0.409497
C	0.758426	2.416391	-1.87417	N	2.45597	3.984691	-1.434344
O	-3.28271	2.078543	-0.38736	H	3.25249	4.572069	-1.629895
O	1.560218	2.530801	-0.9476	H	1.664494	4.027197	-2.055148
N	0.768526	3.230403	-2.9498	O	0.738915	4.530726	1.590564
H	1.459294	3.963556	-3.00609	H	0.179094	5.296126	1.799674
H	0.095173	3.147673	-3.69377	H	-0.495633	-3.360647	1.717644
H	-1.50439	-4.49378	0.103206	O	-1.20082	-0.318486	5.566106
O	-1.52466	3.481235	-0.33419	H	-1.78057	0.371095	5.92913
H	-2.22746	4.150312	-0.29616				

Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.99394	-2.615646	-0.96669	N	-2.387799	-2.967465	-0.780101
H	-4.154637	-3.163919	-0.798079	H	-1.521407	-3.48669	-0.666255
C	-4.959459	-1.409867	-0.144032	C	-2.305465	-1.712868	-0.035966
H	-5.784827	-0.760494	-0.443211	H	-3.179431	-1.106777	-0.284145
C	-5.095933	-1.677308	1.378324	C	-2.267597	-1.896559	1.499753
C	-3.629169	-0.690734	-0.397487	C	-1.033283	-0.979377	-0.486706
H	-6.002173	-2.269812	1.538006	H	-3.048671	-2.608134	1.790825
H	-4.246315	-2.269386	1.727639	H	-1.317939	-2.328875	1.824209
C	-5.265548	-0.394707	2.17958	C	-2.547047	-0.633562	2.278545
O	-2.587978	-1.320793	-0.594648	O	-0.004917	-1.601515	-0.761244
O	-6.043666	0.488959	1.811838	O	-3.093349	0.356389	1.838142
N	-4.526814	-0.281461	3.302451	N	-1.10982	0.364021	-0.523047
H	-4.626663	0.541187	3.878202	H	-1.953389	0.824975	-0.207176
H	-3.891517	-1.00321	3.601634	C	0.03689	1.195175	-0.850933
N	-3.672574	0.65458	-0.337307	H	0.937031	0.768125	-0.40336
H	-4.541591	1.117314	-0.102852	C	0.278339	1.290138	-2.375817
C	-2.476558	1.474028	-0.442982	C	-0.196632	2.573041	-0.259693
H	-1.65632	0.992954	0.094761	H	0.136262	0.280773	-2.772005
C	-2.018333	1.667153	-1.907697	H	-0.46621	1.939422	-2.841161
C	-2.767607	2.813773	0.207619	C	1.709144	1.727823	-2.770713
H	-2.131047	0.694908	-2.395318	O	-1.256562	2.968441	0.177499
H	-2.669557	2.376266	-2.42297	O	2.655654	1.196207	-2.133881

C	-0.533947	2.075837	-2.064231	O	1.806278	2.541787	-3.726806
O	-3.870631	3.20137	0.530522	O	0.907421	3.329937	-0.305368
O	0.296028	1.471801	-1.335761	H	0.689334	4.211013	0.039597
O	-0.277417	2.943503	-2.940051	H	-3.138915	-3.544577	-0.414723
O	-1.658111	3.548838	0.357352	O	-2.147212	-0.733683	3.558393
H	-1.908763	4.408879	0.731974	H	-2.3873	0.086278	4.020443
H	-5.789015	-3.192493	-0.709753				

Asn-Cys

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.888251	-2.4099	-0.65284	N	-2.200369	-1.760254	-1.269446
H	-2.011838	-2.771293	-0.286335	H	-1.689801	-2.638797	-1.254148
C	-3.158865	-1.098031	-0.074058	C	-2.451124	-1.276613	0.087175
H	-4.023301	-0.66537	-0.582163	H	-3.224052	-0.503711	0.023644
C	-3.471683	-1.124568	1.446035	C	-2.936744	-2.352339	1.077049
C	-1.938198	-0.202557	-0.31183	C	-1.215981	-0.559864	0.659246
H	-4.277511	-1.846989	1.610086	H	-3.736008	-2.921991	0.592657
H	-2.59788	-1.4746	2.001416	H	-2.134934	-3.048922	1.325389
C	-3.976286	0.214801	1.96478	C	-3.537512	-1.772329	2.334339
O	-0.795398	-0.657314	-0.342972	O	-1.075102	-0.399136	1.87019
O	-4.791014	0.883012	1.322454	O	-4.283282	-0.815988	2.364592
N	-3.491944	0.62146	3.155156	N	-0.346256	-0.106775	-0.271216
H	-3.820788	1.489136	3.551738	H	-0.560129	-0.352285	-1.231934
H	-2.822759	0.078451	3.676109	C	0.882592	0.596631	0.053041
N	-2.200454	1.119167	-0.428723	H	0.89957	0.7273	1.135577
H	-3.152861	1.454751	-0.353991	C	2.103763	-0.205056	-0.403069
C	-1.139568	2.101732	-0.532042	C	0.821652	1.981158	-0.595676
H	-0.289677	1.774921	0.069936	H	2.05618	-1.196358	0.049399
C	-0.693056	2.23069	-2.007387	H	2.111703	-0.318657	-1.487215
C	-1.656173	3.425268	0.015219	S	3.707112	0.504809	0.145257
H	-0.455962	1.226237	-2.353457	O	1.40191	2.295817	-1.610259
H	-1.510113	2.635087	-2.606318	H	3.703192	1.564045	-0.684202
S	0.820164	3.274562	-2.2129	O	0.009825	2.804207	0.08276
O	-2.825359	3.731244	0.069454	H	-0.039791	3.652282	-0.388102
H	1.181033	2.744984	-3.395381	H	-3.074513	-1.931549	-1.753891
H	-3.619013	-3.064406	-0.391508	O	-3.212422	-2.475503	3.435264
O	-0.654008	4.222765	0.402378	H	-3.668456	-2.077357	4.194438
H	-1.022051	5.076456	0.684914				

Asn-Gln

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.879903	-3.819748	-0.346005	N	-2.324325	-0.763706	3.986893
H	-1.044699	-4.046686	0.187054	H	-1.589329	-0.671252	4.682656
C	-2.397212	-2.524611	0.084431	C	-2.400811	0.452217	3.185034
H	-3.197535	-2.226122	-0.595968	H	-3.098174	0.282778	2.361731
C	-2.976114	-2.517935	1.524077	C	-2.88212	1.697744	3.974078
C	-1.260526	-1.498912	0.005617	C	-1.006406	0.746045	2.619021
H	-3.712097	-3.325178	1.595082	H	-3.747865	1.411781	4.582214
H	-2.183752	-2.730913	2.246175	H	-2.107849	2.031752	4.671897

C	-3.713183	-1.227404	1.853915	C	-3.33393	2.858502	3.110087
O	-0.091267	-1.81269	0.232026	O	0.014994	0.471136	3.246861
O	-4.466789	-0.693736	1.035544	O	-3.531597	2.79601	1.916216
N	-3.502467	-0.710385	3.081162	N	-0.977681	1.371808	1.420537
H	-3.995872	0.125739	3.356253	H	-1.854988	1.733922	1.06779
H	-2.886765	-1.146272	3.748165	C	0.251621	1.954061	0.91795
N	-1.638532	-0.232741	-0.270559	H	1.018204	1.178841	0.860021
H	-2.619382	-0.017526	-0.397739	C	-0.001614	2.540975	-0.482566
C	-0.694566	0.870389	-0.266145	C	0.750713	3.031828	1.8852
H	0.047494	0.693725	0.515754	H	-0.443054	1.750803	-1.092796
C	0.031263	0.980389	-1.629114	H	-0.742835	3.343353	-0.406049
C	-1.454073	2.145083	0.062707	C	1.259683	3.05984	-1.173319
H	0.411894	-0.01652	-1.854963	O	0.035813	3.725902	2.570279
H	-0.701814	1.233191	-2.401278	H	1.695276	3.900852	-0.630225
C	1.195704	1.973255	-1.647372	H	2.02434	2.274579	-1.196168
O	-2.637764	2.307948	-0.13432	C	0.993449	3.452649	-2.622092
H	0.84845	2.998759	-1.512708	O	0.130012	2.902438	-3.305996
H	1.877741	1.758272	-0.816311	N	1.788136	4.42778	-3.11753
C	2.01922	1.846116	-2.923084	H	1.70789	4.682884	-4.090082
O	2.281794	0.752405	-3.42514	H	2.50449	4.868847	-2.563993
N	2.466822	3.005127	-3.455524	H	-3.197361	-0.915769	4.481893
H	3.06273	2.976938	-4.268967	O	2.088295	3.142608	1.855199
H	2.260031	3.89999	-3.043186	H	2.353023	3.867965	2.444322
O	-0.64834	3.088256	0.568777	O	-3.563949	4.022313	3.74521
H	-1.166255	3.898168	0.708708	H	-3.36896	3.957182	4.690885
H	-2.563683	-4.54758	-0.163107				

Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.21535	-2.75801	-1.001343	N	-4.149436	-0.283245	-0.241771
H	-2.452499	-3.205202	-0.500027	H	-3.892906	-0.928048	-0.984495
C	-3.519806	-1.473895	-0.378795	C	-3.24332	-0.41188	0.898632
H	-4.226576	-0.937068	-1.015329	H	-3.702125	0.113482	1.742549
C	-4.15299	-1.588685	1.034415	C	-2.964538	-1.861468	1.34087
C	-2.221323	-0.665178	-0.270415	C	-1.913885	0.318336	0.638227
H	-5.029973	-2.238744	0.957842	H	-3.922774	-2.386552	1.406836
H	-3.4465	-2.063026	1.720114	H	-2.347142	-2.384465	0.609315
C	-4.645846	-0.247821	1.558356	C	-2.341878	-1.952427	2.712243
O	-1.137145	-1.214438	-0.067701	O	-0.89479	0.027832	1.270216
O	-5.315849	0.50618	0.847916	O	-2.683558	-1.291459	3.670718
N	-4.311307	0.066266	2.826362	N	-1.971268	1.296766	-0.281358
H	-4.630408	0.938938	3.21986	H	-2.844005	1.408899	-0.783259
H	-3.756434	-0.545989	3.401814	C	-0.816032	2.082571	-0.673143
N	-2.367198	0.673407	-0.349801	H	-0.157549	2.181654	0.191043
H	-3.288781	1.06753	-0.488333	C	-0.044066	1.399465	-1.830037
C	-1.259323	1.595295	-0.154406	C	-1.301003	3.46098	-1.087363
H	-0.544841	1.133658	0.528735	H	0.149405	0.375145	-1.505519
C	-0.551996	1.913295	-1.494515	H	-0.706501	1.334972	-2.698339
C	-1.806939	2.85981	0.484599	C	1.272924	2.072829	-2.20658

H	-0.295114	0.951744	-1.942578	O	-2.373984	3.680059	-1.606748
H	-1.274258	2.390783	-2.163538	H	1.10536	3.082738	-2.591572
C	0.705245	2.76847	-1.360814	H	1.900996	2.196715	-1.316468
O	-2.916832	3.301589	0.279718	C	2.113342	1.311913	-3.258577
H	0.468753	3.763047	-0.973385	O	3.181291	1.882554	-3.616468
H	1.387737	2.320619	-0.628232	O	1.689449	0.201146	-3.674139
C	1.507019	2.958546	-2.669464	H	-5.099613	-0.508328	0.032228
O	2.466148	3.77707	-2.602948	O	-0.386626	4.412484	-0.8501
O	1.165963	2.293904	-3.683212	H	-0.723286	5.25753	-1.191158
H	-4.019657	-3.374733	-0.941822	O	-1.396904	-2.908671	2.790617
O	-0.907354	3.458031	1.277452	H	-1.075973	-2.941733	3.706407
H	-1.28903	4.288146	1.607826				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.938514	-2.774289	-0.589538	N	1.658145	-0.705395	-0.377812
H	-1.052669	-3.093113	-0.206448	H	1.514304	-0.45675	0.597152
C	-2.256169	-1.453185	-0.053605	C	0.425533	-0.541514	-1.147952
H	-3.128953	-1.065226	-0.582705	H	0.565875	-1.055569	-2.10439
C	-2.581199	-1.447093	1.461364	C	-0.836066	-1.120154	-0.480676
C	-1.06141	-0.527376	-0.314259	C	0.194615	0.93479	-1.510679
H	-3.344468	-2.210679	1.646477	H	-0.602377	-2.130114	-0.12913
H	-1.69613	-1.73076	2.03746	H	-1.131348	-0.526312	0.38534
C	-3.165343	-0.127986	1.951123	C	-1.995665	-1.266062	-1.435333
O	0.096858	-0.947993	-0.31807	O	-0.92747	1.360582	-1.786989
O	-3.88091	0.572379	1.229557	O	-1.903663	-1.66305	-2.578068
N	-2.872097	0.216586	3.221219	N	1.307341	1.6958	-1.548256
H	-3.282675	1.050399	3.614133	H	2.155417	1.266382	-1.202052
H	-2.299991	-0.362147	3.814543	C	1.263471	3.10238	-1.837959
N	-1.36165	0.77437	-0.493744	C	0.891286	3.952251	-0.630538
H	-2.318567	1.088682	-0.384661	H	2.23651	3.437805	-2.202029
C	-0.330117	1.77717	-0.619631	H	0.53317	3.301824	-2.625191
C	-0.943334	3.156364	-0.679849	O	0.697125	3.542589	0.489296
H	0.366715	1.743957	0.224568	H	1.963107	-1.672394	-0.396431
H	0.268138	1.623603	-1.522999	O	0.810412	5.248627	-0.976718
O	-2.128685	3.393955	-0.615255	H	0.582465	5.767262	-0.188332
O	0.002746	4.095754	-0.813003	O	-3.177864	-0.970971	-0.862374
H	-0.424924	4.966872	-0.845213	H	-3.878777	-1.132111	-1.514752
H	-2.647953	-3.444473	-0.309502				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.713806	-2.850714	2.144005	N	-2.115086	-0.070384	2.868403
H	-1.699879	-2.314289	3.007182	H	-2.079429	0.477465	3.723751
C	-2.228942	-2.021248	1.058458	C	-2.789848	0.693041	1.823974
H	-2.096884	-2.56092	0.118267	H	-2.707172	0.141794	0.884495
C	-3.7312	-1.666327	1.195324	C	-4.291679	0.949702	2.104707
C	-1.411353	-0.723661	1.009269	C	-2.085187	2.048949	1.686154
H	-4.278954	-2.593411	1.397152	H	-4.761549	0.002527	2.392242

H	-3.888614	-1.013044	2.05828	H	-4.422356	1.629823	2.949812
C	-4.353305	-1.065041	-0.060302	C	-5.07516	1.4598	0.918355
O	-0.913577	-0.235896	2.020993	O	-1.621517	2.629631	2.663833
O	-3.872849	-1.245814	-1.184153	O	-4.724812	1.384885	-0.242047
N	-5.479164	-0.350089	0.126856	N	-2.065594	2.560579	0.430899
H	-5.960335	0.031922	-0.673426	H	-2.571358	2.052722	-0.283613
H	-5.873146	-0.199411	1.041498	C	-1.676753	3.931214	0.142775
N	-1.324936	-0.155406	-0.219256	H	-1.228141	4.326061	1.057353
H	-1.882474	-0.574349	-0.956474	C	-0.654409	3.992201	-1.00921
C	-0.788842	1.177743	-0.438726	C	-2.935192	4.763656	-0.12928
H	-0.303514	1.478744	0.492076	H	0.079587	3.207207	-0.819659
C	0.234095	1.182038	-1.5905	H	-1.157987	3.74702	-1.949315
C	-1.954361	2.144742	-0.674458	C	0.085201	5.285255	-1.127336
H	0.90313	0.336626	-1.421032	O	-3.129446	5.435074	-1.119588
H	-0.288405	1.000661	-2.53481	N	-0.473616	6.46136	-1.580586
C	1.070865	2.416911	-1.678709	C	1.397688	5.603524	-0.860726
O	-2.130634	2.797352	-1.681051	H	-1.447043	6.572894	-1.828111
N	0.609075	3.636147	-2.128466	C	0.490819	7.417843	-1.565926
C	2.396033	2.636507	-1.3777	N	1.643993	6.934226	-1.137091
H	-0.346475	3.82316	-2.398616	H	2.169844	4.943818	-0.494751
C	1.639541	4.520058	-2.078661	H	0.301488	8.4346	-1.872695
N	2.744057	3.949182	-1.629932	O	-3.820297	4.656539	0.869603
H	3.109803	1.91863	-1.002779	H	-4.605043	5.185224	0.651611
H	1.531766	5.55127	-2.376544	H	-2.631618	-0.920176	3.072441
O	-2.787725	2.171253	0.372734	O	-6.251769	1.990721	1.286921
H	-3.528339	2.765394	0.169407	H	-6.727456	2.270505	0.487551
H	-2.323161	-3.649008	2.2929				

Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.477432	-3.531417	-0.770217	N	-2.476188	-2.718159	-1.351746
H	-1.675815	-3.803821	-0.207663	H	-1.61075	-3.073825	-0.953416
C	-3.037935	-2.287604	-0.250832	C	-3.252453	-2.025937	-0.314886
H	-3.798078	-1.930723	-0.948906	H	-4.20009	-1.713479	-0.758224
C	-3.705792	-2.425675	1.142636	C	-3.540475	-2.893941	0.919753
C	-1.912028	-1.250736	-0.15923	C	-2.433942	-0.791001	0.081391
H	-4.434071	-3.241081	1.087747	H	-4.01777	-3.827942	0.60581
H	-2.957317	-2.702366	1.889534	H	-2.597277	-3.16268	1.406448
C	-4.479156	-1.17877	1.547798	C	-4.434608	-2.22189	1.938423
O	-0.756335	-1.577707	0.115495	O	-1.430898	-0.903632	0.789187
O	-5.19404	-0.579099	0.740619	O	-4.905953	-1.11478	1.81615
N	-4.344076	-0.775247	2.827322	N	-2.844724	0.383788	-0.430315
H	-4.864487	0.026896	3.149776	H	-3.700509	0.42953	-0.963973
H	-3.76135	-1.266199	3.485651	C	-2.145647	1.630485	-0.174761
N	-2.287342	0.031566	-0.346412	H	-1.779371	1.615026	0.854125
H	-3.26299	0.247207	-0.506729	C	-0.918616	1.807566	-1.125627
C	-1.361299	1.138638	-0.181973	C	-3.151638	2.761117	-0.306616
H	-0.678071	0.899063	0.635596	H	-0.396659	0.847387	-1.047727
C	-0.51021	1.371744	-1.471763	C	-1.357005	2.005684	-2.581791

C	-2.163504	2.367621	0.208771	C	0.04611	2.899813	-0.634148
H	-0.129949	0.371827	-1.708367	O	-4.205215	2.676344	-0.900216
C	-1.376526	1.852013	-2.642447	H	-1.823737	2.985966	-2.725117
C	0.70332	2.279463	-1.210507	H	-0.501062	1.94364	-3.256009
O	-3.34521	2.516801	-0.014224	H	-2.07347	1.239516	-2.888742
H	-1.721871	2.879108	-2.484767	H	-0.411843	3.884327	-0.769735
H	-0.8117	1.83067	-3.576082	H	0.198956	2.776581	0.444189
H	-2.254645	1.214791	-2.774098	C	1.408882	2.864492	-1.335703
H	0.36612	3.307278	-1.044044	H	1.322411	3.075501	-2.404863
H	1.189408	1.960512	-0.281411	H	2.082111	3.611737	-0.906498
C	1.734836	2.253823	-2.344546	H	1.882657	1.88344	-1.22479
H	1.325861	2.653126	-3.276434	O	-2.729219	3.882703	0.290517
H	2.608718	2.857225	-2.083681	H	-3.385942	4.581604	0.135976
H	2.078804	1.232654	-2.539793	H	-2.993497	-3.521561	-1.696425
O	-1.40336	3.29292	0.809644	O	-4.711797	-2.932794	3.05299
H	-1.95245	4.07351	0.990443	H	-4.277546	-3.797488	3.03679
H	-3.162268	-4.277968	-0.703341				
Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.349379	-2.602456	-0.148683	N	-0.389429	-2.480516	1.803827
H	-0.521094	-2.796043	0.407833	H	0.453617	-2.360383	2.358692
C	-1.871051	-1.283686	0.196336	C	-0.905501	-1.174207	1.406901
H	-2.658967	-1.024241	-0.51394	H	-1.723492	-1.324855	0.698705
C	-2.47503	-1.193426	1.622715	C	-1.437775	-0.324312	2.587408
C	-0.730717	-0.265021	0.078326	C	0.22454	-0.39908	0.71899
H	-3.212557	-1.995545	1.727774	H	-2.074194	-0.955424	3.217441
H	-1.695323	-1.363384	2.369524	H	-0.620548	0.02164	3.225555
C	-3.217933	0.113065	1.86425	C	-2.289991	0.854519	2.181848
O	0.434812	-0.570346	0.335662	O	1.397218	-0.522487	1.070944
O	-3.9603	0.595122	1.004704	O	-2.76767	1.035404	1.07981
N	-3.025824	0.702779	3.061531	N	-0.156722	0.459383	-0.253004
H	-3.52439	1.552703	3.279063	H	-1.147538	0.642292	-0.34863
H	-2.420207	0.30809	3.762655	C	0.771649	1.434361	-0.794673
N	-1.104476	0.984937	-0.265806	H	1.645955	0.910265	-1.18075
H	-2.081893	1.186755	-0.433818	C	0.073688	2.222238	-1.921156
C	-0.162626	2.090778	-0.318994	C	1.241911	2.378676	0.313125
H	0.613119	1.911649	0.424742	H	-0.286822	1.484804	-2.647242
C	0.47419	2.201659	-1.727558	H	-0.80997	2.710235	-1.494055
C	-0.904333	3.366576	0.0387	C	0.929104	3.2706	-2.652424
H	0.895575	1.214318	-1.944447	O	0.561448	2.737196	1.246902
H	-0.336205	2.368171	-2.445312	H	1.287299	4.001002	-1.917774
C	1.565707	3.268267	-1.914503	C	2.150259	2.648117	-3.343499
O	-2.079091	3.560043	-0.185443	C	0.053737	4.018588	-3.668107
H	1.13496	4.251435	-1.69321	H	1.837869	1.876717	-4.056561
C	2.761309	3.047154	-0.976992	H	2.706575	3.410003	-3.89706
C	2.021497	3.274761	-3.380847	H	2.8393	2.192354	-2.628724
H	3.192839	2.05169	-1.131266	H	-0.804701	4.492745	-3.182677
H	3.54437	3.785523	-1.172417	H	0.628595	4.797975	-4.176347

H	2.481501	3.136427	0.075445	H	-0.327732	3.331495	-4.431838
H	1.182569	3.459741	-4.058688	H	-1.068031	-2.966029	2.382067
H	2.772597	4.051539	-3.551522	O	2.500061	2.799764	0.107495
H	2.467856	2.311368	-3.652304	H	2.731319	3.434652	0.805029
H	-2.035505	-3.318255	0.06954	O	-2.504063	1.690937	3.209786
O	-0.096819	4.276606	0.60023	H	-3.081901	2.410439	2.906844
H	-0.604691	5.090727	0.752173				
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.599702	-3.464517	1.060419	N	-1.6903	-2.826102	0.195725
H	-0.645402	-3.559976	0.726431	H	-0.827069	-3.336109	0.362178
C	-2.166923	-2.214752	0.550669	C	-1.584521	-1.484135	0.762224
H	-2.489716	-2.296324	-0.498147	H	-2.466475	-0.913493	0.464521
C	-3.406324	-1.849305	1.408626	C	-1.496121	-1.459556	2.307558
C	-1.058226	-1.1418	0.545429	C	-0.327326	-0.825078	0.177046
H	-3.818571	-2.775971	1.811493	H	-2.246153	-2.146894	2.715067
H	-3.105385	-1.243424	2.269577	H	-0.521343	-1.829424	2.64111
C	-4.489154	-1.083146	0.666828	C	-1.779117	-0.104019	2.924101
O	0.126544	-1.447347	0.706683	O	0.697292	-1.479285	-0.0238
O	-4.223287	-0.208034	-0.166652	O	-2.250783	0.838507	2.32901
N	-5.760236	-1.397222	0.978647	N	-0.410876	0.498451	-0.060265
H	-6.515113	-0.881841	0.551343	H	-1.248134	1.000583	0.205507
H	-5.987891	-2.115339	1.646734	C	0.730525	1.270058	-0.521271
N	-1.468206	0.122392	0.325794	H	1.63523	0.871455	-0.057009
H	-2.451062	0.279184	0.087173	C	0.876423	1.178205	-2.060964
C	-0.522235	1.214386	0.196785	C	0.543102	2.708921	-0.070169
H	0.337339	1.002962	0.833725	H	0.824128	0.112849	-2.301168
C	-0.037406	1.367301	-1.266191	H	0.008114	1.65681	-2.525775
C	-1.185029	2.493657	0.680831	C	2.177367	1.762504	-2.616433
H	0.315176	0.377726	-1.571024	O	-0.531292	3.222134	0.152102
H	-0.898785	1.611905	-1.896709	H	2.225934	2.83741	-2.421979
C	1.080465	2.394197	-1.463186	H	3.029723	1.309979	-2.096918
O	-2.365711	2.739129	0.575945	C	2.305375	1.511387	-4.123806
H	0.726701	3.395887	-1.201809	H	2.26621	0.435185	-4.32531
H	1.907653	2.166224	-0.781336	H	1.460148	1.971754	-4.647364
C	1.595735	2.398977	-2.907523	C	3.610233	2.083273	-4.659445
H	1.96156	1.401074	-3.172858	H	3.669713	3.162226	-4.519035
H	0.775268	2.638138	-3.592956	H	4.479524	1.618281	-4.194471
C	2.716806	3.414999	-3.075291	N	3.740091	1.838736	-6.143084
H	2.380366	4.430899	-2.868911	H	2.973575	2.271827	-6.662625
H	3.568375	3.188084	-2.433962	H	4.613276	2.222327	-6.510145
N	3.240712	3.418922	-4.490621	H	3.73045	0.839373	-6.359289
H	2.509744	3.668682	-5.160093	O	1.710286	3.359446	0.022786
H	4.002807	4.089958	-4.605079	H	1.533248	4.285055	0.259105
H	3.600212	2.500105	-4.758891	H	-2.440949	-3.340287	0.646145
H	-2.131128	-4.252725	0.70534	O	-1.509084	0.024538	4.23859
O	-0.294905	3.349231	1.207625	H	-1.13594	-0.788904	4.607037
H	-0.757012	4.170564	1.443683				

Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.602011	-3.254409	-0.740085	N	-0.391398	-2.35859	2.878343
H	-1.769357	-3.589987	-0.263481	H	0.082717	-1.997893	3.70179
C	-3.012123	-1.976078	-0.16695	C	-1.202224	-1.304599	2.27681
H	-3.806655	-1.555885	-0.787288	H	-1.592282	-1.669029	1.323649
C	-3.55202	-2.076015	1.283607	C	-2.40047	-0.857634	3.150733
C	-1.807247	-1.027545	-0.186937	C	-0.300549	-0.090685	2.02327
H	-4.327222	-2.849196	1.300851	H	-2.916728	-1.749282	3.523309
H	-2.755566	-2.397555	1.959986	H	-2.063148	-0.307163	4.032768
C	-4.214279	-0.790367	1.76013	C	-3.444226	-0.044533	2.422907
O	-0.653942	-1.444205	-0.073734	O	0.630061	0.190876	2.776594
O	-4.917369	-0.11264	1.005763	O	-3.528954	0.080554	1.217517
N	-4.000465	-0.445707	3.045751	N	-0.625351	0.671078	0.953349
H	-4.453683	0.374959	3.419062	H	-1.515375	0.487561	0.507015
H	-3.429868	-1.001556	3.66174	C	-0.020199	1.974333	0.761519
N	-2.104409	0.286401	-0.282945	H	1.065383	1.864288	0.737751
H	-3.071891	0.580626	-0.33296	C	-0.51255	2.569411	-0.573097
C	-1.081253	1.313288	-0.216763	C	-0.371757	2.894899	1.933782
H	-0.292574	0.9775	0.459019	H	-0.314029	1.820926	-1.345675
C	-0.469218	1.569114	-1.618876	H	-1.597417	2.708487	-0.522231
C	-1.706635	2.577869	0.348791	C	0.170054	3.885895	-0.942379
H	-0.174581	0.587109	-1.99778	O	-1.405697	2.84782	2.558708
H	-1.252586	1.953822	-2.278739	H	-0.068775	4.672969	-0.224726
C	0.738487	2.504703	-1.610339	H	1.256124	3.76293	-0.967475
O	-2.878793	2.864633	0.250395	S	-0.393537	4.434559	-2.600542
H	0.459086	3.515621	-1.308868	C	0.534355	6.003254	-2.714794
H	1.503124	2.139874	-0.918748	H	1.608694	5.816159	-2.66609
S	1.470039	2.590917	-3.291993	H	0.288761	6.45024	-3.679041
C	2.81218	3.785473	-2.964427	H	0.235909	6.682923	-1.914426
H	3.500931	3.390437	-2.215244	O	0.598074	3.793872	2.164046
H	3.346281	3.93234	-3.904216	H	0.309604	4.386671	2.87731
H	2.401451	4.739666	-2.628991	H	-0.981248	-3.128115	3.178953
O	-0.795835	3.360261	0.942905	O	-4.320881	0.514311	3.271704
H	-1.230298	4.178439	1.235835	H	-4.986761	0.996668	2.754592
H	-3.330502	-3.948009	-0.602325				
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.41605	-3.175913	0.617888	N	-2.855706	-0.625237	2.579844
H	-0.622418	-3.132562	1.251461	H	-2.796571	-0.157765	3.480277
C	-2.122073	-1.898671	0.630541	C	-2.946321	0.366097	1.513751
H	-2.875096	-1.909548	-0.160356	H	-2.875803	-0.148772	0.553204
C	-2.847365	-1.587896	1.966488	C	-4.262714	1.186	1.524488
C	-1.110609	-0.782286	0.34575	C	-1.768852	1.337687	1.658886
H	-3.486242	-2.443262	2.20896	H	-5.102198	0.498023	1.675862
H	-2.116835	-1.484969	2.772949	H	-4.273303	1.881052	2.369884
C	-3.763184	-0.37532	1.872848	C	-4.551109	1.933192	0.237201

O	0.061922	-0.86201	0.713443	O	-1.319406	1.645128	2.761761
O	-4.47039	-0.181712	0.880372	O	-3.955079	1.769815	-0.80505
N	-3.76364	0.461485	2.929904	N	-1.298921	1.871252	0.508678
H	-4.382232	1.258731	2.927956	H	-1.846915	1.720112	-0.329149
H	-3.186208	0.303229	3.739634	C	-0.378976	2.991641	0.532781
N	-1.609827	0.306252	-0.27843	H	0.520092	2.712014	1.083602
H	-2.589033	0.334173	-0.533258	C	-0.003913	3.371006	-0.919631
C	-0.808544	1.489784	-0.523051	C	-1.019418	4.185792	1.245394
H	-0.095739	1.607874	0.293623	H	0.388841	2.465157	-1.389807
C	-0.023393	1.362161	-1.863151	H	-0.918602	3.648068	-1.451936
C	-1.731133	2.695875	-0.560078	C	1.010807	4.486431	-1.009736
H	0.513764	0.41291	-1.797674	O	-2.191332	4.476834	1.170171
H	-0.748913	1.275421	-2.676013	C	0.615041	5.793272	-1.31466
C	0.942942	2.492326	-2.120273	C	2.366577	4.231482	-0.767128
O	-2.879649	2.660427	-0.944433	H	-0.431637	6.003977	-1.508772
C	0.645269	3.501862	-3.042271	C	1.551758	6.827636	-1.369986
C	2.153265	2.558742	-1.417207	C	3.305613	5.261517	-0.82087
H	-0.287169	3.46244	-3.596057	H	2.687963	3.220795	-0.536333
C	1.533324	4.558281	-3.256173	H	1.228253	7.834615	-1.608472
C	3.042446	3.61302	-1.625644	C	2.899893	6.564724	-1.121231
H	2.400061	1.778523	-0.704121	H	4.35168	5.047317	-0.632635
H	1.287424	5.331016	-3.97596	H	3.629	7.365799	-1.165226
C	2.73408	4.618021	-2.546643	O	-0.11738	4.899087	1.93383
H	3.975569	3.64816	-1.074498	H	-0.560706	5.675531	2.313097
H	3.425326	5.436675	-2.711821	H	-3.686149	-1.20883	2.591466
O	-1.115394	3.812005	-0.154767	O	-5.572641	2.80848	0.269225
H	-1.724893	4.560874	-0.263116	H	-5.970496	2.860628	1.149896
H	-2.027437	-3.916173	0.948048				

Asn-Pro							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.077513	-2.442822	-0.992343	N	-0.759764	0.157854	-2.761064
H	-0.205229	-2.880386	-0.707048	H	-0.199118	-0.39725	-3.4021
C	-1.658282	-1.694603	0.131326	C	-0.056405	0.323639	-1.482825
H	-2.639355	-1.333063	-0.17993	H	-0.731301	0.832971	-0.793186
C	-1.837757	-2.519675	1.41222	C	0.387121	-0.994549	-0.836875
C	-0.754005	-0.482756	0.398333	C	1.161183	1.224783	-1.743017
H	-2.471967	-3.381858	1.180126	H	-0.478335	-1.659624	-0.743955
H	-0.872548	-2.901149	1.751229	H	1.118695	-1.498949	-1.473599
C	-2.526643	-1.734755	2.518764	C	0.968025	-0.806104	0.547833
O	0.088821	-0.49771	1.303581	O	2.287427	0.742964	-1.911664
O	-3.348756	-0.849978	2.272392	O	0.884499	0.213297	1.193578
N	-2.206003	-2.084938	3.783552	N	0.948377	2.552313	-1.812425
H	-2.659746	-1.620759	4.55564	C	-0.343349	3.256088	-1.709769
H	-1.518481	-2.792368	3.985122	C	2.049239	3.451307	-2.165323
N	-0.902164	0.590747	-0.401862	H	-0.595869	3.422784	-0.6575
C	-1.802563	0.721354	-1.561692	H	-1.132408	2.672473	-2.180196
C	-0.025399	1.751439	-0.239592	C	-0.069114	4.57766	-2.434226
H	-2.805003	1.009067	-1.227709	C	1.405678	4.856959	-2.110715

H	-1.861672	-0.220638	-2.103711	H	2.415844	3.220377	-3.167884
C	-1.144906	1.838809	-2.377358	C	3.251419	3.362684	-1.243065
C	-0.542693	2.752472	-1.300055	H	-0.732735	5.37658	-2.102183
H	1.012692	1.470515	-0.43004	H	-0.201017	4.444419	-3.511626
C	-0.052769	2.363159	1.149337	H	1.496956	5.266692	-1.101265
H	-1.857711	2.356793	-3.019687	H	1.888006	5.542503	-2.806279
H	-0.35271	1.422537	-3.005934	O	4.393708	3.510692	-1.619657
H	-1.322833	3.382624	-0.864696	O	2.914743	3.192046	0.044535
H	0.257382	3.395988	-1.663618	H	3.727141	3.193205	0.575173
O	0.912135	2.877306	1.672058	H	-1.628759	-0.347893	-2.618254
O	-1.275306	2.354815	1.703178	O	1.597877	-1.871963	1.087743
H	-1.223557	2.802423	2.562509	H	1.606325	-2.622583	0.477317
H	-1.7026	-3.194941	-1.266655				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.830458	-3.363075	0.473504	N	0.430387	-0.824805	-2.504372
H	-0.018882	-3.449598	1.079189	H	0.985319	-1.515671	-2.00674
C	-1.183231	-1.953648	0.321619	C	0.279697	0.394697	-1.712609
H	-1.955403	-1.871148	-0.446215	H	-0.56884	0.947719	-2.129584
C	-1.726668	-1.298417	1.615491	C	0.010464	0.12586	-0.203546
C	0.063631	-1.194152	-0.147476	C	1.491287	1.316022	-1.91799
H	-2.481422	-1.968392	2.042093	H	-0.602303	-0.771122	-0.128494
H	-0.93092	-1.210083	2.361216	H	0.958175	-0.076127	0.30713
C	-2.412049	0.047994	1.407192	C	-0.722767	1.21175	0.576032
O	1.19996	-1.552892	0.158192	O	1.701438	2.288253	-1.16872
O	-2.775492	0.442065	0.29359	O	-1.699886	0.964333	1.259316
N	-2.628154	0.770375	2.522924	N	2.275746	1.024862	-2.955826
H	-3.117068	1.65024	2.455311	H	2.028317	0.201465	-3.496181
H	-2.33848	0.450439	3.433116	C	3.445403	1.802297	-3.315867
N	-0.174166	-0.083875	-0.884228	H	3.29566	2.840008	-3.019076
H	-1.130605	0.259427	-0.890006	C	4.68286	1.242013	-2.590168
C	0.900376	0.830688	-1.20947	C	3.629887	1.717407	-4.825395
H	1.683339	0.302363	-1.755085	H	4.469799	1.260059	-1.515949
C	0.333214	1.950073	-2.0906	H	4.839276	0.202596	-2.901879
C	1.514413	1.423844	0.063148	O	5.797776	2.059944	-2.917431
H	-0.124856	1.491244	-2.974018	O	3.404127	0.716394	-5.468469
H	-0.441426	2.4917	-1.533389	H	6.58429	1.689579	-2.501832
O	1.40561	2.812017	-2.448258	H	-0.474007	-1.244203	-2.687879
O	0.869194	1.772126	1.025593	O	4.083557	2.859424	-5.348534
H	1.049048	3.5547	-2.947789	H	4.22169	2.732954	-6.302174
O	2.846931	1.535366	-0.020289	O	-0.245689	2.44919	0.501087
H	3.173383	1.95075	0.794734	H	0.55638	2.473813	-0.1109
H	-1.592661	-3.86852	0.914161				
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.074373	-3.623279	0.464807	N	1.796743	-1.831594	-0.456458
H	-1.403804	-3.830412	1.199905	H	2.563992	-1.864795	0.209083

C	-2.24994	-2.176673	0.354573	C	1.479819	-0.4438	-0.775259
H	-2.841157	-1.967471	-0.53949	H	0.757078	-0.431571	-1.594034
C	-2.975983	-1.537611	1.563485	C	0.875923	0.354639	0.409261
C	-0.865567	-1.535049	0.192492	C	2.768538	0.256137	-1.223912
H	-3.846064	-2.158811	1.803679	H	0.130251	-0.273065	0.910346
H	-2.331355	-1.549483	2.447418	H	1.64592	0.579165	1.15397
C	-3.507387	-0.130403	1.312664	C	0.158082	1.628785	0.011422
O	0.144498	-2.045069	0.677197	O	3.862939	-0.056857	-0.758472
O	-3.616994	0.345158	0.178258	O	-0.127023	1.936701	-1.124891
N	-3.890505	0.549899	2.410874	N	2.60638	1.256332	-2.12007
H	-4.289802	1.47055	2.308643	H	1.66193	1.574358	-2.302488
H	-3.802678	0.164179	3.33715	C	3.670215	2.191775	-2.396259
N	-0.845748	-0.3696	-0.492904	H	4.612962	1.647571	-2.477665
H	-1.737871	0.079281	-0.675629	C	3.425227	2.930275	-3.722724
C	0.338897	0.450697	-0.548154	C	3.828022	3.179981	-1.234738
H	1.211957	-0.194125	-0.666834	H	4.238869	3.652087	-3.847744
C	0.290031	1.413831	-1.746846	C	3.388756	1.985633	-4.918476
C	0.535829	1.218385	0.76297	O	2.182916	3.625949	-3.550686
H	1.197548	2.02526	-1.709043	O	3.098191	3.245916	-0.274169
C	0.221082	0.681309	-3.081725	H	2.593654	1.245612	-4.807645
O	-0.860376	2.242441	-1.530222	H	3.211574	2.555116	-5.834721
O	-0.250496	1.249127	1.679139	H	4.344608	1.465298	-5.022516
H	-0.670074	0.052983	-3.136872	H	1.96104	4.077679	-4.372725
H	0.190152	1.405513	-3.900127	H	0.9978	-2.28693	-0.026665
H	1.105718	0.053588	-3.218354	O	4.902704	3.96599	-1.410323
H	-0.959609	2.84058	-2.279535	H	4.966315	4.577565	-0.659022
H	-2.952367	-4.062779	0.722703	O	-0.220607	2.438295	1.018207
O	1.719358	1.855657	0.775744	H	0.064239	2.094181	1.876684
H	1.804207	2.334617	1.615802				

Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.187528	-2.400155	1.565583	N	-2.2066	-3.0971	1.9153
H	-1.816699	-1.860949	2.343333	H	-2.74603	-2.5423	2.574054
C	-3.256646	-1.648379	0.915927	C	-2.17607	-2.43132	0.617657
H	-3.538137	-2.166608	-0.003174	H	-1.4828	-2.96964	-0.03234
C	-4.536537	-1.491437	1.778652	C	-3.55292	-2.37203	-0.09317
C	-2.724332	-0.254758	0.563648	C	-1.67033	-0.9981	0.824706
H	-4.840588	-2.488174	2.114375	H	-4.03399	-3.35288	-0.00681
H	-4.315926	-0.898577	2.670226	H	-4.2135	-1.65691	0.407744
C	-5.710481	-0.921523	0.994353	C	-3.48618	-2.05765	-1.57467
O	-1.884442	0.313417	1.26383	O	-1.92528	-0.36751	1.849928
O	-5.940986	-1.278198	-0.164211	O	-2.46796	-2.02472	-2.23062
N	-6.482064	-0.021077	1.6358	N	-0.97791	-0.46243	-0.20483
H	-7.293525	0.35548	1.168908	H	-0.98228	-0.97084	-1.08048
H	-6.294148	0.268904	2.581581	C	-0.66048	0.951835	-0.23434
N	-3.277719	0.322662	-0.523645	H	-0.07886	1.211182	0.650868
H	-3.994378	-0.165763	-1.045483	C	0.158346	1.263172	-1.51187
C	-2.949408	1.680891	-0.910597	C	-1.94253	1.785061	-0.2191

H	-2.795795	2.274692	-0.008975	H	1.018186	0.585041	-1.50444
C	-1.641607	1.724197	-1.764774	H	-0.45058	1.006655	-2.38398
C	-4.112572	2.258781	-1.691763	C	0.614828	2.684215	-1.60277
H	-0.943537	1.056681	-1.251695	O	-2.96044	1.481461	-0.79931
H	-1.846337	1.287585	-2.745926	C	0.141246	3.648991	-2.45886
C	-1.04373	3.086646	-1.891696	C	1.616071	3.319237	-0.78496
O	-4.90516	1.596875	-2.32721	H	-0.61517	3.574234	-3.22469
C	-0.967748	3.872065	-3.015971	N	0.785152	4.845072	-2.22244
C	-0.446061	3.845097	-0.822639	C	1.696208	4.677257	-1.2031
H	-1.307213	3.668497	-4.019705	C	2.453138	2.874028	0.252813
N	-0.360414	5.073155	-2.710915	H	0.623842	5.699871	-2.72986
C	-0.027988	5.088202	-1.374086	C	2.581343	5.58677	-0.61616
C	-0.223459	3.588117	0.541743	C	3.33461	3.774887	0.839764
H	-0.175103	5.812237	-3.369111	H	2.415628	1.843446	0.58872
C	0.60169	6.069783	-0.602376	H	2.629252	6.617209	-0.94882
C	0.401593	4.562725	1.312157	C	3.396603	5.118458	0.409615
H	-0.535356	2.645241	0.979259	H	3.986338	3.444282	1.640704
H	0.915788	7.011198	-1.038268	H	4.093589	5.798064	0.886907
C	0.809061	5.79063	0.745387	O	-1.79703	2.917625	0.483058
H	0.581185	4.381057	2.366053	H	-2.61695	3.43304	0.410576
H	1.293819	6.530597	1.372406	H	-2.65666	-4.00357	1.836954
O	-4.140249	3.595303	-1.633089	O	-4.66205	-1.83834	-2.1915
H	-4.86051	3.915776	-2.200866	H	-5.40398	-1.88835	-1.57202
H	-2.551606	-3.268724	1.944784				

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.749734	-2.200547	1.889927	N	0.793159	-1.875901	1.442151
H	-1.125535	-2.034458	2.819471	H	0.213496	-1.866065	2.276964
C	-1.517312	-1.441828	0.905774	C	0.103739	-1.184063	0.357918
H	-1.000171	-1.49947	-0.054774	H	0.798868	-1.06739	-0.476969
C	-2.961413	-1.961698	0.697531	C	-1.153628	-1.925745	-0.16046
C	-1.559336	0.026074	1.351963	C	-0.316687	0.202464	0.860962
H	-2.918333	-3.052424	0.602299	H	-0.905509	-2.983646	-0.301158
H	-3.574575	-1.750278	1.578749	H	-1.96233	-1.894849	0.574224
C	-3.650066	-1.446761	-0.562285	C	-1.670853	-1.439724	-1.493343
O	-1.468212	0.35304	2.535568	O	-0.619267	0.39852	2.037044
O	-3.031897	-0.900786	-1.48275	O	-1.072148	-0.715198	-2.263144
N	-4.979282	-1.655055	-0.624174	N	-0.376174	1.170631	-0.080562
H	-5.484318	-1.383262	-1.454128	H	-0.276238	0.884789	-1.046142
H	-5.4847	-2.112522	0.117448	C	-1.000401	2.444188	0.194385
N	-1.737387	0.923343	0.358765	H	-0.582019	2.852657	1.116199
H	-1.969861	0.555549	-0.55807	C	-0.747471	3.440824	-0.962555
C	-1.973948	2.319804	0.636926	C	-2.504529	2.274913	0.409569
H	-1.184682	2.694078	1.292276	H	-1.209764	3.048854	-1.873549
C	-1.976804	3.142217	-0.67563	H	-1.263192	4.370856	-0.713926
C	-3.304669	2.521797	1.359783	C	0.724807	3.69251	-1.188486
H	-2.808896	2.803256	-1.300208	O	-3.160151	1.330502	0.035625
H	-2.172753	4.183873	-0.412091	C	1.405993	3.103018	-2.257116

C	-0.673218	3.019138	-1.428764	C	1.453518	4.503181	-0.307672
O	-4.247205	1.76639	1.313491	H	0.867067	2.475912	-2.959796
C	-0.555131	2.176764	-2.538102	C	2.773701	3.307589	-2.447212
C	0.464801	3.720443	-1.008354	C	2.817662	4.716804	-0.481732
H	-1.420625	1.624924	-2.890212	H	0.948182	4.977001	0.52779
C	0.65871	2.02871	-3.210931	H	3.28489	2.843793	-3.284314
C	1.683229	3.583694	-1.667177	C	3.481832	4.115382	-1.555259
H	0.399747	4.384581	-0.152538	H	3.375564	5.347451	0.200209
H	0.729958	1.371498	-4.071188	O	4.822911	4.359528	-1.681428
C	1.782165	2.732282	-2.771914	H	5.173109	3.894513	-2.45098
H	2.559453	4.130514	-1.33967	O	-3.022835	3.338921	1.044797
O	3.003475	2.634059	-3.382705	H	-3.982897	3.21763	1.123908
H	2.955242	2.017282	-4.12324	H	0.955655	-2.846802	1.194493
H	-0.828268	-3.195324	1.703511	O	-2.885789	-1.939692	-1.767651
O	-3.316681	3.687623	2.028772	H	-3.157855	-1.624504	-2.645144
H	-4.192936	3.806284	2.429615				

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.50876	-3.51384	-0.51618	N	-3.61224	-2.38805	-0.86489
H	-1.58822	-3.91829	-0.36675	H	-2.93648	-3.1391	-0.97583
C	-2.59861	-2.23505	0.181603	C	-3.08309	-1.38596	0.056625
H	-3.52835	-1.743	-0.1119	H	-3.75404	-0.52413	0.050537
C	-2.5974	-2.35496	1.728934	C	-2.95147	-1.88263	1.516093
C	-1.41097	-1.36491	-0.24658	C	-1.70098	-0.95464	-0.45612
H	-3.38946	-3.05503	2.012624	H	-3.87219	-2.40685	1.796293
H	-1.64762	-2.7753	2.06939	H	-2.14075	-2.60846	1.617458
C	-2.91582	-1.03449	2.415452	C	-2.7768	-0.77922	2.532009
O	-0.31134	-1.85754	-0.50384	O	-0.94755	-1.7571	-1.00982
O	-3.83154	-0.31131	2.014595	O	-3.02048	0.39478	2.344202
N	-2.15063	-0.70542	3.475707	N	-1.36383	0.329366	-0.22382
H	-2.34236	0.14874	3.977599	H	-1.98961	0.919059	0.309391
H	-1.40063	-1.29451	3.798659	C	-0.05498	0.857658	-0.56821
N	-1.64246	-0.03581	-0.26629	H	0.689067	0.074151	-0.40969
H	-2.54798	0.317741	0.014918	C	0.00892	1.289716	-2.06798
C	-0.58838	0.927018	-0.53505	C	0.250533	2.008158	0.374848
H	0.34035	0.55556	-0.09657	H	-0.38865	0.419566	-2.59983
C	-0.35966	1.111513	-2.06911	C	-0.8942	2.492476	-2.36234
C	-0.95573	2.230137	0.15307	C	1.443615	1.523339	-2.55213
H	-0.27574	0.08452	-2.43812	O	-0.58685	2.644032	0.977131
C	-1.55665	1.777531	-2.75653	H	-0.51504	3.401117	-1.88323
C	0.953635	1.834565	-2.38535	H	-0.9327	2.676856	-3.43891
O	-2.08126	2.545467	0.472634	H	-1.91593	2.324258	-2.01228
H	-1.66114	2.823177	-2.44884	H	2.085213	0.665683	-2.32973
H	-1.42096	1.763312	-3.8409	H	1.446113	1.675967	-3.63473
H	-2.49197	1.260411	-2.52724	H	1.886477	2.407087	-2.08677
H	1.802086	1.358933	-1.88474	O	1.563829	2.264493	0.444497
H	1.138002	1.807404	-3.46267	H	1.697929	3.037153	1.017805
H	0.921917	2.881853	-2.07574	H	-4.46274	-2.79607	-0.48969

H	-3.19072	-4.1656	-0.14079	O	-2.34319	-1.25043	3.713806
O	0.112947	3.015562	0.343046	H	-2.28851	-0.50907	4.339061
H	-0.18445	3.851541	0.738425				

Table S14.B. Succinimide Formation XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions							
NH_3							
Product Structure							
Atom	X	Y	Z				
N	-1.133326	-0.563263	0.000024				
H	-0.744703	-1.50246	-0.000031				
H	-0.744689	-0.093642	0.813368				
H	-0.7447	-0.093681	-0.813362				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.891127	-2.884246	0.251026	N	-1.042902	-2.775176	1.359843
H	-0.956162	-2.907849	0.649126	H	-0.736188	-2.253319	2.176226
C	-2.478588	-1.564604	0.463042	C	-1.904821	-1.960734	0.520089
H	-3.41318	-1.505706	-0.098634	H	-2.289833	-2.60121	-0.280449
C	-2.79954	-1.243788	1.946244	C	-3.081068	-1.196656	1.168428
C	-1.501839	-0.510341	-0.071776	C	-1.116766	-0.859026	-0.199821
H	-3.401492	-2.066112	2.346382	H	-4.052559	-1.6718	1.032706
H	-1.875284	-1.200716	2.528218	H	-2.918291	-1.06206	2.241714
C	-3.632141	0.020374	2.107956	C	-3.069578	0.171844	0.524872
O	-0.282102	-0.672645	-0.008889	O	-0.015218	-0.942138	-0.698557
O	-4.563417	0.276189	1.34013	O	-3.894511	1.056175	0.631215
N	-3.30323	0.830859	3.134184	N	-1.902406	0.288036	-0.224191
H	-3.852308	1.660376	3.303569	C	-1.504711	1.5079	-0.912134
H	-2.545178	0.619918	3.7626	H	-0.505306	1.305213	-1.310538
N	-2.065964	0.613276	-0.561733	C	-2.444024	1.855738	-2.072693
H	-3.071102	0.728352	-0.521814	C	-1.298399	2.621602	0.114935
C	-1.268481	1.74318	-1.003132	H	-3.444149	2.088802	-1.70865
H	-0.413474	1.851669	-0.330768	H	-2.054195	2.712883	-2.620564
C	-0.748766	1.561198	-2.442252	H	-2.501534	1.003354	-2.751868
C	-2.106086	3.005279	-0.898769	O	-1.10025	2.440047	1.293432
H	-1.584144	1.477638	-3.141561	H	-1.555907	-3.581316	1.701205
H	-0.121346	2.40522	-2.732476	O	-1.298401	3.832155	-0.460924
H	-0.157105	0.646245	-2.487801	H	-1.10317	4.49529	0.220986
O	-3.305202	3.031904	-0.731085				
H	-2.441316	-3.592356	0.727048				
O	-1.351788	4.103353	-1.047044				
H	-1.928241	4.883985	-1.013008				
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z

N	-2.773546	-3.901166	-0.30998	N	-2.617216	-4.351801	1.003787
H	-1.928572	-4.250817	0.13375	H	-2.349071	-4.282302	1.981622
C	-3.10055	-2.585205	0.229565	C	-2.660843	-3.038532	0.383934
H	-3.922862	-2.165011	-0.353524	H	-3.06396	-3.161739	-0.626596
C	-3.538223	-2.600081	1.71833	C	-3.420004	-1.895512	1.097852
C	-1.86956	-1.682668	0.085495	C	-1.25322	-2.463758	0.179004
H	-4.352688	-3.324062	1.822226	H	-4.402568	-1.681585	0.67746
H	-2.711732	-2.941934	2.346497	H	-3.548962	-2.112474	2.162073
C	-4.087038	-1.258237	2.182489	C	-2.522033	-0.685894	0.977264
O	-0.72548	-2.130539	0.169856	O	-0.259879	-3.046354	-0.196158
O	-4.850731	-0.599152	1.471981	O	-2.759279	0.465721	1.281809
N	-3.699212	-0.838623	3.403629	N	-1.297393	-1.103796	0.47051
H	-4.064922	0.0289	3.76687	C	-0.162598	-0.209091	0.26998
H	-3.076424	-1.377563	3.983016	H	0.695195	-0.870475	0.109446
N	-2.130799	-0.368653	-0.082071	C	-0.354243	0.695797	-0.955326
H	-3.089989	-0.045666	-0.100873	C	0.140664	0.568644	1.552825
C	-1.077282	0.629542	-0.114478	H	-0.822558	0.089896	-1.735949
H	-0.282896	0.323254	0.569179	H	-1.050242	1.498573	-0.701782
C	-0.488752	0.763664	-1.540442	C	0.965572	1.268841	-1.479703
C	-1.65723	1.948554	0.370655	O	0.434795	1.739449	1.591353
H	-0.208521	-0.24916	-1.842288	H	1.452887	1.853343	-0.695212
H	-1.283382	1.095538	-2.21615	H	1.64068	0.451199	-1.75445
C	0.72584	1.688894	-1.644231	C	0.730656	2.154601	-2.701281
O	-2.825048	2.255799	0.282517	H	0.266324	1.569929	-3.500754
H	0.436799	2.719935	-1.421738	H	0.058849	2.980288	-2.442495
H	1.483158	1.399227	-0.908572	N	2.007692	2.68443	-3.186877
C	1.334451	1.626898	-3.043952	H	2.796101	2.649133	-2.557331
H	1.697669	0.61461	-3.244126	C	2.185742	3.301151	-4.354181
H	0.575965	1.876632	-3.7939	N	1.147427	3.530226	-5.163721
N	2.45757	2.562883	-3.144696	N	3.414197	3.683457	-4.724638
H	2.538929	3.270964	-2.429894	H	0.199954	3.441132	-4.835806
C	3.310098	2.626566	-4.166676	H	1.281109	3.968596	-6.060812
N	3.172364	1.811448	-5.215998	H	4.228422	3.359178	-4.227999
N	4.324355	3.498987	-4.136495	H	3.56521	4.175874	-5.589779
H	2.351923	1.241691	-5.336245	H	-3.538463	-4.776235	0.979622
H	3.841137	1.821956	-5.969003	O	0.102172	-0.226792	2.632464
H	4.50134	4.065217	-3.322918	H	0.325184	0.303548	3.414349
H	4.925069	3.627231	-4.934182				
H	-3.518851	-4.558759	-0.103005				
O	-0.712844	2.749963	0.880646				
H	-1.120632	3.597466	1.124567				
Asn-Asn							
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.022756	-3.639036	-0.157895	N	-0.114507	-4.044523	0.700107
H	-0.159107	-3.602377	0.376757	H	-0.051479	-3.816724	1.688332
C	-1.8483	-2.479092	0.165658	C	-0.921035	-3.065744	-0.006236
H	-2.698823	-2.456163	-0.518764	H	-1.053697	-3.422118	-1.033465
C	-2.407633	-2.481632	1.612055	C	-2.299446	-2.667906	0.570751
C	-1.005493	-1.215256	-0.040783	C	-0.192996	-1.72329	-0.151065

H	-2.898975	-3.445453	1.781146	H	-3.14477	-3.167045	0.0977
H	-1.58869	-2.402408	2.331983	H	-2.345563	-2.868503	1.645354
C	-3.467009	-1.411751	1.839413	C	-2.390252	-1.171545	0.377893
O	0.209617	-1.207226	0.15903	O	0.981182	-1.533666	-0.378647
O	-4.301762	-1.141013	0.972054	O	-3.348207	-0.44393	0.543205
N	-3.447903	-0.792448	3.036788	N	-1.137417	-0.710221	-0.012395
H	-4.159074	-0.10928	3.250767	C	-0.828972	0.697604	-0.188452
H	-2.771937	-1.020642	3.747448	H	0.245085	0.751776	-0.39225
N	-1.688033	-0.109868	-0.410768	C	-1.571113	1.311425	-1.384231
H	-2.696919	-0.143207	-0.492118	C	-1.030359	1.427347	1.140697
C	-1.037051	1.177687	-0.53865	H	-1.575827	0.572864	-2.191325
H	-0.30742	1.299241	0.265828	H	-2.608781	1.526313	-1.131871
C	-0.277738	1.300052	-1.883225	C	-0.850516	2.539971	-1.932401
C	-2.087651	2.268695	-0.404333	O	-0.912157	0.906122	2.224029
H	0.277524	0.368305	-2.013825	O	0.375609	2.636893	-1.90239
H	-0.983078	1.388936	-2.711896	N	-1.641543	3.477582	-2.491381
C	0.758426	2.416391	-1.874167	H	-1.219115	4.282971	-2.927679
O	-3.28271	2.078543	-0.38736	H	-2.644983	3.394689	-2.506062
O	1.560218	2.530801	-0.947595	H	-0.546049	-4.960398	0.634824
N	0.768526	3.230403	-2.9498	O	-1.29889	2.726553	0.959651
H	1.459294	3.963556	-3.006089	H	-1.363866	3.155327	1.828359
H	0.095173	3.147673	-3.693769				
H	-1.504394	-4.493778	0.103206				
O	-1.524662	3.481235	-0.334189				
H	-2.227458	4.150312	-0.296163				
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.99394	-2.615646	-0.96669	N	-4.621989	-3.535013	-0.763109
H	-4.154637	-3.163919	-0.798079	H	-4.365086	-3.586074	0.218791
C	-4.959459	-1.409867	-0.144032	C	-4.932237	-2.167932	-1.144843
H	-5.784827	-0.760494	-0.443211	H	-5.305271	-2.186863	-2.174353
C	-5.095933	-1.677308	1.378324	C	-5.905241	-1.345795	-0.269706
C	-3.629169	-0.690734	-0.397487	C	-3.673727	-1.291745	-1.198442
H	-6.002173	-2.269812	1.538006	H	-6.920064	-1.285953	-0.662657
H	-4.246315	-2.269386	1.727639	H	-5.959114	-1.752565	0.744396
C	-5.265548	-0.394707	2.17958	C	-5.288467	0.03245	-0.183902
O	-2.587978	-1.320793	-0.594648	O	-2.576708	-1.598096	-1.613673
O	-6.043666	0.488959	1.811838	O	-5.773522	1.044701	0.280799
N	-4.526814	-0.281461	3.302451	N	-4.006056	-0.03244	-0.714432
H	-4.626663	0.541187	3.878202	C	-3.085339	1.096907	-0.722967
H	-3.891517	-1.00321	3.601634	H	-2.130533	0.710094	-1.092835
N	-3.672574	0.65458	-0.337307	C	-3.517481	2.221775	-1.671156
H	-4.541591	1.117314	-0.102852	C	-2.81385	1.519882	0.718351
C	-2.476558	1.474028	-0.442982	H	-3.988147	1.757262	-2.543504
H	-1.65632	0.992954	0.094761	H	-4.26236	2.867523	-1.209031
C	-2.018333	1.667153	-1.907697	C	-2.338957	3.071828	-2.211626
C	-2.767607	2.813773	0.207619	O	-2.848003	0.767108	1.665905
H	-2.131047	0.694908	-2.395318	O	-1.204415	2.529205	-2.25186

H	-2.669557	2.376266	-2.42297	O	-2.637571	4.227695	-2.610012
C	-0.533947	2.075837	-2.064231	O	-2.477138	2.812877	0.816192
O	-3.870631	3.20137	0.530522	H	-2.266479	3.002534	1.744666
O	0.296028	1.471801	-1.335761	H	-5.44121	-4.121271	-0.884234
O	-0.277417	2.943503	-2.940051				
O	-1.658111	3.548838	0.357352				
H	-1.908763	4.408879	0.731974				
H	-5.789015	-3.192493	-0.709753				
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.888251	-2.4099	-0.65284	N	-2.432049	-2.725908	0.969617
H	-2.011838	-2.771293	-0.286335	H	-1.832365	-2.451721	1.74267
C	-3.158865	-1.098031	-0.074058	C	-3.108095	-1.57372	0.402654
H	-4.023301	-0.66537	-0.582163	H	-3.82651	-1.940339	-0.338517
C	-3.471683	-1.124568	1.446035	C	-3.823308	-0.579175	1.346956
C	-1.938198	-0.202557	-0.31183	C	-2.148419	-0.682707	-0.39636
H	-4.277511	-1.846989	1.610086	H	-4.901298	-0.722604	1.416164
H	-2.59788	-1.4746	2.001416	H	-3.409131	-0.632913	2.358147
C	-3.976286	0.214801	1.96478	C	-3.504908	0.789583	0.791972
O	-0.795398	-0.657314	-0.342972	O	-1.244294	-1.024516	-1.124914
O	-4.791014	0.883012	1.322454	O	-3.967892	1.865328	1.112598
N	-3.491944	0.62146	3.155156	N	-2.516741	0.643473	-0.176152
H	-3.820788	1.489136	3.551738	C	-1.913064	1.765977	-0.886047
H	-2.822759	0.078451	3.676109	H	-1.024703	1.359066	-1.377407
N	-2.200454	1.119167	-0.428723	C	-2.871124	2.33473	-1.941602
H	-3.152861	1.454751	-0.353991	C	-1.418946	2.826426	0.100867
C	-1.139568	2.101732	-0.532042	H	-3.324877	1.50192	-2.480022
H	-0.289677	1.774921	0.069936	H	-3.662973	2.914254	-1.470046
C	-0.693056	2.23069	-2.007387	S	-2.050317	3.338175	-3.239493
C	-1.656173	3.425268	0.015219	O	-1.572626	4.016635	-0.03768
H	-0.455962	1.226237	-2.353457	H	-1.722397	4.37661	-2.450761
H	-1.510113	2.635087	-2.606318	H	-3.113362	-3.379905	1.340247
S	0.820164	3.274562	-2.2129	O	-0.741301	2.272648	1.115314
O	-2.825359	3.731244	0.069454	H	-0.429228	2.979918	1.702755
H	1.181033	2.744984	-3.395381				
H	-3.619013	-3.064406	-0.391508				
O	-0.654008	4.222765	0.402378				
H	-1.022051	5.076456	0.684914				
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.879903	-3.819748	-0.346005	N	0.013409	-4.753899	-1.071706
H	-1.044699	-4.046686	0.187054	H	-0.082809	-5.151975	-0.141624
C	-2.397212	-2.524611	0.084431	C	-0.794998	-3.555075	-1.208139
H	-3.197535	-2.226122	-0.595968	H	-0.745118	-3.237645	-2.255145
C	-2.976114	-2.517935	1.524077	C	-2.274526	-3.590755	-0.760809
C	-1.260526	-1.498912	0.005617	C	-0.208434	-2.379976	-0.414913
H	-3.712097	-3.325178	1.595082	H	-2.986549	-3.703385	-1.578204

H	-2.183752	-2.730913	2.246175	H	-2.449046	-4.400706	-0.046654
C	-3.713183	-1.227404	1.853915	C	-2.500767	-2.281629	-0.039798
O	-0.091267	-1.81269	0.232026	O	0.95757	-2.073682	-0.293995
O	-4.466789	-0.693736	1.035544	O	-3.546323	-1.811385	0.360909
N	-3.502467	-0.710385	3.081162	N	-1.26665	-1.666681	0.137048
H	-3.995872	0.125739	3.356253	C	-1.098695	-0.413177	0.859578
H	-2.886765	-1.146272	3.748165	H	-0.01531	-0.273911	0.944266
N	-1.638532	-0.232741	-0.270559	C	-1.705132	0.773404	0.0864
H	-2.619382	-0.017526	-0.397739	C	-1.588338	-0.617363	2.297027
C	-0.694566	0.870389	-0.266145	H	-1.541642	0.584361	-0.975614
H	0.047494	0.693725	0.515754	H	-2.784077	0.803294	0.244497
C	0.031263	0.980389	-1.629114	C	-1.069234	2.119125	0.442638
C	-1.454073	2.145083	0.062707	O	-1.52148	-1.67116	2.885289
H	0.411894	-0.01652	-1.854963	H	-1.242659	2.375555	1.488262
H	-0.701814	1.233191	-2.401278	H	0.017469	2.065398	0.30322
C	1.195704	1.973255	-1.647372	C	-1.563933	3.236861	-0.467458
O	-2.637764	2.307948	-0.13432	O	-1.875431	3.040051	-1.642668
H	0.84845	2.998759	-1.512708	N	-1.612459	4.46751	0.090436
H	1.877741	1.758272	-0.816311	H	-1.867966	5.258851	-0.480439
C	2.01922	1.846116	-2.923084	H	-1.34819	4.632124	1.047986
O	2.281794	0.752405	-3.42514	O	-2.049601	0.511982	2.848436
N	2.466822	3.005127	-3.455524	H	-2.292852	0.327154	3.770164
H	3.06273	2.976938	-4.268967	H	-0.301236	-5.459726	-1.729158
H	2.260031	3.89999	-3.043186				
O	-0.64834	3.088256	0.568777				
H	-1.166255	3.898168	0.708708				
H	-2.563683	-4.54758	-0.163107				
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.21535	-2.75801	-1.001343	N	-4.005998	-2.782859	0.877514
H	-2.452499	-3.205202	-0.500027	H	-3.258324	-3.173842	1.44402
C	-3.519806	-1.473895	-0.378795	C	-3.896649	-1.336286	0.8012
H	-4.226576	-0.937068	-1.015329	H	-4.785031	-0.963333	0.280653
C	-4.15299	-1.588685	1.034415	C	-3.697009	-0.527333	2.103137
C	-2.221323	-0.665178	-0.270415	C	-2.717064	-0.898579	-0.077382
H	-5.029973	-2.238744	0.957842	H	-4.603413	-0.0521	2.478006
H	-3.4465	-2.063026	1.720114	H	-3.292349	-1.157817	2.900217
C	-4.645846	-0.247821	1.558356	C	-2.656893	0.516092	1.763921
O	-1.137145	-1.214438	-0.067701	O	-2.351796	-1.386072	-1.125069
O	-5.315849	0.50618	0.847916	O	-2.284126	1.455127	2.438735
N	-4.311307	0.066266	2.826362	N	-2.128497	0.212897	0.515691
H	-4.630408	0.938938	3.21986	C	-1.068723	0.991654	-0.123486
H	-3.756434	-0.545989	3.401814	H	-0.712723	0.362001	-0.945681
N	-2.367198	0.673407	-0.349801	C	-1.591256	2.323394	-0.680074
H	-3.288781	1.06753	-0.488333	C	0.119523	1.146128	0.827001
C	-1.259323	1.595295	-0.154406	H	-2.57154	2.129659	-1.120744
H	-0.544841	1.133658	0.528735	H	-1.744899	3.022137	0.143531
C	-0.551996	1.913295	-1.494515	C	-0.675456	2.932395	-1.740928

C	-1.806939	2.85981	0.484599	O	0.751664	2.163195	0.984276
H	-0.295114	0.951744	-1.942578	H	0.312696	3.139734	-1.324032
H	-1.274258	2.390783	-2.163538	H	-0.517202	2.214948	-2.555506
C	0.705245	2.76847	-1.360814	C	-1.19842	4.237391	-2.382709
O	-2.916832	3.301589	0.279718	O	-0.419015	4.784664	-3.212272
H	0.468753	3.763047	-0.973385	O	-2.339469	4.654256	-2.049916
H	1.387737	2.320619	-0.628232	H	-4.880044	-3.040057	1.324029
C	1.507019	2.958546	-2.669464	O	0.423684	-0.015729	1.431182
O	2.466148	3.77707	-2.602948	H	1.194482	0.129394	2.00289
O	1.165963	2.293904	-3.683212				
H	-4.019657	-3.374733	-0.941822				
O	-0.907354	3.458031	1.277452				
H	-1.28903	4.288146	1.607826				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.938514	-2.774289	-0.589538	N	-2.244467	-2.276168	1.594067
H	-1.052669	-3.093113	-0.206448	H	-2.545563	-1.666659	2.349387
C	-2.256169	-1.453185	-0.053605	C	-2.322002	-1.592595	0.314927
H	-3.128953	-1.065226	-0.582705	H	-2.094789	-2.324361	-0.467437
C	-2.581199	-1.447093	1.461364	C	-3.621116	-0.840271	-0.058219
C	-1.06141	-0.527376	-0.314259	C	-1.235854	-0.51832	0.178579
H	-3.344468	-2.210679	1.646477	H	-4.269865	-1.38258	-0.745874
H	-1.69613	-1.73076	2.03746	H	-4.204152	-0.597545	0.834916
C	-3.165343	-0.127986	1.951123	C	-3.16427	0.460876	-0.678939
O	0.096858	-0.947993	-0.31807	O	-0.080519	-0.571826	0.539926
O	-3.88091	0.572379	1.229557	O	-3.832911	1.305085	-1.238862
N	-2.872097	0.216586	3.221219	N	-1.790355	0.568288	-0.486658
H	-3.282675	1.050399	3.614133	C	-1.03282	1.73861	-0.852113
H	-2.299991	-0.362147	3.814543	C	-1.043278	2.787124	0.249334
N	-1.36165	0.77437	-0.493744	H	-0.000551	1.451187	-1.056132
H	-2.318567	1.088682	-0.384661	H	-1.456541	2.175544	-1.757458
C	-0.330117	1.77717	-0.619631	O	-1.615423	2.680188	1.307306
C	-0.943334	3.156364	-0.679849	O	-0.325195	3.856869	-0.119211
H	0.366715	1.743957	0.224568	H	-0.347025	4.511511	0.59767
H	0.268138	1.623603	-1.522999	H	-2.866183	-3.077922	1.595749
O	-2.128685	3.393955	-0.615255				
O	0.002746	4.095754	-0.813003				
H	-0.424924	4.966872	-0.845213				
H	-2.647953	-3.444473	-0.309502				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.713806	-2.850714	2.144005	N	-1.632554	-2.881646	2.741376
H	-1.699879	-2.314289	3.007182	H	-1.608939	-2.285599	3.564134
C	-2.228942	-2.021248	1.058458	C	-2.11161	-2.148907	1.583182
H	-2.096884	-2.56092	0.118267	H	-2.227621	-2.863807	0.761761
C	-3.7312	-1.666327	1.195324	C	-3.403518	-1.307138	1.705877
C	-1.411353	-0.723661	1.009269	C	-1.070883	-1.140464	1.079244

H	-4.278954	-2.593411	1.397152	H	-4.290462	-1.786311	1.291816
H	-3.888614	-1.013044	2.05828	H	-3.611568	-1.05621	2.750159
C	-4.353305	-1.065041	-0.060302	C	-3.107548	-0.019545	0.972856
O	-0.913577	-0.235896	2.020993	O	0.12824	-1.285303	0.997263
O	-3.872849	-1.245814	-1.184153	O	-3.867005	0.885134	0.690565
N	-5.479164	-0.350089	0.126856	N	-1.748901	0.008173	0.678684
H	-5.960335	0.031922	-0.673426	C	-1.095692	1.134099	0.024166
H	-5.873146	-0.199411	1.041498	H	-0.022289	0.959061	0.144273
N	-1.324936	-0.155406	-0.219256	C	-1.443667	1.194212	-1.481278
H	-1.882474	-0.574349	-0.956474	C	-1.402162	2.43637	0.766328
C	-0.788842	1.177743	-0.438726	H	-1.478968	0.164526	-1.841251
H	-0.303514	1.478744	0.492076	H	-2.44581	1.613882	-1.594587
C	0.234095	1.182038	-1.5905	C	-0.449924	1.926877	-2.321704
C	-1.954361	2.144742	-0.674458	O	-1.627156	3.495881	0.226006
H	0.90313	0.336626	-1.421032	N	-0.262303	3.292084	-2.291509
H	-0.288405	1.000661	-2.53481	C	0.436064	1.473294	-3.272596
C	1.070865	2.416911	-1.678709	H	-0.739395	3.918228	-1.657306
O	-2.130634	2.797352	-1.681051	C	0.70377	3.602452	-3.194325
N	0.609075	3.636147	-2.128466	N	1.150992	2.523514	-3.813931
C	2.396033	2.636507	-1.3777	H	0.585281	0.453983	-3.595286
H	-0.346475	3.82316	-2.398616	H	1.039613	4.614662	-3.356756
C	1.639541	4.520058	-2.078661	O	-1.335228	2.28156	2.092474
N	2.744057	3.949182	-1.629932	H	-1.511003	3.137525	2.516067
H	3.109803	1.91863	-1.002779	H	-2.262202	-3.649416	2.949864
H	1.531766	5.55127	-2.376544				
O	-2.787725	2.171253	0.372734				
H	-3.528339	2.765394	0.169407				
H	-2.323161	-3.649008	2.2929				

Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.477432	-3.531417	-0.770217	N	-1.832738	-4.186777	0.82438
H	-1.675815	-3.803821	-0.207663	H	-2.129082	-3.947429	1.76656
C	-3.037935	-2.287604	-0.250832	C	-2.03303	-3.06687	-0.079173
H	-3.798078	-1.930723	-0.948906	H	-1.800736	-3.411607	-1.092688
C	-3.705792	-2.425675	1.142636	C	-3.395265	-2.343643	-0.092314
C	-1.912028	-1.250736	-0.15923	C	-1.037974	-1.933481	0.188474
H	-4.434071	-3.241081	1.087747	H	-4.060673	-2.650529	-0.89877
H	-2.957317	-2.702366	1.889534	H	-3.922211	-2.487631	0.855697
C	-4.479156	-1.17877	1.547798	C	-3.064358	-0.87179	-0.212835
O	-0.756335	-1.577707	0.115495	O	0.131603	-2.03554	0.490011
O	-5.19404	-0.579099	0.740619	O	-3.833399	0.038388	-0.436184
N	-4.344076	-0.775247	2.827322	N	-1.693822	-0.718545	-0.007277
H	-4.864487	0.026896	3.149776	C	-0.978063	0.548743	0.085226
H	-3.76135	-1.266199	3.485651	H	0.074075	0.261416	0.142787
N	-2.287342	0.031566	-0.346412	C	-1.157316	1.478109	-1.166639
H	-3.26299	0.247207	-0.506729	C	-1.280899	1.218296	1.420512
C	-1.361299	1.138638	-0.181973	H	-1.586874	0.833212	-1.939426
H	-0.678071	0.899063	0.635596	C	-2.118176	2.655787	-0.942902

C	-0.51021	1.371744	-1.471763	C	0.226794	1.943331	-1.660679
C	-2.163504	2.367621	0.208771	O	-2.136974	0.879411	2.202805
H	-0.129949	0.371827	-1.708367	H	-1.657512	3.424758	-0.317275
C	-1.376526	1.852013	-2.642447	H	-2.376796	3.114855	-1.898866
C	0.70332	2.279463	-1.210507	H	-3.044356	2.323995	-0.473989
O	-3.34521	2.516801	-0.014224	H	0.698441	2.546138	-0.875846
H	-1.721871	2.879108	-2.484767	H	0.86079	1.06031	-1.800883
H	-0.8117	1.83067	-3.576082	C	0.185965	2.736779	-2.970096
H	-2.254645	1.214791	-2.774098	H	-0.327848	3.694056	-2.852271
H	0.36612	3.307278	-1.044044	H	1.199606	2.94746	-3.321975
H	1.189408	1.960512	-0.281411	H	-0.330436	2.172598	-3.754088
C	1.734836	2.253823	-2.344546	O	-0.437635	2.240729	1.634929
H	1.325861	2.653126	-3.276434	H	-0.662861	2.655786	2.483224
H	2.608718	2.857225	-2.083681	H	-2.400288	-4.974045	0.52818
H	2.078804	1.232654	-2.539793				
O	-1.40336	3.29292	0.809644				
H	-1.95245	4.07351	0.990443				
H	-3.162268	-4.277968	-0.703341				
Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.349379	-2.602456	-0.148683	N	-2.044941	-3.946433	0.845242
H	-0.521094	-2.796043	0.407833	H	-2.475247	-3.77977	1.750635
C	-1.871051	-1.283686	0.196336	C	-2.321054	-2.85122	-0.068133
H	-2.658967	-1.024241	-0.51394	H	-1.945406	-3.139335	-1.055694
C	-2.47503	-1.193426	1.622715	C	-3.772621	-2.337774	-0.208634
C	-0.730717	-0.265021	0.078326	C	-1.528837	-1.589513	0.299123
H	-3.212557	-1.995545	1.727774	H	-4.291967	-2.7001	-1.095641
H	-1.695323	-1.363384	2.369524	H	-4.370453	-2.607751	0.666788
C	-3.217933	0.113065	1.86425	C	-3.657353	-0.830968	-0.242556
O	0.434812	-0.570346	0.335662	O	-0.379534	-1.517381	0.675951
O	-3.9603	0.595122	1.004704	O	-4.524043	-0.012723	-0.477349
N	-3.025824	0.702779	3.061531	N	-2.35257	-0.488787	0.089477
H	-3.52439	1.552703	3.279063	C	-1.883283	0.889557	0.20361
H	-2.420207	0.30809	3.762655	H	-0.922704	0.814107	0.720938
N	-1.104476	0.984937	-0.265806	C	-1.697516	1.553247	-1.168639
H	-2.081893	1.186755	-0.433818	C	-2.793966	1.687723	1.137928
C	-0.162626	2.090778	-0.318994	H	-1.310281	0.790865	-1.852888
H	0.613119	1.911649	0.424742	H	-2.679187	1.852868	-1.542041
C	0.47419	2.201659	-1.727558	C	-0.73653	2.757029	-1.171352
C	-0.904333	3.366576	0.0387	O	-3.158303	2.822233	0.94099
H	0.895575	1.214318	-1.944447	H	-1.042896	3.439777	-0.372107
H	-0.336205	2.368171	-2.445312	C	0.71743	2.331166	-0.919991
C	1.565707	3.268267	-1.914503	C	-0.853559	3.505386	-2.50597
O	-2.079091	3.560043	-0.185443	H	1.062197	1.653842	-1.70948
H	1.13496	4.251435	-1.69321	H	1.378025	3.202904	-0.913064
C	2.761309	3.047154	-0.976992	H	0.84454	1.818731	0.037797
C	2.021497	3.274761	-3.380847	H	-1.873751	3.864012	-2.672733
H	3.192839	2.05169	-1.131266	H	-0.182069	4.368663	-2.530661

H	3.54437	3.785523	-1.172417	H	-0.585959	2.84935	-3.342345
H	2.481501	3.136427	0.075445	H	-2.443261	-4.806554	0.483379
H	1.182569	3.459741	-4.058688	O	-3.092447	0.993667	2.248761
H	2.772597	4.051539	-3.551522	H	-3.648322	1.549423	2.818191
H	2.467856	2.311368	-3.652304				
H	-2.035505	-3.318255	0.06954				
O	-0.096819	4.276606	0.60023				
H	-0.604691	5.090727	0.752173				
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.599702	-3.464517	1.060419	N	-1.527467	-3.317575	2.309417
H	-0.645402	-3.559976	0.726431	H	-0.582599	-3.625467	2.524519
C	-2.166923	-2.214752	0.550669	C	-1.52341	-2.606373	1.033971
H	-2.489716	-2.296324	-0.498147	H	-1.199234	-3.228307	0.186068
C	-3.406324	-1.849305	1.408626	C	-2.859372	-1.93023	0.691177
C	-1.058226	-1.1418	0.545429	C	-0.530058	-1.448626	1.089698
H	-3.818571	-2.775971	1.811493	H	-3.422781	-2.420716	-0.102008
H	-3.105385	-1.243424	2.269577	H	-3.498184	-1.863502	1.576274
C	-4.489154	-1.083146	0.666828	C	-2.491478	-0.521313	0.276591
O	0.126544	-1.447347	0.706683	O	0.608952	-1.489366	1.505763
O	-4.223287	-0.208034	-0.166652	O	-3.20829	0.335017	-0.197677
N	-5.760236	-1.397222	0.978647	N	-1.142282	-0.324542	0.5583
H	-6.515113	-0.881841	0.551343	C	-0.461511	0.947185	0.360266
H	-5.987891	-2.115339	1.646734	H	0.536419	0.807646	0.79043
N	-1.468206	0.122392	0.325794	C	-0.323334	1.303618	-1.13399
H	-2.451062	0.279184	0.087173	C	-1.136683	1.998611	1.247535
C	-0.522235	1.214386	0.196785	H	-0.222008	0.360411	-1.678153
H	0.337339	1.002962	0.833725	H	-1.242517	1.777113	-1.484153
C	-0.037406	1.367301	-1.266191	C	0.891896	2.185525	-1.439328
C	-1.185029	2.493657	0.680831	O	-1.684319	1.74285	2.294189
H	0.315176	0.377726	-1.571024	H	0.830468	3.119658	-0.875795
H	-0.898785	1.611905	-1.896709	H	1.802478	1.671216	-1.110897
C	1.080465	2.394197	-1.463186	C	0.993885	2.497094	-2.93693
O	-2.365711	2.739129	0.575945	H	1.044589	1.563037	-3.50748
H	0.726701	3.395887	-1.201809	H	0.093534	3.028989	-3.263884
H	1.907653	2.166224	-0.781336	C	2.223102	3.344149	-3.234229
C	1.595735	2.398977	-2.907523	H	2.183735	4.309876	-2.730286
H	1.96156	1.401074	-3.172858	H	3.145829	2.836619	-2.952826
H	0.775268	2.638138	-3.592956	N	2.333211	3.637728	-4.710678
C	2.716806	3.414999	-3.075291	H	1.505676	4.127659	-5.057866
H	2.380366	4.430899	-2.868911	H	3.144592	4.224214	-4.915909
H	3.568375	3.188084	-2.433962	H	2.431772	2.778751	-5.256249
N	3.240712	3.418922	-4.490621	H	-2.092055	-4.158054	2.227942
H	2.509744	3.668682	-5.160093	O	-1.008493	3.2388	0.760345
H	4.002807	4.089958	-4.605079	H	-1.410157	3.859243	1.390192
H	3.600212	2.500105	-4.758891				
H	-2.131128	-4.252725	0.70534				
O	-0.294905	3.349231	1.207625				

H	-0.757012	4.170564	1.443683				
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.602011	-3.254409	-0.740085	N	-1.672857	-4.463812	-1.137311
H	-1.769357	-3.589987	-0.263481	H	-0.689856	-4.629942	-0.939997
C	-3.012123	-1.976078	-0.16695	C	-2.158759	-3.305052	-0.408682
H	-3.806655	-1.555885	-0.787288	H	-3.240459	-3.241791	-0.567454
C	-3.55202	-2.076015	1.283607	C	-1.860928	-3.189781	1.104425
C	-1.807247	-1.027545	-0.186937	C	-1.600304	-1.998203	-0.986831
H	-4.327222	-2.849196	1.300851	H	-2.702794	-3.449366	1.746161
H	-2.755566	-2.397555	1.959986	H	-1.013644	-3.82031	1.388886
C	-4.214279	-0.790367	1.76013	C	-1.459329	-1.749059	1.32116
O	-0.653942	-1.444205	-0.073734	O	-1.451726	-1.704768	-2.152435
O	-4.917369	-0.11264	1.005763	O	-1.257703	-1.169498	2.369304
N	-4.000465	-0.445707	3.045751	N	-1.308455	-1.149021	0.076495
H	-4.453683	0.374959	3.419062	C	-0.879773	0.234208	-0.099954
H	-3.429868	-1.001556	3.66174	H	-0.635035	0.323683	-1.163537
N	-2.104409	0.286401	-0.282945	C	-1.996376	1.226132	0.263033
H	-3.071891	0.580626	-0.33296	C	0.425575	0.491528	0.656813
C	-1.081253	1.313288	-0.216763	H	-2.934399	0.809876	-0.113515
H	-0.292574	0.9775	0.459019	H	-2.075777	1.29228	1.349953
C	-0.469218	1.569114	-1.618876	C	-1.769047	2.608499	-0.3496
C	-1.706635	2.577869	0.348791	O	0.664356	1.489607	1.293346
H	-0.174581	0.587109	-1.99778	H	-0.834389	3.043152	0.006472
H	-1.252586	1.953822	-2.278739	H	-1.733579	2.542123	-1.440929
C	0.738487	2.504703	-1.610339	S	-3.1433	3.732644	0.115732
O	-2.878793	2.864633	0.250395	C	-2.58003	5.245684	-0.738035
H	0.459086	3.515621	-1.308868	H	-2.513671	5.074857	-1.814186
H	1.503124	2.139874	-0.918748	H	-3.321945	6.020585	-0.540277
S	1.470039	2.590917	-3.291993	H	-1.61111	5.564826	-0.349438
C	2.81218	3.785473	-2.964427	O	1.304318	-0.506263	0.476141
H	3.500931	3.390437	-2.215244	H	2.121854	-0.287185	0.951555
H	3.346281	3.93234	-3.904216	H	-2.177644	-5.293445	-0.843544
H	2.401451	4.739666	-2.628991				
O	-0.795835	3.360261	0.942905				
H	-1.230298	4.178439	1.235835				
H	-3.330502	-3.948009	-0.602325				
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.41605	-3.175913	0.617888	N	-1.393587	-3.480604	0.938172
H	-0.622418	-3.132562	1.251461	H	-1.376603	-3.260584	1.93001
C	-2.122073	-1.898671	0.630541	C	-1.720368	-2.304956	0.151224
H	-2.875096	-1.909548	-0.160356	H	-1.841272	-2.625052	-0.889284
C	-2.847365	-1.587896	1.966488	C	-2.936782	-1.440358	0.556198
C	-1.110609	-0.782286	0.34575	C	-0.561891	-1.299473	0.116945
H	-3.486242	-2.443262	2.20896	H	-3.835201	-1.628358	-0.031262
H	-2.116835	-1.484969	2.772949	H	-3.186284	-1.584073	1.611622

C	-3.763184	-0.37532	1.872848	C	-2.479035	-0.010286	0.38101
O	0.061922	-0.86201	0.713443	O	0.623778	-1.532835	0.030001
O	-4.47039	-0.181712	0.880372	O	-3.140053	1.006948	0.435911
N	-3.76364	0.461485	2.929904	N	-1.106052	-0.020519	0.162903
H	-4.382232	1.258731	2.927956	C	-0.312756	1.190954	0.021133
H	-3.186208	0.303229	3.739634	H	0.728118	0.853863	0.006379
N	-1.609827	0.306252	-0.27843	C	-0.626039	1.928057	-1.303659
H	-2.589033	0.334173	-0.533258	C	-0.448602	2.015846	1.304206
C	-0.808544	1.489784	-0.523051	H	-0.809779	1.148531	-2.048438
H	-0.095739	1.607874	0.293623	H	-1.552829	2.490758	-1.193463
C	-0.023393	1.362161	-1.863151	C	0.49362	2.820929	-1.793545
C	-1.731133	2.695875	-0.560078	O	-0.619056	1.528593	2.397622
H	0.513764	0.41291	-1.797674	C	0.322447	4.204859	-1.898022
H	-0.748913	1.275421	-2.676013	C	1.720914	2.265623	-2.180233
C	0.942942	2.492326	-2.120273	H	-0.620196	4.648677	-1.597675
O	-2.879649	2.660427	-0.944433	C	1.352288	5.018856	-2.374246
C	0.645269	3.501862	-3.042271	C	2.75528	3.074741	-2.65129
C	2.153265	2.558742	-1.417207	H	1.868396	1.191697	-2.119552
H	-0.287169	3.46244	-3.596057	H	1.200496	6.089944	-2.448607
C	1.533324	4.558281	-3.256173	C	2.573811	4.456653	-2.749796
C	3.042446	3.61302	-1.625644	H	3.697556	2.626846	-2.946553
H	2.400061	1.778523	-0.704121	H	3.375172	5.087155	-3.118051
H	1.287424	5.331016	-3.97596	O	-0.3045	3.327302	1.088123
C	2.73408	4.618021	-2.546643	H	-0.350468	3.785833	1.942977
H	3.975569	3.64816	-1.074498	H	-2.102552	-4.19415	0.805535
H	3.425326	5.436675	-2.711821				
O	-1.115394	3.812005	-0.154767				
H	-1.724893	4.560874	-0.263116				
H	-2.027437	-3.916173	0.948048				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.830458	-3.363075	0.473504	N	-1.12055	-3.26675	1.227952
H	-0.018882	-3.449598	1.079189	H	-0.78307	-2.9773	2.14175
C	-1.183231	-1.953648	0.321619	C	-1.373278	-2.11562	0.379721
H	-1.955403	-1.871148	-0.446215	H	-1.839606	-2.477591	-0.542833
C	-1.726668	-1.298417	1.615491	C	-2.206095	-0.938018	0.938402
C	0.063631	-1.194152	-0.147476	C	-0.06846	-1.448872	-0.075317
H	-2.481422	-1.968392	2.042093	H	-3.245497	-0.929449	0.611007
H	-0.93092	-1.210083	2.361216	H	-2.196484	-0.935261	2.032339
C	-2.412049	0.047994	1.407192	C	-1.492471	0.308609	0.469325
O	1.19996	-1.552892	0.158192	O	0.964133	-1.985492	-0.409914
O	-2.775492	0.442065	0.29359	O	-1.854771	1.464864	0.548881
N	-2.628154	0.770375	2.522924	N	-0.272029	-0.072129	-0.0776
H	-3.117068	1.65024	2.455311	C	0.722821	0.885297	-0.526933
H	-2.33848	0.450439	3.433116	H	1.593499	0.295253	-0.831475
N	-0.174166	-0.083875	-0.884228	C	0.251382	1.675659	-1.759743
H	-1.130605	0.259427	-0.890006	C	1.180612	1.724353	0.669783
C	0.900376	0.830688	-1.20947	H	-0.415055	1.027443	-2.339203

H	1.683339	0.302363	-1.755085	H	-0.303702	2.565655	-1.457652
C	0.333214	1.950073	-2.0906	O	1.410002	2.012579	-2.517238
C	1.514413	1.423844	0.063148	O	1.175449	1.319684	1.809095
H	-0.124856	1.491244	-2.974018	H	1.192092	2.743634	-3.105094
H	-0.441426	2.4917	-1.533389	O	1.624184	2.933212	0.310392
O	1.40561	2.812017	-2.448258	H	1.93224	3.394929	1.107322
O	0.869194	1.772126	1.025593	H	-1.982	-3.780727	1.379856
H	1.049048	3.5547	-2.947789				
O	2.846931	1.535366	-0.020289				
H	3.173383	1.95075	0.794734				
H	-1.592661	-3.86852	0.914161				
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.074373	-3.623279	0.464807	N	-2.294208	-3.991687	-0.404589
H	-1.403804	-3.830412	1.199905	H	-1.902524	-3.96673	0.532928
C	-2.24994	-2.176673	0.354573	C	-2.524657	-2.647733	-0.90472
H	-2.841157	-1.967471	-0.53949	H	-3.048826	-2.73406	-1.862772
C	-2.975983	-1.537611	1.563485	C	-3.266181	-1.629693	-0.013354
C	-0.865567	-1.535049	0.192492	C	-1.21492	-1.928651	-1.242377
H	-3.846064	-2.158811	1.803679	H	-4.323749	-1.512801	-0.248864
H	-2.331355	-1.549483	2.447418	H	-3.182908	-1.902554	1.042838
C	-3.507387	-0.130403	1.312664	C	-2.536531	-0.317511	-0.205725
O	0.144498	-2.045069	0.677197	O	-0.214152	-2.402521	-1.734306
O	-3.616994	0.345158	0.178258	O	-2.86161	0.772406	0.207566
N	-3.890505	0.549899	2.410874	N	-1.363762	-0.580615	-0.920741
H	-4.289802	1.47055	2.308643	C	-0.323664	0.391596	-1.227908
H	-3.802678	0.164179	3.33715	H	0.570222	-0.206178	-1.439741
N	-0.845748	-0.3696	-0.492904	C	-0.590328	1.21317	-2.501368
H	-1.737871	0.079281	-0.675629	C	0.053363	1.173458	0.031273
C	0.338897	0.450697	-0.548154	H	0.288952	1.852572	-2.637321
H	1.211957	-0.194125	-0.666834	C	-0.755216	0.319311	-3.728748
C	0.290031	1.413831	-1.746846	O	-1.748479	2.017819	-2.286435
C	0.535829	1.218385	0.76297	O	0.012785	0.705004	1.144435
H	1.197548	2.02526	-1.709043	H	-1.628471	-0.32872	-3.623307
C	0.221082	0.681309	-3.081725	H	-0.896638	0.940954	-4.616366
O	-0.860376	2.242441	-1.530222	H	0.13014	-0.301732	-3.88421
O	-0.250496	1.249127	1.679139	H	-1.899471	2.544998	-3.079491
H	-0.670074	0.052983	-3.136872	H	-3.17469	-4.492025	-0.342683
H	0.190152	1.405513	-3.900127	O	0.530517	2.393319	-0.244786
H	1.105718	0.053588	-3.218354	H	0.829226	2.797728	0.585883
H	-0.959609	2.84058	-2.279535				
H	-2.952367	-4.062779	0.722703				
O	1.719358	1.855657	0.775744				
H	1.804207	2.334617	1.615802				
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.187528	-2.400155	1.565583	N	-1.064645	-2.673648	2.405632

H	-1.816699	-1.860949	2.343333	H	-1.603765	-2.408274	3.225236
C	-3.256646	-1.648379	0.915927	C	-1.655213	-2.12503	1.196973
H	-3.538137	-2.166608	-0.003174	H	-1.106215	-2.535788	0.343184
C	-4.536537	-1.491437	1.778652	C	-3.172779	-2.299806	0.955747
C	-2.724332	-0.254758	0.563648	C	-1.447761	-0.60763	1.103114
H	-4.840588	-2.488174	2.114375	H	-3.424229	-3.087413	0.245559
H	-4.315926	-0.898577	2.670226	H	-3.698947	-2.509166	1.89148
C	-5.710481	-0.921523	0.994353	C	-3.649731	-0.959328	0.445413
O	-1.884442	0.313417	1.26383	O	-0.449221	0.024275	1.370669
O	-5.940986	-1.278198	-0.164211	O	-4.738196	-0.666475	-0.007289
N	-6.482064	-0.021077	1.6358	N	-2.617584	-0.04302	0.60476
H	-7.293525	0.35548	1.168908	C	-2.72507	1.368287	0.251473
H	-6.294148	0.268904	2.581581	H	-1.875789	1.849447	0.744549
N	-3.277719	0.322662	-0.523645	C	-2.630216	1.600811	-1.27214
H	-3.994378	-0.165763	-1.045483	C	-3.977628	1.987762	0.871921
C	-2.949408	1.680891	-0.910597	H	-1.934131	0.851413	-1.661998
H	-2.795795	2.274692	-0.008975	H	-3.603153	1.409526	-1.726222
C	-1.641607	1.724197	-1.764774	C	-2.137543	2.972121	-1.615955
C	-4.112572	2.258781	-1.691763	O	-4.739803	2.725661	0.29677
H	-0.943537	1.056681	-1.251695	C	-2.84353	3.998313	-2.19439
H	-1.846337	1.287585	-2.745926	C	-0.803103	3.470107	-1.392913
C	-1.04373	3.086646	-1.891696	H	-3.875997	4.02942	-2.504127
O	-4.90516	1.596875	-2.32721	N	-2.030746	5.102164	-2.347634
C	-0.967748	3.872065	-3.015971	C	-0.773615	4.812589	-1.864908
C	-0.446061	3.845097	-0.822639	C	0.365572	2.911883	-0.844717
H	-1.307213	3.668497	-4.019705	H	-2.315953	5.979676	-2.750754
N	-0.360414	5.073155	-2.710915	C	0.38081	5.598873	-1.803247
C	-0.027988	5.088202	-1.374086	C	1.515452	3.691516	-0.780845
C	-0.223459	3.588117	0.541743	H	0.368679	1.893433	-0.471414
H	-0.175103	5.812237	-3.369111	H	0.384794	6.619311	-2.168877
C	0.60169	6.069783	-0.602376	C	1.522584	5.021429	-1.255402
C	0.401593	4.562725	1.312157	H	2.423585	3.274798	-0.359531
H	-0.535356	2.645241	0.979259	H	2.43467	5.604197	-1.191763
H	0.915788	7.011198	-1.038268	O	-4.096035	1.65601	2.168841
C	0.809061	5.79063	0.745387	H	-4.890651	2.085417	2.524328
H	0.581185	4.381057	2.366053	H	-1.069979	-3.687382	2.363719
H	1.293819	6.530597	1.372406				
O	-4.140249	3.595303	-1.633089				
H	-4.86051	3.915776	-2.200866				
H	-2.551606	-3.268724	1.944784				
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.749734	-2.200547	1.889927	N	-1.579584	-2.315952	1.207972
H	-1.125535	-2.034458	2.819471	H	-2.246775	-2.335684	1.974242
C	-1.517312	-1.441828	0.905774	C	-1.801176	-1.159839	0.358071
H	-1.000171	-1.49947	-0.054774	H	-1.136523	-1.24965	-0.508149
C	-2.961413	-1.961698	0.697531	C	-3.231694	-0.85065	-0.137285
C	-1.559336	0.026074	1.351963	C	-1.370828	0.14433	1.040284

H	-2.918333	-3.052424	0.602299	H	-3.438098	-1.189674	-1.152055
H	-3.574575	-1.750278	1.578749	H	-3.980034	-1.292227	0.527412
C	-3.650066	-1.446761	-0.562285	C	-3.360957	0.652949	-0.047622
O	-1.468212	0.35304	2.535568	O	-0.39997	0.329931	1.740413
O	-3.031897	-0.900786	-1.48275	O	-4.235536	1.35988	-0.505034
N	-4.979282	-1.655055	-0.624174	N	-2.281169	1.134969	0.684751
H	-5.484318	-1.383262	-1.454128	C	-2.087977	2.537982	1.007674
H	-5.4847	-2.112522	0.117448	H	-1.195964	2.573462	1.641207
N	-1.737387	0.923343	0.358765	C	-1.827023	3.398477	-0.255454
H	-1.969861	0.555549	-0.55807	C	-3.233104	3.027346	1.891754
C	-1.973948	2.319804	0.636926	H	-2.739786	3.437684	-0.850678
H	-1.184682	2.694078	1.292276	H	-1.604516	4.411715	0.080785
C	-1.976804	3.142217	-0.67563	C	-0.682333	2.842321	-1.068575
C	-3.304669	2.521797	1.359783	O	-3.977454	2.307755	2.514654
H	-2.808896	2.803256	-1.300208	C	-0.915042	1.979955	-2.144663
H	-2.172753	4.183873	-0.412091	C	0.646448	3.127767	-0.728326
C	-0.673218	3.019138	-1.428764	H	-1.933983	1.744822	-2.433195
O	-4.247205	1.76639	1.313491	C	0.13876	1.410354	-2.860244
C	-0.555131	2.176764	-2.538102	C	1.709847	2.569967	-1.432343
C	0.464801	3.720443	-1.008354	H	0.855886	3.795426	0.101274
H	-1.420625	1.624924	-2.890212	H	-0.062817	0.743896	-3.692465
C	0.65871	2.02871	-3.210931	C	1.45599	1.704776	-2.500588
C	1.683229	3.583694	-1.667177	H	2.735545	2.796537	-1.166592
H	0.399747	4.384581	-0.152538	O	2.53781	1.182386	-3.156607
H	0.729958	1.371498	-4.071188	H	2.244932	0.602454	-3.8699
C	1.782165	2.732282	-2.771914	H	-1.716601	-3.168413	0.675153
H	2.559453	4.130514	-1.33967	O	-3.277068	4.366377	1.941425
O	3.003475	2.634059	-3.382705	H	-3.982322	4.627409	2.555708
H	2.955242	2.017282	-4.12324				
H	-0.828268	-3.195324	1.703511				
O	-3.316681	3.687623	2.028772				
H	-4.192936	3.806284	2.429615				

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.50876	-3.51384	-0.51618	N	-1.121495	-4.32416	-0.054759
H	-1.58822	-3.91829	-0.36675	H	-0.850217	-4.173554	0.912926
C	-2.59861	-2.23505	0.181603	C	-1.678691	-3.111766	-0.6288
H	-3.52835	-1.743	-0.1119	H	-2.054206	-3.358535	-1.627878
C	-2.5974	-2.35496	1.728934	C	-2.770523	-2.345053	0.144707
C	-1.41097	-1.36491	-0.24658	C	-0.605377	-2.044865	-0.866293
H	-3.38946	-3.05503	2.012624	H	-3.787604	-2.550966	-0.187479
H	-1.64762	-2.7753	2.06939	H	-2.713169	-2.560498	1.215957
C	-2.91582	-1.03449	2.415452	C	-2.439797	-0.880593	-0.045334
O	-0.31134	-1.85754	-0.50384	O	0.532239	-2.215541	-1.248227
O	-3.83154	-0.31131	2.014595	O	-3.135064	0.071378	0.237449
N	-2.15063	-0.70542	3.475707	N	-1.164487	-0.79431	-0.602391
H	-2.34236	0.14874	3.977599	C	-0.410828	0.432099	-0.837413
H	-1.40063	-1.29451	3.798659	H	0.487635	0.099365	-1.361753

N	-1.64246	-0.03581	-0.26629	C	-1.145012	1.470788	-1.756922
H	-2.54798	0.317741	0.014918	C	0.086994	0.997884	0.487132
C	-0.58838	0.927018	-0.53505	H	-1.943638	0.9014	-2.240431
H	0.34035	0.55556	-0.09657	C	-1.784011	2.651843	-1.012262
C	-0.35966	1.111513	-2.06911	C	-0.188128	1.973876	-2.847158
C	-0.95573	2.230137	0.15307	O	-0.24416	0.619966	1.585715
H	-0.27574	0.08452	-2.43812	H	-1.019451	3.321957	-0.610576
C	-1.55665	1.777531	-2.75653	H	-2.395526	3.229864	-1.71015
C	0.953635	1.834565	-2.38535	H	-2.422987	2.313492	-0.19715
O	-2.08126	2.545467	0.472634	H	0.202308	1.148552	-3.449436
H	-1.66114	2.823177	-2.44884	H	-0.708075	2.665844	-3.515019
H	-1.42096	1.763312	-3.8409	H	0.658565	2.505744	-2.403239
H	-2.49197	1.260411	-2.52724	H	-1.821946	-5.058243	-0.053591
H	1.802086	1.358933	-1.88474	O	0.982575	1.975238	0.27363
H	1.138002	1.807404	-3.46267	H	1.271506	2.323803	1.13249
H	0.921917	2.881853	-2.07574				
H	-3.19072	-4.1656	-0.14079				
O	0.112947	3.015562	0.343046				
H	-0.18445	3.851541	0.738425				

Table S14.C. Succinimide Hydrolysis into Asp-X XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions							
H_2O							
Reactant Structure							
Atom	X	Y	Z				
O	-0.999631	0.482902	0				
H	-0.03661	0.526297	0				
H	-1.280189	1.405171	0				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.042902	-2.775176	1.359843	N	-0.686569	-1.643772	0.223108
H	-0.736188	-2.253319	2.176226	H	-0.383147	-2.167004	1.039497
C	-1.904821	-1.960734	0.520089	C	-2.147407	-1.702916	0.114768
H	-2.289833	-2.60121	-0.280449	H	-2.521987	-2.719075	-0.046106
C	-3.081068	-1.196656	1.168428	C	-2.773191	-1.184051	1.433816
C	-1.116766	-0.859026	-0.199821	C	-2.679393	-0.926432	-1.102315
H	-4.052559	-1.6718	1.032706	H	-2.490272	-1.87125	2.232431
H	-2.918291	-1.06206	2.241714	H	-2.380055	-0.196998	1.67752
C	-3.069578	0.171844	0.524872	C	-4.290565	-1.162056	1.367583
O	-0.015218	-0.942138	-0.698557	O	-3.525082	-1.461354	-1.821251
O	-3.894511	1.056175	0.631215	O	-4.864316	-0.02907	0.951053
N	-1.902406	0.288036	-0.224191	N	-2.26073	0.337056	-1.360854
C	-1.504711	1.5079	-0.912134	C	-1.305272	1.179812	-0.663606
H	-0.505306	1.305213	-1.310538	H	-0.729902	0.539435	0.01274
C	-2.444024	1.855738	-2.072693	C	-0.34002	1.834545	-1.659901

C	-1.298399	2.621602	0.114935	C	-2.026896	2.183529	0.230805
H	-3.444149	2.088802	-1.70865	H	-0.880752	2.465285	-2.370629
H	-2.054195	2.712883	-2.620564	H	0.393676	2.44871	-1.139399
H	-2.501534	1.003354	-2.751868	H	0.181389	1.051441	-2.212094
O	-1.10025	2.440047	1.293432	O	-3.169275	2.057851	0.637384
H	-1.555907	-3.581316	1.701205	H	-0.258485	-2.092588	-0.581667
O	-1.298401	3.832155	-0.460924	O	-1.257982	3.210773	0.582634
H	-1.10317	4.49529	0.220986	H	-1.751275	3.77881	1.197825
				O	-4.97508	-2.123742	1.648348
				H	-2.711837	0.748963	-2.169229
				H	-4.209124	0.688081	0.772893

Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.617216	-4.351801	1.003787	N	-3.009589	-4.26148	0.19562
H	-2.349071	-4.282302	1.981622	H	-2.252229	-4.736558	0.678908
C	-2.660843	-3.038532	0.383934	C	-3.035816	-2.855068	0.584744
H	-3.06396	-3.161739	-0.626596	H	-3.768772	-2.339106	-0.039819
C	-3.420004	-1.895512	1.097852	C	-3.415626	-2.621395	2.06765
C	-1.25322	-2.463758	0.179004	C	-1.642139	-2.262193	0.328957
H	-4.402568	-1.681585	0.67746	H	-4.288059	-3.238189	2.309898
H	-3.548962	-2.112474	2.162073	H	-2.615267	-2.947021	2.737366
C	-2.522033	-0.685894	0.977264	C	-3.803195	-1.200774	2.403139
O	-0.259879	-3.046354	-0.196158	O	-0.625807	-2.936765	0.473501
O	-2.759279	0.465721	1.281809	O	-4.049135	-0.325782	1.597486
N	-1.297393	-1.103796	0.47051	N	-1.630883	-0.953983	-0.022344
C	-0.162598	-0.209091	0.26998	C	-0.412163	-0.163814	-0.134737
H	0.695195	-0.870475	0.109446	H	0.419999	-0.868962	-0.093855
C	-0.354243	0.695797	-0.955326	C	-0.38151	0.63125	-1.440606
C	0.140664	0.568644	1.552825	C	-0.321864	0.737573	1.10254
H	-0.822558	0.089896	-1.735949	H	-0.613762	-0.064499	-2.251557
H	-1.050242	1.498573	-0.701782	H	-1.172704	1.387063	-1.419799
C	0.965572	1.268841	-1.479703	C	0.975089	1.293413	-1.698796
O	0.434795	1.739449	1.591353	O	-0.512621	1.932258	1.109054
H	1.452887	1.853343	-0.695212	H	1.232622	1.958761	-0.869403
H	1.64068	0.451199	-1.75445	H	1.753114	0.52487	-1.761809
C	0.730656	2.154601	-2.701281	C	0.95527	2.097452	-2.996397
H	0.266324	1.569929	-3.500754	H	0.691382	1.446718	-3.836119
H	0.058849	2.980288	-2.442495	H	0.2052	2.892488	-2.925878
N	2.007692	2.68443	-3.186877	N	2.27516	2.685446	-3.243409
H	2.796101	2.649133	-2.557331	H	2.976931	2.57705	-2.526076
C	2.185742	3.301151	-4.354181	C	2.608416	3.379081	-4.330194
N	1.147427	3.530226	-5.163721	N	1.701621	3.621778	-5.281064
N	3.414197	3.683457	-4.724638	N	3.859088	3.839258	-4.473894
H	0.199954	3.441132	-4.835806	H	0.724203	3.432743	-5.133916
H	1.281109	3.968596	-6.060812	H	1.943462	4.164914	-6.094031
H	4.228422	3.359178	-4.227999	H	4.598589	3.509483	-3.874256
H	3.56521	4.175874	-5.589779	H	4.136653	4.314741	-5.317504
H	-3.538463	-4.776235	0.979622	H	-3.876362	-4.716929	0.463793

O	0.102172	-0.226792	2.632464	O	-0.039741	0.026291	2.205567
H	0.325184	0.303548	3.414349	H	-0.047456	0.62353	2.971295
				O	-3.880869	-1.006298	3.729326
				H	-4.164885	-0.0916	3.891196
				H	-2.515371	-0.46174	-0.018603
Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.114507	-4.044523	0.700107	N	-0.194641	-3.986025	0.103945
H	-0.051479	-3.816724	1.688332	H	0.381145	-4.039723	-0.731391
C	-0.921035	-3.065744	-0.006236	C	-1.138846	-2.881543	-0.026132
H	-1.053697	-3.422118	-1.033465	H	-1.68266	-3.005508	-0.965174
C	-2.299446	-2.667906	0.570751	C	-2.154604	-2.944892	1.131152
C	-0.192996	-1.72329	-0.151065	C	-0.449274	-1.499097	-0.014429
H	-3.14477	-3.167045	0.0977	H	-2.445219	-3.991756	1.270811
H	-2.345563	-2.868503	1.645354	H	-1.693067	-2.622139	2.06996
C	-2.390252	-1.171545	0.377893	C	-3.431773	-2.165918	0.895218
O	0.981182	-1.533666	-0.378647	O	0.613399	-1.322781	0.57589
O	-3.348207	-0.44393	0.543205	O	-4.25278	-2.03644	1.952747
N	-1.137417	-0.710221	-0.012395	N	-1.115597	-0.518395	-0.670814
C	-0.828972	0.697604	-0.188452	C	-0.752428	0.883013	-0.57496
H	0.245085	0.751776	-0.39225	H	0.247237	0.926279	-0.136648
C	-1.571113	1.311425	-1.384231	C	-0.727481	1.558832	-1.945895
C	-1.030359	1.427347	1.140697	C	-1.676173	1.622162	0.397298
H	-1.575827	0.572864	-2.191325	H	-0.141169	0.929149	-2.621306
H	-2.608781	1.526313	-1.131871	H	-1.735121	1.636468	-2.359445
C	-0.850516	2.539971	-1.932401	C	-0.043501	2.92034	-1.902611
O	-0.912157	0.906122	2.224029	O	-2.190561	2.694225	0.174364
O	0.375609	2.636893	-1.90239	O	0.88175	3.153474	-1.124753
N	-1.641543	3.477582	-2.491381	N	-0.480052	3.825603	-2.802748
H	-1.219115	4.282971	-2.927679	H	-0.033602	4.728759	-2.850426
H	-2.644983	3.394689	-2.506062	H	-1.254066	3.639146	-3.419257
H	-0.546049	-4.960398	0.634824	H	0.448013	-3.788132	0.867831
O	-1.29889	2.726553	0.959651	O	-1.837514	0.945701	1.54516
H	-1.363866	3.155327	1.828359	H	-2.421138	1.458354	2.127273
				O	-3.770691	-1.693917	-0.168202
				H	-2.04129	-0.745511	-1.013511
				H	-3.880215	-2.447208	2.745812
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.621989	-3.535013	-0.763109	N	-5.566453	-3.229187	-1.662452
H	-4.365086	-3.586074	0.218791	H	-4.885791	-3.638682	-1.028418
C	-4.932237	-2.167932	-1.144843	C	-5.702581	-1.803693	-1.383233
H	-5.305271	-2.186863	-2.174353	H	-6.32432	-1.354127	-2.160521
C	-5.905241	-1.345795	-0.269706	C	-6.349268	-1.490248	-0.008931
C	-3.673727	-1.291745	-1.198442	C	-4.307431	-1.16804	-1.412278
H	-6.920064	-1.285953	-0.662657	H	-7.223021	-2.138802	0.122165
H	-5.959114	-1.752565	0.744396	H	-5.656231	-1.730819	0.802927

C	-5.288467	0.03245	-0.183902	C	-6.851687	-0.068615	0.144708
O	-2.576708	-1.598096	-1.613673	O	-3.31357	-1.787092	-1.033946
O	-5.773522	1.044701	0.280799	O	-7.210014	0.305893	1.387079
N	-4.006056	-0.03244	-0.714432	N	-4.257187	0.118687	-1.823985
C	-3.085339	1.096907	-0.722967	C	-3.073191	0.927361	-1.598921
H	-2.130533	0.710094	-1.092835	H	-2.203498	0.427045	-2.024592
C	-3.517481	2.221775	-1.671156	C	-3.228372	2.302537	-2.27124
C	-2.81385	1.519882	0.718351	C	-2.841068	1.092385	-0.095484
H	-3.988147	1.757262	-2.543504	H	-3.615076	2.122845	-3.279487
H	-4.26236	2.867523	-1.209031	H	-3.961621	2.908075	-1.733629
C	-2.338957	3.071828	-2.211626	C	-1.896446	3.07835	-2.43092
O	-2.848003	0.767108	1.665905	O	-3.695966	0.978005	0.754141
O	-1.204415	2.529205	-2.25186	O	-0.941145	2.442898	-2.946758
O	-2.637571	4.227695	-2.610012	O	-1.897059	4.283706	-2.068928
O	-2.477138	2.812877	0.816192	O	-1.568109	1.417263	0.179572
H	-2.266479	3.002534	1.744666	H	-1.487763	1.557493	1.137033
H	-5.44121	-4.121271	-0.884234	H	-6.450323	-3.704932	-1.511185
				O	-6.988715	0.718794	-0.765756
				H	-5.141356	0.600531	-1.927071
				H	-7.045545	-0.39808	2.03048
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.432049	-2.725908	0.969617	N	-2.36359	-2.416809	0.317138
H	-1.832365	-2.451721	1.74267	H	-1.649206	-2.691331	0.984859
C	-3.108095	-1.57372	0.402654	C	-2.627234	-0.989796	0.436182
H	-3.82651	-1.940339	-0.338517	H	-3.369579	-0.720831	-0.319404
C	-3.823308	-0.579175	1.346956	C	-3.21498	-0.50516	1.803213
C	-2.148419	-0.682707	-0.39636	C	-1.322768	-0.233805	0.167475
H	-4.901298	-0.722604	1.416164	H	-3.502671	0.543676	1.726837
H	-3.409131	-0.632913	2.358147	H	-4.107702	-1.100884	2.006993
C	-3.504908	0.789583	0.791972	C	-2.262493	-0.630862	2.965713
O	-1.244294	-1.024516	-1.124914	O	-0.259053	-0.627262	0.636407
O	-3.967892	1.865328	1.112598	O	-2.07028	-1.912275	3.337972
N	-2.516741	0.643473	-0.176152	N	-1.443493	0.902152	-0.564059
C	-1.913064	1.765977	-0.886047	C	-0.320459	1.782052	-0.860515
H	-1.024703	1.359066	-1.377407	H	0.553112	1.347797	-0.374278
C	-2.871124	2.33473	-1.941602	C	-0.091083	1.884389	-2.369548
C	-1.418946	2.826426	0.100867	C	-0.597811	3.143713	-0.218282
H	-3.324877	1.50192	-2.480022	H	0.036304	0.878119	-2.770401
H	-3.662973	2.914254	-1.470046	H	-0.943604	2.349722	-2.864671
S	-2.050317	3.338175	-3.239493	S	1.441439	2.788872	-2.825274
O	-1.572626	4.016635	-0.03768	O	-0.958516	4.130381	-0.818968
H	-1.722397	4.37661	-2.450761	H	1.003641	4.017387	-2.495196
H	-3.113362	-3.379905	1.340247	H	-3.201253	-2.942928	0.545819
O	-0.741301	2.272648	1.115314	O	-0.423758	3.100293	1.109396
H	-0.429228	2.979918	1.702755	H	-0.657305	3.964898	1.485361
				O	-1.718947	0.299085	3.522442
				H	-2.348365	1.142456	-0.943565

				H	-1.43214	-1.924054	4.069746
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	0.013409	-4.753899	-1.071706	N	0.40392	-4.565044	-0.997246
H	-0.082809	-5.151975	-0.141624	H	0.47393	-4.883687	-0.034732
C	-0.794998	-3.555075	-1.208139	C	-0.627535	-3.538899	-1.103049
H	-0.745118	-3.237645	-2.255145	H	-0.59367	-3.113513	-2.108402
C	-2.274526	-3.590755	-0.760809	C	-2.065154	-4.062201	-0.850584
C	-0.208434	-2.379976	-0.414913	C	-0.321858	-2.442496	-0.07557
H	-2.986549	-3.703385	-1.578204	H	-2.199734	-4.996373	-1.407548
H	-2.449046	-4.400706	-0.046654	H	-2.203131	-4.307257	0.207044
C	-2.500767	-2.281629	-0.039798	C	-3.167867	-3.130794	-1.313321
O	0.95757	-2.073682	-0.293995	O	0.193984	-2.703807	1.010099
O	-3.546323	-1.811385	0.360909	O	-4.418725	-3.450294	-0.933435
N	-1.26665	-1.666681	0.137048	N	-0.700863	-1.190589	-0.418599
C	-1.098695	-0.413177	0.859578	C	-0.714779	-0.125611	0.565224
H	-0.01531	-0.273911	0.944266	H	0.281027	-0.029832	1.002428
C	-1.705132	0.773404	0.0864	C	-1.109509	1.194487	-0.121468
C	-1.588338	-0.617363	2.297027	C	-1.688696	-0.471546	1.695663
H	-1.541642	0.584361	-0.975614	H	-0.444087	1.329481	-0.976319
H	-2.784077	0.803294	0.244497	H	-2.127865	1.103746	-0.513807
C	-1.069234	2.119125	0.442638	C	-1.006608	2.420601	0.787268
O	-1.52148	-1.67116	2.885289	O	-2.693869	-1.130059	1.561205
H	-1.242659	2.375555	1.488262	H	-1.709994	2.361036	1.619715
H	0.017469	2.065398	0.30322	H	-0.003989	2.475672	1.226987
C	-1.563933	3.236861	-0.467458	C	-1.211314	3.715949	0.010596
O	-1.875431	3.040051	-1.642668	O	-0.818136	3.854485	-1.148144
N	-1.612459	4.46751	0.090436	N	-1.825968	4.713485	0.68439
H	-1.867966	5.258851	-0.480439	H	-1.932782	5.61412	0.24286
H	-1.34819	4.632124	1.047986	H	-2.142517	4.604527	1.634082
O	-2.049601	0.511982	2.848436	O	-1.31101	0.080831	2.85964
H	-2.292852	0.327154	3.770164	H	-1.982349	-0.121498	3.53168
H	-0.301236	-5.459726	-1.729158	H	0.164508	-5.368623	-1.569362
				O	-3.001823	-2.159589	-2.01857
				H	-1.293061	-1.094067	-1.234223
				H	-4.430416	-4.238587	-0.372038
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.005998	-2.782859	0.877514	N	-2.805088	-2.066325	-0.388966
H	-3.258324	-3.173842	1.44402	H	-1.888427	-1.638378	-0.47908
C	-3.896649	-1.336286	0.8012	C	-3.710846	-1.247474	0.428506
H	-4.785031	-0.963333	0.280653	H	-4.608711	-1.843398	0.592332
C	-3.697009	-0.527333	2.103137	C	-3.141995	-0.897229	1.821927
C	-2.717064	-0.898579	-0.077382	C	-4.237897	-0.098575	-0.457271
H	-4.603413	-0.0521	2.478006	H	-3.036433	-1.834519	2.3783
H	-3.292349	-1.157817	2.900217	H	-2.135726	-0.47557	1.768249
C	-2.656893	0.516092	1.763921	C	-3.990402	0.051421	2.64093

O	-2.351796	-1.386072	-1.125069	O	-5.366486	-0.191191	-0.940239
O	-2.284126	1.455127	2.438735	O	-3.60321	0.247386	3.918389
N	-2.128497	0.212897	0.515691	N	-3.445389	0.952736	-0.788723
C	-1.068723	0.991654	-0.123486	C	-2.11406	1.319228	-0.332844
H	-0.712723	0.362001	-0.945681	H	-1.593863	0.440008	0.037463
C	-1.591256	2.323394	-0.680074	C	-1.300355	1.91196	-1.498325
C	0.119523	1.146128	0.827001	C	-2.221375	2.344401	0.798562
H	-2.57154	2.129659	-1.120744	H	-1.278646	1.164049	-2.29329
H	-1.744899	3.022137	0.143531	H	-1.834438	2.782894	-1.89036
C	-0.675456	2.932395	-1.740928	C	0.123651	2.301792	-1.106933
O	0.751664	2.163195	0.984276	O	-2.897844	3.34454	0.742584
H	0.312696	3.139734	-1.324032	H	0.121934	3.077853	-0.334657
H	-0.517202	2.214948	-2.555506	H	0.643281	1.443259	-0.665541
C	-1.19842	4.237391	-2.382709	C	0.999066	2.817633	-2.273341
O	-0.419015	4.784664	-3.212272	O	2.144228	3.236239	-1.94787
O	-2.339469	4.654256	-2.049916	O	0.522465	2.777107	-3.437596
H	-4.880044	-3.040057	1.324029	H	-2.659187	-2.96799	0.055052
O	0.423684	-0.015729	1.431182	O	-1.464669	2.014056	1.85823
H	1.194482	0.129394	2.00289	H	-1.547168	2.708835	2.5327
				O	-4.958878	0.642404	2.223763
				H	-3.906578	1.632308	-1.380899
				H	-2.813242	-0.26761	4.134778

Asn-Gly

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.244467	-2.276168	1.594067	N	-3.76232	2.895395	1.395995
H	-2.545563	-1.666659	2.349387	H	-4.299658	2.898136	0.533957
C	-2.322002	-1.592595	0.314927	C	-3.236152	1.547886	1.632491
H	-2.094789	-2.324361	-0.467437	H	-2.848719	1.522178	2.655211
C	-3.621116	-0.840271	-0.058219	C	-4.254871	0.397092	1.524237
C	-1.235854	-0.51832	0.178579	C	-2.040025	1.270457	0.701316
H	-4.269865	-1.38258	-0.745874	H	-3.790792	-0.535759	1.850614
H	-4.204152	-0.597545	0.834916	H	-5.083358	0.604869	2.209384
C	-3.16427	0.460876	-0.678939	C	-4.857634	0.2316	0.143617
O	-0.080519	-0.571826	0.539926	O	-2.064032	0.342191	-0.107302
O	-3.832911	1.305085	-1.238862	O	-5.170336	-1.024722	-0.236729
N	-1.790355	0.568288	-0.486658	N	-0.961271	2.087138	0.795938
C	-1.03282	1.73861	-0.852113	C	-0.703479	3.068273	1.822066
C	-1.043278	2.787124	0.249334	C	-0.226862	2.462569	3.133442
H	-0.000551	1.451187	-1.056132	H	0.053297	3.770486	1.468774
H	-1.456541	2.175544	-1.757458	H	-1.60788	3.647947	2.022347
O	-1.615423	2.680188	1.307306	O	-0.215488	1.282838	3.398981
O	-0.325195	3.856869	-0.119211	O	0.161229	3.424842	3.986159
H	-0.347025	4.511511	0.59767	H	0.432133	3.010556	4.821455
H	-2.866183	-3.077922	1.595749	H	-4.400171	3.148776	2.143967
				O	-5.126596	1.147115	-0.603282
				H	-0.183216	1.814128	0.210919
				H	-4.891514	-1.671007	0.426325

Asn-His

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.632554	-2.881646	2.741376	N	-1.417365	-3.019279	2.131476
H	-1.608939	-2.285599	3.564134	H	-0.874489	-2.6139	2.888884
C	-2.11161	-2.148907	1.583182	C	-2.212113	-1.98238	1.483029
H	-2.227621	-2.863807	0.761761	H	-2.6897	-2.414231	0.600789
C	-3.403518	-1.307138	1.705877	C	-3.32223	-1.382522	2.38423
C	-1.070883	-1.140464	1.079244	C	-1.267528	-0.851354	1.052184
H	-4.290462	-1.786311	1.291816	H	-3.839528	-2.203323	2.893753
H	-3.611568	-1.05621	2.750159	H	-2.883517	-0.757207	3.168322
C	-3.107548	-0.019545	0.972856	C	-4.38922	-0.603436	1.640741
O	0.12824	-1.285303	0.997263	O	-0.277315	-0.559726	1.717495
O	-3.867005	0.885134	0.690565	O	-5.264171	0.082992	2.398976
N	-1.748901	0.008173	0.678684	N	-1.63822	-0.191459	-0.07159
C	-1.095692	1.134099	0.024166	C	-1.008853	1.044375	-0.504952
H	-0.022289	0.959061	0.144273	H	-0.101273	1.157332	0.093035
C	-1.443667	1.194212	-1.481278	C	-0.643711	0.990081	-2.002053
C	-1.402162	2.43637	0.766328	C	-1.916203	2.229551	-0.155285
H	-1.478968	0.164526	-1.841251	H	-0.208468	0.006061	-2.184006
H	-2.44581	1.613882	-1.594587	H	-1.559355	1.056521	-2.597544
C	-0.449924	1.926877	-2.321704	C	0.351371	2.013468	-2.444222
O	-1.627156	3.495881	0.226006	O	-2.279289	3.085134	-0.933569
N	-0.262303	3.292084	-2.291509	N	0.08062	3.359844	-2.566322
C	0.436064	1.473294	-3.272596	C	1.66812	1.887156	-2.825342
H	-0.739395	3.918228	-1.657306	H	-0.801569	3.78929	-2.324177
C	0.70377	3.602452	-3.194325	C	1.21065	3.978064	-2.997917
N	1.150992	2.523514	-3.813931	N	2.197434	3.115475	-3.170093
H	0.585281	0.453983	-3.595286	H	2.251223	0.979973	-2.874469
H	1.039613	4.614662	-3.356756	H	1.258796	5.042347	-3.167334
O	-1.335228	2.28156	2.092474	O	-2.27469	2.212284	1.134571
H	-1.511003	3.137525	2.516067	H	-2.852347	2.973033	1.309066
H	-2.262202	-3.649416	2.949864	H	-2.022437	-3.728508	2.533037
				O	-4.521157	-0.585949	0.436556
				H	-2.535882	-0.433272	-0.47269
				H	-5.062508	-0.001523	3.341819
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.832738	-4.186777	0.82438	N	-1.86303	-4.022643	0.038337
H	-2.129082	-3.947429	1.76656	H	-1.694766	-3.990928	1.040076
C	-2.03303	-3.06687	-0.079173	C	-2.28436	-2.7082	-0.432485
H	-1.800736	-3.411607	-1.092688	H	-2.323952	-2.725416	-1.523926
C	-3.395265	-2.343643	-0.092314	C	-3.675801	-2.266951	0.092528
C	-1.037974	-1.933481	0.188474	C	-1.249984	-1.672716	0.025266
H	-4.060673	-2.650529	-0.89877	H	-4.370462	-3.108348	-0.009559
H	-3.922211	-2.487631	0.855697	H	-3.623837	-2.032529	1.160016
C	-3.064358	-0.87179	-0.212835	C	-4.300354	-1.109852	-0.661374
O	0.131603	-2.03554	0.490011	O	-0.641628	-1.796942	1.08741
O	-3.833399	0.038388	-0.436184	O	-5.389993	-0.551346	-0.103585

N	-1.693822	-0.718545	-0.007277	N	-1.102294	-0.598627	-0.781585
C	-0.978063	0.548743	0.085226	C	-0.400558	0.586691	-0.327786
H	0.074075	0.261416	0.142787	H	0.599472	0.295805	-0.001707
C	-1.157316	1.478109	-1.166639	C	-0.271206	1.61286	-1.488833
C	-1.280899	1.218296	1.420512	C	-1.121411	1.178228	0.886198
H	-1.586874	0.833212	-1.939426	H	0.083621	1.016767	-2.338652
C	-2.118176	2.655787	-0.942902	C	-1.622688	2.241103	-1.865001
C	0.226794	1.943331	-1.660679	C	0.804613	2.672746	-1.189347
O	-2.136974	0.879411	2.202805	O	-2.298762	1.040921	1.127627
H	-1.657512	3.424758	-0.317275	H	-1.962606	2.930523	-1.085813
H	-2.376796	3.114855	-1.898866	H	-1.536383	2.80411	-2.795564
H	-3.044356	2.323995	-0.473989	H	-2.406443	1.493038	-2.007969
H	0.698441	2.546138	-0.875846	H	0.465267	3.317539	-0.372547
H	0.86079	1.06031	-1.800883	H	1.706294	2.165701	-0.828648
C	0.185965	2.736779	-2.970096	C	1.170528	3.531192	-2.405274
H	-0.327848	3.694056	-2.852271	H	0.33015	4.144063	-2.741089
H	1.199606	2.94746	-3.321975	H	1.99405	4.207983	-2.161798
H	-0.330436	2.172598	-3.754088	H	1.487982	2.906295	-3.246681
O	-0.437635	2.240729	1.634929	O	-0.289187	1.90199	1.652532
H	-0.662861	2.655786	2.483224	H	-0.800376	2.288935	2.3819
H	-2.400288	-4.974045	0.52818	H	-2.592293	-4.708783	-0.128236
				O	-3.913221	-0.692226	-1.731172
				H	-1.768069	-0.500207	-1.536546
				H	-5.60066	-0.95679	0.749557

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.044941	-3.946433	0.845242	N	-1.781728	-4.217354	0.481162
H	-2.475247	-3.77977	1.750635	H	-1.76226	-4.095772	1.490013
C	-2.321054	-2.85122	-0.068133	C	-2.479214	-3.094917	-0.137128
H	-1.945406	-3.139335	-1.055694	H	-2.373333	-3.174511	-1.221159
C	-3.772621	-2.337774	-0.208634	C	-3.99216	-3.032507	0.195258
C	-1.528837	-1.589513	0.299123	C	-1.822476	-1.795861	0.345575
H	-4.291967	-2.7001	-1.095641	H	-4.416286	-4.036993	0.08666
H	-4.370453	-2.607751	0.666788	H	-4.142729	-2.742262	1.239714
C	-3.657353	-0.830968	-0.242556	C	-4.801623	-2.129009	-0.713537
O	-0.379534	-1.517381	0.675951	O	-1.364179	-1.6918	1.482852
O	-4.524043	-0.012723	-0.477349	O	-6.070825	-1.885965	-0.336558
N	-2.35257	-0.488787	0.089477	N	-1.828434	-0.769828	-0.533615
C	-1.883283	0.889557	0.20361	C	-1.472383	0.573182	-0.114828
H	-0.922704	0.814107	0.720938	H	-0.474209	0.550616	0.322459
C	-1.697516	1.553247	-1.168639	C	-1.50342	1.508541	-1.339959
C	-2.793966	1.687723	1.137928	C	-2.443988	1.059242	0.962271
H	-1.310281	0.790865	-1.852888	H	-0.837354	1.068984	-2.091016
H	-2.679187	1.852868	-1.542041	H	-2.51672	1.485687	-1.757261
C	-0.73653	2.757029	-1.171352	C	-1.08791	2.968933	-1.094386
O	-3.158303	2.822233	0.94099	O	-3.616517	0.766129	1.01532
H	-1.042896	3.439777	-0.372107	H	-1.75774	3.399255	-0.340964
C	0.71743	2.331166	-0.919991	C	0.352871	3.086773	-0.577937

C	-0.853559	3.505386	-2.50597	C	-1.265553	3.770257	-2.391992
H	1.062197	1.653842	-1.70948	H	1.053865	2.626432	-1.283468
H	1.378025	3.202904	-0.913064	H	0.634106	4.13767	-0.464277
H	0.84454	1.818731	0.037797	H	0.482511	2.604993	0.393905
H	-1.873751	3.864012	-2.672733	H	-2.296759	3.72008	-2.754568
H	-0.182069	4.368663	-2.530661	H	-1.012186	4.822726	-2.236083
H	-0.585959	2.84935	-3.342345	H	-0.611504	3.381268	-3.180561
H	-2.443261	-4.806554	0.483379	H	-2.268652	-5.086551	0.286601
O	-3.092447	0.993667	2.248761	O	-1.846862	1.889244	1.832519
H	-3.648322	1.549423	2.818191	H	-2.513356	2.208295	2.462644
				O	-4.398986	-1.652425	-1.752038
				H	-2.393687	-0.876133	-1.366512
				H	-6.279259	-2.311836	0.507203

Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.527467	-3.317575	2.309417	N	-3.56232	-1.024615	1.154042
H	-0.582599	-3.625467	2.524519	H	-3.567454	-0.42178	1.971603
C	-1.52341	-2.606373	1.033971	C	-2.486962	-2.014094	1.261501
H	-1.199234	-3.228307	0.186068	H	-2.390262	-2.449427	2.262263
C	-2.859372	-1.93023	0.691177	C	-2.749027	-3.162155	0.262455
C	-0.530058	-1.448626	1.089698	C	-1.123207	-1.389433	0.940208
H	-3.422781	-2.420716	-0.102008	H	-3.747666	-3.564475	0.456274
H	-3.498184	-1.863502	1.576274	H	-2.720378	-2.789532	-0.761898
C	-2.491478	-0.521313	0.276591	C	-1.787973	-4.314613	0.445166
O	0.608952	-1.489366	1.505763	O	-0.075313	-1.957797	1.253977
O	-3.20829	0.335017	-0.197677	O	-1.069788	-4.57139	-0.662439
N	-1.142282	-0.324542	0.5583	N	-1.152683	-0.22585	0.266175
C	-0.461511	0.947185	0.360266	C	0.058388	0.457365	-0.135174
H	0.536419	0.807646	0.79043	H	0.693657	-0.23407	-0.69409
C	-0.323334	1.303618	-1.13399	C	-0.301225	1.664542	-1.021226
C	-1.136683	1.998611	1.247535	C	0.843846	0.912368	1.096966
H	-0.222008	0.360411	-1.678153	H	-0.919095	1.28608	-1.841736
H	-1.242517	1.777113	-1.484153	H	-0.920842	2.356725	-0.440588
C	0.891896	2.185525	-1.439328	C	0.912813	2.400463	-1.594329
O	-1.684319	1.74285	2.294189	O	0.348538	1.32704	2.118862
H	0.830468	3.119658	-0.875795	H	1.514715	2.824026	-0.784642
H	1.802478	1.671216	-1.110897	H	1.555444	1.688727	-2.12404
C	0.993885	2.497094	-2.93693	C	0.49088	3.520844	-2.552249
H	1.044589	1.563037	-3.50748	H	-0.090226	3.099574	-3.379903
H	0.093534	3.028989	-3.263884	H	-0.157067	4.232393	-2.028692
C	2.223102	3.344149	-3.234229	C	1.70998	4.248577	-3.101305
H	2.183735	4.309876	-2.730286	H	2.280813	4.739429	-2.313187
H	3.145829	2.836619	-2.952826	H	2.370903	3.578054	-3.650185
N	2.333211	3.637728	-4.710678	N	1.303228	5.331727	-4.070293
H	1.505676	4.127659	-5.057866	H	0.695002	6.022731	-3.625476
H	3.144592	4.224214	-4.915909	H	2.116437	5.831499	-4.435304
H	2.431772	2.778751	-5.256249	H	0.796562	4.947019	-4.8707
H	-2.092055	-4.158054	2.227942	H	-4.467846	-1.482181	1.129479

O	-1.008493	3.2388	0.760345	O	2.168764	0.843196	0.888216
H	-1.410157	3.859243	1.390192	H	2.624148	1.194339	1.670823
				O	-1.686345	-4.965311	1.462467
				H	-2.06277	0.180571	0.089213
				H	-0.488717	-5.328012	-0.48016
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.672857	-4.463812	-1.137311	N	-2.098986	-4.572427	-0.971069
H	-0.689856	-4.629942	-0.939997	H	-2.868846	-4.49467	-1.629578
C	-2.158759	-3.305052	-0.408682	C	-2.034084	-3.364859	-0.153879
H	-3.240459	-3.241791	-0.567454	H	-3.017298	-3.198162	0.29111
C	-1.860928	-3.189781	1.104425	C	-1.018025	-3.578266	0.984732
C	-1.600304	-1.998203	-0.986831	C	-1.623654	-2.117851	-0.963633
H	-2.702794	-3.449366	1.746161	H	-1.159355	-4.58938	1.381301
H	-1.013644	-3.82031	1.388886	H	0.0069	-3.533412	0.602017
C	-1.459329	-1.749059	1.32116	C	-1.165739	-2.623803	2.151096
O	-1.451726	-1.704768	-2.152435	O	-0.20433	-2.680938	3.090264
O	-1.257703	-1.169498	2.369304	O	-2.089744	-1.855612	2.307835
N	-1.308455	-1.149021	0.076495	N	-2.075372	-0.932189	-0.494313
C	-0.879773	0.234208	-0.099954	C	-1.558101	0.318434	-1.013664
H	-0.635035	0.323683	-1.163537	H	-1.699516	0.342083	-2.095684
C	-1.996376	1.226132	0.263033	C	-2.320506	1.490213	-0.362793
C	0.425575	0.491528	0.656813	C	-0.055353	0.420258	-0.73676
H	-2.934399	0.809876	-0.113515	H	-3.385485	1.306062	-0.53137
H	-2.075777	1.29228	1.349953	H	-2.151303	1.468144	0.71888
C	-1.769047	2.608499	-0.3496	C	-1.937151	2.858046	-0.926425
O	0.664356	1.489607	1.293346	O	0.501354	-0.059779	0.223189
H	-0.834389	3.043152	0.006472	H	-0.897292	3.10347	-0.702729
H	-1.733579	2.542123	-1.440929	H	-2.068411	2.878626	-2.011565
S	-3.1433	3.732644	0.115732	S	-3.001795	4.156562	-0.185581
C	-2.58003	5.245684	-0.738035	C	-2.274692	5.62162	-0.997916
H	-2.513671	5.074857	-1.814186	H	-2.377566	5.547854	-2.082151
H	-3.321945	6.020585	-0.540277	H	-2.826937	6.491994	-0.641016
H	-1.61111	5.564826	-0.349438	H	-1.222129	5.725275	-0.727738
O	1.304318	-0.506263	0.476141	O	0.572321	1.144021	-1.677142
H	2.121854	-0.287185	0.951555	H	1.508958	1.225238	-1.433271
H	-2.177644	-5.293445	-0.843544	H	-1.257273	-4.636049	-1.539761
				O	-0.903795	-2.205614	-1.957304
				H	-2.486375	-0.931185	0.431546
				H	0.479295	-3.327566	2.863885
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.393587	-3.480604	0.938172	N	-1.521044	-3.09535	0.970608
H	-1.376603	-3.260584	1.93001	H	-1.364675	-2.8086	1.931356
C	-1.720368	-2.304956	0.151224	C	-2.072722	-2.010833	0.172038
H	-1.841272	-2.625052	-0.889284	H	-2.064382	-2.326985	-0.873829
C	-2.936782	-1.440358	0.556198	C	-3.549647	-1.596008	0.474819

C	-0.561891	-1.299473	0.116945	C	-1.15944	-0.794841	0.347522
H	-3.835201	-1.628358	-0.031262	H	-3.872093	-0.849675	-0.251992
H	-3.186284	-1.584073	1.611622	H	-4.174434	-2.484982	0.348755
C	-2.479035	-0.010286	0.38101	C	-3.772898	-1.006655	1.851865
O	0.623778	-1.532835	0.030001	O	-0.764179	-0.458458	1.462764
O	-3.140053	1.006948	0.435911	O	-3.741411	-1.861834	2.898891
N	-1.106052	-0.020519	0.162903	N	-0.842302	-0.109802	-0.77078
C	-0.312756	1.190954	0.021133	C	-0.028864	1.090604	-0.719777
H	0.728118	0.853863	0.006379	H	0.87807	0.882353	-0.14989
C	-0.626039	1.928057	-1.303659	C	0.345986	1.520463	-2.157569
C	-0.448602	2.015846	1.304206	C	-0.78266	2.221378	-0.016457
H	-0.809779	1.148531	-2.048438	H	0.829892	0.661233	-2.630323
H	-1.552829	2.490758	-1.193463	H	-0.575476	1.727814	-2.709436
C	0.49362	2.820929	-1.793545	C	1.262809	2.720914	-2.198416
O	-0.619056	1.528593	2.397622	O	-1.956725	2.462648	-0.175945
C	0.322447	4.204859	-1.898022	C	0.76149	3.997465	-2.47539
C	1.720914	2.265623	-2.180233	C	2.630619	2.575503	-1.933781
H	-0.620196	4.648677	-1.597675	H	-0.295429	4.123718	-2.686003
C	1.352288	5.018856	-2.374246	C	1.606908	5.109109	-2.482098
C	2.75528	3.074741	-2.65129	C	3.478403	3.683123	-1.939218
H	1.868396	1.191697	-2.119552	H	3.033455	1.58974	-1.724026
H	1.200496	6.089944	-2.448607	H	1.202663	6.091288	-2.699685
C	2.573811	4.456653	-2.749796	C	2.967716	4.955027	-2.212286
H	3.697556	2.626846	-2.946553	H	4.535243	3.553692	-1.734729
H	3.375172	5.087155	-3.118051	H	3.625894	5.816381	-2.218851
O	-0.3045	3.327302	1.088123	O	0.028976	2.947824	0.764598
H	-0.350468	3.785833	1.942977	H	-0.478545	3.688816	1.134258
H	-2.102552	-4.19415	0.805535	H	-2.109621	-3.920737	0.950218
				O	-3.976775	0.166017	2.063711
				H	-1.227686	-0.398302	-1.657509
				H	-3.613878	-2.774866	2.607007

Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.12055	-3.26675	1.227952	N	-0.283399	-3.3178	1.068972
H	-0.78307	-2.9773	2.14175	H	0.111917	-2.860018	1.885983
C	-1.373278	-2.11562	0.379721	C	-1.269082	-2.453652	0.407181
H	-1.839606	-2.477591	-0.542833	H	-1.754769	-3.043985	-0.370054
C	-2.206095	-0.938018	0.938402	C	-2.356452	-1.913477	1.354894
C	-0.06846	-1.448872	-0.075317	C	-0.493464	-1.374107	-0.364015
H	-3.245497	-0.929449	0.611007	H	-2.875505	-2.764899	1.808474
H	-2.196484	-0.935261	2.032339	H	-1.924865	-1.355156	2.193226
C	-1.492471	0.308609	0.469325	C	-3.392509	-1.049289	0.665022
O	0.964133	-1.985492	-0.409914	O	-0.194158	-1.525128	-1.54609
O	-1.854771	1.464864	0.548881	O	-3.412589	-0.823792	-0.522393
N	-0.272029	-0.072129	-0.0776	N	-0.120198	-0.279638	0.339559
C	0.722821	0.885297	-0.526933	C	0.664029	0.782357	-0.25243
H	1.593499	0.295253	-0.831475	H	1.408318	0.359314	-0.931997
C	0.251382	1.675659	-1.759743	C	-0.243036	1.733846	-1.083191

C	1.180612	1.724353	0.669783	C	1.381401	1.531231	0.854872
H	-0.415055	1.027443	-2.339203	H	-0.872282	1.10052	-1.708168
H	-0.303702	2.565655	-1.457652	H	-0.890219	2.306031	-0.407309
O	1.410002	2.012579	-2.517238	O	0.481666	2.576454	-1.960944
O	1.175449	1.319684	1.809095	O	1.205076	1.354154	2.038702
H	1.192092	2.743634	-3.105094	H	1.038346	3.16831	-1.440097
O	1.624184	2.933212	0.310392	O	2.218424	2.455908	0.357038
H	1.93224	3.394929	1.107322	H	2.616796	2.949669	1.092844
H	-1.982	-3.780727	1.379856	H	-0.732044	-4.16673	1.400015
				O	-4.350009	-0.514868	1.451404
				H	-0.32304	-0.19578	1.324899
				H	-4.231882	-0.764035	2.378985
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.294208	-3.991687	-0.404589	N	-0.815212	-1.793149	2.039587
H	-1.902524	-3.96673	0.532928	H	-1.449392	-1.727467	2.829978
C	-2.524657	-2.647733	-0.90472	C	-1.553973	-2.24014	0.858203
H	-3.048826	-2.73406	-1.862772	H	-0.815791	-2.508683	0.094921
C	-3.266181	-1.629693	-0.013354	C	-2.455357	-3.474333	1.047974
C	-1.21492	-1.928651	-1.242377	C	-2.379203	-1.076184	0.279833
H	-4.323749	-1.512801	-0.248864	H	-2.841932	-3.802377	0.080967
H	-3.182908	-1.902554	1.042838	H	-1.845488	-4.290989	1.448343
C	-2.536531	-0.317511	-0.205725	C	-3.596415	-3.256416	2.021322
O	-0.214152	-2.402521	-1.734306	O	-3.594729	-1.179231	0.106314
O	-2.86161	0.772406	0.207566	O	-3.534786	-2.556571	3.008413
N	-1.363762	-0.580615	-0.920741	N	-1.720673	0.058062	-0.051168
C	-0.323664	0.391596	-1.227908	C	-0.310565	0.348764	0.057566
H	0.570222	-0.206178	-1.439741	H	0.28604	-0.549726	-0.086
C	-0.590328	1.21317	-2.501368	C	0.092962	1.366624	-1.049679
C	0.053363	1.173458	0.031273	C	0.045627	0.942608	1.415201
H	0.288952	1.852572	-2.637321	H	1.124201	1.677279	-0.85028
C	-0.755216	0.319311	-3.728748	C	0.001375	0.757284	-2.439712
O	-1.748479	2.017819	-2.286435	O	-0.777681	2.501546	-1.026551
O	0.012785	0.705004	1.144435	O	-0.70329	1.605231	2.097491
H	-1.628471	-0.32872	-3.623307	H	-1.019172	0.431916	-2.653893
H	-0.896638	0.940954	-4.616366	H	0.294861	1.499687	-3.184202
H	0.13014	-0.301732	-3.88421	H	0.668621	-0.103476	-2.521737
H	-1.899471	2.544998	-3.079491	H	-0.650688	2.993249	-0.205452
H	-3.17469	-4.492025	-0.342683	H	-0.100133	-2.471667	2.280253
O	0.530517	2.393319	-0.244786	O	1.341553	0.747177	1.706526
H	0.829226	2.797728	0.585883	H	1.546047	1.2107	2.534492
				O	-4.732074	-3.946709	1.788515
				H	-2.304278	0.821451	-0.370126
				H	-4.673304	-4.447724	0.963563
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.064645	-2.673648	2.405632	N	-1.669844	-2.831264	2.128843

H	-1.603765	-2.408274	3.225236	H	-1.785647	-2.366705	3.023411
C	-1.655213	-2.12503	1.196973	C	-2.53812	-2.258512	1.110881
H	-1.106215	-2.535788	0.343184	H	-2.239315	-2.671019	0.144179
C	-3.172779	-2.299806	0.955747	C	-4.067724	-2.556737	1.241309
C	-1.447761	-0.60763	1.103114	C	-2.318369	-0.743241	1.111521
H	-3.424229	-3.087413	0.245559	H	-4.590107	-2.156796	0.371682
H	-3.698947	-2.509166	1.89148	H	-4.193869	-3.643335	1.242148
C	-3.649731	-0.959328	0.445413	C	-4.728485	-1.967786	2.470061
O	-0.449221	0.024275	1.370669	O	-2.267629	-0.113594	2.167401
O	-4.738196	-0.666475	-0.007289	O	-5.49341	-1.031639	2.446909
N	-2.617584	-0.04302	0.60476	N	-2.217835	-0.145977	-0.093604
C	-2.72507	1.368287	0.251473	C	-2.067479	1.291855	-0.220435
H	-1.875789	1.849447	0.744549	H	-1.24235	1.621202	0.412368
C	-2.630216	1.600811	-1.27214	C	-1.776886	1.651287	-1.697961
C	-3.977628	1.987762	0.871921	C	-3.335205	2.010436	0.241657
H	-1.934131	0.851413	-1.661998	H	-0.89212	1.078559	-1.995827
H	-3.603153	1.409526	-1.726222	H	-2.614813	1.302689	-2.309104
C	-2.137543	2.972121	-1.615955	C	-1.553298	3.113299	-1.921102
O	-4.739803	2.725661	0.29677	O	-4.459212	1.649729	-0.022219
C	-2.84353	3.998313	-2.19439	C	-2.406561	3.988584	-2.549108
C	-0.803103	3.470107	-1.392913	C	-0.41768	3.887523	-1.489792
H	-3.875997	4.02942	-2.504127	H	-3.364542	3.800858	-3.008661
N	-2.030746	5.102164	-2.347634	N	-1.871644	5.258734	-2.534449
C	-0.773615	4.812589	-1.864908	C	-0.652574	5.231783	-1.893788
C	0.365572	2.911883	-0.844717	C	0.772081	3.577795	-0.808393
H	-2.315953	5.979676	-2.750754	H	-2.301033	6.07236	-2.943953
C	0.38081	5.598873	-1.803247	C	0.261593	6.258172	-1.636928
C	1.515452	3.691516	-0.780845	C	1.683876	4.595062	-0.550096
H	0.368679	1.893433	-0.471414	H	0.978077	2.561282	-0.49133
H	0.384794	6.619311	-2.168877	H	0.065741	7.276007	-1.95381
C	1.522584	5.021429	-1.255402	C	1.429945	5.9223	-0.960021
H	2.423585	3.274798	-0.359531	H	2.605735	4.369561	-0.025816
H	2.43467	5.604197	-1.191763	H	2.159704	6.694407	-0.74381
O	-4.096035	1.65601	2.168841	O	-3.05381	3.120802	0.937958
H	-4.890651	2.085417	2.524328	H	-3.88751	3.570689	1.152011
H	-1.069979	-3.687382	2.363719	H	-1.810964	-3.829537	2.236499
				O	-4.437572	-2.541627	3.659181
				H	-2.309635	-0.69911	-0.932717
				H	-3.844872	-3.298019	3.550784
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.579584	-2.315952	1.207972	N	-3.325767	-0.106811	-1.56427
H	-2.246775	-2.335684	1.974242	H	-2.409136	-0.416284	-1.875231
C	-1.801176	-1.159839	0.358071	C	-3.474483	-0.258029	-0.118774
H	-1.136523	-1.24965	-0.508149	H	-4.518603	-0.02158	0.115528
C	-3.231694	-0.85065	-0.137285	C	-3.233239	-1.676304	0.455372
C	-1.370828	0.14433	1.040284	C	-2.659493	0.822288	0.614003
H	-3.438098	-1.189674	-1.152055	H	-3.474941	-1.667818	1.521597

H	-3.980034	-1.292227	0.527412	H	-3.916742	-2.360035	-0.046363
C	-3.360957	0.652949	-0.047622	C	-1.82936	-2.232707	0.286293
O	-0.39997	0.329931	1.740413	O	-2.095981	0.594048	1.696344
O	-4.235536	1.35988	-0.505034	O	-1.562491	-3.154138	-0.459889
N	-2.281169	1.134969	0.684751	N	-2.64666	2.018128	0.012328
C	-2.087977	2.537982	1.007674	C	-1.844448	3.132522	0.462686
H	-1.195964	2.573462	1.641207	H	-1.492812	2.905873	1.46944
C	-1.827023	3.398477	-0.255454	C	-0.611537	3.360136	-0.464056
C	-3.233104	3.027346	1.891754	C	-2.688633	4.395734	0.518502
H	-2.739786	3.437684	-0.850678	H	-0.971052	3.663711	-1.451738
H	-1.604516	4.411715	0.080785	H	-0.036443	4.192683	-0.053385
C	-0.682333	2.842321	-1.068575	C	0.235196	2.116426	-0.573192
O	-3.977454	2.307755	2.514654	O	-3.762206	4.540411	-0.019755
C	-0.915042	1.979955	-2.144663	C	0.06838	1.222986	-1.636032
C	0.646448	3.127767	-0.728326	C	1.166735	1.791064	0.421126
H	-1.933983	1.744822	-2.433195	H	-0.641208	1.45319	-2.423493
C	0.13876	1.410354	-2.860244	C	0.796106	0.034892	-1.707339
C	1.709847	2.569967	-1.432343	C	1.901992	0.61085	0.364755
H	0.855886	3.795426	0.101274	H	1.315858	2.466547	1.257258
H	-0.062817	0.743896	-3.692465	H	0.649276	-0.647871	-2.537663
C	1.45599	1.704776	-2.500588	C	1.710695	-0.274872	-0.699029
H	2.735545	2.796537	-1.166592	H	2.61853	0.362186	1.138486
O	2.53781	1.182386	-3.156607	O	2.447495	-1.42761	-0.697852
H	2.244932	0.602454	-3.8699	H	2.215734	-1.969194	-1.461983
H	-1.716601	-3.168413	0.675153	H	-4.015408	-0.668248	-2.052348
O	-3.277068	4.366377	1.941425	O	-2.065453	5.359943	1.21356
H	-3.982322	4.627409	2.555708	H	-2.608847	6.16429	1.187283
				O	-0.872181	-1.670081	1.029011
				H	-3.076649	2.060385	-0.903869
				H	-1.236493	-0.868455	1.483825
Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.121495	-4.32416	-0.054759	N	-2.07841	-1.816651	2.622999
H	-0.850217	-4.173554	0.912926	H	-2.522878	-0.904955	2.579081
C	-1.678691	-3.111766	-0.6288	C	-2.034053	-2.441025	1.296383
H	-2.054206	-3.358535	-1.627878	H	-1.702758	-3.47007	1.438848
C	-2.770523	-2.345053	0.144707	C	-3.387094	-2.538236	0.548208
C	-0.605377	-2.044865	-0.866293	C	-0.896576	-1.812601	0.47081
H	-3.787604	-2.550966	-0.187479	H	-3.237244	-2.939074	-0.461217
H	-2.713169	-2.560498	1.215957	H	-4.011443	-3.268422	1.074363
C	-2.439797	-0.880593	-0.045334	C	-4.195454	-1.263895	0.422851
O	0.532239	-2.215541	-1.248227	O	0.108353	-2.465825	0.179763
O	-3.135064	0.071378	0.237449	O	-3.810173	-0.151805	0.72294
N	-1.164487	-0.79431	-0.602391	N	-1.044482	-0.523976	0.108552
C	-0.410828	0.432099	-0.837413	C	-0.028613	0.176995	-0.649216
H	0.487635	0.099365	-1.361753	H	0.236156	-0.420215	-1.525073
C	-1.145012	1.470788	-1.756922	C	-0.574929	1.548592	-1.13475
C	0.086994	0.997884	0.487132	C	1.242042	0.332258	0.186536

H	-1.943638	0.9014	-2.240431	H	-1.521274	1.30379	-1.63114
C	-1.784011	2.651843	-1.012262	C	-0.869281	2.5224	0.015496
C	-0.188128	1.973876	-2.847158	C	0.346975	2.190578	-2.178453
O	-0.24416	0.619966	1.585715	O	1.277611	0.459616	1.38861
H	-1.019451	3.321957	-0.610576	H	0.052368	2.825174	0.520583
H	-2.395526	3.229864	-1.71015	H	-1.347922	3.422293	-0.378618
H	-2.422987	2.313492	-0.19715	H	-1.536572	2.095371	0.768386
H	0.202308	1.148552	-3.449436	H	0.550837	1.507543	-3.007483
H	-0.708075	2.665844	-3.515019	H	-0.126042	3.087882	-2.585231
H	0.658565	2.505744	-2.403239	H	1.303757	2.485063	-1.739551
H	-1.821946	-5.058243	-0.053591	H	-2.636441	-2.385914	3.252246
O	0.982575	1.975238	0.27363	O	2.340332	0.349522	-0.5891
H	1.271506	2.323803	1.13249	H	3.113576	0.499717	-0.021429
				O	-5.441703	-1.398514	-0.059243
				H	-1.903652	-0.049564	0.360052
				H	-5.651291	-2.321533	-0.262442

Table S14.D. Succinimide Hydrolysis into iso-Asp-X XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions							
H_2O							
Reactant Structure							
Atom	X	Y	Z				
O	-0.999631	0.482902	0				
H	-0.03661	0.526297	0				
H	-1.280189	1.405171	0				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.042902	-2.775176	1.359843	N	-2.774077	-1.945286	2.227494
H	-0.736188	-2.253319	2.176226	H	-2.470263	-2.76505	2.745084
C	-1.904821	-1.960734	0.520089	C	-1.975601	-1.802483	1.015333
H	-2.289833	-2.60121	-0.280449	H	-2.060743	-2.715576	0.424291
C	-3.081068	-1.196656	1.168428	C	-2.52706	-0.63359	0.171593
C	-1.116766	-0.859026	-0.199821	C	-0.490829	-1.563833	1.305348
H	-4.052559	-1.6718	1.032706	H	-3.617182	-0.723886	0.182235
H	-2.918291	-1.06206	2.241714	H	-2.27381	0.311078	0.648104
C	-3.069578	0.171844	0.524872	C	-2.109575	-0.693841	-1.289993
O	-0.015218	-0.942138	-0.698557	O	0.29491	-1.916204	0.275593
O	-3.894511	1.056175	0.631215	O	-2.093747	-1.771561	-1.887385
N	-1.902406	0.288036	-0.224191	N	-1.806828	0.454668	-1.949688
C	-1.504711	1.5079	-0.912134	C	-1.79506	1.839753	-1.501743
H	-0.505306	1.305213	-1.310538	H	-1.479691	2.420236	-2.373083
C	-2.444024	1.855738	-2.072693	C	-3.172798	2.383796	-1.078358
C	-1.298399	2.621602	0.114935	C	-0.703053	2.100344	-0.46103
H	-3.444149	2.088802	-1.70865	H	-3.543361	1.906336	-0.171203
H	-2.054195	2.712883	-2.620564	H	-3.110101	3.457443	-0.900559

H	-2.501534	1.003354	-2.751868	H	-3.885619	2.200231	-1.883686
O	-1.10025	2.440047	1.293432	O	0.037912	1.269372	0.008275
H	-1.555907	-3.581316	1.701205	H	-2.609688	-1.152429	2.843214
O	-1.298401	3.832155	-0.460924	O	-0.651163	3.404098	-0.141619
H	-1.10317	4.49529	0.220986	H	0.060992	3.534883	0.505103
				O	-0.06138	-1.103274	2.340234
				H	-1.574626	0.302174	-2.921281
				H	1.209499	-1.672581	0.491843
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.617216	-4.351801	1.003787	N	-3.606785	-4.693253	1.703665
H	-2.349071	-4.282302	1.981622	H	-4.536768	-4.286267	1.754508
C	-2.660843	-3.038532	0.383934	C	-2.595305	-3.640389	1.580995
H	-3.06396	-3.161739	-0.626596	H	-1.626376	-4.119601	1.434718
C	-3.420004	-1.895512	1.097852	C	-2.856021	-2.651814	0.412661
C	-1.25322	-2.463758	0.179004	C	-2.504652	-2.920304	2.921816
H	-4.402568	-1.681585	0.67746	H	-2.952189	-3.238931	-0.503155
H	-3.548962	-2.112474	2.162073	H	-3.798196	-2.129265	0.58904
C	-2.522033	-0.685894	0.977264	C	-1.759398	-1.610878	0.299503
O	-0.259879	-3.046354	-0.196158	O	-3.675472	-2.355466	3.263284
O	-2.759279	0.465721	1.281809	O	-1.516915	-2.877195	3.619458
N	-1.297393	-1.103796	0.47051	N	-0.860238	-1.784852	-0.695541
C	-0.162598	-0.209091	0.26998	C	0.266837	-0.882698	-0.895623
H	0.695195	-0.870475	0.109446	H	0.949428	-1.400632	-1.57689
C	-0.354243	0.695797	-0.955326	C	-0.152785	0.455929	-1.523263
C	0.140664	0.568644	1.552825	C	1.059906	-0.699122	0.404418
H	-0.822558	0.089896	-1.735949	H	-0.90846	0.231039	-2.281065
H	-1.050242	1.498573	-0.701782	H	-0.630423	1.071892	-0.757993
C	0.965572	1.268841	-1.479703	C	1.009653	1.210919	-2.174742
O	0.434795	1.739449	1.591353	O	1.498681	0.35462	0.803765
H	1.452887	1.853343	-0.695212	H	1.783197	1.421779	-1.432664
H	1.64068	0.451199	-1.75445	H	1.458395	0.589126	-2.957954
C	0.730656	2.154601	-2.701281	C	0.528444	2.523028	-2.789269
H	0.266324	1.569929	-3.500754	H	-0.243255	2.323441	-3.540486
H	0.058849	2.980288	-2.442495	H	0.095297	3.157836	-2.009686
N	2.007692	2.68443	-3.186877	N	1.65043	3.22828	-3.416398
H	2.796101	2.649133	-2.557331	H	2.545748	2.762561	-3.431394
C	2.185742	3.301151	-4.354181	C	1.567305	4.423862	-3.997175
N	1.147427	3.530226	-5.163721	N	0.402628	5.07637	-4.035624
N	3.414197	3.683457	-4.724638	N	2.651936	4.976687	-4.555882
H	0.199954	3.441132	-4.835806	H	-0.442962	4.668505	-3.674713
H	1.281109	3.968596	-6.060812	H	0.328864	5.978033	-4.477696
H	4.228422	3.359178	-4.227999	H	3.560246	4.554307	-4.452128
H	3.56521	4.175874	-5.589779	H	2.618766	5.908064	-4.937478
H	-3.538463	-4.776235	0.979622	H	-3.586594	-5.285352	0.878784
O	0.102172	-0.226792	2.632464	O	1.282599	-1.871041	1.021187
H	0.325184	0.303548	3.414349	H	1.80737	-1.699373	1.81924
				O	-1.663863	-0.683174	1.105482

				H	-0.962992	-2.564023	-1.32629
				H	-3.575038	-1.93032	4.129819
Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.114507	-4.044523	0.700107	N	-1.136249	-4.547417	0.019377
H	-0.051479	-3.816724	1.688332	H	-0.505434	-5.172879	-0.472616
C	-0.921035	-3.065744	-0.006236	C	-0.618237	-3.183793	0.000122
H	-1.053697	-3.422118	-1.033465	H	-0.559842	-2.858825	-1.041823
C	-2.299446	-2.667906	0.570751	C	-1.61037	-2.263314	0.75457
C	-0.192996	-1.72329	-0.151065	C	0.79611	-3.009874	0.560696
H	-3.14477	-3.167045	0.0977	H	-2.610201	-2.651371	0.553724
H	-2.345563	-2.868503	1.645354	H	-1.460604	-2.343224	1.8368
C	-2.390252	-1.171545	0.377893	C	-1.675791	-0.777588	0.420142
O	0.981182	-1.533666	-0.378647	O	1.154094	-3.963906	1.423371
O	-3.348207	-0.44393	0.543205	O	-2.699096	-0.14129	0.684727
N	-1.137417	-0.710221	-0.012395	N	-0.604335	-0.191316	-0.156105
C	-0.828972	0.697604	-0.188452	C	-0.592837	1.231012	-0.446756
H	0.245085	0.751776	-0.39225	H	0.4299	1.486699	-0.736395
C	-1.571113	1.311425	-1.384231	C	-1.512481	1.598582	-1.620552
C	-1.030359	1.427347	1.140697	C	-0.844563	2.032718	0.836583
H	-1.575827	0.572864	-2.191325	H	-1.37159	0.842175	-2.398407
H	-2.608781	1.526313	-1.131871	H	-2.557988	1.56531	-1.316989
C	-0.850516	2.539971	-1.932401	C	-1.147234	2.937187	-2.250008
O	-0.912157	0.906122	2.224029	O	-0.393814	1.731779	1.917521
O	0.375609	2.636893	-1.90239	O	0.016308	3.338138	-2.29395
N	-1.641543	3.477582	-2.491381	N	-2.170521	3.624598	-2.798163
H	-1.219115	4.282971	-2.927679	H	-1.983452	4.494554	-3.273077
H	-2.644983	3.394689	-2.506062	H	-3.123499	3.305347	-2.737393
H	-0.546049	-4.960398	0.634824	H	-1.196666	-4.891775	0.973634
O	-1.29889	2.726553	0.959651	O	-1.563563	3.144951	0.621295
H	-1.363866	3.155327	1.828359	H	-1.635241	3.63118	1.458326
				O	1.524551	-2.079516	0.266325
				H	0.270863	-0.702088	-0.21786
				H	2.044112	-3.764565	1.757719
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.621989	-3.535013	-0.763109	N	-4.972912	-3.235323	-1.55686
H	-4.365086	-3.586074	0.218791	H	-4.704518	-3.809433	-2.349964
C	-4.932237	-2.167932	-1.144843	C	-5.745285	-2.081113	-2.006458
H	-5.305271	-2.186863	-2.174353	H	-6.675384	-2.456299	-2.44016
C	-5.905241	-1.345795	-0.269706	C	-6.165466	-1.176597	-0.819379
C	-3.673727	-1.291745	-1.198442	C	-5.114588	-1.185013	-3.084785
H	-6.920064	-1.285953	-0.662657	H	-7.036551	-0.59081	-1.116403
H	-5.959114	-1.752565	0.744396	H	-6.484383	-1.823742	0.002439
C	-5.288467	0.03245	-0.183902	C	-5.19826	-0.145205	-0.233583
O	-2.576708	-1.598096	-1.613673	O	-3.800846	-1.359947	-3.232753
O	-5.773522	1.044701	0.280799	O	-5.634448	0.723739	0.524773

N	-4.006056	-0.03244	-0.714432	N	-3.886372	-0.203094	-0.559018
C	-3.085339	1.096907	-0.722967	C	-2.969406	0.8946	-0.275758
H	-2.130533	0.710094	-1.092835	H	-1.974997	0.526249	-0.543232
C	-3.517481	2.221775	-1.671156	C	-3.263966	2.134671	-1.128459
C	-2.81385	1.519882	0.718351	C	-2.896703	1.129366	1.234009
H	-3.988147	1.757262	-2.543504	H	-4.25961	2.51819	-0.901933
H	-4.26236	2.867523	-1.209031	H	-2.5557	2.926921	-0.873872
C	-2.338957	3.071828	-2.211626	C	-3.161418	1.909696	-2.652732
O	-2.848003	0.767108	1.665905	O	-2.894495	0.241964	2.057091
O	-1.204415	2.529205	-2.25186	O	-2.576267	0.852052	-3.065444
O	-2.637571	4.227695	-2.610012	O	-3.636634	2.805552	-3.377069
O	-2.477138	2.812877	0.816192	O	-2.749577	2.42469	1.558525
H	-2.266479	3.002534	1.744666	H	-2.646557	2.481724	2.522132
H	-5.44121	-4.121271	-0.884234	H	-4.107307	-2.95676	-1.105996
				O	-5.759101	-0.34167	-3.677323
				H	-3.348605	-0.468444	-3.431476
				H	-3.568524	-0.847161	-1.266215
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.432049	-2.725908	0.969617	N	-3.880227	-0.757353	2.553541
H	-1.832365	-2.451721	1.74267	H	-4.060105	-1.23903	3.424933
C	-3.108095	-1.57372	0.402654	C	-3.787971	-1.628602	1.394245
H	-3.82651	-1.940339	-0.338517	H	-4.623369	-2.334162	1.445064
C	-3.823308	-0.579175	1.346956	C	-3.956411	-0.833885	0.092349
C	-2.148419	-0.682707	-0.39636	C	-2.544267	-2.537193	1.292081
H	-4.901298	-0.722604	1.416164	H	-3.95384	-1.515003	-0.76234
H	-3.409131	-0.632913	2.358147	H	-4.922643	-0.325159	0.106184
C	-3.504908	0.789583	0.791972	C	-2.838865	0.177206	-0.105084
O	-1.244294	-1.024516	-1.124914	O	-1.737526	-2.607399	2.36092
O	-3.967892	1.865328	1.112598	O	-1.816024	0.170422	0.583282
N	-2.516741	0.643473	-0.176152	N	-3.017832	1.073399	-1.101358
C	-1.913064	1.765977	-0.886047	C	-2.028735	2.09363	-1.421816
H	-1.024703	1.359066	-1.377407	H	-2.304912	2.49838	-2.398944
C	-2.871124	2.33473	-1.941602	C	-2.030431	3.231043	-0.388591
C	-1.418946	2.826426	0.100867	C	-0.636015	1.479481	-1.607632
H	-3.324877	1.50192	-2.480022	H	-3.066601	3.49655	-0.176292
H	-3.662973	2.914254	-1.470046	H	-1.559588	2.906792	0.537885
S	-2.050317	3.338175	-3.239493	S	-1.258917	4.793816	-0.966721
O	-1.572626	4.016635	-0.03768	O	0.389265	1.945655	-1.166532
H	-1.722397	4.37661	-2.450761	H	0.005781	4.339449	-1.011789
H	-3.113362	-3.379905	1.340247	H	-3.101541	-0.114401	2.637957
O	-0.741301	2.272648	1.115314	O	-0.676409	0.389229	-2.387302
H	-0.429228	2.979918	1.702755	H	0.229576	0.058665	-2.496917
				O	-2.316617	-3.220607	0.318259
				H	-3.865071	1.044703	-1.647572
				H	-2.034621	-1.976276	3.035217
Asn-Gln							
Reactant Structure				Product Structure			

Atom	X	Y	Z	Atom	X	Y	Z
N	0.013409	-4.753899	-1.071706	N	-0.323422	-4.712727	-2.511596
H	-0.082809	-5.151975	-0.141624	H	0.50575	-4.815328	-3.088762
C	-0.794998	-3.555075	-1.208139	C	-0.119569	-3.673199	-1.508852
H	-0.745118	-3.237645	-2.255145	H	0.0507	-2.728381	-2.031631
C	-2.274526	-3.590755	-0.760809	C	-1.405374	-3.542258	-0.651077
C	-0.208434	-2.379976	-0.414913	C	1.100114	-3.861031	-0.602321
H	-2.986549	-3.703385	-1.578204	H	-2.243717	-3.787777	-1.303971
H	-2.449046	-4.400706	-0.046654	H	-1.409449	-4.285552	0.153858
C	-2.500767	-2.281629	-0.039798	C	-1.754324	-2.195024	-0.027488
O	0.95757	-2.073682	-0.293995	O	1.528322	-5.12356	-0.529947
O	-3.546323	-1.811385	0.360909	O	-2.936002	-1.909791	0.186694
N	-1.26665	-1.666681	0.137048	N	-0.750863	-1.352798	0.29119
C	-1.098695	-0.413177	0.859578	C	-1.008968	-0.057357	0.903923
H	-0.01531	-0.273911	0.944266	H	-0.038797	0.301137	1.263042
C	-1.705132	0.773404	0.0864	C	-1.565679	0.963066	-0.105201
C	-1.588338	-0.617363	2.297027	C	-1.834234	-0.262728	2.183837
H	-1.541642	0.584361	-0.975614	H	-1.037136	0.803657	-1.046426
H	-2.784077	0.803294	0.244497	H	-2.622122	0.758405	-0.286877
C	-1.069234	2.119125	0.442638	C	-1.364356	2.421026	0.322708
O	-1.52148	-1.67116	2.885289	O	-1.598751	-1.129596	2.994803
H	-1.242659	2.375555	1.488262	H	-1.90138	2.639311	1.246101
H	0.017469	2.065398	0.30322	H	-0.300415	2.605016	0.515437
C	-1.563933	3.236861	-0.467458	C	-1.771366	3.38852	-0.780077
O	-1.875431	3.040051	-1.642668	O	-1.481726	3.19164	-1.961524
N	-1.612459	4.46751	0.090436	N	-2.450655	4.48836	-0.383861
H	-1.867966	5.258851	-0.480439	H	-2.70485	5.18532	-1.06743
H	-1.34819	4.632124	1.047986	H	-2.687778	4.653053	0.580626
O	-2.049601	0.511982	2.848436	O	-2.801971	0.650771	2.351549
H	-2.292852	0.327154	3.770164	H	-3.238316	0.47666	3.20101
H	-0.301236	-5.459726	-1.729158	H	-0.47534	-5.612914	-2.065138
				O	1.624393	-2.95119	0.014518
				H	0.211066	-1.666125	0.205459
				H	2.277935	-5.163165	0.086672
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.005998	-2.782859	0.877514	N	-3.212712	-2.911848	1.724475
H	-3.258324	-3.173842	1.44402	H	-2.996121	-3.480572	0.911341
C	-3.896649	-1.336286	0.8012	C	-3.979442	-1.736264	1.335434
H	-4.785031	-0.963333	0.280653	H	-4.311645	-1.230307	2.247553
C	-3.697009	-0.527333	2.103137	C	-3.166117	-0.705363	0.497849
C	-2.717064	-0.898579	-0.077382	C	-5.244165	-2.191538	0.59104
H	-4.603413	-0.0521	2.478006	H	-2.151874	-0.694632	0.902716
H	-3.292349	-1.157817	2.900217	H	-3.07444	-1.035074	-0.543111
C	-2.656893	0.516092	1.763921	C	-3.72355	0.708885	0.518935
O	-2.351796	-1.386072	-1.125069	O	-5.412324	-3.330046	0.205911
O	-2.284126	1.455127	2.438735	O	-4.894153	0.9456	0.873204
N	-2.128497	0.212897	0.515691	N	-2.918961	1.715094	0.139635

C	-1.068723	0.991654	-0.123486	C	-1.524358	1.63	-0.272178
H	-0.712723	0.362001	-0.945681	H	-1.369832	0.720911	-0.853572
C	-1.591256	2.323394	-0.680074	C	-1.181788	2.84846	-1.154701
C	0.119523	1.146128	0.827001	C	-0.607311	1.592287	0.952027
H	-2.57154	2.129659	-1.120744	H	-1.909429	2.868061	-1.969231
H	-1.744899	3.022137	0.143531	H	-1.330818	3.761299	-0.570373
C	-0.675456	2.932395	-1.740928	C	0.232577	2.819493	-1.729531
O	0.751664	2.163195	0.984276	O	-0.787312	2.231377	1.962402
H	0.312696	3.139734	-1.324032	H	0.981841	2.839536	-0.931892
H	-0.517202	2.214948	-2.555506	H	0.402972	1.884801	-2.274402
C	-1.19842	4.237391	-2.382709	C	0.560794	3.988122	-2.688078
O	-0.419015	4.784664	-3.212272	O	-0.314452	4.874639	-2.868909
O	-2.339469	4.654256	-2.049916	O	1.707781	3.951143	-3.212764
H	-4.880044	-3.040057	1.324029	H	-2.333684	-2.634192	2.148997
O	0.423684	-0.015729	1.431182	O	0.443513	0.780219	0.758708
H	1.194482	0.129394	2.00289	H	1.023076	0.828536	1.537021
				O	-6.162924	-1.254292	0.377404
				H	-3.329203	2.638381	0.204208
				H	-5.807744	-0.357226	0.656619

Asn-Gly

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.244467	-2.276168	1.594067	N	-3.17543	0.611804	3.325044
H	-2.545563	-1.666659	2.349387	H	-3.005138	0.11674	4.194205
C	-2.322002	-1.592595	0.314927	C	-2.929709	-0.256591	2.182393
H	-2.094789	-2.324361	-0.467437	H	-3.562386	-1.140482	2.28103
C	-3.621116	-0.840271	-0.058219	C	-3.357567	0.432842	0.854626
C	-1.235854	-0.51832	0.178579	C	-1.517377	-0.84054	2.062915
H	-4.269865	-1.38258	-0.745874	H	-2.918448	-0.094934	0.00275
H	-4.204152	-0.597545	0.834916	H	-4.440458	0.355976	0.771764
C	-3.16427	0.460876	-0.678939	C	-3.042348	1.922012	0.749464
O	-0.080519	-0.571826	0.539926	O	-0.544685	0.029452	2.408533
O	-3.832911	1.305085	-1.238862	O	-1.281165	-1.96461	1.681401
N	-1.790355	0.568288	-0.486658	N	-1.733614	2.28119	0.80528
C	-1.03282	1.73861	-0.852113	C	-1.343087	3.663739	0.9051
C	-1.043278	2.787124	0.249334	C	-1.478506	4.208023	2.320507
H	-0.000551	1.451187	-1.056132	H	-0.303323	3.780185	0.593725
H	-1.456541	2.175544	-1.757458	H	-1.954806	4.27834	0.243167
O	-1.615423	2.680188	1.307306	O	-1.810534	3.564626	3.290054
O	-0.325195	3.856869	-0.119211	O	-1.16845	5.511959	2.361738
H	-0.347025	4.511511	0.59767	H	-1.251423	5.825722	3.276924
H	-2.866183	-3.077922	1.595749	H	-2.571322	1.430914	3.317963
				O	-3.937256	2.753058	0.602128
				H	0.315713	-0.40603	2.292032
				H	-1.046425	1.588868	1.065653

Asn-His

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.632554	-2.881646	2.741376	N	-2.370174	-3.453051	2.342664

H	-1.608939	-2.285599	3.564134	H	-2.782415	-3.362008	3.266913
C	-2.11161	-2.148907	1.583182	C	-1.790226	-2.185683	1.906621
H	-2.227621	-2.863807	0.761761	H	-1.41677	-2.323876	0.889351
C	-3.403518	-1.307138	1.705877	C	-2.797424	-0.990628	1.904091
C	-1.070883	-1.140464	1.079244	C	-0.573787	-1.82449	2.747104
H	-4.290462	-1.786311	1.291816	H	-3.782058	-1.39851	1.672129
H	-3.611568	-1.05621	2.750159	H	-2.873191	-0.550578	2.904579
C	-3.107548	-0.019545	0.972856	C	-2.589182	0.14823	0.910221
O	0.12824	-1.285303	0.997263	O	-0.584159	-2.354741	3.970906
O	-3.867005	0.885134	0.690565	O	-3.561564	0.748946	0.444969
N	-1.748901	0.008173	0.678684	N	-1.324387	0.482073	0.579396
C	-1.095692	1.134099	0.024166	C	-1.031013	1.553189	-0.359878
H	-0.022289	0.959061	0.144273	H	0.03411	1.77092	-0.242301
C	-1.443667	1.194212	-1.481278	C	-1.306789	1.148152	-1.827367
C	-1.402162	2.43637	0.766328	C	-1.75362	2.850643	0.02129
H	-1.478968	0.164526	-1.841251	H	-1.021761	0.096824	-1.92459
H	-2.44581	1.613882	-1.594587	H	-2.376995	1.216336	-2.019951
C	-0.449924	1.926877	-2.321704	C	-0.568064	1.966033	-2.83449
O	-1.627156	3.495881	0.226006	O	-2.338286	3.574246	-0.74934
N	-0.262303	3.292084	-2.291509	N	0.785348	1.816126	-3.073564
C	0.436064	1.473294	-3.272596	C	-0.961061	2.9628	-3.695785
H	-0.739395	3.918228	-1.657306	H	1.400767	1.151012	-2.629534
C	0.70377	3.602452	-3.194325	C	1.142751	2.701054	-4.042895
N	1.150992	2.523514	-3.813931	N	0.107442	3.415111	-4.446008
H	0.585281	0.453983	-3.595286	H	-1.950276	3.379192	-3.801999
H	1.039613	4.614662	-3.356756	H	2.153602	2.776801	-4.411855
O	-1.335228	2.28156	2.092474	O	-1.596407	3.1352	1.326389
H	-1.511003	3.137525	2.516067	H	-2.047042	3.97501	1.508991
H	-2.262202	-3.649416	2.949864	H	-3.119924	-3.7145	1.709837
				O	0.306106	-1.076733	2.360816
				H	-0.548302	0.018724	1.042664
				H	0.193297	-2.033091	4.456516

Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.83274	-4.18678	0.82438	N	-2.084057	-3.90613	0.500314
H	-2.12908	-3.94743	1.76656	H	-3.006492	-4.265236	0.716218
C	-2.03303	-3.06687	-0.07917	C	-2.148354	-2.735132	-0.368745
H	-1.80074	-3.41161	-1.09269	H	-2.049138	-2.992892	-1.427246
C	-3.39527	-2.34364	-0.09231	C	-3.392784	-1.872432	-0.163061
C	-1.03797	-1.93348	0.188474	C	-0.97653	-1.763166	-0.014055
H	-4.06067	-2.65053	-0.89877	H	-4.209961	-2.095254	-0.847796
H	-3.92221	-2.48763	0.855697	H	-3.767787	-1.965327	0.862236
C	-3.06436	-0.87179	-0.21284	C	-2.908433	-0.443341	-0.33523
O	0.131603	-2.03554	0.490011	O	-0.587611	-1.91394	1.306316
O	-3.8334	0.038388	-0.43618	O	-3.619306	0.53617	-0.509233
N	-1.69382	-0.71855	-0.00728	N	-1.545221	-0.439119	-0.253291
C	-0.97806	0.548743	0.085226	C	-0.701477	0.740061	-0.148163
H	0.074075	0.261416	0.142787	H	0.320293	0.35837	-0.176734

C	-1.15732	1.478109	-1.16664	C	-0.853495	1.748249	-1.344951
C	-1.2809	1.218296	1.420512	C	-0.849767	1.402073	1.217945
H	-1.58687	0.833212	-1.93943	H	-1.406652	1.193353	-2.10847
C	-2.11818	2.655787	-0.9429	C	-1.658522	3.010012	-1.001351
C	0.226794	1.943331	-1.66068	C	0.537051	2.082057	-1.918629
O	-2.13697	0.879411	2.202805	O	-1.741704	1.220143	2.011418
H	-1.65751	3.424758	-0.31728	H	-1.081691	3.683455	-0.360887
H	-2.3768	3.114855	-1.89887	H	-1.911783	3.555369	-1.912539
H	-3.04436	2.323995	-0.47399	H	-2.590475	2.751107	-0.498863
H	0.698441	2.546138	-0.87585	H	1.125442	2.593273	-1.147535
H	0.86079	1.06031	-1.80088	H	1.057243	1.14204	-2.136688
C	0.185965	2.736779	-2.9701	C	0.499633	2.933322	-3.191594
H	-0.32785	3.694056	-2.85227	H	0.105322	3.93487	-3.002123
H	1.199606	2.94746	-3.32198	H	1.504662	3.04765	-3.607245
H	-0.33044	2.172598	-3.75409	H	-0.128282	2.465131	-3.957321
O	-0.43764	2.240729	1.634929	O	0.176973	2.244804	1.441549
H	-0.66286	2.655786	2.483224	H	0.039471	2.674651	2.300926
H	-2.40029	-4.97405	0.52818	H	-1.554574	-4.659072	0.074978
				O	0.182464	-1.960693	-0.793832
				H	-0.040949	-1.847883	-1.727308
				H	-0.960366	-2.787053	1.564812

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.044941	-3.946433	0.845242	N	-2.596084	-4.991211	1.077513
H	-2.475247	-3.77977	1.750635	H	-3.32496	-5.475998	1.592606
C	-2.321054	-2.85122	-0.068133	C	-2.714726	-3.538638	1.263283
H	-1.945406	-3.139335	-1.055694	H	-2.673576	-3.330612	2.332598
C	-3.772621	-2.337774	-0.208634	C	-1.552407	-2.839685	0.559377
C	-1.528837	-1.589513	0.299123	C	-4.086605	-3.04896	0.802637
H	-4.291967	-2.7001	-1.095641	H	-0.616362	-3.209591	0.988336
H	-4.370453	-2.607751	0.666788	H	-1.539883	-3.097264	-0.503347
C	-3.657353	-0.830968	-0.242556	C	-1.596106	-1.328784	0.719851
O	-0.379534	-1.517381	0.675951	O	-5.063529	-2.987241	1.517937
O	-4.524043	-0.012723	-0.477349	O	-2.354743	-0.770276	1.514866
N	-2.35257	-0.488787	0.089477	N	-0.734344	-0.631865	-0.052835
C	-1.883283	0.889557	0.20361	C	-0.647122	0.822014	-0.005412
H	-0.922704	0.814107	0.720938	H	0.261897	1.080299	-0.554938
C	-1.697516	1.553247	-1.168639	C	-1.854507	1.51354	-0.668719
C	-2.793966	1.687723	1.137928	C	-0.344203	1.253737	1.437673
H	-1.310281	0.790865	-1.852888	H	-2.158096	0.88578	-1.513041
H	-2.679187	1.852868	-1.542041	H	-2.686751	1.517227	0.037386
C	-0.73653	2.757029	-1.171352	C	-1.587121	2.939003	-1.189484
O	-3.158303	2.822233	0.94099	O	0.453822	0.687757	2.150692
H	-1.042896	3.439777	-0.372107	H	-1.112282	3.517522	-0.390314
C	0.71743	2.331166	-0.919991	C	-0.651822	2.938625	-2.407965
C	-0.853559	3.505386	-2.50597	C	-2.9181	3.619446	-1.537485
H	1.062197	1.653842	-1.70948	H	-1.102486	2.383936	-3.238864
H	1.378025	3.202904	-0.913064	H	-0.462662	3.960399	-2.750032

H	0.84454	1.818731	0.037797	H	0.318985	2.483613	-2.190983
H	-1.873751	3.864012	-2.672733	H	-3.572991	3.681389	-0.663049
H	-0.182069	4.368663	-2.530661	H	-2.754579	4.634479	-1.911793
H	-0.585959	2.84935	-3.342345	H	-3.447943	3.057498	-2.315445
H	-2.443261	-4.806554	0.483379	H	-2.708177	-5.239312	0.097857
O	-3.092447	0.993667	2.248761	O	-1.003928	2.358378	1.8156
H	-3.648322	1.549423	2.818191	H	-0.718834	2.585959	2.715177
				O	-4.128198	-2.77563	-0.515504
				H	-0.115772	-1.128078	-0.674895
				H	-5.039141	-2.539745	-0.753288
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.527467	-3.317575	2.309417	N	-2.532956	-3.846178	1.068179
H	-0.582599	-3.625467	2.524519	H	-3.142712	-3.990977	1.868078
C	-1.52341	-2.606373	1.033971	C	-1.711372	-2.656753	1.260944
H	-1.199234	-3.228307	0.186068	H	-1.063529	-2.549434	0.386873
C	-2.859372	-1.93023	0.691177	C	-2.634708	-1.412331	1.350378
C	-0.530058	-1.448626	1.089698	C	-0.764306	-2.694749	2.463743
H	-3.422781	-2.420716	-0.102008	H	-3.512302	-1.628341	0.740367
H	-3.498184	-1.863502	1.576274	H	-2.99384	-1.270244	2.37565
C	-2.491478	-0.521313	0.276591	C	-2.113851	-0.066155	0.857107
O	0.608952	-1.489366	1.505763	O	0.206947	-1.968499	2.576201
O	-3.20829	0.335017	-0.197677	O	-2.901835	0.762425	0.39194
N	-1.142282	-0.324542	0.5583	N	-0.794217	0.187977	0.962929
C	-0.461511	0.947185	0.360266	C	-0.221988	1.454102	0.52729
H	0.536419	0.807646	0.79043	H	0.791306	1.47967	0.94106
C	-0.323334	1.303618	-1.13399	C	-0.127099	1.561421	-1.006158
C	-1.136683	1.998611	1.247535	C	-0.94956	2.60517	1.239207
H	-0.222008	0.360411	-1.678153	H	0.134851	0.56523	-1.374296
H	-1.242517	1.777113	-1.484153	H	-1.109241	1.806792	-1.415228
C	0.891896	2.185525	-1.439328	C	0.92705	2.5629	-1.48938
O	-1.684319	1.74285	2.294189	O	-1.21123	2.594507	2.420976
H	0.830468	3.119658	-0.875795	H	0.702203	3.561476	-1.106057
H	1.802478	1.671216	-1.110897	H	1.90679	2.278789	-1.087021
C	0.993885	2.497094	-2.93693	C	1.002729	2.611501	-3.020031
H	1.044589	1.563037	-3.50748	H	1.232593	1.614578	-3.412738
H	0.093534	3.028989	-3.263884	H	0.029296	2.905731	-3.42833
C	2.223102	3.344149	-3.234229	C	2.066482	3.598037	-3.479385
H	2.183735	4.309876	-2.730286	H	1.8485	4.614237	-3.151256
H	3.145829	2.836619	-2.952826	H	3.060199	3.319619	-3.128642
N	2.333211	3.637728	-4.710678	N	2.146336	3.645413	-4.985933
H	1.505676	4.127659	-5.057866	H	1.254182	3.925847	-5.398747
H	3.144592	4.224214	-4.915909	H	2.853496	4.311258	-5.303815
H	2.431772	2.778751	-5.256249	H	2.388885	2.732069	-5.375775
H	-2.092055	-4.158054	2.227942	H	-1.947511	-4.673201	1.000666
O	-1.008493	3.2388	0.760345	O	-1.212012	3.652178	0.443231
H	-1.410157	3.859243	1.390192	H	-1.626648	4.344544	0.982686
				O	-1.109978	-3.586681	3.394956

				H	-0.481375	-3.524996	4.133104
				H	-0.196886	-0.473121	1.449991
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.672857	-4.463812	-1.137311	N	-2.306725	-3.999034	-1.563735
H	-0.689856	-4.629942	-0.939997	H	-3.223378	-4.144828	-1.97638
C	-2.158759	-3.305052	-0.408682	C	-2.2271	-2.669956	-0.94191
H	-3.240459	-3.241791	-0.567454	H	-3.023631	-2.604092	-0.197013
C	-1.860928	-3.189781	1.104425	C	-0.863913	-2.499502	-0.259295
C	-1.600304	-1.998203	-0.986831	C	-2.470095	-1.583483	-1.99104
H	-2.702794	-3.449366	1.746161	H	-0.697453	-3.373928	0.369652
H	-1.013644	-3.82031	1.388886	H	-0.079017	-2.4588	-1.018087
C	-1.459329	-1.749059	1.32116	C	-0.817755	-1.280562	0.649297
O	-1.451726	-1.704768	-2.152435	O	-3.777071	-1.456086	-2.272148
O	-1.257703	-1.169498	2.369304	O	-1.230017	-1.32251	1.809957
N	-1.308455	-1.149021	0.076495	N	-0.300404	-0.151455	0.114942
C	-0.879773	0.234208	-0.099954	C	-0.274536	1.111789	0.835372
H	-0.635035	0.323683	-1.163537	H	0.382991	1.768936	0.25847
C	-1.996376	1.226132	0.263033	C	-1.656886	1.773749	0.966182
C	0.425575	0.491528	0.656813	C	0.407845	0.980392	2.196483
H	-2.934399	0.809876	-0.113515	H	-2.272998	1.171336	1.637704
H	-2.075777	1.29228	1.349953	H	-1.526316	2.750044	1.438026
C	-1.769047	2.608499	-0.3496	C	-2.393958	1.912946	-0.364987
O	0.664356	1.489607	1.293346	O	0.059646	1.569571	3.194674
H	-0.834389	3.043152	0.006472	H	-2.543819	0.935599	-0.825897
H	-1.733579	2.542123	-1.440929	H	-3.374418	2.363887	-0.198972
S	-3.1433	3.732644	0.115732	S	-1.469515	2.949018	-1.572898
C	-2.58003	5.245684	-0.738035	C	-2.442921	2.57514	-3.072704
H	-2.513671	5.074857	-1.814186	H	-3.486475	2.862766	-2.931898
H	-3.321945	6.020585	-0.540277	H	-2.014392	3.160053	-3.88769
H	-1.61111	5.564826	-0.349438	H	-2.370007	1.512065	-3.307811
O	1.304318	-0.506263	0.476141	O	1.503059	0.204767	2.145476
H	2.121854	-0.287185	0.951555	H	1.90889	0.199098	3.026933
H	-2.177644	-5.293445	-0.843544	H	-1.624885	-4.083877	-2.313612
				O	-1.607659	-0.940985	-2.553565
				H	-3.883044	-0.813979	-2.992963
				H	-0.07666	-0.141313	-0.869442
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.393587	-3.480604	0.938172	N	-2.567287	-3.760336	0.098992
H	-1.376603	-3.260584	1.93001	H	-3.004891	-4.016635	0.97954
C	-1.720368	-2.304956	0.151224	C	-1.686152	-2.608293	0.275569
H	-1.841272	-2.625052	-0.889284	H	-1.289876	-2.338848	-0.705961
C	-2.936782	-1.440358	0.556198	C	-2.392776	-1.356657	0.885215
C	-0.561891	-1.299473	0.116945	C	-0.477586	-2.976658	1.123648
H	-3.835201	-1.628358	-0.031262	H	-3.418318	-1.352574	0.512889
H	-3.186284	-1.584073	1.611622	H	-2.461822	-1.450399	1.974538

C	-2.479035	-0.010286	0.38101	C	-1.848393	0.034806	0.574761
O	0.623778	-1.532835	0.030001	O	0.587971	-2.391647	1.059145
O	-3.140053	1.006948	0.435911	O	-2.613243	1.003496	0.556966
N	-1.106052	-0.020519	0.162903	N	-0.527297	0.168854	0.337699
C	-0.312756	1.190954	0.021133	C	0.066662	1.463099	0.040238
H	0.728118	0.853863	0.006379	H	1.148394	1.320863	0.112974
C	-0.626039	1.928057	-1.303659	C	-0.271337	1.946119	-1.390384
C	-0.448602	2.015846	1.304206	C	-0.263693	2.4452	1.173602
H	-0.809779	1.148531	-2.048438	H	-0.222697	1.056801	-2.025127
H	-1.552829	2.490758	-1.193463	H	-1.300849	2.302965	-1.41368
C	0.49362	2.820929	-1.793545	C	0.675806	2.992544	-1.937083
O	-0.619056	1.528593	2.397622	O	-0.19107	2.152749	2.34618
C	0.322447	4.204859	-1.898022	C	0.237292	4.287978	-2.231635
C	1.720914	2.265623	-2.180233	C	2.017448	2.669641	-2.184365
H	-0.620196	4.648677	-1.597675	H	-0.796187	4.554505	-2.040863
C	1.352288	5.018856	-2.374246	C	1.113859	5.239721	-2.75669
C	2.75528	3.074741	-2.65129	C	2.899845	3.618002	-2.70328
H	1.868396	1.191697	-2.119552	H	2.375295	1.665671	-1.977049
H	1.200496	6.089944	-2.448607	H	0.753528	6.238082	-2.979175
C	2.573811	4.456653	-2.749796	C	2.449963	4.908931	-2.99163
H	3.697556	2.626846	-2.946553	H	3.933633	3.347784	-2.888057
H	3.375172	5.087155	-3.118051	H	3.132545	5.646915	-3.397703
O	-0.3045	3.327302	1.088123	O	-0.577338	3.673909	0.743193
H	-0.350468	3.785833	1.942977	H	-0.722836	4.238223	1.51961
H	-2.102552	-4.19415	0.805535	H	-3.315968	-3.515432	-0.541813
				O	-0.708536	-3.963875	1.991068
				H	0.086913	-0.630556	0.454426
				H	0.089036	-4.099566	2.528667
Asn-Ser							
Reactant Structure				Product Structure			
N	-1.12055	-3.26675	1.227952	N	-1.953434	-4.041002	0.682012
H	-0.78307	-2.9773	2.14175	H	-1.114103	-4.549084	0.948464
C	-1.373278	-2.11562	0.379721	C	-1.626482	-2.64543	0.372164
H	-1.839606	-2.477591	-0.542833	H	-2.566513	-2.104684	0.247607
C	-2.206095	-0.938018	0.938402	C	-0.762671	-1.944138	1.444553
C	-0.06846	-1.448872	-0.075317	C	-0.914709	-2.672307	-0.979538
H	-3.245497	-0.929449	0.611007	H	-1.274028	-2.039174	2.402642
H	-2.196484	-0.935261	2.032339	H	0.204545	-2.448107	1.50824
C	-1.492471	0.308609	0.469325	C	-0.597021	-0.46069	1.165258
O	0.964133	-1.985492	-0.409914	O	0.281635	-2.818717	-1.117204
O	-1.854771	1.464864	0.548881	O	-1.763997	-2.551034	-2.006862
N	-0.272029	-0.072129	-0.0776	N	0.461882	-0.114536	0.393333
C	0.722821	0.885297	-0.526933	C	0.673965	1.248847	-0.056938
H	1.593499	0.295253	-0.831475	H	1.679714	1.297841	-0.484087
C	0.251382	1.675659	-1.759743	C	-0.322815	1.639537	-1.167411
C	1.180612	1.724353	0.669783	C	0.713413	2.192914	1.150584
H	-0.415055	1.027443	-2.339203	H	-0.318286	0.837192	-1.906741
H	-0.303702	2.565655	-1.457652	H	-1.330577	1.720313	-0.750727
O	1.410002	2.012579	-2.517238	O	0.061207	2.822995	-1.855104

O	1.175449	1.319684	1.809095	O	1.305315	1.95648	2.176062
H	1.192092	2.743634	-3.105094	H	-0.054281	3.56823	-1.25302
O	1.624184	2.933212	0.310392	O	0.073155	3.35436	0.922065
H	1.93224	3.394929	1.107322	H	0.182603	3.928142	1.697393
H	-1.982	-3.780727	1.379856	H	-2.58618	-4.078176	1.475088
				O	-1.393828	0.378666	1.587445
				H	1.055648	-0.84164	0.022984
				H	-1.262124	-2.622144	-2.835755
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.294208	-3.991687	-0.404589	N	-1.137389	-3.010104	2.039006
H	-1.902524	-3.96673	0.532928	H	-0.633595	-3.719976	2.560756
C	-2.524657	-2.647733	-0.90472	C	-1.254797	-3.397606	0.62955
H	-3.048826	-2.73406	-1.862772	H	-1.720693	-4.386556	0.60196
C	-3.266181	-1.629693	-0.013354	C	-2.183616	-2.437989	-0.139488
C	-1.21492	-1.928651	-1.242377	C	0.112423	-3.575015	-0.039021
H	-4.323749	-1.512801	-0.248864	H	-2.096101	-2.630475	-1.211724
H	-3.182908	-1.902554	1.042838	H	-3.208134	-2.647997	0.162669
C	-2.536531	-0.317511	-0.205725	C	-1.959174	-0.954047	0.132645
O	-0.214152	-2.402521	-1.734306	O	0.781129	-4.604383	0.497045
O	-2.86161	0.772406	0.207566	O	0.575551	-2.885329	-0.92745
N	-1.363762	-0.580615	-0.920741	N	-0.808293	-0.436903	-0.343208
C	-0.323664	0.391596	-1.227908	C	-0.263223	0.890008	-0.090894
H	0.570222	-0.206178	-1.439741	H	0.567507	1.00433	-0.790434
C	-0.590328	1.21317	-2.501368	C	-1.215781	2.093402	-0.355313
C	0.053363	1.173458	0.031273	C	0.364304	1.060946	1.293155
H	0.288952	1.852572	-2.637321	H	-0.568865	2.973528	-0.358867
C	-0.755216	0.319311	-3.728748	C	-1.916528	1.969974	-1.705491
O	-1.748479	2.017819	-2.286435	O	-2.131948	2.298552	0.711211
O	0.012785	0.705004	1.144435	O	1.034496	2.024419	1.586319
H	-1.628471	-0.32872	-3.623307	H	-2.594347	1.113555	-1.716676
H	-0.896638	0.940954	-4.616366	H	-2.499049	2.874589	-1.890948
H	0.13014	-0.301732	-3.88421	H	-1.190938	1.848843	-2.514805
H	-1.899471	2.544998	-3.079491	H	-2.575256	1.43484	0.853029
H	-3.17469	-4.492025	-0.342683	H	-0.617402	-2.141167	2.134692
O	0.530517	2.393319	-0.244786	O	0.112287	0.053528	2.142893
H	0.829226	2.797728	0.585883	H	0.544928	0.254325	2.98893
				O	-2.810201	-0.294758	0.743936
				H	1.657198	-4.662258	0.082069
				H	-0.184701	-1.101175	-0.791239
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.064645	-2.673648	2.405632	N	-3.032144	-1.920589	2.99817
H	-1.603765	-2.408274	3.225236	H	-2.796041	-2.209726	3.941972
C	-1.655213	-2.12503	1.196973	C	-2.138335	-2.562932	2.027131
H	-1.106215	-2.535788	0.343184	H	-2.210252	-3.642442	2.18476
C	-3.172779	-2.299806	0.955747	C	-2.586978	-2.278568	0.579697

C	-1.447761	-0.60763	1.103114	C	-0.669127	-2.210466	2.281977
H	-3.424229	-3.087413	0.245559	H	-1.7905	-2.567786	-0.110366
H	-3.698947	-2.509166	1.89148	H	-3.461927	-2.891814	0.370114
C	-3.649731	-0.959328	0.445413	C	-3.004713	-0.836046	0.312878
O	-0.449221	0.024275	1.370669	O	0.042464	-1.523646	1.574695
O	-4.738196	-0.666475	-0.007289	O	-0.239851	-2.74383	3.43469
N	-2.617584	-0.04302	0.60476	N	-2.023574	0.089982	0.374959
C	-2.72507	1.368287	0.251473	C	-2.284157	1.514458	0.245177
H	-1.875789	1.849447	0.744549	H	-1.378939	2.017368	0.597184
C	-2.630216	1.600811	-1.27214	C	-2.563549	1.959849	-1.209053
C	-3.977628	1.987762	0.871921	C	-3.389737	1.96152	1.207301
H	-1.934131	0.851413	-1.661998	H	-1.93337	1.334679	-1.848967
H	-3.603153	1.409526	-1.726222	H	-3.601415	1.73644	-1.457411
C	-2.137543	2.972121	-1.615955	C	-2.252517	3.404542	-1.454254
O	-4.739803	2.725661	0.29677	O	-4.282614	2.729045	0.939902
C	-2.84353	3.998313	-2.19439	C	-3.139223	4.435863	-1.644685
C	-0.803103	3.470107	-1.392913	C	-0.934969	3.985231	-1.526181
H	-3.875997	4.02942	-2.504127	H	-4.217283	4.418103	-1.649941
N	-2.030746	5.102164	-2.347634	N	-2.455861	5.619983	-1.832504
C	-0.773615	4.812589	-1.864908	C	-1.101822	5.379179	-1.763486
C	0.365572	2.911883	-0.844717	C	0.366189	3.462994	-1.420697
H	-2.315953	5.979676	-2.750754	H	-2.884285	6.517139	-1.991721
C	0.38081	5.598873	-1.803247	C	-0.014888	6.249087	-1.89185
C	1.515452	3.691516	-0.780845	C	1.450593	4.324617	-1.546883
H	0.368679	1.893433	-0.471414	H	0.522878	2.403876	-1.246185
H	0.384794	6.619311	-2.168877	H	-0.16195	7.307561	-2.073604
C	1.522584	5.021429	-1.255402	C	1.261141	5.704467	-1.779185
H	2.423585	3.274798	-0.359531	H	2.459055	3.934212	-1.467064
H	2.43467	5.604197	-1.191763	H	2.125808	6.351839	-1.873067
O	-4.096035	1.65601	2.168841	O	-3.215519	1.442047	2.440711
H	-4.890651	2.085417	2.524328	H	-3.924052	1.779338	3.011692
H	-1.069979	-3.687382	2.363719	H	-2.942339	-0.907477	2.963353
				O	-4.176662	-0.53009	0.081521
				H	0.676295	-2.461907	3.5904
				H	-1.090254	-0.221675	0.616744

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.579584	-2.315952	1.207972	N	-2.337464	-1.974781	-1.164329
H	-2.246775	-2.335684	1.974242	H	-1.50441	-2.343399	-1.613988
C	-1.801176	-1.159839	0.358071	C	-1.962272	-1.150575	-0.027303
H	-1.136523	-1.24965	-0.508149	H	-1.278745	-0.378067	-0.389866
C	-3.231694	-0.85065	-0.137285	C	-3.22074	-0.458154	0.593968
C	-1.370828	0.14433	1.040284	C	-1.194753	-1.909775	1.054578
H	-3.438098	-1.189674	-1.152055	H	-4.082585	-0.701466	-0.024285
H	-3.980034	-1.292227	0.527412	H	-3.415199	-0.827119	1.604459
C	-3.360957	0.652949	-0.047622	C	-3.105979	1.060074	0.629273
O	-0.39997	0.329931	1.740413	O	-1.02245	-3.105157	1.090011
O	-4.235536	1.35988	-0.505034	O	-0.715801	-1.070993	1.999487

N	-2.281169	1.134969	0.684751	N	-2.124447	1.546815	1.424849
C	-2.087977	2.537982	1.007674	C	-1.702246	2.932395	1.405421
H	-1.195964	2.573462	1.641207	H	-0.839392	2.993205	2.074948
C	-1.827023	3.398477	-0.255454	C	-1.251872	3.43121	0.000768
C	-3.233104	3.027346	1.891754	C	-2.752697	3.837197	2.050195
H	-2.739786	3.437684	-0.850678	H	-2.133196	3.670502	-0.593081
H	-1.604516	4.411715	0.080785	H	-0.692541	4.3577	0.146559
C	-0.682333	2.842321	-1.068575	C	-0.414561	2.403628	-0.724981
O	-3.977454	2.307755	2.514654	O	-3.662818	3.464578	2.752349
C	-0.915042	1.979955	-2.144663	C	-0.864088	1.830189	-1.917729
C	0.646448	3.127767	-0.728326	C	0.809754	1.959695	-0.205321
H	-1.933983	1.744822	-2.433195	H	-1.814958	2.142227	-2.334833
C	0.13876	1.410354	-2.860244	C	-0.126961	0.843818	-2.576852
C	1.709847	2.569967	-1.432343	C	1.55259	0.970591	-0.842836
H	0.855886	3.795426	0.101274	H	1.188503	2.38279	0.719405
H	-0.062817	0.743896	-3.692465	H	-0.498891	0.407806	-3.498035
C	1.45599	1.704776	-2.500588	C	1.082255	0.407306	-2.033475
H	2.735545	2.796537	-1.166592	H	2.493587	0.626678	-0.430271
O	2.53781	1.182386	-3.156607	O	1.849159	-0.566485	-2.61446
H	2.244932	0.602454	-3.8699	H	1.426194	-0.883375	-3.421761
H	-1.716601	-3.168413	0.675153	H	-2.871204	-2.781885	-0.851672
O	-3.277068	4.366377	1.941425	O	-2.510731	5.133904	1.78718
H	-3.982322	4.627409	2.555708	H	-3.171269	5.667426	2.25768
				O	-3.838816	1.789591	-0.037513
				H	-1.534367	0.885225	1.907699
				H	-0.258866	-1.58594	2.683768

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.121495	-4.32416	-0.054759	N	-3.845045	-3.308743	0.853744
H	-0.850217	-4.173554	0.912926	H	-4.017746	-4.03826	0.168773
C	-1.678691	-3.111766	-0.6288	C	-2.547519	-2.687591	0.616711
H	-2.054206	-3.358535	-1.627878	H	-2.569471	-2.235159	-0.379197
C	-2.770523	-2.345053	0.144707	C	-2.313641	-1.562655	1.665131
C	-0.605377	-2.044865	-0.866293	C	-1.345593	-3.637894	0.594131
H	-3.787604	-2.550966	-0.187479	H	-3.295701	-1.233434	2.002371
H	-2.713169	-2.560498	1.215957	H	-1.787454	-1.953127	2.54271
C	-2.439797	-0.880593	-0.045334	C	-1.589578	-0.299479	1.204286
O	0.532239	-2.215541	-1.248227	O	-0.236458	-3.306866	0.214823
O	-3.135064	0.071378	0.237449	O	-1.616811	-4.866523	1.03977
N	-1.164487	-0.79431	-0.602391	N	-0.517533	-0.459773	0.403134
C	-0.410828	0.432099	-0.837413	C	0.272463	0.641543	-0.136721
H	0.487635	0.099365	-1.361753	H	1.2748	0.228341	-0.291481
C	-1.145012	1.470788	-1.756922	C	-0.233753	1.100201	-1.527733
C	0.086994	0.997884	0.487132	C	0.512449	1.685042	0.964646
H	-1.943638	0.9014	-2.240431	H	-0.282185	0.162794	-2.095973
C	-1.784011	2.651843	-1.012262	C	-1.642762	1.705211	-1.532334
C	-0.188128	1.973876	-2.847158	C	0.781815	2.004415	-2.242218
O	-0.24416	0.619966	1.585715	O	1.000929	1.396935	2.035336

H	-1.019451	3.321957	-0.610576	H	-1.668779	2.655817	-0.996975
H	-2.395526	3.229864	-1.71015	H	-1.95906	1.884396	-2.564076
H	-2.422987	2.313492	-0.19715	H	-2.368785	1.034244	-1.069875
H	0.202308	1.148552	-3.449436	H	1.782188	1.559658	-2.241898
H	-0.708075	2.665844	-3.515019	H	0.481016	2.146715	-3.283757
H	0.658565	2.505744	-2.403239	H	0.845218	2.987474	-1.772089
H	-1.821946	-5.058243	-0.053591	H	-3.861491	-3.761574	1.763499
O	0.982575	1.975238	0.27363	O	0.23201	2.947048	0.612199
H	1.271506	2.323803	1.13249	H	0.474174	3.524274	1.354308
				O	-1.976745	0.808803	1.583233
				H	-0.22396	-1.405424	0.17379
				H	-0.801406	-5.394035	1.010707

Table S14.E. Isoimide Formation XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions							
NH_3							
Product Structure							
Atom	X	Y	Z				
N	-1.133326	-0.563263	0.000024				
H	-0.744703	-1.50246	-0.000031				
H	-0.744689	-0.093642	0.813368				
H	-0.7447	-0.093681	-0.813362				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.891127	-2.884246	0.251026	N	-1.807882	-2.438342	-0.867872
H	-0.956162	-2.907849	0.649126	H	-1.207004	-3.206044	-0.579699
C	-2.478588	-1.564604	0.463042	C	-2.065254	-1.543932	0.203586
H	-3.41318	-1.505706	-0.098634	C	-2.776582	-1.823895	1.503468
C	-2.79954	-1.243788	1.946244	C	-1.664967	-0.265381	0.222698
C	-1.501839	-0.510341	-0.071776	H	-3.821172	-2.132513	1.387401
H	-3.401492	-2.066112	2.346382	H	-2.288425	-2.573892	2.136992
H	-1.875284	-1.200716	2.528218	C	-2.724787	-0.476223	2.194155
C	-3.632141	0.020374	2.107956	O	-2.042961	0.408065	1.391906
O	-0.282102	-0.672645	-0.008889	O	-3.165404	-0.127749	3.257867
O	-4.563417	0.276189	1.34013	N	-0.882987	0.472428	-0.638615
N	-3.30323	0.830859	3.134184	H	-0.672258	-0.080277	-1.463679
H	-3.852308	1.660376	3.303569	C	-1.283142	1.839423	-0.96295
H	-2.545178	0.619918	3.7626	H	-1.472495	2.373088	-0.030769
N	-2.065964	0.613276	-0.561733	C	-0.1588	2.548336	-1.730263
H	-3.071102	0.728352	-0.521814	C	-2.567033	1.882329	-1.79307
C	-1.268481	1.74318	-1.003132	H	0.061541	2.022589	-2.663605
H	-0.413474	1.851669	-0.330768	H	-0.445886	3.573466	-1.968444
C	-0.748766	1.561198	-2.442252	H	0.743254	2.565179	-1.116697
C	-2.106086	3.005279	-0.898769	O	-2.983114	0.970677	-2.471338

H	-1.584144	1.477638	-3.141561	H	-2.665868	-2.853237	-1.220758
H	-0.121346	2.40522	-2.732476	O	-3.173566	3.078463	-1.703242
H	-0.157105	0.646245	-2.487801	H	-3.956422	3.075394	-2.278074
O	-3.305202	3.031904	-0.731085				
H	-2.441316	-3.592356	0.727048				
O	-1.351788	4.103353	-1.047044				
H	-1.928241	4.883985	-1.013008				
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.773546	-3.901166	-0.30998	N	-3.925407	-3.019957	-0.755598
H	-1.928572	-4.250817	0.13375	H	-3.85229	-4.002934	-0.50657
C	-3.10055	-2.585205	0.229565	C	-3.617042	-2.178292	0.344255
H	-3.922862	-2.165011	-0.353524	C	-4.336497	-2.065945	1.664999
C	-3.538223	-2.600081	1.71833	C	-2.566427	-1.34794	0.379076
C	-1.86956	-1.682668	0.085495	H	-5.376028	-1.731045	1.582891
H	-4.352688	-3.324062	1.822226	H	-4.340876	-2.98742	2.258884
H	-2.711732	-2.941934	2.346497	C	-3.522847	-1.009479	2.38506
C	-4.087038	-1.258237	2.182489	O	-2.477395	-0.627311	1.577201
O	-0.72548	-2.130539	0.169856	O	-3.670974	-0.51862	3.472961
O	-4.850731	-0.599152	1.471981	N	-1.520261	-1.142492	-0.495508
N	-3.699212	-0.838623	3.403629	H	-1.665089	-1.703835	-1.329741
H	-4.064922	0.0289	3.76687	C	-1.142142	0.235542	-0.815496
H	-3.076424	-1.377563	3.983016	H	-1.013508	0.784009	0.118008
N	-2.130799	-0.368653	-0.082071	C	0.188413	0.223177	-1.588449
H	-3.089989	-0.045666	-0.100873	C	-2.228287	0.929865	-1.640732
C	-1.077282	0.629542	-0.114478	H	0.904703	-0.323853	-0.969256
H	-0.282896	0.323254	0.569179	H	0.053584	-0.350774	-2.511968
C	-0.488752	0.763664	-1.540442	C	0.734703	1.615982	-1.914135
C	-1.65723	1.948554	0.370655	O	-2.890038	0.378956	-2.49111
H	-0.208521	-0.24916	-1.842288	H	0.048551	2.149489	-2.57916
H	-1.283382	1.095538	-2.21615	H	0.82265	2.206988	-0.996747
C	0.72584	1.688894	-1.644231	C	2.10346	1.514899	-2.58403
O	-2.825048	2.255799	0.282517	H	2.809024	1.024007	-1.906708
H	0.436799	2.719935	-1.421738	H	2.028048	0.916546	-3.498318
H	1.483158	1.399227	-0.908572	N	2.604975	2.852041	-2.912573
C	1.334451	1.626898	-3.043952	H	1.973161	3.630699	-2.797485
H	1.697669	0.61461	-3.244126	C	3.803983	3.106435	-3.434516
H	0.575965	1.876632	-3.7939	N	4.665108	2.112642	-3.667218
N	2.45757	2.562883	-3.144696	N	4.150359	4.365033	-3.735294
H	2.538929	3.270964	-2.429894	H	4.407319	1.149111	-3.536169
C	3.310098	2.626566	-4.166676	H	5.569072	2.296547	-4.071186
N	3.172364	1.811448	-5.215998	H	3.571132	5.140193	-3.455671
N	4.324355	3.498987	-4.136495	H	5.080811	4.579875	-4.055478
H	2.351923	1.241691	-5.336245	H	-4.875672	-2.869959	-1.083094
H	3.841137	1.821956	-5.969003	O	-2.349855	2.230066	-1.329305
H	4.50134	4.065217	-3.322918	H	-3.019339	2.629318	-1.909582
H	4.925069	3.627231	-4.934182				
H	-3.518851	-4.558759	-0.103005				

O	-0.712844	2.749963	0.880646				
H	-1.120632	3.597466	1.124567				
Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.022756	-3.639036	-0.157895	N	-3.149386	-2.30362	0.368802
H	-0.159107	-3.602377	0.376757	H	-3.026965	-3.311868	0.413378
C	-1.8483	-2.479092	0.165658	C	-2.116385	-1.620346	1.061159
H	-2.698823	-2.456163	-0.518764	C	-1.784827	-1.672196	2.53151
C	-2.407633	-2.481632	1.612055	C	-1.223361	-0.8165	0.469064
C	-1.005493	-1.215256	-0.040783	H	-2.586263	-1.312672	3.185813
H	-2.898975	-3.445453	1.781146	H	-1.491924	-2.663752	2.89624
H	-1.58869	-2.402408	2.331983	C	-0.599245	-0.733392	2.6268
C	-3.467009	-1.411751	1.839413	O	-0.30288	-0.263849	1.368302
O	0.209617	-1.207226	0.15903	O	0.047944	-0.38834	3.579916
O	-4.301762	-1.141013	0.972054	N	-0.988053	-0.512165	-0.855297
N	-3.447903	-0.792448	3.036788	H	-1.710132	-0.934662	-1.431011
H	-4.159074	-0.10928	3.250767	C	-0.724597	0.878685	-1.211209
H	-2.771937	-1.020642	3.747448	H	0.038449	1.275056	-0.541468
N	-1.688033	-0.109868	-0.410768	C	-0.181363	0.950331	-2.652004
H	-2.696919	-0.143207	-0.492118	C	-1.980283	1.746598	-1.08436
C	-1.037051	1.177687	-0.53865	H	0.581302	0.173127	-2.745305
H	-0.30742	1.299241	0.265828	H	-0.971977	0.727096	-3.372333
C	-0.277738	1.300052	-1.883225	C	0.511096	2.276538	-2.94623
C	-2.087651	2.268695	-0.404333	O	-3.112027	1.320561	-1.101076
H	0.277524	0.368305	-2.013825	O	1.390798	2.708876	-2.202922
H	-0.983078	1.388936	-2.711896	N	0.129142	2.913784	-4.071647
C	0.758426	2.416391	-1.874167	H	0.581747	3.778929	-4.325717
O	-3.28271	2.078543	-0.38736	H	-0.603984	2.563785	-4.66637
O	1.560218	2.530801	-0.947595	H	-4.061759	-2.100361	0.76757
N	0.768526	3.230403	-2.9498	O	-1.675568	3.049626	-0.982299
H	1.459294	3.963556	-3.006089	H	-2.500437	3.562127	-0.955284
H	0.095173	3.147673	-3.693769				
H	-1.504394	-4.493778	0.103206				
O	-1.524662	3.481235	-0.334189				
H	-2.227458	4.150312	-0.296163				
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.99394	-2.615646	-0.96669	N	-5.066713	-1.93482	-1.371556
H	-4.154637	-3.163919	-0.798079	H	-4.961427	-2.945999	-1.366163
C	-4.959459	-1.409867	-0.144032	C	-4.759022	-1.368747	-0.106957
H	-5.784827	-0.760494	-0.443211	C	-5.463203	-1.585176	1.208737
C	-5.095933	-1.677308	1.378324	C	-3.724943	-0.544807	0.11177
C	-3.629169	-0.690734	-0.397487	H	-6.510564	-1.264407	1.216712
H	-6.002173	-2.269812	1.538006	H	-5.441055	-2.619507	1.571915
H	-4.246315	-2.269386	1.727639	C	-4.661762	-0.707866	2.149168
C	-5.265548	-0.394707	2.17958	O	-3.636052	-0.123109	1.445607
O	-2.587978	-1.320793	-0.594648	O	-4.805904	-0.489019	3.323401

O	-6.043666	0.488959	1.811838	N	-2.697402	-0.112834	-0.696747
N	-4.526814	-0.281461	3.302451	H	-2.85275	-0.440425	-1.645047
H	-4.626663	0.541187	3.878202	C	-2.311627	1.300275	-0.648088
H	-3.891517	-1.00321	3.601634	H	-2.077065	1.566222	0.381625
N	-3.672574	0.65458	-0.337307	C	-1.059463	1.527726	-1.512046
H	-4.541591	1.117314	-0.102852	C	-3.442938	2.200937	-1.145319
C	-2.476558	1.474028	-0.442982	H	-0.334294	0.762889	-1.220823
H	-1.65632	0.992954	0.094761	H	-1.30631	1.385652	-2.567073
C	-2.018333	1.667153	-1.907697	C	-0.409105	2.914938	-1.287144
C	-2.767607	2.813773	0.207619	O	-4.23674	1.888688	-2.005553
H	-2.131047	0.694908	-2.395318	O	-0.033644	3.162446	-0.111267
H	-2.669557	2.376266	-2.42297	O	-0.295706	3.665814	-2.290999
C	-0.533947	2.075837	-2.064231	O	-3.449221	3.39788	-0.536321
O	-3.870631	3.20137	0.530522	H	-4.153338	3.939749	-0.929039
O	0.296028	1.471801	-1.335761	H	-6.026767	-1.740974	-1.642422
O	-0.277417	2.943503	-2.940051				
O	-1.658111	3.548838	0.357352				
H	-1.908763	4.408879	0.731974				
H	-5.789015	-3.192493	-0.709753				
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.888251	-2.4099	-0.65284	N	-3.265565	-1.256197	-1.715681
H	-2.011838	-2.771293	-0.286335	H	-3.046508	-2.21842	-1.960265
C	-3.158865	-1.098031	-0.074058	C	-2.911281	-0.963728	-0.373581
H	-4.023301	-0.66537	-0.582163	C	-3.463774	-1.565801	0.89383
C	-3.471683	-1.124568	1.446035	C	-1.963683	-0.083251	-0.026483
C	-1.938198	-0.202557	-0.31183	H	-4.536141	-1.397544	1.038897
H	-4.277511	-1.846989	1.610086	H	-3.289225	-2.642993	0.998354
H	-2.59788	-1.4746	2.001416	C	-2.687819	-0.826026	1.965369
C	-3.976286	0.214801	1.96478	O	-1.800571	0.032364	1.358334
O	-0.795398	-0.657314	-0.342972	O	-2.750552	-0.899522	3.163946
O	-4.791014	0.883012	1.322454	N	-1.069064	0.648298	-0.776803
N	-3.491944	0.62146	3.155156	H	-1.209482	0.463109	-1.765387
H	-3.820788	1.489136	3.551738	C	-0.873444	2.079034	-0.475259
H	-2.822759	0.078451	3.676109	H	-0.820849	2.187055	0.607469
N	-2.200454	1.119167	-0.428723	C	0.430686	2.549628	-1.112602
H	-3.152861	1.454751	-0.353991	C	-2.081815	2.863159	-0.98993
C	-1.139568	2.101732	-0.532042	H	1.246793	1.933379	-0.734384
H	-0.289677	1.774921	0.069936	H	0.393388	2.448095	-2.197636
C	-0.693056	2.23069	-2.007387	S	0.876049	4.279207	-0.685341
C	-1.656173	3.425268	0.015219	O	-2.151733	3.394052	-2.076819
H	-0.455962	1.226237	-2.353457	H	-0.060012	4.877194	-1.444791
H	-1.510113	2.635087	-2.606318	H	-4.262165	-1.132813	-1.871995
S	0.820164	3.274562	-2.2129	O	-3.099062	2.822679	-0.115762
O	-2.825359	3.731244	0.069454	H	-3.871736	3.257183	-0.513351
H	1.181033	2.744984	-3.395381				
H	-3.619013	-3.064406	-0.391508				
O	-0.654008	4.222765	0.402378				

H	-1.022051	5.076456	0.684914				
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.879903	-3.819748	-0.346005	N	-2.405637	-3.272387	-0.813647
H	-1.044699	-4.046686	0.187054	H	-2.276636	-4.117653	-0.263582
C	-2.397212	-2.524611	0.084431	C	-2.813433	-2.179744	-0.005484
H	-3.197535	-2.226122	-0.595968	C	-4.081046	-2.035022	0.798681
C	-2.976114	-2.517935	1.524077	C	-2.073251	-1.081493	0.196396
C	-1.260526	-1.498912	0.005617	H	-4.997564	-2.051729	0.199331
H	-3.712097	-3.325178	1.595082	H	-4.201959	-2.78112	1.592848
H	-2.183752	-2.730913	2.246175	C	-3.911566	-0.663663	1.421055
C	-3.713183	-1.227404	1.853915	O	-2.695291	-0.149415	1.037509
O	-0.091267	-1.81269	0.232026	O	-4.644591	-0.038265	2.140913
O	-4.466789	-0.693736	1.035544	N	-0.793605	-0.743728	-0.189763
N	-3.502467	-0.710385	3.081162	H	-0.423411	-1.469015	-0.796913
H	-3.995872	0.125739	3.356253	C	-0.56036	0.599401	-0.7253
H	-2.886765	-1.146272	3.748165	H	-0.976681	1.32624	-0.027071
N	-1.638532	-0.232741	-0.270559	C	0.954538	0.830519	-0.85973
H	-2.619382	-0.017526	-0.397739	C	-1.247328	0.780146	-2.080862
C	-0.694566	0.870389	-0.266145	H	1.40018	0.626791	0.114979
H	0.047494	0.693725	0.515754	H	1.364853	0.099703	-1.565043
C	0.031263	0.980389	-1.629114	C	1.325821	2.248338	-1.30155
C	-1.454073	2.145083	0.062707	O	-1.337717	-0.089988	-2.917286
H	0.411894	-0.01652	-1.854963	H	0.950218	2.466176	-2.303543
H	-0.701814	1.233191	-2.401278	H	0.866055	2.980311	-0.62733
C	1.195704	1.973255	-1.647372	C	2.829866	2.483962	-1.23483
O	-2.637764	2.307948	-0.13432	O	3.525829	2.012901	-0.334596
H	0.84845	2.998759	-1.512708	N	3.347971	3.265392	-2.208326
H	1.877741	1.758272	-0.816311	H	4.328411	3.501226	-2.182373
C	2.01922	1.846116	-2.923084	H	2.780832	3.654274	-2.943808
O	2.281794	0.752405	-3.42514	O	-1.720667	2.025394	-2.249651
N	2.466822	3.005127	-3.455524	H	-2.105369	2.095366	-3.139242
H	3.06273	2.976938	-4.268967	H	-3.098708	-3.487637	-1.524972
H	2.260031	3.89999	-3.043186				
O	-0.64834	3.088256	0.568777				
H	-1.166255	3.898168	0.708708				
H	-2.563683	-4.54758	-0.163107				
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.21535	-2.75801	-1.001343	N	-4.163187	-1.284624	-1.338603
H	-2.452499	-3.205202	-0.500027	H	-4.315922	-2.279251	-1.193616
C	-3.519806	-1.473895	-0.378795	C	-3.981218	-0.59884	-0.109572
H	-4.226576	-0.937068	-1.015329	C	-4.962608	-0.440607	1.024429
C	-4.15299	-1.588685	1.034415	C	-2.839385	0.003972	0.2491
C	-2.221323	-0.665178	-0.270415	H	-5.878531	0.096008	0.754771
H	-5.029973	-2.238744	0.957842	H	-5.268256	-1.382547	1.495012
H	-3.4465	-2.063026	1.720114	C	-4.17157	0.383343	2.020381

C	-4.645846	-0.247821	1.558356	O	-2.914742	0.608289	1.511977
O	-1.137145	-1.214438	-0.067701	O	-4.486898	0.816959	3.097392
O	-5.315849	0.50618	0.847916	N	-1.596852	0.062908	-0.342614
N	-4.311307	0.066266	2.826362	H	-1.632029	-0.396642	-1.24761
H	-4.630408	0.938938	3.21986	C	-0.911424	1.358949	-0.407148
H	-3.756434	-0.545989	3.401814	H	-0.870287	1.776373	0.599336
N	-2.367198	0.673407	-0.349801	C	0.517499	1.151905	-0.93893
H	-3.288781	1.06753	-0.488333	C	-1.671595	2.333754	-1.306558
C	-1.259323	1.595295	-0.154406	H	0.996316	0.413925	-0.29251
H	-0.544841	1.133658	0.528735	H	0.460187	0.70812	-1.938236
C	-0.551996	1.913295	-1.494515	C	1.357554	2.426805	-0.981093
C	-1.806939	2.85981	0.484599	O	-2.186316	2.025762	-2.359037
H	-0.295114	0.951744	-1.942578	H	0.921496	3.164838	-1.661662
H	-1.274258	2.390783	-2.163538	H	1.36907	2.905096	0.00522
C	0.705245	2.76847	-1.360814	C	2.829503	2.223723	-1.409484
O	-2.916832	3.301589	0.279718	O	3.514256	3.279251	-1.513914
H	0.468753	3.763047	-0.973385	O	3.236253	1.049942	-1.614391
H	1.387737	2.320619	-0.628232	H	-4.972211	-0.933903	-1.843815
C	1.507019	2.958546	-2.669464	O	-1.695292	3.581952	-0.810355
O	2.466148	3.77707	-2.602948	H	-2.153945	4.15886	-1.443528
O	1.165963	2.293904	-3.683212				
H	-4.019657	-3.374733	-0.941822				
O	-0.907354	3.458031	1.277452				
H	-1.28903	4.288146	1.607826				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.938514	-2.774289	-0.589538	N	-1.390207	-1.868693	-1.769079
H	-1.052669	-3.093113	-0.206448	H	-0.674367	-2.585114	-1.686187
C	-2.256169	-1.453185	-0.053605	C	-1.65392	-1.251416	-0.518639
H	-3.128953	-1.065226	-0.582705	C	-2.03919	-1.907654	0.783327
C	-2.581199	-1.447093	1.461364	C	-1.636509	0.073773	-0.319342
C	-1.06141	-0.527376	-0.314259	H	-2.99094	-2.451289	0.752826
H	-3.344468	-2.210679	1.646477	H	-1.287138	-2.598343	1.179599
H	-1.69613	-1.73076	2.03746	C	-2.172347	-0.719559	1.714837
C	-3.165343	-0.127986	1.951123	O	-1.934876	0.432	1.002689
O	0.096858	-0.947993	-0.31807	O	-2.437593	-0.674706	2.887425
O	-3.88091	0.572379	1.229557	N	-1.472857	1.136174	-1.176614
N	-2.872097	0.216586	3.221219	H	-1.271168	0.810326	-2.11602
H	-3.282675	1.050399	3.614133	C	-0.592258	2.219339	-0.755807
H	-2.299991	-0.362147	3.814543	C	-0.432576	3.226168	-1.871041
N	-1.36165	0.77437	-0.493744	H	-1.004336	2.722709	0.120079
H	-2.318567	1.088682	-0.384661	H	0.418061	1.877815	-0.48579
C	-0.330117	1.77717	-0.619631	O	-0.786931	3.059045	-3.016144
C	-0.943334	3.156364	-0.679849	O	0.191949	4.33143	-1.436061
H	0.366715	1.743957	0.224568	H	0.316574	4.933761	-2.187348
H	0.268138	1.623603	-1.522999	H	-2.218174	-2.323169	-2.145438
O	-2.128685	3.393955	-0.615255				
O	0.002746	4.095754	-0.813003				

H	-0.424924	4.966872	-0.845213				
H	-2.647953	-3.444473	-0.309502				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.713806	-2.850714	2.144005	N	-0.51819	-2.31233	0.658894
H	-1.699879	-2.314289	3.007182	H	-0.54901	-2.775728	1.563323
C	-2.228942	-2.021248	1.058458	C	-1.382358	-1.188072	0.616876
H	-2.096884	-2.56092	0.118267	C	-2.884617	-1.155884	0.743454
C	-3.7312	-1.666327	1.195324	C	-0.958093	0.074794	0.477809
C	-1.411353	-0.723661	1.009269	H	-3.411576	-1.711279	-0.039761
H	-4.278954	-2.593411	1.397152	H	-3.267811	-1.513904	1.706162
H	-3.888614	-1.013044	2.05828	C	-3.186636	0.322887	0.602607
C	-4.353305	-1.065041	-0.060302	O	-2.001778	1.006635	0.461131
O	-0.913577	-0.235896	2.020993	O	-4.237754	0.907176	0.604243
O	-3.872849	-1.245814	-1.184153	N	0.304722	0.622123	0.445076
N	-5.479164	-0.350089	0.126856	H	1.005932	-0.107988	0.524444
H	-5.960335	0.031922	-0.673426	C	0.633879	1.638571	-0.570463
H	-5.873146	-0.199411	1.041498	H	-0.19846	2.340791	-0.618088
N	-1.324936	-0.155406	-0.219256	C	1.917059	2.373732	-0.157742
H	-1.882474	-0.574349	-0.956474	C	0.765669	0.952402	-1.931467
C	-0.788842	1.177743	-0.438726	H	1.762595	2.742899	0.857466
H	-0.303514	1.478744	0.492076	H	2.742761	1.656062	-0.123776
C	0.234095	1.182038	-1.5905	C	2.268943	3.531384	-1.034319
C	-1.954361	2.144742	-0.674458	O	1.812794	0.618805	-2.44663
H	0.90313	0.336626	-1.421032	N	2.827067	3.403107	-2.289895
H	-0.288405	1.000661	-2.53481	C	2.149565	4.889062	-0.844152
C	1.070865	2.416911	-1.678709	H	3.023457	2.52569	-2.750346
O	-2.130634	2.797352	-1.681051	C	3.014323	4.650368	-2.795604
N	0.609075	3.636147	-2.128466	N	2.616324	5.580328	-1.945177
C	2.396033	2.636507	-1.3777	H	1.761088	5.396423	0.025867
H	-0.346475	3.82316	-2.398616	H	3.438202	4.820286	-3.772889
C	1.639541	4.520058	-2.078661	O	-0.434707	0.689126	-2.465755
N	2.744057	3.949182	-1.629932	H	-0.310103	0.183532	-3.286059
H	3.109803	1.91863	-1.002779	H	-0.778774	-3.006834	-0.035763
H	1.531766	5.55127	-2.376544				
O	-2.787725	2.171253	0.372734				
H	-3.528339	2.765394	0.169407				
H	-2.323161	-3.649008	2.2929				
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.477432	-3.531417	-0.770217	N	-3.253726	-2.905894	-1.605582
H	-1.675815	-3.803821	-0.207663	H	-2.928852	-3.867566	-1.548033
C	-3.037935	-2.287604	-0.250832	C	-3.253466	-2.277324	-0.333278
H	-3.798078	-1.930723	-0.948906	C	-4.049492	-2.65081	0.891819
C	-3.705792	-2.425675	1.142636	C	-2.475057	-1.233995	-0.014769
C	-1.912028	-1.250736	-0.15923	H	-5.134779	-2.583405	0.760621
H	-4.434071	-3.241081	1.087747	H	-3.834392	-3.651439	1.284998

H	-2.957317	-2.702366	1.889534	C	-3.598638	-1.609912	1.896597
C	-4.479156	-1.17877	1.547798	O	-2.655873	-0.802381	1.306614
O	-0.756335	-1.577707	0.115495	O	-3.93665	-1.42991	3.037044
O	-5.19404	-0.579099	0.740619	N	-1.476309	-0.581692	-0.705054
N	-4.344076	-0.775247	2.827322	H	-1.424122	-0.964798	-1.643605
H	-4.864487	0.026896	3.149776	C	-1.474054	0.884742	-0.701067
H	-3.76135	-1.266199	3.485651	H	-1.675728	1.217362	0.317056
N	-2.287342	0.031566	-0.346412	C	-0.077032	1.429195	-1.111217
H	-3.26299	0.247207	-0.506729	C	-2.582321	1.428643	-1.60287
C	-1.361299	1.138638	-0.181973	H	0.611443	0.935893	-0.415028
H	-0.678071	0.899063	0.635596	C	0.315441	1.030544	-2.540712
C	-0.51021	1.371744	-1.471763	C	0.025817	2.948541	-0.878742
C	-2.163504	2.367621	0.208771	O	-2.974941	0.880231	-2.608915
H	-0.129949	0.371827	-1.708367	H	-0.339465	1.503772	-3.278311
C	-1.376526	1.852013	-2.642447	H	1.340107	1.339447	-2.754462
C	0.70332	2.279463	-1.210507	H	0.272596	-0.050902	-2.692655
O	-3.34521	2.516801	-0.014224	H	-0.58394	3.476345	-1.619996
H	-1.721871	2.879108	-2.484767	H	-0.407217	3.186705	0.098973
H	-0.8117	1.83067	-3.576082	C	1.463097	3.479165	-0.925773
H	-2.254645	1.214791	-2.774098	H	1.912609	3.35816	-1.914735
H	0.36612	3.307278	-1.044044	H	1.486643	4.545035	-0.682836
H	1.189408	1.960512	-0.281411	H	2.097633	2.956469	-0.202434
C	1.734836	2.253823	-2.344546	O	-3.070567	2.600289	-1.163375
H	1.325861	2.653126	-3.276434	H	-3.739605	2.913055	-1.794596
H	2.608718	2.857225	-2.083681	H	-4.187043	-2.934702	-2.006563
H	2.078804	1.232654	-2.539793				
O	-1.40336	3.29292	0.809644				
H	-1.95245	4.07351	0.990443				
H	-3.162268	-4.277968	-0.703341				

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.349379	-2.602456	-0.148683	N	-2.205334	-1.849941	-1.047677
H	-0.521094	-2.796043	0.407833	H	-2.025474	-2.815147	-0.783766
C	-1.871051	-1.283686	0.196336	C	-2.110072	-0.977275	0.067209
H	-2.658967	-1.024241	-0.51394	C	-2.953769	-0.964566	1.317213
C	-2.47503	-1.193426	1.622715	C	-1.184022	-0.016515	0.188262
C	-0.730717	-0.265021	0.078326	H	-4.016808	-0.769484	1.139866
H	-3.212557	-1.995545	1.727774	H	-2.890244	-1.880251	1.916811
H	-1.695323	-1.363384	2.369524	C	-2.354077	0.187925	2.09739
C	-3.217933	0.113065	1.86425	O	-1.299733	0.706197	1.38371
O	0.434812	-0.570346	0.335662	O	-2.663488	0.652123	3.16315
O	-3.9603	0.595122	1.004704	N	-0.099801	0.328585	-0.589508
N	-3.025824	0.702779	3.061531	H	-0.089391	-0.246096	-1.426977
H	-3.52439	1.552703	3.279063	C	0.120667	1.747113	-0.88807
H	-2.420207	0.30809	3.762655	H	0.09806	2.297666	0.051074
N	-1.104476	0.984937	-0.265806	C	1.494314	1.909932	-1.565202
H	-2.081893	1.186755	-0.433818	C	-0.977896	2.29365	-1.800456
C	-0.162626	2.090778	-0.318994	H	2.234201	1.474315	-0.885309

H	0.613119	1.911649	0.424742	H	1.495606	1.298245	-2.47492
C	0.47419	2.201659	-1.727558	C	1.909744	3.348282	-1.919269
C	-0.904333	3.366576	0.0387	O	-1.466234	1.67548	-2.720077
H	0.895575	1.214318	-1.944447	H	1.155612	3.773979	-2.592655
H	-0.336205	2.368171	-2.445312	C	2.005357	4.247764	-0.678769
C	1.565707	3.268267	-1.914503	C	3.246381	3.321682	-2.67395
O	-2.079091	3.560043	-0.185443	H	2.719996	3.83413	0.041829
H	1.13496	4.251435	-1.69321	H	2.350022	5.248281	-0.95555
C	2.761309	3.047154	-0.976992	H	1.041784	4.359617	-0.176082
C	2.021497	3.274761	-3.380847	H	3.182028	2.709087	-3.578351
H	3.192839	2.05169	-1.131266	H	3.54706	4.3311	-2.969024
H	3.54437	3.785523	-1.172417	H	4.039523	2.906999	-2.041598
H	2.481501	3.136427	0.075445	H	-3.133709	-1.826448	-1.460345
H	1.182569	3.459741	-4.058688	O	-1.33077	3.549764	-1.482228
H	2.772597	4.051539	-3.551522	H	-1.997272	3.856847	-2.119127
H	2.467856	2.311368	-3.652304				
H	-2.035505	-3.318255	0.06954				
O	-0.096819	4.276606	0.60023				
H	-0.604691	5.090727	0.752173				

Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.599702	-3.464517	1.060419	N	-1.988977	0.295861	3.734979
H	-0.645402	-3.559976	0.726431	H	-1.260096	-0.111845	3.157616
C	-2.166923	-2.214752	0.550669	C	-2.828731	1.145967	3.017588
H	-2.489716	-2.296324	-0.498147	C	-4.224527	1.48111	3.45557
C	-3.406324	-1.849305	1.408626	C	-2.539642	1.880847	1.934659
C	-1.058226	-1.1418	0.545429	H	-4.90216	0.622226	3.458755
H	-3.818571	-2.775971	1.811493	H	-4.275469	1.940503	4.448197
H	-3.105385	-1.243424	2.269577	C	-4.668835	2.481527	2.402395
C	-4.489154	-1.083146	0.666828	O	-3.648538	2.697144	1.538269
O	0.126544	-1.447347	0.706683	O	-5.734695	3.037571	2.286216
O	-4.223287	-0.208034	-0.166652	N	-1.380323	2.094694	1.20018
N	-5.760236	-1.397222	0.978647	H	-0.5496	1.984419	1.771103
H	-6.515113	-0.881841	0.551343	C	-1.259124	1.389547	-0.076903
H	-5.987891	-2.115339	1.646734	H	-2.153531	1.598456	-0.667857
N	-1.468206	0.122392	0.325794	C	-0.019374	1.904587	-0.832025
H	-2.451062	0.279184	0.087173	C	-1.169106	-0.123784	0.129989
C	-0.522235	1.214386	0.196785	H	-0.127928	2.991016	-0.897343
H	0.337339	1.002962	0.833725	H	0.869797	1.707659	-0.22166
C	-0.037406	1.367301	-1.266191	C	0.172322	1.317021	-2.233213
C	-1.185029	2.493657	0.680831	O	-0.636165	-0.653131	1.082109
H	0.315176	0.377726	-1.571024	H	0.338171	0.23716	-2.17323
H	-0.898785	1.611905	-1.896709	H	-0.741115	1.462032	-2.820467
C	1.080465	2.394197	-1.463186	C	1.356014	1.970903	-2.956281
O	-2.365711	2.739129	0.575945	H	1.179502	3.04757	-3.054443
H	0.726701	3.395887	-1.201809	H	2.266784	1.843786	-2.360839
H	1.907653	2.166224	-0.781336	C	1.557744	1.356862	-4.334623
C	1.595735	2.398977	-2.907523	H	1.792145	0.294075	-4.276847

H	1.96156	1.401074	-3.172858	H	0.684236	1.491689	-4.972141
H	0.775268	2.638138	-3.592956	N	2.713927	2.009481	-5.053342
C	2.716806	3.414999	-3.075291	H	3.585725	1.909218	-4.528501
H	2.380366	4.430899	-2.868911	H	2.864446	1.594655	-5.974959
H	3.568375	3.188084	-2.433962	H	2.553117	3.009662	-5.191505
N	3.240712	3.418922	-4.490621	H	-2.49226	-0.436306	4.220704
H	2.509744	3.668682	-5.160093	O	-1.721771	-0.812558	-0.878634
H	4.002807	4.089958	-4.605079	H	-1.592782	-1.762134	-0.717456
H	3.600212	2.500105	-4.758891				
H	-2.131128	-4.252725	0.70534				
O	-0.294905	3.349231	1.207625				
H	-0.757012	4.170564	1.443683				
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.602011	-3.254409	-0.740085	N	-3.412941	-2.44574	-0.872782
H	-1.769357	-3.589987	-0.263481	H	-3.39134	-3.391583	-0.500537
C	-3.012123	-1.976078	-0.16695	C	-3.435894	-1.477058	0.163668
H	-3.806655	-1.555885	-0.787288	C	-4.493295	-1.262179	1.217258
C	-3.55202	-2.076015	1.283607	C	-2.452469	-0.594936	0.385413
C	-1.807247	-1.027545	-0.186937	H	-5.476487	-0.99183	0.81759
H	-4.327222	-2.849196	1.300851	H	-4.642321	-2.114588	1.890349
H	-2.755566	-2.397555	1.959986	C	-3.93096	-0.094977	2.003365
C	-4.214279	-0.790367	1.76013	O	-2.711481	0.2522	1.470944
O	-0.653942	-1.444205	-0.073734	O	-4.382929	0.500301	2.945677
O	-4.917369	-0.11264	1.005763	N	-1.209882	-0.430305	-0.189843
N	-4.000465	-0.445707	3.045751	H	-1.106754	-1.086337	-0.958738
H	-4.453683	0.374959	3.419062	C	-0.791184	0.923371	-0.560348
H	-3.429868	-1.001556	3.66174	H	-0.950763	1.580562	0.294702
N	-2.104409	0.286401	-0.282945	C	0.707393	0.903715	-0.918464
H	-3.071891	0.580626	-0.33296	C	-1.610445	1.451001	-1.740324
C	-1.081253	1.313288	-0.216763	H	1.229268	0.476789	-0.058104
H	-0.292574	0.9775	0.459019	H	0.859656	0.225046	-1.764327
C	-0.469218	1.569114	-1.618876	C	1.273387	2.285692	-1.245216
C	-1.706635	2.577869	0.348791	O	-1.97899	0.767448	-2.668554
H	-0.174581	0.587109	-1.99778	H	0.814464	2.702693	-2.144516
H	-1.252586	1.953822	-2.278739	H	1.098168	2.979924	-0.418883
C	0.738487	2.504703	-1.610339	S	3.081652	2.168543	-1.533851
O	-2.878793	2.864633	0.250395	C	3.424075	3.917258	-1.933819
H	0.459086	3.515621	-1.308868	H	3.163934	4.560174	-1.090847
H	1.503124	2.139874	-0.918748	H	4.493831	3.996551	-2.131961
S	1.470039	2.590917	-3.291993	H	2.868037	4.221757	-2.822515
C	2.81218	3.785473	-2.964427	O	-1.856803	2.766926	-1.640855
H	3.500931	3.390437	-2.215244	H	-2.338577	3.055987	-2.433815
H	3.346281	3.93234	-3.904216	H	-4.239318	-2.380281	-1.460608
H	2.401451	4.739666	-2.628991				
O	-0.795835	3.360261	0.942905				
H	-1.230298	4.178439	1.235835				
H	-3.330502	-3.948009	-0.602325				

Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.41605	-3.175913	0.617888	N	-2.554845	-2.496469	-0.829825
H	-0.622418	-3.132562	1.251461	H	-2.436672	-3.424111	-0.430803
C	-2.122073	-1.898671	0.630541	C	-2.649468	-1.502829	0.178525
H	-2.875096	-1.909548	-0.160356	C	-3.705123	-1.352294	1.245064
C	-2.847365	-1.587896	1.966488	C	-1.747673	-0.528264	0.35561
C	-1.110609	-0.782286	0.34575	H	-4.714996	-1.184799	0.855775
H	-3.486242	-2.443262	2.20896	H	-3.765207	-2.193431	1.94551
H	-2.116835	-1.484969	2.772949	C	-3.239352	-0.114823	1.98569
C	-3.763184	-0.37532	1.872848	O	-2.065462	0.325069	1.42043
O	0.061922	-0.86201	0.713443	O	-3.728804	0.465878	2.918308
O	-4.47039	-0.181712	0.880372	N	-0.536779	-0.265673	-0.250399
N	-3.76364	0.461485	2.929904	H	-0.383256	-0.935189	-0.99905
H	-4.382232	1.258731	2.927956	C	-0.260624	1.1092	-0.674535
H	-3.186208	0.303229	3.739634	H	-0.442752	1.775497	0.167989
N	-1.609827	0.306252	-0.27843	C	1.218641	1.219138	-1.106446
H	-2.589033	0.334173	-0.533258	C	-1.168979	1.522784	-1.834949
C	-0.808544	1.489784	-0.523051	H	1.81766	0.880028	-0.25769
H	-0.095739	1.607874	0.293623	H	1.390074	0.521243	-1.931369
C	-0.023393	1.362161	-1.863151	C	1.617476	2.618736	-1.51396
C	-1.731133	2.695875	-0.560078	O	-1.415848	0.810293	-2.782445
H	0.513764	0.41291	-1.797674	C	1.713725	2.975041	-2.863863
H	-0.748913	1.275421	-2.676013	C	1.869172	3.594448	-0.540417
C	0.942942	2.492326	-2.120273	H	1.525486	2.228503	-3.628522
O	-2.879649	2.660427	-0.944433	C	2.04889	4.278969	-3.235976
C	0.645269	3.501862	-3.042271	C	2.204036	4.897855	-0.907336
C	2.153265	2.558742	-1.417207	H	1.804402	3.330536	0.510465
H	-0.287169	3.46244	-3.596057	H	2.120605	4.5373	-4.286548
C	1.533324	4.558281	-3.256173	C	2.29343	5.244676	-2.258303
C	3.042446	3.61302	-1.625644	H	2.398288	5.640245	-0.141346
H	2.400061	1.778523	-0.704121	H	2.555463	6.256856	-2.544809
H	1.287424	5.331016	-3.97596	O	-1.652006	2.765629	-1.693322
C	2.73408	4.618021	-2.546643	H	-2.185109	2.983739	-2.475979
H	3.975569	3.64816	-1.074498	H	-3.395084	-2.527404	-1.400634
H	3.425326	5.436675	-2.711821				
O	-1.115394	3.812005	-0.154767				
H	-1.724893	4.560874	-0.263116				
H	-2.027437	-3.916173	0.948048				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.830458	-3.363075	0.473504	N	-1.413736	-2.023155	-1.053024
H	-0.018882	-3.449598	1.079189	H	-1.298564	-3.018701	-0.882344
C	-1.183231	-1.953648	0.321619	C	-1.029751	-1.252818	0.074777
H	-1.955403	-1.871148	-0.446215	C	-1.629248	-1.256955	1.458728
C	-1.726668	-1.298417	1.615491	C	-0.001917	-0.394297	0.078133
C	0.063631	-1.194152	-0.147476	H	-2.680024	-0.950341	1.492796

H	-2.481422	-1.968392	2.042093	H	-1.556565	-2.21802	1.980951
H	-0.93092	-1.210083	2.361216	C	-0.780794	-0.228303	2.179277
C	-2.412049	0.047994	1.407192	O	0.177717	0.242551	1.312135
O	1.19996	-1.552892	0.158192	O	-0.842399	0.179497	3.308869
O	-2.775492	0.442065	0.29359	N	0.95348	-0.095851	-0.872025
N	-2.628154	0.770375	2.522924	H	0.756966	-0.620438	-1.720137
H	-3.117068	1.65024	2.455311	C	1.230136	1.314259	-1.152507
H	-2.33848	0.450439	3.433116	H	1.338658	1.849736	-0.21029
N	-0.174166	-0.083875	-0.884228	C	2.540166	1.404	-1.939118
H	-1.130605	0.259427	-0.890006	C	0.09718	1.946617	-1.965874
C	0.900376	0.830688	-1.20947	H	3.337268	0.969606	-1.327201
H	1.683339	0.302363	-1.755085	H	2.446599	0.821287	-2.863879
C	0.333214	1.950073	-2.0906	O	2.781848	2.778755	-2.221847
C	1.514413	1.423844	0.063148	O	-0.390523	1.423906	-2.943398
H	-0.124856	1.491244	-2.974018	H	3.559648	2.846266	-2.786184
H	-0.441426	2.4917	-1.533389	O	-0.301392	3.127346	-1.474625
O	1.40561	2.812017	-2.448258	H	-1.008739	3.47826	-2.04133
O	0.869194	1.772126	1.025593	H	-2.391419	-1.876492	-1.288196
H	1.049048	3.5547	-2.947789				
O	2.846931	1.535366	-0.020289				
H	3.173383	1.95075	0.794734				
H	-1.592661	-3.86852	0.914161				
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.074373	-3.623279	0.464807	N	-3.818829	0.421766	-1.520285
H	-1.403804	-3.830412	1.199905	H	-4.43474	-0.326524	-1.827053
C	-2.24994	-2.176673	0.354573	C	-3.251854	0.14724	-0.24829
H	-2.841157	-1.967471	-0.53949	C	-3.959392	-0.026948	1.072015
C	-2.975983	-1.537611	1.563485	C	-1.940179	-0.028272	-0.036633
C	-0.865567	-1.535049	0.192492	H	-4.515	0.856284	1.405838
H	-3.846064	-2.158811	1.803679	H	-4.653043	-0.875405	1.109523
H	-2.331355	-1.549483	2.447418	C	-2.807203	-0.282648	2.022097
C	-3.507387	-0.130403	1.312664	O	-1.633019	-0.283553	1.306354
O	0.144498	-2.045069	0.677197	O	-2.802421	-0.46887	3.210546
O	-3.616994	0.345158	0.178258	N	-0.86756	-0.094575	-0.892668
N	-3.890505	0.549899	2.410874	H	-1.149303	0.129771	-1.840388
H	-4.289802	1.47055	2.308643	C	0.39225	0.526633	-0.518819
H	-3.802678	0.164179	3.33715	H	0.654952	0.221734	0.495399
N	-0.845748	-0.3696	-0.492904	C	1.524272	0.055776	-1.451923
H	-1.737871	0.079281	-0.675629	C	0.310402	2.056875	-0.526461
C	0.338897	0.450697	-0.548154	H	2.436741	0.577573	-1.14353
H	1.211957	-0.194125	-0.666834	C	1.749856	-1.449604	-1.388456
C	0.290031	1.413831	-1.746846	O	1.143221	0.487935	-2.76557
C	0.535829	1.218385	0.76297	O	-0.606585	2.70159	-0.978412
H	1.197548	2.02526	-1.709043	H	0.846031	-1.989039	-1.676055
C	0.221082	0.681309	-3.081725	H	2.561215	-1.73103	-2.065285
O	-0.860376	2.242441	-1.530222	H	2.034888	-1.749547	-0.376233
O	-0.250496	1.249127	1.679139	H	1.805139	0.186267	-3.397716

H	-0.670074	0.052983	-3.136872	H	-4.374692	1.272436	-1.504993
H	0.190152	1.405513	-3.900127	O	1.396081	2.606816	0.045064
H	1.105718	0.053588	-3.218354	H	1.312292	3.573396	0.005717
H	-0.959609	2.84058	-2.279535				
H	-2.952367	-4.062779	0.722703				
O	1.719358	1.855657	0.775744				
H	1.804207	2.334617	1.615802				
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.187528	-2.400155	1.565583	N	-2.217661	-3.101106	-0.156411
H	-1.816699	-1.860949	2.343333	H	-1.647624	-3.840234	0.246609
C	-3.256646	-1.648379	0.915927	C	-2.612628	-2.153391	0.822945
H	-3.538137	-2.166608	-0.003174	C	-3.47404	-2.373349	2.041157
C	-4.536537	-1.491437	1.778652	C	-2.225116	-0.870995	0.822029
C	-2.724332	-0.254758	0.563648	H	-4.49411	-2.702387	1.815823
H	-4.840588	-2.488174	2.114375	H	-3.059751	-3.082489	2.767361
H	-4.315926	-0.898577	2.670226	C	-3.516261	-0.989803	2.658469
C	-5.710481	-0.921523	0.994353	O	-2.747907	-0.14062	1.897758
O	-1.884442	0.313417	1.26383	O	-4.086248	-0.591634	3.639939
O	-5.940986	-1.278198	-0.164211	N	-1.349492	-0.168402	0.021485
N	-6.482064	-0.021077	1.6358	H	-1.008917	-0.775318	-0.718747
H	-7.293525	0.35548	1.168908	C	-1.77471	1.137539	-0.489101
H	-6.294148	0.268904	2.581581	H	-2.134577	1.735391	0.347073
N	-3.277719	0.322662	-0.523645	C	-0.570721	1.843693	-1.153098
H	-3.994378	-0.165763	-1.045483	C	-2.903735	0.991334	-1.510341
C	-2.949408	1.680891	-0.910597	H	0.217453	1.894895	-0.395631
H	-2.795795	2.274692	-0.008975	H	-0.202109	1.208518	-1.964362
C	-1.641607	1.724197	-1.764774	C	-0.899804	3.206611	-1.676954
C	-4.112572	2.258781	-1.691763	O	-2.903206	0.168905	-2.399613
H	-0.943537	1.056681	-1.251695	C	-1.02343	3.576908	-2.994791
H	-1.846337	1.287585	-2.745926	C	-1.194208	4.380187	-0.89455
C	-1.04373	3.086646	-1.891696	H	-0.886605	2.98699	-3.88782
O	-4.90516	1.596875	-2.32721	N	-1.375855	4.907358	-3.079463
C	-0.967748	3.872065	-3.015971	C	-1.488351	5.429566	-1.80997
C	-0.446061	3.845097	-0.822639	C	-1.233459	4.64728	0.485006
H	-1.307213	3.668497	-4.019705	H	-1.512664	5.417037	-3.937152
N	-0.360414	5.073155	-2.710915	C	-1.817087	6.720212	-1.383936
C	-0.027988	5.088202	-1.374086	C	-1.559693	5.929076	0.913469
C	-0.223459	3.588117	0.541743	H	-1.009704	3.867464	1.204822
H	-0.175103	5.812237	-3.369111	H	-2.037812	7.507059	-2.095908
C	0.60169	6.069783	-0.602376	C	-1.849914	6.954697	-0.012773
C	0.401593	4.562725	1.312157	H	-1.593199	6.148435	1.974764
H	-0.535356	2.645241	0.979259	H	-2.102274	7.944255	0.351351
H	0.915788	7.011198	-1.038268	O	-3.892702	1.876933	-1.319269
C	0.809061	5.79063	0.745387	H	-4.557561	1.756145	-2.01762
H	0.581185	4.381057	2.366053	H	-3.022444	-3.551005	-0.58375
H	1.293819	6.530597	1.372406				
O	-4.140249	3.595303	-1.633089				

H	-4.86051	3.915776	-2.200866				
H	-2.551606	-3.268724	1.944784				
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.749734	-2.200547	1.889927	N	-0.858914	-1.233634	-0.298535
H	-1.125535	-2.034458	2.819471	H	-0.499641	-1.44541	0.628083
C	-1.517312	-1.441828	0.905774	C	-2.207749	-0.795499	-0.246854
H	-1.000171	-1.49947	-0.054774	C	-3.397047	-1.487675	0.370602
C	-2.961413	-1.961698	0.697531	C	-2.640477	0.348217	-0.795064
C	-1.559336	0.026074	1.351963	H	-3.649612	-2.451859	-0.086427
H	-2.918333	-3.052424	0.602299	H	-3.311143	-1.656341	1.449439
H	-3.574575	-1.750278	1.578749	C	-4.51687	-0.50156	0.104361
C	-3.650066	-1.446761	-0.562285	O	-4.010589	0.563549	-0.604835
O	-1.468212	0.35304	2.535568	O	-5.679555	-0.540257	0.408941
O	-3.031897	-0.900786	-1.48275	N	-2.007933	1.302842	-1.557085
N	-4.979282	-1.655055	-0.624174	H	-1.015049	1.099926	-1.598852
H	-5.484318	-1.383262	-1.454128	C	-2.289254	2.708517	-1.278858
H	-5.4847	-2.112522	0.117448	H	-2.451181	2.881481	-0.209346
N	-1.737387	0.923343	0.358765	C	-1.102258	3.592344	-1.742351
H	-1.969861	0.555549	-0.55807	C	-3.539375	3.174388	-2.01863
C	-1.973948	2.319804	0.636926	H	-0.970287	3.4587	-2.819558
H	-1.184682	2.694078	1.292276	H	-1.380387	4.634915	-1.571144
C	-1.976804	3.142217	-0.67563	C	0.176356	3.257748	-1.009518
C	-3.304669	2.521797	1.359783	O	-3.940873	2.744298	-3.073872
H	-2.808896	2.803256	-1.300208	C	1.207572	2.550554	-1.635295
H	-2.172753	4.183873	-0.412091	C	0.344902	3.618034	0.335493
C	-0.673218	3.019138	-1.428764	H	1.109647	2.265818	-2.677796
O	-4.247205	1.76639	1.313491	C	2.373044	2.205214	-0.947614
C	-0.555131	2.176764	-2.538102	C	1.499603	3.282906	1.034148
C	0.464801	3.720443	-1.008354	H	-0.437502	4.170991	0.845042
H	-1.420625	1.624924	-2.890212	H	3.161916	1.656395	-1.450963
C	0.65871	2.02871	-3.210931	C	2.518797	2.572021	0.39104
C	1.683229	3.583694	-1.667177	H	1.626552	3.56753	2.071835
H	0.399747	4.384581	-0.152538	O	3.632688	2.27068	1.125876
H	0.729958	1.371498	-4.071188	H	4.269533	1.790786	0.582467
C	1.782165	2.732282	-2.771914	H	-0.757573	-2.078845	-0.854304
H	2.559453	4.130514	-1.33967	O	-4.122301	4.19573	-1.364407
O	3.003475	2.634059	-3.382705	H	-4.871284	4.513846	-1.893755
H	2.955242	2.017282	-4.12324				
H	-0.828268	-3.195324	1.703511				
O	-3.316681	3.687623	2.028772				
H	-4.192936	3.806284	2.429615				
Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.508764	-3.513843	-0.516176	N	-3.36288	-2.443965	-0.81557
H	-1.588223	-3.918286	-0.366745	H	-3.226691	-3.444001	-0.937954
C	-2.598611	-2.235046	0.181603	C	-2.635015	-1.950281	0.298144

H	-3.528348	-1.743	-0.111899	C	-2.787603	-2.322741	1.751421
C	-2.5974	-2.354963	1.728934	C	-1.632257	-1.066335	0.204262
C	-1.410966	-1.364905	-0.246575	H	-3.769979	-2.08803	2.17506
H	-3.389464	-3.055034	2.012624	H	-2.585128	-3.377211	1.973188
H	-1.647623	-2.775303	2.06939	C	-1.7341	-1.45974	2.415886
C	-2.91582	-1.034491	2.415452	O	-1.072033	-0.742965	1.447819
O	-0.311335	-1.857536	-0.503836	O	-1.439951	-1.3442	3.576637
O	-3.831542	-0.311314	2.014595	N	-0.998453	-0.499464	-0.880348
N	-2.150634	-0.705417	3.475707	H	-1.475772	-0.790842	-1.727408
H	-2.342355	0.14874	3.977599	C	-0.736148	0.942566	-0.856005
H	-1.400633	-1.294507	3.798659	H	-0.326979	1.194286	0.122446
N	-1.642464	-0.035807	-0.266285	C	0.325604	1.317162	-1.926548
H	-2.547982	0.317741	0.014918	C	-2.03132	1.733108	-1.042724
C	-0.588375	0.927018	-0.53505	H	1.170187	0.657064	-1.701759
H	0.34035	0.55556	-0.096571	C	-0.13823	1.032252	-3.361337
C	-0.359657	1.111513	-2.069107	C	0.800043	2.768461	-1.778335
C	-0.955728	2.230137	0.15307	O	-2.973125	1.355466	-1.703943
H	-0.275736	0.08452	-2.438121	H	-0.996125	1.65406	-3.633596
C	-1.556654	1.777531	-2.756527	H	0.671878	1.254743	-4.060546
C	0.953635	1.834565	-2.385353	H	-0.416567	-0.014436	-3.509472
O	-2.081263	2.545467	0.472634	H	1.128229	2.981056	-0.757073
H	-1.661144	2.823177	-2.44884	H	1.641798	2.951647	-2.450967
H	-1.420962	1.763312	-3.840897	H	0.008657	3.478756	-2.032626
H	-2.491966	1.260411	-2.52724	H	-4.3618	-2.295336	-0.702462
H	1.802086	1.358933	-1.884738	O	-2.007441	2.912111	-0.399282
H	1.138002	1.807404	-3.462667	H	-2.83655	3.383182	-0.585388
H	0.921917	2.881853	-2.075742				
H	-3.190723	-4.165595	-0.140792				
O	0.112947	3.015562	0.343046				
H	-0.184445	3.851541	0.738425				

Table S14.F. Isoimide Hydrolysis into Asp-X XYZ Coordinates (Implicit solvation, ε = 80)

All Reactions			
H_2O			
Reactant Structure			
Atom	X	Y	Z
O	-0.999631	0.482902	0
H	-0.03661	0.526297	0
H	-1.280189	1.405171	0

Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.807882	-2.438342	-0.867872	N	-2.674286	-1.236602	0.118869
H	-1.207004	-3.206044	-0.579699	H	-1.998271	-1.239167	0.878314
C	-2.065254	-1.543932	0.203586	C	-3.564933	-0.078924	0.22164
C	-2.776582	-1.823895	1.503468	C	-4.098906	0.206237	1.631005

C	-1.664967	-0.265381	0.222698	C	-2.922425	1.190322	-0.358445
H	-3.821172	-2.132513	1.387401	H	-3.277865	0.33627	2.342649
H	-2.288425	-2.573892	2.136992	H	-4.668122	1.140506	1.64167
C	-2.724787	-0.476223	2.194155	C	-5.007798	-0.886573	2.133007
O	-2.042961	0.408065	1.391906	O	-3.433303	2.301291	-0.202845
O	-3.165404	-0.127749	3.257867	O	-5.295435	-0.734286	3.439486
N	-0.882987	0.472428	-0.638615	N	-1.793	0.994631	-1.065858
H	-0.672258	-0.080277	-1.463679	H	-1.507754	0.033172	-1.204543
C	-1.283142	1.839423	-0.96295	C	-1.128086	2.070536	-1.763118
H	-1.472495	2.373088	-0.030769	H	-1.040189	2.925453	-1.088878
C	-0.1588	2.548336	-1.730263	C	0.26828	1.63252	-2.224869
C	-2.567033	1.882329	-1.79307	C	-1.948079	2.535762	-2.967528
H	0.061541	2.022589	-2.663605	H	0.201344	0.782662	-2.909533
H	-0.445886	3.573466	-1.968444	H	0.77099	2.453609	-2.736625
H	0.743254	2.565179	-1.116697	H	0.86518	1.340659	-1.358874
O	-2.983114	0.970677	-2.471338	O	-2.782818	1.880381	-3.546183
H	-2.665868	-2.853237	-1.220758	H	-3.216788	-2.089209	0.206394
O	-3.173566	3.078463	-1.703242	O	-1.591558	3.778252	-3.337323
H	-3.956422	3.075394	-2.278074	H	-2.095095	4.022246	-4.130628
				O	-5.453532	-1.796592	1.466158
				H	-5.898143	-1.44748	3.705658
				H	-4.421937	-0.275858	-0.431038
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.925407	-3.019957	-0.755598	N	-3.91028	-1.789416	-0.124624
H	-3.85229	-4.002934	-0.50657	H	-3.391228	-2.626559	-0.373056
C	-3.617042	-2.178292	0.344255	C	-3.636275	-1.383341	1.251113
C	-4.336497	-2.065945	1.664999	C	-3.472164	-2.54901	2.260437
C	-2.566427	-1.34794	0.379076	C	-2.394353	-0.477223	1.344962
H	-5.376028	-1.731045	1.582891	H	-2.654067	-3.195211	1.939123
H	-4.340876	-2.98742	2.258884	H	-3.2269	-2.139684	3.24303
C	-3.522847	-1.009479	2.38506	C	-4.722235	-3.394066	2.333129
O	-2.477395	-0.627311	1.577201	O	-1.916972	-0.147517	2.431354
O	-3.670974	-0.51862	3.472961	O	-5.771259	-2.877571	3.011752
N	-1.520261	-1.142492	-0.495508	N	-1.895857	-0.061045	0.166993
H	-1.665089	-1.703835	-1.329741	H	-2.414882	-0.322283	-0.662443
C	-1.142142	0.235542	-0.815496	C	-0.77167	0.845808	0.09173
H	-1.013508	0.784009	0.118008	H	0.048219	0.448902	0.694838
C	0.188413	0.223177	-1.588449	C	-0.322857	0.977664	-1.375309
C	-2.228287	0.929865	-1.640732	C	-1.148438	2.213654	0.667194
H	0.904703	-0.323853	-0.969256	H	-0.160657	-0.037486	-1.750397
H	0.053584	-0.350774	-2.511968	H	-1.143041	1.411566	-1.957439
C	0.734703	1.615982	-1.914135	C	0.953349	1.801244	-1.566355
O	-2.890038	0.378956	-2.49111	O	-2.238557	2.727015	0.572913
H	0.048551	2.149489	-2.57916	H	0.801201	2.82978	-1.226857
H	0.82265	2.206988	-0.996747	H	1.762962	1.376224	-0.964201
C	2.10346	1.514899	-2.58403	C	1.367247	1.813857	-3.036191
H	2.809024	1.024007	-1.906708	H	1.54126	0.790679	-3.383516

H	2.028048	0.916546	-3.498318	H	0.566858	2.252892	-3.641234
N	2.604975	2.852041	-2.912573	N	2.596206	2.59281	-3.208033
H	1.973161	3.630699	-2.797485	H	2.961672	3.078291	-2.402098
C	3.803983	3.106435	-3.434516	C	3.249598	2.730137	-4.360783
N	4.665108	2.112642	-3.667218	N	2.775416	2.16706	-5.475964
N	4.150359	4.365033	-3.735294	N	4.388635	3.432687	-4.407141
H	4.407319	1.149111	-3.536169	H	1.853633	1.764989	-5.510378
H	5.569072	2.296547	-4.071186	H	3.258266	2.278455	-6.352766
H	3.571132	5.140193	-3.455671	H	4.848991	3.728788	-3.561684
H	5.080811	4.579875	-4.055478	H	4.907215	3.51837	-5.26642
H	-4.875672	-2.869959	-1.083094	H	-4.893551	-1.994885	-0.258528
O	-2.349855	2.230066	-1.329305	O	-0.096167	2.803639	1.257335
H	-3.019339	2.629318	-1.909582	H	-0.36427	3.687378	1.558065
				O	-4.847305	-4.47136	1.797664
				H	-4.46399	-0.743687	1.575422
				H	-5.547227	-2.035524	3.431827

Asn-Asn

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.149386	-2.30362	0.368802	N	-2.232504	-2.587521	-0.733181
H	-3.026965	-3.311868	0.413378	H	-1.406906	-2.923266	-0.243922
C	-2.116385	-1.620346	1.061159	C	-3.092994	-1.81559	0.163492
C	-1.784827	-1.672196	2.53151	C	-3.322935	-2.442837	1.545548
C	-1.223361	-0.8165	0.469064	C	-2.603114	-0.367877	0.324639
H	-2.586263	-1.312672	3.185813	H	-2.36566	-2.625194	2.045874
H	-1.491924	-2.663752	2.89624	H	-3.884357	-1.75338	2.184161
C	-0.599245	-0.733392	2.6268	C	-4.098893	-3.739321	1.466461
O	-0.30288	-0.263849	1.368302	O	-3.087433	0.384269	1.170745
O	0.047944	-0.38834	3.579916	O	-4.641076	-4.160903	0.470347
N	-0.988053	-0.512165	-0.855297	N	-1.636242	0.006936	-0.538441
H	-1.710132	-0.934662	-1.431011	H	-1.402133	-0.665314	-1.259506
C	-0.724597	0.878685	-1.211209	C	-1.163662	1.366724	-0.620364
H	0.038449	1.275056	-0.541468	H	-1.151774	1.790717	0.385906
C	-0.181363	0.950331	-2.652004	C	0.270634	1.411652	-1.182216
C	-1.980283	1.746598	-1.08436	C	-2.116105	2.224735	-1.459335
H	0.581302	0.173127	-2.745305	H	0.830974	0.597472	-0.714108
H	-0.971977	0.727096	-3.372333	H	0.274875	1.234402	-2.260082
C	0.511096	2.276538	-2.94623	C	1.004681	2.696163	-0.808858
O	-3.112027	1.320561	-1.101076	O	-3.052629	1.807811	-2.098439
O	1.390798	2.708876	-2.202922	O	0.982339	3.129361	0.341911
N	0.129142	2.913784	-4.071647	N	1.710634	3.283405	-1.795986
H	0.581747	3.778929	-4.325717	H	2.247487	4.112689	-1.591551
H	-0.603984	2.563785	-4.66637	H	1.702213	2.938967	-2.741992
H	-4.061759	-2.100361	0.76757	H	-2.73385	-3.406129	-1.060641
O	-1.675568	3.049626	-0.982299	O	-1.769974	3.52118	-1.405855
H	-2.500437	3.562127	-0.955284	H	-2.375598	4.028729	-1.970134
				O	-4.189229	-4.449815	2.610396
				H	-4.066677	-1.722763	-0.328489
				H	-3.718049	-4.014572	3.335012

Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-5.066713	-1.93482	-1.371556	N	-5.824712	0.628534	0.5937
H	-4.961427	-2.945999	-1.366163	H	-6.008325	-0.156112	-0.026304
C	-4.759022	-1.368747	-0.106957	C	-4.80288	0.27992	1.582752
C	-5.463203	-1.585176	1.208737	C	-4.981609	-1.092206	2.245078
C	-3.724943	-0.544807	0.11177	C	-3.383682	0.398901	1.006353
H	-6.510564	-1.264407	1.216712	H	-5.026147	-1.887475	1.494787
H	-5.441055	-2.619507	1.571915	H	-4.12545	-1.320278	2.886908
C	-4.661762	-0.707866	2.149168	C	-6.221756	-1.162274	3.098771
O	-3.636052	-0.123109	1.445607	O	-2.400683	-0.019109	1.623182
O	-4.805904	-0.489019	3.323401	O	-6.915866	-0.219255	3.415904
N	-2.697402	-0.112834	-0.696747	N	-3.292084	1.013461	-0.187172
H	-2.85275	-0.440425	-1.645047	H	-4.14696	1.403535	-0.563136
C	-2.311627	1.300275	-0.648088	C	-2.014993	1.291226	-0.810942
H	-2.077065	1.566222	0.381625	H	-1.421315	0.377024	-0.843695
C	-1.059463	1.527726	-1.512046	C	-2.221603	1.800689	-2.24868
C	-3.442938	2.200937	-1.145319	C	-1.242549	2.329008	0.004373
H	-0.334294	0.762889	-1.220823	H	-2.923613	1.115038	-2.733217
H	-1.30631	1.385652	-2.567073	H	-2.671031	2.796079	-2.232582
C	-0.409105	2.914938	-1.287144	C	-0.921353	1.802464	-3.091498
O	-4.23674	1.888688	-2.005553	O	-1.745855	3.211729	0.661843
O	-0.033644	3.162446	-0.111267	O	-0.32212	0.699833	-3.18418
O	-0.295706	3.665814	-2.290999	O	-0.591612	2.891592	-3.628829
O	-3.449221	3.39788	-0.536321	O	0.085287	2.176346	-0.128248
H	-4.153338	3.939749	-0.929039	H	0.525319	2.893464	0.356371
H	-6.026767	-1.740974	-1.642422	H	-6.696509	0.837819	1.068191
				O	-6.480195	-2.421688	3.499059
				H	-7.272321	-2.408243	4.060396
				H	-4.845369	1.041902	2.36811
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.265565	-1.256197	-1.715681	N	-3.804639	-0.641783	0.002536
H	-3.046508	-2.21842	-1.960265	H	-3.537596	-1.434488	-0.57371
C	-2.911281	-0.963728	-0.373581	C	-2.881265	-0.459994	1.119121
C	-3.463774	-1.565801	0.89383	C	-2.354943	-1.770162	1.756602
C	-1.963683	-0.083251	-0.026483	C	-1.675999	0.42351	0.732413
H	-4.536141	-1.397544	1.038897	H	-1.851778	-2.369053	0.996351
H	-3.289225	-2.642993	0.998354	H	-1.633091	-1.523927	2.538275
C	-2.687819	-0.826026	1.965369	C	-3.484482	-2.598514	2.322301
O	-1.800571	0.032364	1.358334	O	-0.697598	0.527771	1.468377
O	-2.750552	-0.899522	3.163946	O	-4.027729	-2.177563	3.486764
N	-1.069064	0.648298	-0.776803	N	-1.819724	1.079159	-0.439304
H	-1.209482	0.463109	-1.765387	H	-2.684916	0.902247	-0.939345
C	-0.873444	2.079034	-0.475259	C	-0.82216	1.986285	-0.980155
H	-0.820849	2.187055	0.607469	H	0.016558	1.990046	-0.283008
C	0.430686	2.549628	-1.112602	C	-0.361252	1.522187	-2.36342

C	-2.081815	2.863159	-0.98993	C	-1.423994	3.393743	-1.011994
H	1.246793	1.933379	-0.734384	H	-0.004906	0.494477	-2.283791
H	0.393388	2.448095	-2.197636	H	-1.183757	1.550256	-3.078511
S	0.876049	4.279207	-0.685341	S	1.056994	2.479258	-3.032645
O	-2.151733	3.394052	-2.076819	O	-1.839147	3.946412	-2.0055
H	-0.060012	4.877194	-1.444791	H	0.375456	3.608655	-3.296818
H	-4.262165	-1.132813	-1.871995	H	-4.749093	-0.810497	0.328575
O	-3.099062	2.822679	-0.115762	O	-1.470313	3.933622	0.213995
H	-3.871736	3.257183	-0.513351	H	-1.902809	4.80142	0.157012
				O	-3.944465	-3.579936	1.7856
				H	-3.404562	0.125074	1.882985
				H	-3.559959	-1.410643	3.845909
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.405637	-3.272387	-0.813647	N	-2.819112	-2.395601	-0.863774
H	-2.276636	-4.117653	-0.263582	H	-2.035801	-2.995241	-0.617227
C	-2.813433	-2.179744	-0.005484	C	-3.22454	-1.574737	0.278893
C	-4.081046	-2.035022	0.798681	C	-3.315493	-2.321464	1.61561
C	-2.073251	-1.081493	0.196396	C	-2.332004	-0.334645	0.434706
H	-4.997564	-2.051729	0.199331	H	-2.367414	-2.812152	1.85605
H	-4.201959	-2.78112	1.592848	H	-3.516967	-1.621043	2.431433
C	-3.911566	-0.663663	1.421055	C	-4.412284	-3.355452	1.622146
O	-2.695291	-0.149415	1.037509	O	-2.391995	0.386494	1.432694
O	-4.644591	-0.038265	2.140913	O	-5.270322	-3.480275	0.773828
N	-0.793605	-0.743728	-0.189763	N	-1.514579	-0.07605	-0.603523
H	-0.423411	-1.469015	-0.796913	H	-1.600916	-0.679846	-1.411577
C	-0.56036	0.599401	-0.7253	C	-0.68285	1.106413	-0.645094
H	-0.976681	1.32624	-0.027071	H	-0.088577	1.159716	0.270298
C	0.954538	0.830519	-0.85973	C	0.250653	1.027847	-1.866407
C	-1.247328	0.780146	-2.080862	C	-1.549317	2.36687	-0.706182
H	1.40018	0.626791	0.114979	H	0.786351	0.07807	-1.809792
H	1.364853	0.099703	-1.565043	H	-0.356231	1.006344	-2.777584
C	1.325821	2.248338	-1.30155	C	1.268101	2.167924	-1.941409
O	-1.337717	-0.089988	-2.917286	O	-2.606624	2.452977	-1.285924
H	0.950218	2.466176	-2.303543	H	0.776988	3.133665	-2.075437
H	0.866055	2.980311	-0.62733	H	1.829496	2.228547	-1.001944
C	2.829866	2.483962	-1.23483	C	2.293421	1.93346	-3.04442
O	3.525829	2.012901	-0.334596	O	2.720463	0.809777	-3.311806
N	3.347971	3.265392	-2.208326	N	2.726705	3.038728	-3.690053
H	4.328411	3.501226	-2.182373	H	3.447329	2.950413	-4.390383
H	2.780832	3.654274	-2.943808	H	2.379434	3.958445	-3.472539
O	-1.720667	2.025394	-2.249651	O	-0.964533	3.396166	-0.071078
H	-2.105369	2.095366	-3.139242	H	-1.518365	4.185698	-0.185611
H	-3.098708	-3.487637	-1.524972	H	-3.584092	-3.00619	-1.129888
				O	-4.347097	-4.143284	2.711887
				H	-5.084104	-4.774478	2.678289
				H	-4.216515	-1.172449	0.048084
Asn-Glu							

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.163187	-1.284624	-1.338603	N	-2.542693	-3.102864	-1.509173
H	-4.315922	-2.279251	-1.193616	H	-2.08959	-3.576926	-0.733538
C	-3.981218	-0.59884	-0.109572	C	-3.161602	-1.87079	-1.034808
C	-4.962608	-0.440607	1.024429	H	-3.616135	-1.371499	-1.894006
C	-2.839385	0.003972	0.2491	C	-4.304514	-2.028166	0.018949
H	-5.878531	0.096008	0.754771	C	-2.062233	-0.982868	-0.449053
H	-5.268256	-1.382547	1.495012	H	-4.764744	-1.057493	0.206268
C	-4.17157	0.383343	2.020381	H	-5.057581	-2.6941	-0.410072
O	-2.914742	0.608289	1.511977	C	-3.871209	-2.587736	1.35138
O	-4.486898	0.816959	3.097392	O	-1.249156	-1.434449	0.358322
N	-1.596852	0.062908	-0.342614	O	-3.865601	-1.972986	2.396399
H	-1.632029	-0.396642	-1.24761	N	-2.056439	0.308737	-0.835608
C	-0.911424	1.358949	-0.407148	C	-1.11286	1.268379	-0.28828
H	-0.870287	1.776373	0.599336	H	-0.100068	0.877434	-0.406615
C	0.517499	1.151905	-0.93893	C	-1.248718	2.608922	-1.034942
C	-1.671595	2.333754	-1.306558	C	-1.368819	1.460506	1.206484
H	0.996316	0.413925	-0.29251	H	-1.117047	2.404997	-2.100376
H	0.460187	0.70812	-1.938236	H	-2.268893	2.983612	-0.905704
C	1.357554	2.426805	-0.981093	C	-0.241977	3.668529	-0.592701
O	-2.186316	2.025762	-2.359037	O	-2.464291	1.511005	1.717149
H	0.921496	3.164838	-1.661662	H	-0.386257	3.932968	0.459121
H	1.36907	2.905096	0.00522	H	0.778058	3.274161	-0.661898
C	2.829503	2.223723	-1.409484	C	-0.285183	4.983109	-1.405474
O	3.514256	3.279251	-1.513914	O	0.507814	5.885302	-1.017542
O	3.236253	1.049942	-1.614391	O	-1.08481	5.060522	-2.374812
H	-4.972211	-0.933903	-1.843815	H	-3.255672	-3.73347	-1.863076
O	-1.695292	3.581952	-0.810355	O	-0.22458	1.618767	1.891479
H	-2.153945	4.15886	-1.443528	H	-0.444129	1.797324	2.820467
				O	-3.500669	-3.882313	1.272233
				H	-2.771944	0.642531	-1.463645
				H	-3.221827	-4.171948	2.155975
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.390207	-1.868693	-1.769079	N	-3.62171	-0.877501	0.729752
H	-0.674367	-2.585114	-1.686187	H	-3.569877	-1.460596	-0.100388
C	-1.65392	-1.251416	-0.518639	C	-2.298641	-0.647466	1.303519
C	-2.03919	-1.907654	0.783327	C	-1.335662	-1.860805	1.24295
C	-1.636509	0.073773	-0.319342	C	-1.596843	0.570632	0.671333
H	-2.99094	-2.451289	0.752826	H	-1.202401	-2.169222	0.205146
H	-1.287138	-2.598343	1.179599	H	-0.363757	-1.565997	1.644788
C	-2.172347	-0.719559	1.714837	C	-1.885821	-3.041506	2.007426
O	-1.934876	0.432	1.002689	O	-0.420922	0.832957	0.923318
O	-2.437593	-0.674706	2.887425	O	-2.3945	-4.010566	1.49253
N	-1.472857	1.136174	-1.176614	N	-2.368845	1.315747	-0.142902
H	-1.271168	0.810326	-2.11602	H	-3.342749	1.047658	-0.205012
C	-0.592258	2.219339	-0.755807	C	-1.904339	2.546121	-0.722159

C	-0.432576	3.226168	-1.871041	C	-1.994565	3.728958	0.232229
H	-1.004336	2.722709	0.120079	H	-0.862147	2.44504	-1.032737
H	0.418061	1.877815	-0.48579	H	-2.490194	2.781908	-1.612705
O	-0.786931	3.059045	-3.016144	O	-2.457652	3.702666	1.347776
O	0.191949	4.33143	-1.436061	O	-1.486716	4.833353	-0.341122
H	0.316574	4.933761	-2.187348	H	-1.566265	5.572684	0.283057
H	-2.218174	-2.323169	-2.145438	H	-4.232162	-1.346327	1.388985
				O	-1.829831	-2.974136	3.356868
				H	-2.442435	-0.357679	2.349817
				H	-1.37015	-2.177646	3.657277
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.51819	-2.31233	0.658894	N	-2.005993	-2.73553	0.018378
H	-0.54901	-2.775728	1.563323	H	-1.101426	-2.907389	0.448641
C	-1.382358	-1.188072	0.616876	C	-2.824729	-1.854835	0.850577
C	-2.884617	-1.155884	0.743454	H	-3.858687	-1.946991	0.504928
C	-0.958093	0.074794	0.477809	C	-2.781192	-2.191921	2.356117
H	-3.411576	-1.711279	-0.039761	C	-2.464428	-0.376433	0.626403
H	-3.267811	-1.513904	1.706162	H	-3.011121	-3.256917	2.462463
C	-3.186636	0.322887	0.602607	H	-1.782912	-2.02238	2.761323
O	-2.001778	1.006635	0.461131	C	-3.766495	-1.451327	3.226405
O	-4.237754	0.907176	0.604243	O	-2.808937	0.489263	1.429702
N	0.304722	0.622123	0.445076	O	-3.514598	-0.973151	4.311904
H	1.005932	-0.107988	0.524444	N	-1.787762	-0.125311	-0.514391
C	0.633879	1.638571	-0.570463	C	-1.370053	1.201549	-0.927488
H	-0.19846	2.340791	-0.618088	H	-1.673567	1.88879	-0.13505
C	1.917059	2.373732	-0.157742	C	0.156433	1.264675	-1.126033
C	0.765669	0.952402	-1.931467	C	-2.148279	1.583133	-2.189855
H	1.762595	2.742899	0.857466	H	0.610053	0.831909	-0.232506
H	2.742761	1.656062	-0.123776	H	0.431743	0.629414	-1.973237
C	2.268943	3.531384	-1.034319	C	0.704267	2.64371	-1.300146
O	1.812794	0.618805	-2.44663	O	-1.665834	1.714046	-3.29444
N	2.827067	3.403107	-2.289895	N	0.573555	3.387929	-2.45422
C	2.149565	4.889062	-0.844152	C	1.422226	3.449767	-0.446117
H	3.023457	2.52569	-2.750346	H	0.064553	3.092512	-3.275345
C	3.014323	4.650368	-2.795604	C	1.19456	4.580238	-2.257766
N	2.616324	5.580328	-1.945177	N	1.725105	4.654745	-1.049444
H	1.761088	5.396423	0.025867	H	1.738367	3.219678	0.560094
H	3.438202	4.820286	-3.772889	H	1.229299	5.345984	-3.016801
O	-0.434707	0.689126	-2.465755	O	-3.452836	1.737358	-1.933636
H	-0.310103	0.183532	-3.286059	H	-3.913023	1.944595	-2.763452
H	-0.778774	-3.006834	-0.035763	H	-2.456402	-3.636416	-0.097736
				O	-5.008656	-1.445634	2.702232
				H	-5.596784	-0.98467	3.320981
				H	-1.547883	-0.936942	-1.073541
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z

N	-3.253726	-2.905894	-1.605582	N	-3.582246	-2.03336	-0.917624
H	-2.928852	-3.867566	-1.548033	H	-2.8283	-2.68863	-0.730816
C	-3.253466	-2.277324	-0.333278	C	-3.950426	-1.298216	0.291361
C	-4.049492	-2.65081	0.891819	C	-4.092629	-2.164706	1.558127
C	-2.475057	-1.233995	-0.014769	C	-2.976862	-0.140527	0.55706
H	-5.134779	-2.583405	0.760621	H	-4.694062	-3.042576	1.302147
H	-3.834392	-3.651439	1.284998	H	-3.120047	-2.516431	1.905408
C	-3.598638	-1.609912	1.896597	C	-4.828361	-1.463534	2.673875
O	-2.655873	-0.802381	1.306614	O	-2.906829	0.397118	1.664858
O	-3.93665	-1.42991	3.037044	O	-4.292346	-1.710138	3.884111
N	-1.476309	-0.581692	-0.705054	N	-2.243087	0.254089	-0.498308
H	-1.424122	-0.964798	-1.643605	H	-2.393839	-0.246686	-1.364265
C	-1.474054	0.884742	-0.701067	C	-1.328742	1.373049	-0.423156
H	-1.675728	1.217362	0.317056	H	-0.690356	1.241832	0.453621
C	-0.077032	1.429195	-1.111217	C	-0.427674	1.423729	-1.689215
C	-2.582321	1.428643	-1.60287	C	-2.105463	2.674821	-0.218806
H	0.611443	0.935893	-0.415028	H	-0.041194	0.40149	-1.787779
C	0.315441	1.030544	-2.540712	C	-1.219232	1.769746	-2.959611
C	0.025817	2.948541	-0.878742	C	0.782018	2.353434	-1.481802
O	-2.974941	0.880231	-2.608915	O	-3.225346	2.89091	-0.620682
H	-0.339465	1.503772	-3.278311	H	-1.54622	2.813759	-2.945058
H	1.340107	1.339447	-2.754462	H	-0.601141	1.622949	-3.84667
H	0.272596	-0.050902	-2.692655	H	-2.109312	1.146706	-3.07764
H	-0.58394	3.476345	-1.619996	H	0.440421	3.392226	-1.429356
H	-0.407217	3.186705	0.098973	H	1.235374	2.128687	-0.510238
C	1.463097	3.479165	-0.925773	C	1.85071	2.217591	-2.572078
H	1.912609	3.35816	-1.914735	H	1.480536	2.535925	-3.549953
H	1.486643	4.545035	-0.682836	H	2.721046	2.834839	-2.333418
H	2.097633	2.956469	-0.202434	H	2.19014	1.180394	-2.662591
O	-3.070567	2.600289	-1.163375	O	-1.372411	3.584244	0.446432
H	-3.739605	2.913055	-1.794596	H	-1.886841	4.405265	0.510287
H	-4.187043	-2.934702	-2.006563	H	-4.369158	-2.575081	-1.257718
				O	-5.831421	-0.797326	2.526022
				H	-4.84022	-1.268389	4.553072
				H	-4.916936	-0.819478	0.102699

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.205334	-1.849941	-1.047677	N	-2.325101	-1.526949	-0.979111
H	-2.025474	-2.815147	-0.783766	H	-1.498542	-2.119064	-0.975739
C	-2.110072	-0.977275	0.067209	C	-2.599907	-1.012922	0.364042
C	-2.953769	-0.964566	1.317213	C	-2.49044	-2.048399	1.490315
C	-1.184022	-0.016515	0.188262	C	-1.730904	0.209612	0.695659
H	-4.016808	-0.769484	1.139866	H	-1.502842	-2.519657	1.494653
H	-2.890244	-1.880251	1.916811	H	-2.607067	-1.565942	2.465204
C	-2.354077	0.187925	2.09739	C	-3.540675	-3.12465	1.385983
O	-1.299733	0.706197	1.38371	O	-1.676878	0.675099	1.836353
O	-2.663488	0.652123	3.16315	O	-4.499552	-3.106265	0.643159
N	-0.099801	0.328585	-0.589508	N	-1.070116	0.750375	-0.344616

H	-0.089391	-0.246096	-1.426977	H	-1.245779	0.345247	-1.255575
C	0.120667	1.747113	-0.88807	C	-0.278495	1.954789	-0.206932
H	0.09806	2.297666	0.051074	H	0.429244	1.818084	0.611869
C	1.494314	1.909932	-1.565202	C	0.470699	2.223393	-1.527237
C	-0.977896	2.29365	-1.800456	C	-1.173483	3.142646	0.148277
H	2.234201	1.474315	-0.885309	H	1.055999	1.323957	-1.750128
H	1.495606	1.298245	-2.47492	H	-0.275956	2.326759	-2.322839
C	1.909744	3.348282	-1.919269	C	1.40456	3.445419	-1.543175
O	-1.466234	1.67548	-2.720077	O	-2.290076	3.321333	-0.281028
H	1.155612	3.773979	-2.592655	H	0.812013	4.338992	-1.313895
C	2.005357	4.247764	-0.678769	C	2.527852	3.335584	-0.50263
C	3.246381	3.321682	-2.67395	C	1.987144	3.619369	-2.952988
H	2.719996	3.83413	0.041829	H	3.120007	2.428671	-0.669798
H	2.350022	5.248281	-0.95555	H	3.202202	4.193722	-0.575096
H	1.041784	4.359617	-0.176082	H	2.141197	3.306368	0.518592
H	3.182028	2.709087	-3.578351	H	1.196314	3.729231	-3.701204
H	3.54706	4.3311	-2.969024	H	2.626033	4.505705	-3.002553
H	4.039523	2.906999	-2.041598	H	2.595986	2.751486	-3.230541
H	-3.133709	-1.826448	-1.460345	H	-3.099749	-2.10631	-1.284269
O	-1.33077	3.549764	-1.482228	O	-0.54946	4.004347	0.968553
H	-1.997272	3.856847	-2.119127	H	-1.132921	4.766254	1.117092
				O	-3.304041	-4.136012	2.242577
				H	-4.017183	-4.788495	2.150881
				H	-3.625331	-0.62873	0.356148

Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.988977	0.295861	3.734979	N	-4.358816	-0.552771	0.573917
H	-1.260096	-0.111845	3.157616	H	-4.612787	-0.092867	1.442732
C	-2.828731	1.145967	3.017588	C	-3.297963	-1.536393	0.802493
C	-4.224527	1.48111	3.45557	H	-3.422778	-2.100382	1.73419
C	-2.539642	1.880847	1.934659	C	-3.271621	-2.579038	-0.337173
H	-4.90216	0.622226	3.458755	C	-1.914076	-0.874549	0.921189
H	-4.275469	1.940503	4.448197	H	-2.412881	-3.234018	-0.186173
C	-4.668835	2.481527	2.402395	H	-4.183037	-3.176315	-0.300046
O	-3.648538	2.697144	1.538269	C	-3.128334	-1.928355	-1.694545
O	-5.734695	3.037571	2.286216	O	-0.947847	-1.524338	1.318774
N	-1.380323	2.094694	1.20018	O	-4.268098	-1.965124	-2.409682
H	-0.5496	1.984419	1.771103	N	-1.864819	0.423713	0.561121
C	-1.259124	1.389547	-0.076903	C	-0.626624	1.179043	0.44879
H	-2.153531	1.598456	-0.667857	H	0.16705	0.535702	0.832105
C	-0.019374	1.904587	-0.832025	C	-0.341939	1.576649	-1.001419
C	-1.169106	-0.123784	0.129989	C	-0.746789	2.389807	1.376904
H	-0.127928	2.991016	-0.897343	H	-0.412013	0.667034	-1.604179
H	0.869797	1.707659	-0.22166	H	-1.126865	2.257613	-1.345859
C	0.172322	1.317021	-2.233213	C	1.032577	2.227194	-1.181806
O	-0.636165	-0.653131	1.082109	O	-1.09028	3.497327	1.030251
H	0.338171	0.23716	-2.17323	H	1.097588	3.134346	-0.572067
H	-0.741115	1.462032	-2.820467	H	1.809826	1.543636	-0.820885

C	1.356014	1.970903	-2.956281	C	1.307155	2.581883	-2.647582
H	1.179502	3.04757	-3.054443	H	1.252618	1.676889	-3.262717
H	2.266784	1.843786	-2.360839	H	0.535422	3.268873	-3.012013
C	1.557744	1.356862	-4.334623	C	2.678558	3.223088	-2.803146
H	1.792145	0.294075	-4.276847	H	2.75858	4.156047	-2.244998
H	0.684236	1.491689	-4.972141	H	3.478471	2.553838	-2.486849
N	2.713927	2.009481	-5.053342	N	2.957145	3.566051	-4.246391
H	3.585725	1.909218	-4.528501	H	2.276745	4.237262	-4.608884
H	2.864446	1.594655	-5.974959	H	3.884747	3.979783	-4.359675
H	2.553117	3.009662	-5.191505	H	2.915803	2.737105	-4.843351
H	-2.49226	-0.436306	4.220704	H	-5.199186	-1.003848	0.227395
O	-1.721771	-0.812558	-0.878634	O	-0.4611	2.068455	2.649035
H	-1.592782	-1.762134	-0.717456	H	-0.604436	2.85056	3.206876
				O	-2.109904	-1.415786	-2.105813
				H	-2.72017	0.807474	0.174276
				H	-4.111569	-1.519533	-3.258482

Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.412941	-2.44574	-0.872782	N	-3.875225	-1.546984	-0.883489
H	-3.39134	-3.391583	-0.500537	H	-3.264376	-2.336096	-1.07303
C	-3.435894	-1.477058	0.163668	C	-3.742168	-1.090657	0.496898
C	-4.493295	-1.262179	1.217258	C	-3.541059	-2.214946	1.545903
C	-2.452469	-0.594936	0.385413	C	-2.605951	-0.062978	0.655821
H	-5.476487	-0.99183	0.81759	H	-2.657924	-2.800346	1.286086
H	-4.642321	-2.114588	1.890349	H	-3.382512	-1.762687	2.527294
C	-3.93096	-0.094977	2.003365	C	-4.723292	-3.154231	1.57957
O	-2.711481	0.2522	1.470944	O	-2.249985	0.337041	1.764975
O	-4.382929	0.500301	2.945677	O	-4.742836	-4.244282	1.055768
N	-1.209882	-0.430305	-0.189843	N	-2.062044	0.377609	-0.493054
H	-1.106754	-1.086337	-0.958738	H	-2.490703	0.052774	-1.351161
C	-0.791184	0.923371	-0.560348	C	-1.044064	1.404986	-0.50673
H	-0.950763	1.580562	0.294702	H	-0.239279	1.118533	0.173888
C	0.707393	0.903715	-0.918464	C	-0.487819	1.552548	-1.937087
C	-1.610445	1.451001	-1.740324	C	-1.619148	2.733798	-0.009517
H	1.229268	0.476789	-0.058104	H	-0.15778	0.558898	-2.254052
H	0.859656	0.225046	-1.764327	H	-1.300421	1.857997	-2.604203
C	1.273387	2.285692	-1.245216	C	0.675725	2.538438	-2.036655
O	-1.97899	0.767448	-2.668554	O	-2.748338	3.116213	-0.208754
H	0.814464	2.702693	-2.144516	H	0.357158	3.555095	-1.797864
H	1.098168	2.979924	-0.418883	H	1.477198	2.259983	-1.347206
S	3.081652	2.168543	-1.533851	S	1.349567	2.537659	-3.743494
C	3.424075	3.917258	-1.933819	C	2.653873	3.798977	-3.536198
H	3.163934	4.560174	-1.090847	H	3.37908	3.478342	-2.785954
H	4.493831	3.996551	-2.131961	H	3.153458	3.903693	-4.500218
H	2.868037	4.221757	-2.822515	H	2.216695	4.757164	-3.249253
O	-1.856803	2.766926	-1.640855	O	-0.694051	3.454074	0.64523
H	-2.338577	3.055987	-2.433815	H	-1.083675	4.309011	0.891411
H	-4.239318	-2.380281	-1.460608	H	-4.822643	-1.846457	-1.082085

				O	-5.836208	-2.711589	2.207077
				H	-4.648621	-0.528532	0.745516
				H	-5.693134	-1.850518	2.624148
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.554845	-2.496469	-0.829825	N	-3.147753	-1.512656	0.138708
H	-2.436672	-3.424111	-0.430803	H	-2.660118	-2.04362	-0.577842
C	-2.649468	-1.502829	0.178525	C	-2.26119	-1.213792	1.26272
C	-3.705123	-1.352294	1.245064	H	-2.890773	-0.895921	2.09923
C	-1.747673	-0.528264	0.35561	C	-1.405011	-2.412115	1.725298
H	-4.714996	-1.184799	0.855775	C	-1.360568	-0.005668	0.957493
H	-3.765207	-2.193431	1.94551	H	-2.082608	-3.253746	1.901576
C	-3.239352	-0.114823	1.98569	H	-0.699696	-2.706287	0.947147
O	-2.065462	0.325069	1.42043	C	-0.628239	-2.212643	3.003267
O	-3.728804	0.465878	2.918308	O	-0.3385	0.208444	1.612835
N	-0.536779	-0.265673	-0.250399	O	0.518566	-2.563376	3.184045
H	-0.383256	-0.935189	-0.99905	N	-1.793371	0.798691	-0.030049
C	-0.260624	1.1092	-0.674535	C	-1.0732	1.984508	-0.44151
H	-0.442752	1.775497	0.167989	H	-0.614378	2.441154	0.43597
C	1.218641	1.219138	-1.106446	C	0.044673	1.628814	-1.468544
C	-1.168979	1.522784	-1.834949	C	-2.063717	2.959491	-1.054781
H	1.81766	0.880028	-0.25769	H	0.640411	0.845535	-0.993708
H	1.390074	0.521243	-1.931369	H	-0.431211	1.19298	-2.350814
C	1.617476	2.618736	-1.51396	C	0.92313	2.794712	-1.850456
O	-1.415848	0.810293	-2.782445	O	-3.052148	2.625362	-1.6707
C	1.713725	2.975041	-2.863863	C	0.759352	3.450485	-3.075754
C	1.869172	3.594448	-0.540417	C	1.908065	3.255806	-0.966812
H	1.525486	2.228503	-3.628522	H	0.001979	3.103317	-3.771167
C	2.04889	4.278969	-3.235976	C	1.557829	4.545723	-3.412002
C	2.204036	4.897855	-0.907336	C	2.706647	4.350777	-1.297259
H	1.804402	3.330536	0.510465	H	2.050674	2.752304	-0.015822
H	2.120605	4.5373	-4.286548	H	1.41859	5.040604	-4.36666
C	2.29343	5.244676	-2.258303	C	2.532855	5.000505	-2.522369
H	2.398288	5.640245	-0.141346	H	3.465592	4.693578	-0.602849
H	2.555463	6.256856	-2.544809	H	3.154524	5.849931	-2.781799
O	-1.652006	2.765629	-1.693322	O	-1.696051	4.232718	-0.870134
H	-2.185109	2.983739	-2.475979	H	-2.322138	4.809028	-1.338957
H	-3.395084	-2.527404	-1.400634	H	-3.932177	-2.077849	0.444525
				O	-1.381447	-1.667509	3.979955
				H	-0.835792	-1.595729	4.778886
				H	-2.618581	0.507858	-0.541066
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.413736	-2.023155	-1.053024	N	-1.415886	-1.682143	-0.981022
H	-1.298564	-3.018701	-0.882344	H	-0.629202	-2.32469	-0.947987
C	-1.029751	-1.252818	0.074777	C	-1.444869	-0.82501	0.201449
C	-1.629248	-1.256955	1.458728	C	-1.232645	-1.557953	1.541449

C	-0.001917	-0.394297	0.078133	C	-0.435098	0.328124	0.077733
H	-2.680024	-0.950341	1.492796	H	-1.892114	-2.430455	1.559022
H	-1.556565	-2.21802	1.980951	H	-0.20446	-1.918726	1.616001
C	-0.780794	-0.228303	2.179277	C	-1.622255	-0.713159	2.738435
O	0.177717	0.242551	1.312135	O	-0.021312	0.923093	1.073905
O	-0.842399	0.179497	3.308869	O	-0.79695	-0.721935	3.805078
N	0.95348	-0.095851	-0.872025	N	-0.085455	0.645424	-1.183637
H	0.756966	-0.620438	-1.720137	H	-0.44033	0.053811	-1.926005
C	1.230136	1.314259	-1.152507	C	0.82971	1.721394	-1.500101
H	1.338658	1.849736	-0.21029	H	0.750456	2.496082	-0.737691
C	2.540166	1.404	-1.939118	C	2.274897	1.191333	-1.529614
C	0.09718	1.946617	-1.965874	C	0.452008	2.29479	-2.859073
H	3.337268	0.969606	-1.327201	H	2.475913	0.731903	-0.556006
H	2.446599	0.821287	-2.863879	H	2.357729	0.422887	-2.30746
O	2.781848	2.778755	-2.221847	O	3.147257	2.286072	-1.782689
O	-0.390523	1.423906	-2.943398	O	0.079619	1.615229	-3.790169
H	3.559648	2.846266	-2.786184	H	4.051525	1.956416	-1.827367
O	-0.301392	3.127346	-1.474625	O	0.596465	3.622758	-2.914226
H	-1.008739	3.47826	-2.04133	H	0.382983	3.921774	-3.813923
H	-2.391419	-1.876492	-1.288196	H	-2.2584	-2.243699	-1.036147
				O	-2.658155	-0.089949	2.801761
				H	0.00972	-1.220439	3.616951
				H	-2.428195	-0.345022	0.236841

Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.818829	0.421766	-1.520285	N	-3.222619	-2.169628	-1.305364
H	-4.43474	-0.326524	-1.827053	H	-2.533591	-2.916695	-1.313037
C	-3.251854	0.14724	-0.24829	C	-3.267145	-1.511018	-0.001304
C	-3.959392	-0.026948	1.072015	C	-3.309297	-2.468016	1.206607
C	-1.940179	-0.028272	-0.036633	C	-2.106774	-0.516658	0.162535
H	-4.515	0.856284	1.405838	H	-4.068311	-3.230983	1.007597
H	-4.653043	-0.875405	1.109523	H	-2.352863	-2.97546	1.339744
C	-2.807203	-0.282648	2.022097	C	-3.725848	-1.785712	2.486777
O	-1.633019	-0.283553	1.306354	O	-1.763641	-0.11741	1.276842
O	-2.802421	-0.46887	3.210546	O	-3.024535	-2.21196	3.554204
N	-0.86756	-0.094575	-0.892668	N	-1.530328	-0.114992	-0.985373
H	-1.149303	0.129771	-1.840388	H	-1.914529	-0.482685	-1.846645
C	0.39225	0.526633	-0.518819	C	-0.480418	0.867427	-1.040697
H	0.654952	0.221734	0.495399	H	0.051877	0.863827	-0.086717
C	1.524272	0.055776	-1.451923	C	0.527241	0.536667	-2.157218
C	0.310402	2.056875	-0.526461	C	-1.053603	2.276471	-1.217547
H	2.436741	0.577573	-1.14353	H	1.272152	1.338652	-2.174994
C	1.749856	-1.449604	-1.388456	C	1.219756	-0.803046	-1.936873
O	1.143221	0.487935	-2.76557	O	-0.232887	0.554032	-3.373563
O	-0.606585	2.70159	-0.978412	O	-2.219699	2.543106	-1.385676
H	0.846031	-1.989039	-1.676055	H	0.492945	-1.61692	-1.896195
H	2.561215	-1.73103	-2.065285	H	1.917813	-0.998257	-2.755256
H	2.034888	-1.749547	-0.376233	H	1.788422	-0.789336	-1.003188

H	1.805139	0.186267	-3.397716	H	0.344662	0.312855	-4.106605
H	-4.374692	1.272436	-1.504993	H	-4.119882	-2.589564	-1.522298
O	1.396081	2.606816	0.045064	O	-0.082176	3.202554	-1.144981
H	1.312292	3.573396	0.005717	H	-0.480608	4.07973	-1.264127
				O	-4.632782	-0.984903	2.577337
				H	-3.374448	-1.766929	4.343088
				H	-4.173927	-0.897818	0.025819
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.217661	-3.101106	-0.156411	N	-3.279845	-2.342762	-0.2127
H	-1.647624	-3.840234	0.246609	H	-2.719649	-2.375386	0.635326
C	-2.612628	-2.153391	0.822945	C	-4.436983	-1.463062	-0.03607
C	-3.47404	-2.373349	2.041157	C	-5.192948	-1.641428	1.286477
C	-2.225116	-0.870995	0.822029	C	-4.062846	0.014254	-0.226686
H	-4.49411	-2.702387	1.815823	H	-4.522537	-1.513283	2.141695
H	-3.059751	-3.082489	2.767361	H	-5.971252	-0.879273	1.387178
C	-3.516261	-0.989803	2.658469	C	-5.858986	-2.989706	1.390451
O	-2.747907	-0.14062	1.897758	O	-4.84344	0.923646	0.062327
O	-4.086248	-0.591634	3.639939	O	-5.978219	-3.790147	0.486809
N	-1.349492	-0.168402	0.021485	N	-2.84841	0.239734	-0.762218
H	-1.008917	-0.775318	-0.718747	H	-2.314529	-0.575158	-1.03825
C	-1.77471	1.137539	-0.489101	C	-2.385445	1.573794	-1.075636
H	-2.134577	1.735391	0.347073	H	-2.455367	2.200387	-0.184812
C	-0.570721	1.843693	-1.153098	C	-0.915099	1.50663	-1.557154
C	-2.903735	0.991334	-1.510341	C	-3.255071	2.20769	-2.161624
H	0.217453	1.894895	-0.395631	H	-0.349518	0.997832	-0.769246
H	-0.202109	1.208518	-1.964362	H	-0.873183	0.87441	-2.449047
C	-0.899804	3.206611	-1.676954	C	-0.317113	2.846604	-1.846605
O	-2.903206	0.168905	-2.399613	O	-3.67382	1.621967	-3.134196
C	-1.02343	3.576908	-2.994791	C	-0.014222	3.363818	-3.083163
C	-1.194208	4.380187	-0.89455	C	0.022366	3.863182	-0.884219
H	-0.886605	2.98699	-3.88782	H	-0.122984	2.916102	-4.058829
N	-1.375855	4.907358	-3.079463	N	0.491066	4.639571	-2.948665
C	-1.488351	5.429566	-1.80997	C	0.52773	4.975906	-1.61354
C	-1.233459	4.64728	0.485006	C	-0.046529	3.940298	0.517588
H	-1.512664	5.417037	-3.937152	H	0.800487	5.222706	-3.709013
C	-1.817087	6.720212	-1.383936	C	0.958774	6.147012	-0.98269
C	-1.559693	5.929076	0.913469	C	0.380981	5.102627	1.149426
H	-1.009704	3.867464	1.204822	H	-0.42413	3.105543	1.098041
H	-2.037812	7.507059	-2.095908	H	1.341365	6.984511	-1.554598
C	-1.849914	6.954697	-0.012773	C	0.877577	6.195411	0.405582
H	-1.593199	6.148435	1.974764	H	0.333721	5.175041	2.230212
H	-2.102274	7.944255	0.351351	H	1.202697	7.089135	0.926179
O	-3.892702	1.876933	-1.319269	O	-3.464227	3.513069	-1.935279
H	-4.557561	1.756145	-2.01762	H	-3.965298	3.878597	-2.682487
H	-3.022444	-3.551005	-0.58375	H	-3.59887	-3.289137	-0.390195
				O	-6.336803	-3.214732	2.628817
				H	-6.772096	-4.082581	2.636374

				H	-5.131461	-1.679634	-0.854539
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.858914	-1.233634	-0.298535	N	-0.368638	-1.26566	-2.870788
H	-0.499641	-1.44541	0.628083	H	0.299576	-1.210767	-2.107854
C	-2.207749	-0.795499	-0.246854	C	-1.726492	-1.413445	-2.347434
C	-3.397047	-1.487675	0.370602	C	-1.91257	-2.478307	-1.253771
C	-2.640477	0.348217	-0.795064	C	-2.299909	-0.065365	-1.877762
H	-3.649612	-2.451859	-0.086427	H	-2.971987	-2.579409	-1.003387
H	-3.311143	-1.656341	1.449439	H	-1.577013	-3.449503	-1.630931
C	-4.51687	-0.50156	0.104361	C	-1.15087	-2.171259	0.017841
O	-4.010589	0.563549	-0.604835	O	-3.299514	-0.007891	-1.159307
O	-5.679555	-0.540257	0.408941	O	-0.412851	-1.223874	0.168088
N	-2.007933	1.302842	-1.557085	N	-1.651396	1.019134	-2.339966
H	-1.015049	1.099926	-1.598852	H	-0.843509	0.838383	-2.922465
C	-2.289254	2.708517	-1.278858	C	-2.01086	2.364486	-1.974128
H	-2.451181	2.881481	-0.209346	H	-2.453544	2.341383	-0.975478
C	-1.102258	3.592344	-1.742351	C	-0.759714	3.279892	-1.948427
C	-3.539375	3.174388	-2.01863	C	-3.066961	2.940878	-2.914436
H	-0.970287	3.4587	-2.819558	H	-0.345217	3.340523	-2.959299
H	-1.380387	4.634915	-1.571144	H	-1.087485	4.284028	-1.67201
C	0.176356	3.257748	-1.009518	C	0.285399	2.771669	-0.983104
O	-3.940873	2.744298	-3.073872	O	-3.368684	2.493526	-3.996237
C	1.207572	2.550554	-1.635295	C	1.419138	2.090003	-1.434119
C	0.344902	3.618034	0.335493	C	0.119867	2.932978	0.399082
H	1.109647	2.265818	-2.677796	H	1.576763	1.951172	-2.498586
C	2.373044	2.205214	-0.947614	C	2.363136	1.579848	-0.541724
C	1.499603	3.282906	1.034148	C	1.050779	2.429931	1.303274
H	-0.437502	4.170991	0.845042	H	-0.750547	3.459406	0.777378
H	3.161916	1.656395	-1.450963	H	3.236564	1.053603	-0.912132
C	2.518797	2.572021	0.39104	C	2.177279	1.749144	0.831677
H	1.626552	3.56753	2.071835	H	0.918927	2.560261	2.370823
O	3.632688	2.27068	1.125876	O	3.06114	1.274602	1.763386
H	4.269533	1.790786	0.582467	H	3.796494	0.828525	1.325913
H	-0.757573	-2.078845	-0.854304	H	-0.118453	-2.062552	-3.445324
O	-4.122301	4.19573	-1.364407	O	-3.619248	4.048757	-2.389041
H	-4.871284	4.513846	-1.893755	H	-4.259947	4.407162	-3.024207
				O	-1.31967	-3.035816	1.039678
				H	-2.366329	-1.708746	-3.185662
				H	-1.937047	-3.743608	0.806271
Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.36288	-2.443965	-0.81557	N	-3.647112	-1.772197	-0.152363
H	-3.226691	-3.444001	-0.937954	H	-3.065955	-2.519749	-0.522968
C	-2.635015	-1.950281	0.298144	C	-3.122597	-1.292159	1.126669
C	-2.787603	-2.322741	1.751421	C	-2.714534	-2.391261	2.11722
C	-1.632257	-1.066335	0.204262	C	-1.957152	-0.309763	0.93148

H	-3.769979	-2.08803	2.17506	H	-1.979538	-3.06208	1.658945
H	-2.585128	-3.377211	1.973188	H	-2.23067	-1.948582	2.993635
C	-1.7341	-1.45974	2.415886	C	-3.896646	-3.20515	2.596061
O	-1.072033	-0.742965	1.447819	O	-1.248668	0.049732	1.874516
O	-1.439951	-1.3442	3.576637	O	-5.055159	-2.948939	2.358778
N	-0.998453	-0.499464	-0.880348	N	-1.794268	0.147431	-0.323116
H	-1.475772	-0.790842	-1.727408	H	-2.472914	-0.163049	-1.006299
C	-0.736148	0.942566	-0.856005	C	-0.786187	1.129737	-0.657405
H	-0.326979	1.194286	0.122446	H	0.174009	0.791537	-0.261011
C	0.325604	1.317162	-1.926548	C	-0.660902	1.272375	-2.200045
C	-2.03132	1.733108	-1.042724	C	-1.102792	2.465021	0.017888
H	1.170187	0.657064	-1.701759	H	-0.555204	0.242418	-2.559933
C	-0.13823	1.032252	-3.361337	C	-1.908587	1.887645	-2.850045
C	0.800043	2.768461	-1.778335	C	0.604625	2.0399	-2.601194
O	-2.973125	1.355466	-1.703943	O	-2.212003	2.871676	0.27606
H	-0.996125	1.65406	-3.633596	H	-2.0349	2.931799	-2.549354
H	0.671878	1.254743	-4.060546	H	-1.807723	1.861469	-3.937795
H	-0.416567	-0.014436	-3.509472	H	-2.826729	1.354028	-2.590593
H	1.128229	2.981056	-0.757073	H	1.499147	1.599403	-2.152611
H	1.641798	2.951647	-2.450967	H	0.721223	2.014468	-3.687561
H	0.008657	3.478756	-2.032626	H	0.552034	3.087233	-2.293339
H	-4.3618	-2.295336	-0.702462	H	-4.572942	-2.161999	-0.011986
O	-2.007441	2.912111	-0.399282	O	0.016708	3.166265	0.266975
H	-2.83655	3.383182	-0.585388	H	-0.235784	4.022066	0.649988
				O	-3.60831	-4.284485	3.353684
				H	-3.913319	-0.695823	1.593693
				H	-2.653757	-4.383978	3.478664

Table S15.A. Direct Hydrolysis XYZ Coordinates (Implicit solvation + 1 H_2O, ε = 80)

All Reactions							
H_2O				NH_3			
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
O	-0.999631	0.482902	0	N	-1.133326	-0.563263	0.000024
H	-0.03661	0.526297	0	H	-0.744703	-1.50246	-0.000031
H	-1.280189	1.405171	0	H	-0.744689	-0.093642	0.813368
				H	-0.7447	-0.093681	-0.813362
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.80773	-2.89702	0.322781	N	-1.11264	-2.51925	1.131243
H	-0.8935	-2.8566	0.765271	H	-0.54945	-2.13514	1.885271
C	-2.4982	-1.62759	0.512093	C	-2.37094	-1.783	1.037062
H	-3.41582	-1.63777	-0.0803	H	-2.91318	-2.13963	0.159047
C	-2.89399	-1.33329	1.989232	C	-3.28544	-1.94878	2.273881
C	-1.58617	-0.49828	0.020725	C	-2.02984	-0.2966	0.863952
H	-3.50316	-2.16811	2.345328	H	-3.36877	-3.01519	2.512

H	-1.99508	-1.27759	2.60751	H	-2.85214	-1.46439	3.151822
C	-3.74049	-0.08017	2.096182	C	-4.69498	-1.45717	2.063505
O	-0.36607	-0.54394	0.17892	O	-1.12057	0.222947	1.512483
O	-4.79322	0.018047	1.44587	O	-5.22463	-1.32196	0.976127
N	-3.29073	0.908693	2.885898	N	-2.79988	0.393457	-0.00066
H	-3.79964	1.7833	2.918791	H	-3.58154	-0.06272	-0.45177
H	-2.4151	0.835444	3.377462	C	-2.63825	1.822874	-0.20027
N	-2.21562	0.562616	-0.52842	H	-2.44197	2.292357	0.767138
H	-3.22437	0.567357	-0.60323	C	-1.47511	2.150629	-1.15677
C	-1.50372	1.769975	-0.90598	C	-3.93689	2.392222	-0.73905
H	-0.68459	1.92096	-0.19897	H	-1.6591	1.718829	-2.14319
C	-0.92407	1.686692	-2.33104	H	-1.35378	3.230437	-1.25406
C	-2.44546	2.954284	-0.78719	H	-0.55774	1.724989	-0.74921
H	-1.72519	1.552601	-3.06165	O	-4.84687	1.728599	-1.19226
H	-0.36707	2.593439	-2.5717	H	-1.2922	-3.4939	1.351993
H	-0.25001	0.831005	-2.38509	O	-3.9481	3.726091	-0.68827
O	-3.65244	2.870454	-0.69301	H	-4.77586	4.050051	-1.0799
H	-2.32706	-3.64875	0.765413	O	-5.32661	-1.20842	3.217092
O	-1.78502	4.114275	-0.83356	H	-6.24059	-0.93873	3.028454
H	-2.42561	4.843574	-0.79794	O	-7.22382	0.491987	-0.01236
O	-5.5167	2.70548	1.57376	H	-6.65997	-0.1933	0.382624
H	-5.43496	1.734685	1.473014	H	-6.58919	1.048474	-0.48572
H	-4.979	3.044699	0.844549				

Asn-Arg

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.58109	-4.21239	-0.25604	N	-2.22925	-2.56808	2.631462
H	-1.75237	-4.48694	0.264381	H	-2.54084	-1.93257	3.361089
C	-3.02324	-2.89574	0.183885	C	-2.48712	-1.97585	1.323663
H	-3.8279	-2.56056	-0.47452	H	-2.02577	-2.60525	0.559825
C	-3.5645	-2.86043	1.644081	C	-3.99636	-1.8384	0.980913
C	-1.84376	-1.92251	0.08095	C	-1.83127	-0.58873	1.289662
H	-4.37052	-3.59513	1.719168	H	-4.44618	-2.83482	1.033515
H	-2.77277	-3.15091	2.338671	H	-4.49776	-1.20341	1.712837
C	-4.15725	-1.50722	1.985733	C	-4.21994	-1.30754	-0.41776
O	-0.68826	-2.2829	0.302176	O	-1.79656	0.138404	2.281123
O	-5.04757	-1.01849	1.271802	O	-3.54485	-1.64682	-1.3756
N	-3.66439	-0.86385	3.056292	N	-1.32296	-0.20396	0.096036
H	-3.99544	0.069792	3.265489	H	-1.49969	-0.78058	-0.71508
H	-2.91333	-1.24867	3.605405	C	-0.72524	1.103256	-0.09012
N	-2.17296	-0.64143	-0.19684	H	0.010632	1.269325	0.698648
H	-3.13982	-0.39269	-0.35964	C	-0.04157	1.162427	-1.46803
C	-1.19361	0.430061	-0.18115	C	-1.7767	2.208823	0.016879
H	-0.41897	0.178428	0.545183	H	0.644814	0.312455	-1.52233
C	-0.54338	0.607341	-1.57429	H	-0.80067	1.020813	-2.24481
C	-1.88819	1.704255	0.269473	C	0.728102	2.462827	-1.71227
H	-0.17162	-0.38138	-1.85692	O	-2.88128	2.163397	-0.48233
H	-1.32452	0.876997	-2.29203	H	0.05371	3.323548	-1.68444
C	0.601135	1.622765	-1.61879	H	1.468558	2.604223	-0.91787

O	-3.06473	1.937338	0.085324	C	1.432922	2.429896	-3.06677
H	0.227618	2.627238	-1.40006	H	2.112334	1.572159	-3.11616
H	1.347564	1.380435	-0.85548	H	0.691063	2.329558	-3.86452
C	1.26543	1.618999	-2.99418	N	2.184804	3.670395	-3.27089
H	1.687113	0.629958	-3.19572	H	2.349771	4.254216	-2.46405
H	0.522852	1.842516	-3.76796	C	2.767173	4.027344	-4.41539
N	2.343164	2.610846	-3.04085	N	2.702807	3.228864	-5.48439
H	2.363852	3.31405	-2.31665	N	3.412006	5.197154	-4.49973
C	3.223135	2.729264	-4.03478	H	2.361086	2.284898	-5.41664
N	3.160447	1.916484	-5.09324	H	3.113309	3.506419	-6.36115
N	4.182819	3.660222	-3.97043	H	3.356318	5.876245	-3.75813
H	2.365499	1.32052	-5.25184	H	3.877349	5.475316	-5.34829
H	3.84125	1.979094	-5.83268	O	-1.32079	3.269829	0.686835
H	4.342054	4.183416	-3.12486	H	-1.9991	3.965756	0.676448
H	4.844347	3.778202	-4.72053	H	-2.75621	-3.42964	2.735297
H	-3.30045	-4.90428	-0.07048	O	-5.20178	-0.41409	-0.49426
O	-1.04693	2.553898	0.862708	H	-5.15203	0.057611	-1.36971
H	-1.52458	3.37155	1.081958	O	-4.60568	1.229089	-2.52525
O	-5.25826	1.653988	2.032365	H	-5.22085	1.947442	-2.7139
H	-5.34261	0.742645	1.683452	H	-3.93061	1.613916	-1.93596
H	-4.5648	2.037328	1.477253				

Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.91832	-3.6156	0.168144	N	0.445014	-2.73941	1.792313
H	-0.10409	-3.47257	0.759511	H	1.361793	-2.74785	2.230901
C	-1.80531	-2.46396	0.269113	C	-0.2463	-1.50025	2.121097
H	-2.60376	-2.57206	-0.46831	H	-1.15888	-1.44046	1.523199
C	-2.47287	-2.29451	1.66601	C	-0.65678	-1.37669	3.619225
C	-0.9982	-1.19855	-0.03664	C	0.667021	-0.32124	1.763422
H	-3.00556	-3.22077	1.896911	H	-1.24785	-2.26002	3.876213
H	-1.70321	-2.14442	2.426457	H	0.228076	-1.35444	4.256691
C	-3.497	-1.17657	1.65985	C	-1.52719	-0.16262	3.856463
O	0.177599	-1.08344	0.307194	O	1.891511	-0.40526	1.836029
O	-4.42125	-1.18344	0.831151	O	-2.51865	0.074989	3.186687
N	-3.34254	-0.1853	2.552464	N	0.033849	0.82639	1.424653
H	-3.97479	0.604876	2.525598	H	-0.97669	0.858948	1.405261
H	-2.57075	-0.16975	3.199051	C	0.758981	2.058322	1.199883
N	-1.67891	-0.20262	-0.64653	H	1.654124	2.057835	1.827087
H	-2.65719	-0.3214	-0.87524	C	1.221854	2.197441	-0.27063
C	-1.09147	1.105834	-0.84842	C	-0.10794	3.230538	1.630511
H	-0.46748	1.356473	0.012974	H	1.628722	1.226146	-0.56252
C	-0.19006	1.144835	-2.10686	H	0.373101	2.411188	-0.92332
C	-2.20881	2.131616	-0.94274	C	2.355522	3.202848	-0.43612
H	0.423892	0.241581	-2.07831	O	-1.26515	3.138034	1.986973
H	-0.7968	1.108336	-3.01381	O	3.329069	3.189603	0.316122
C	0.778355	2.321249	-2.09621	N	2.243976	4.06156	-1.46966
O	-3.3863	1.858325	-1.04046	H	2.985125	4.723881	-1.64245
O	1.447506	2.582757	-1.09726	H	1.431594	4.085129	-2.06398

N	0.883161	3.017622	-3.24638	O	0.550973	4.38568	1.552664
H	1.53907	3.782228	-3.30137	H	-0.04544	5.110324	1.803761
H	0.317202	2.812139	-4.05333	H	-0.07253	-3.53593	2.150346
H	-1.39008	-4.45202	0.4974	O	-1.09044	0.632582	4.828516
O	-1.73384	3.378267	-0.93373	H	-1.62688	1.475065	4.839935
H	-2.47312	3.999668	-1.0391	O	-2.33454	3.007351	4.624584
O	-5.55105	1.360064	0.909186	H	-2.04851	3.21591	3.717675
H	-5.30502	0.418564	0.797467	H	-1.97071	3.709895	5.176508
H	-4.96516	1.811705	0.286471				
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.69709	-2.99045	-0.85307	N	-2.17996	-3.1324	-0.87143
H	-3.86947	-3.41083	-0.43862	H	-1.27593	-3.56506	-0.70151
C	-4.88767	-1.65224	-0.30794	C	-2.29735	-1.91775	-0.06919
H	-5.69007	-1.16013	-0.86247	H	-3.21924	-1.40504	-0.35122
C	-5.27398	-1.63028	1.201362	C	-2.33348	-2.17683	1.456808
C	-3.5846	-0.86431	-0.48273	C	-1.09019	-1.02537	-0.39015
H	-6.17651	-2.23383	1.325791	H	-3.07781	-2.95354	1.665279
H	-4.47358	-2.0829	1.791221	H	-1.37284	-2.55362	1.813908
C	-5.60292	-0.22485	1.664151	C	-2.74909	-0.97473	2.266249
O	-2.48683	-1.40672	-0.34882	O	0.033559	-1.51083	-0.53163
O	-6.5151	0.413574	1.115869	O	-3.45077	-0.07255	1.847584
N	-4.85491	0.298486	2.649959	N	-1.33266	0.297223	-0.46313
H	-5.00002	1.264049	2.917387	H	-2.26575	0.647317	-0.29339
H	-4.08481	-0.20755	3.055854	C	-0.27225	1.265059	-0.69333
N	-3.7287	0.45551	-0.71982	H	0.620898	0.962069	-0.1435
H	-4.65442	0.855293	-0.79551	C	0.114716	1.373198	-2.188
C	-2.5951	1.363875	-0.75824	C	-0.73821	2.610418	-0.17321
H	-1.83678	1.017151	-0.0542	H	0.15365	0.348586	-2.56769
C	-1.93807	1.434225	-2.15699	H	-0.65774	1.908307	-2.74405
C	-3.07352	2.736536	-0.32567	C	1.507416	2.000261	-2.43976
H	-1.86318	0.401834	-2.50967	O	-1.89512	2.887278	0.077736
H	-2.57888	1.981254	-2.85146	O	2.447162	1.586506	-1.71196
C	-0.50499	2.019695	-2.1516	O	1.589746	2.834604	-3.37903
O	-4.23888	3.081286	-0.29925	O	0.263829	3.483833	-0.05994
O	0.279622	1.562761	-1.27996	H	-0.0992	4.339379	0.22277
O	-0.23576	2.869457	-3.0403	H	-2.89371	-3.80256	-0.60261
O	-2.06248	3.547974	-0.00992	O	-2.28549	-1.01352	3.521284
H	-2.42204	4.42449	0.20483	H	-2.6192	-0.24161	4.007809
H	-5.48848	-3.58163	-0.61892	O	-3.53318	2.726772	2.483976
O	-6.17138	3.064268	1.904677	H	-3.58941	1.76237	2.381261
H	-6.45826	2.186818	1.577593	H	-2.98923	2.993531	1.728808
H	-5.50505	3.330964	1.255228				
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.69038	-2.56994	-0.53888	N	-2.05095	-1.98515	-1.18003
H	-1.82466	-2.83818	-0.07888	H	-1.50511	-2.83471	-1.0656

C	-3.11917	-1.26406	-0.05628	C	-2.50784	-1.474	0.109624
H	-3.97329	-0.93493	-0.65247	H	-3.27597	-0.72008	-0.09259
C	-3.5549	-1.24934	1.439106	C	-3.111	-2.52802	1.054213
C	-1.96477	-0.27264	-0.23506	C	-1.38948	-0.70401	0.829675
H	-4.34389	-1.99591	1.563169	H	-3.85226	-3.10711	0.493797
H	-2.71232	-1.53683	2.072253	H	-2.34919	-3.2242	1.407855
C	-4.13936	0.091355	1.839881	C	-3.84692	-1.93108	2.227206
O	-0.79064	-0.61667	-0.11773	O	-1.41254	-0.5362	2.048636
O	-5.07287	0.584889	1.186815	O	-4.51537	-0.91456	2.188945
N	-3.59349	0.71793	2.894327	N	-0.43801	-0.19467	0.018733
H	-3.92357	1.642171	3.143348	H	-0.52689	-0.41403	-0.9673
H	-2.80922	0.330109	3.392672	C	0.658523	0.632802	0.494482
N	-2.3335	1.010897	-0.45908	H	0.662048	0.563883	1.583106
H	-3.31338	1.250361	-0.53832	C	1.990056	0.143797	-0.0754
C	-1.36951	2.094134	-0.48396	C	0.360954	2.086404	0.114713
H	-0.53218	1.83186	0.163921	H	2.105879	-0.91251	0.170267
C	-0.85427	2.303818	-1.92541	H	2.014988	0.252568	-1.16005
C	-2.04383	3.347697	0.057032	S	3.457778	0.975639	0.650003
H	-0.46517	1.345779	-2.2668	O	0.904169	2.70093	-0.77317
H	-1.67889	2.610377	-2.57019	H	3.281041	2.164501	0.045772
S	0.509461	3.549737	-2.01156	O	-0.62077	2.597814	0.877635
O	-3.22897	3.577502	-0.05547	H	-0.81818	3.498644	0.572322
H	0.906785	3.214886	-3.25192	H	-2.84009	-2.21262	-1.7747
H	-3.38622	-3.2734	-0.312	O	-3.75372	-2.68548	3.330915
O	-1.1743	4.170837	0.643604	H	-4.28541	-2.2724	4.031154
H	-1.63669	4.980612	0.918384	O	-3.55603	1.740866	1.543587
O	-5.28736	3.230831	2.037697	H	-3.84323	0.843007	1.777301
H	-5.37338	2.329732	1.663538	H	-2.5933	1.712155	1.605212
H	-4.64191	3.650636	1.452436				

Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.69053	-3.91683	1.184279	N	-2.22447	-0.70372	3.921631
H	-1.36859	-3.71739	2.127681	H	-1.5547	-0.53329	4.666853
C	-2.18243	-2.6886	0.56578	C	-2.42825	0.520174	3.152
H	-2.40953	-2.89565	-0.48163	H	-3.06041	0.286198	2.293051
C	-3.46325	-2.12271	1.230132	C	-3.10452	1.658901	3.953829
C	-1.06572	-1.64072	0.640098	C	-1.05374	0.994664	2.660678
H	-4.22748	-2.90662	1.210512	H	-3.96245	1.24802	4.497616
H	-3.26474	-1.88623	2.278572	H	-2.41774	2.055698	4.708584
C	-4.03622	-0.92409	0.494046	C	-3.63409	2.790816	3.101373
O	-0.33862	-1.53806	1.627688	O	-0.05483	0.908446	3.374215
O	-3.98479	-0.8456	-0.74318	O	-3.7181	2.757064	1.889968
N	-4.60337	0.033104	1.245364	N	-1.00905	1.531015	1.422648
H	-4.96045	0.866181	0.799361	H	-1.88069	1.718423	0.946986
H	-4.59145	-0.00384	2.251766	C	0.222337	2.076713	0.883665
N	-0.94874	-0.82302	-0.42979	H	0.995205	1.305845	0.911682
H	-1.66464	-0.85886	-1.1425	C	-0.01251	2.531584	-0.56749
C	0.026088	0.250141	-0.4631	C	0.709939	3.249615	1.736092

H	1.009841	-0.1587	-0.22485	H	-0.39355	1.673797	-1.12514
C	0.043748	0.878403	-1.86751	H	-0.78779	3.304399	-0.57612
C	-0.30143	1.312608	0.587402	C	1.253502	3.051588	-1.25253
H	0.235025	0.078223	-2.58485	O	-0.00675	4.116271	2.192384
H	-0.94804	1.286367	-2.0869	H	1.631543	3.95047	-0.76033
C	1.105742	1.966124	-2.03232	H	2.04822	2.299397	-1.19209
O	-1.41605	1.732312	0.818591	C	1.016387	3.315317	-2.73477
H	0.913642	2.815585	-1.37246	O	0.321382	2.569123	-3.42509
H	2.09191	1.574098	-1.75765	N	1.6366	4.40003	-3.24858
C	1.210061	2.440583	-3.4774	H	1.556828	4.592678	-4.23557
O	0.978283	1.696741	-4.43057	H	2.203858	5.01201	-2.68513
N	1.601347	3.72336	-3.64507	H	-3.0947	-0.99796	4.353878
H	1.750821	4.07525	-4.57845	O	2.038111	3.247256	1.878117
H	1.799444	4.330429	-2.86645	H	2.30382	4.042292	2.369608
O	0.796127	1.774514	1.193815	O	-4.05295	3.890263	3.745822
H	0.542538	2.488122	1.80272	H	-3.93296	3.811873	4.703298
H	-2.44275	-4.59472	1.259587	O	-2.33811	5.053091	0.741604
O	-3.53206	1.912465	-1.18452	H	-3.00948	4.404176	1.001219
H	-2.83679	1.91967	-0.50679	H	-1.55997	4.786884	1.258495
H	-3.77344	0.969962	-1.2426				
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.52678	-2.56927	-1.36222	N	-4.20453	-0.46285	-0.70347
H	-2.7765	-3.13144	-0.96928	H	-3.76677	-1.19101	-1.26137
C	-3.74056	-1.3907	-0.53204	C	-3.54886	-0.33549	0.597802
H	-4.46022	-0.74197	-1.03542	H	-4.20743	0.257958	1.240206
C	-4.29768	-1.71444	0.887104	C	-3.27116	-1.67192	1.312697
C	-2.40629	-0.65589	-0.37129	C	-2.24777	0.478836	0.490367
H	-5.2467	-2.24198	0.762451	H	-4.18535	-2.27284	1.273267
H	-3.60224	-2.37876	1.404632	H	-2.48225	-2.2312	0.807626
C	-4.58306	-0.45839	1.688056	C	-2.93806	-1.50944	2.775426
O	-1.3463	-1.27108	-0.24887	O	-1.37815	0.404944	1.362663
O	-5.39851	0.385249	1.287603	O	-3.5364	-0.74744	3.521083
N	-3.89633	-0.28687	2.828885	N	-2.16403	1.282863	-0.58305
H	-4.03956	0.551523	3.372327	H	-2.91272	1.226536	-1.26317
H	-3.21748	-0.95765	3.15031	C	-1.01646	2.129985	-0.84927
N	-2.49364	0.688009	-0.30295	H	-0.59561	2.450845	0.104999
H	-3.39323	1.139282	-0.39962	C	0.067388	1.369927	-1.65447
C	-1.34851	1.536508	-0.01376	C	-1.5006	3.351028	-1.61192
H	-0.65067	0.969891	0.604778	H	0.267455	0.448206	-1.10471
C	-0.63633	1.977832	-1.31599	H	-0.35807	1.07601	-2.61871
C	-1.84548	2.736095	0.774715	C	1.369626	2.141277	-1.85202
H	-0.43766	1.063787	-1.87901	O	-2.43132	3.346178	-2.38838
H	-1.33608	2.5695	-1.91332	H	1.209708	3.039807	-2.45436
C	0.668165	2.740663	-1.10127	H	1.74585	2.497175	-0.88548
O	-2.95262	3.2158	0.659039	C	2.510606	1.336954	-2.51689
H	0.49061	3.689626	-0.58762	O	3.564145	1.989614	-2.75968
H	1.335157	2.170212	-0.44438	O	2.32146	0.115774	-2.75904

C	1.456999	3.058133	-2.39296	H	-5.17763	-0.72354	-0.58667
O	2.520942	3.718183	-2.22938	O	-0.75509	4.436173	-1.35873
O	0.999542	2.645849	-3.49146	H	-1.07139	5.16643	-1.91596
H	-4.36286	-3.14498	-1.37782	O	-1.97314	-2.32922	3.195061
O	-0.90629	3.230101	1.592204	H	-1.84295	-2.18797	4.167451
H	-1.25807	4.026015	2.024294	O	-2.0934	-1.57283	5.811315
O	-6.9967	0.027561	-0.94579	H	-2.7204	-0.9582	5.390686
H	-6.4315	0.168739	-0.15644	H	-1.39189	-1.02133	6.177757
H	-6.77278	0.748968	-1.54314				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.02736	-2.76395	-0.58666	N	1.594117	-0.74241	-0.64787
H	-1.14423	-3.08954	-0.20307	H	1.556586	-0.54259	0.34774
C	-2.35272	-1.45799	-0.02795	C	0.286174	-0.55242	-1.27086
H	-3.23076	-1.06605	-0.54615	H	0.307493	-1.04958	-2.24614
C	-2.67591	-1.48023	1.495442	C	-0.89859	-1.13161	-0.47062
C	-1.16427	-0.51825	-0.25875	C	0.0356	0.930253	-1.58184
H	-3.48923	-2.19307	1.654873	H	-0.63101	-2.1468	-0.16183
H	-1.80336	-1.82789	2.053139	H	-1.0896	-0.54757	0.43058
C	-3.16132	-0.12769	1.97822	C	-2.15852	-1.26023	-1.2895
O	-0.00293	-0.92426	-0.21886	O	-1.1057	1.35811	-1.79486
O	-4.1219	0.425142	1.418703	O	-2.19467	-1.67396	-2.43213
N	-2.49875	0.445528	2.995788	N	1.129614	1.703869	-1.64183
H	-2.75467	1.380923	3.285808	H	2.002625	1.265806	-1.37573
H	-1.69392	0.009691	3.415712	C	1.060968	3.11525	-1.90963
N	-1.47363	0.783333	-0.44118	C	0.710586	3.937708	-0.67712
H	-2.43891	1.085545	-0.42055	H	2.02076	3.465725	-2.29304
C	-0.45034	1.800892	-0.50733	H	0.307939	3.318029	-2.67417
C	-1.0397	3.169946	-0.26666	O	0.550862	3.503918	0.438741
H	0.323384	1.615432	0.242854	H	1.901351	-1.70337	-0.74838
H	0.053231	1.813319	-1.47996	O	0.604538	5.23792	-0.99837
O	-2.21683	3.396626	-0.08144	H	0.390187	5.740476	-0.19585
O	-0.09456	4.112779	-0.29412	O	-3.26277	-0.91959	-0.60717
H	-0.50791	4.978957	-0.14455	H	-4.03409	-1.06535	-1.1792
H	-2.73844	-3.44201	-0.3312	O	-2.72918	0.769431	-4.03819
O	-4.0623	3.089198	2.217198	H	-2.81637	-0.17785	-3.86908
H	-3.44576	3.433486	1.556301	H	-2.16984	1.061984	-3.29613
H	-4.25218	2.185553	1.890794				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.73845	-3.13342	2.012263	N	-2.24312	-0.10778	3.072019
H	-1.70833	-2.6927	2.927822	H	-2.35472	0.464654	3.904322
C	-2.3591	-2.22665	1.054478	C	-2.78763	0.59101	1.916927
H	-2.28966	-2.67134	0.058997	H	-2.53857	0.024106	1.016694
C	-3.8624	-1.932	1.343849	C	-4.33592	0.768159	1.9525
C	-1.59525	-0.89772	1.085815	C	-2.14166	1.980994	1.837362
H	-4.38595	-2.88928	1.394858	H	-4.78193	-0.22557	2.050353

H	-3.95398	-1.43446	2.311813	H	-4.62968	1.365013	2.81683
C	-4.49974	-1.13367	0.222818	C	-4.8675	1.378529	0.67586
O	-1.22945	-0.40344	2.149896	O	-1.82263	2.60379	2.844061
O	-4.5956	-1.61422	-0.91516	O	-4.56542	0.964047	-0.43332
N	-4.90717	0.114708	0.507276	N	-2.01086	2.477296	0.578188
H	-5.31598	0.681171	-0.22139	H	-2.32754	1.909856	-0.19706
H	-4.83029	0.505964	1.432243	C	-1.5798	3.837928	0.284928
N	-1.41629	-0.30526	-0.11863	H	-1.1225	4.238014	1.188791
H	-1.77942	-0.74324	-0.96326	C	-0.57941	3.850841	-0.88306
C	-0.86733	1.033931	-0.27728	C	-2.84431	4.642815	-0.02415
H	-0.41106	1.322077	0.667999	H	0.248432	3.195844	-0.60616
C	0.175775	1.059065	-1.41126	H	-1.05862	3.419848	-1.76745
C	-2.03833	1.976865	-0.56816	C	-0.03583	5.206959	-1.19317
H	0.966086	0.357499	-1.13883	O	-3.30895	4.777878	-1.1412
H	-0.28912	0.688187	-2.32902	N	-0.73065	6.165347	-1.90367
C	0.777957	2.406433	-1.63899	C	1.163559	5.80527	-0.88277
O	-2.55308	2.103404	-1.66264	H	-1.66417	6.058215	-2.27366
N	0.149433	3.409952	-2.35005	C	0.053033	7.272267	-1.99114
C	1.97071	2.960665	-1.23592	N	1.212428	7.091175	-1.38386
H	-0.76155	3.343586	-2.78071	H	1.987313	5.374229	-0.33434
C	0.964084	4.498141	-2.34837	H	-0.26591	8.167028	-2.50225
N	2.080468	4.263011	-1.68235	O	-3.42044	5.119468	1.076591
H	2.749794	2.487936	-0.65746	H	-4.25422	5.560059	0.840105
H	0.698403	5.419504	-2.84239	H	-2.74626	-0.9754	3.228394
O	-2.46247	2.618654	0.52017	O	-5.65971	2.429191	0.869616
H	-3.23524	3.160836	0.286865	H	-5.86967	2.835761	-0.01793
H	-2.28996	-3.98115	2.10166	O	-5.8189	3.444137	-1.62435
O	-2.75925	-0.63832	-2.7697	H	-5.45274	2.623436	-1.98413
H	-3.54264	-0.95429	-2.27973	H	-5.06163	4.055322	-1.60944
H	-2.80796	0.327322	-2.70915				
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.01329	-3.29598	-1.07912	N	-2.22823	-3.13588	-1.13646
H	-2.19508	-3.7476	-0.67933	H	-1.43716	-3.44561	-0.57792
C	-3.33099	-2.09468	-0.31731	C	-3.11624	-2.30911	-0.31431
H	-4.1267	-1.55771	-0.83773	H	-3.94833	-1.98259	-0.9395
C	-3.81315	-2.37961	1.136292	C	-3.67431	-3.04727	0.91935
C	-2.08011	-1.21359	-0.24893	C	-2.28723	-1.09743	0.134656
H	-4.68609	-3.03539	1.078312	H	-4.09511	-4.00735	0.599869
H	-3.02831	-2.90746	1.682844	H	-2.85814	-3.27247	1.612076
C	-4.25138	-1.11576	1.852165	C	-4.78336	-2.31736	1.646401
O	-0.95393	-1.70144	-0.1481	O	-1.26792	-1.26233	0.808624
O	-5.13818	-0.38822	1.381614	O	-5.44032	-1.40861	1.183561
N	-3.62487	-0.80865	2.998741	N	-2.73934	0.105556	-0.26458
H	-3.87933	0.034348	3.492153	H	-3.60503	0.145927	-0.79459
H	-2.89048	-1.38421	3.377242	C	-2.05341	1.342406	0.058253
N	-2.30982	0.115922	-0.24114	H	-1.41817	1.150973	0.923814
H	-3.25876	0.46261	-0.28341	C	-1.14059	1.814545	-1.11922

C	-1.24689	1.084418	-0.03551	C	-3.0752	2.398324	0.449809
H	-0.51564	0.649682	0.649088	H	-0.55219	0.920337	-1.35692
C	-0.51698	1.428773	-1.37293	C	-1.96096	2.198133	-2.35737
C	-1.85451	2.309336	0.626645	C	-0.15856	2.917514	-0.68807
H	-0.29421	0.44488	-1.80077	O	-4.23561	2.421824	0.091792
C	-1.43707	2.18285	-2.34066	H	-2.53147	3.116492	-2.18482
C	0.822755	2.14558	-1.13558	H	-1.30796	2.367995	-3.21501
O	-3.0306	2.598695	0.586074	H	-2.66427	1.409237	-2.6354
H	-1.63147	3.201545	-1.98913	H	-0.70379	3.851865	-0.52163
H	-0.98335	2.253533	-3.33067	H	0.280832	2.641728	0.277092
H	-2.39742	1.673605	-2.45446	C	0.970104	3.153729	-1.6984
H	0.637898	3.162174	-0.775	H	0.591356	3.525083	-2.65421
H	1.362853	1.627745	-0.33471	H	1.679001	3.893293	-1.31608
C	1.712332	2.195104	-2.3833	H	1.522956	2.228746	-1.89296
H	1.258593	2.78486	-3.18418	O	-2.53785	3.346248	1.22456
H	2.679484	2.64823	-2.14864	H	-3.21189	4.023014	1.403091
H	1.899268	1.188762	-2.7726	H	-2.71659	-3.96841	-1.4527
O	-0.93064	3.056766	1.244241	O	-5.07058	-2.74467	2.887711
H	-1.36397	3.846869	1.606938	H	-4.48339	-3.46432	3.159696
H	-3.78161	-3.95769	-1.02871	O	-5.59898	0.203349	-1.16766
O	-6.68247	-0.92098	-0.85461	H	-5.68993	-0.3734	-0.3896
H	-6.15251	-0.77514	-0.04244	H	-5.40926	1.077963	-0.79302
H	-6.95082	-1.84493	-0.81422				

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.80945	-2.91742	0.310238	N	-0.19533	-2.41491	1.747362
H	-0.10942	-2.85441	1.044593	H	0.546411	-2.19641	2.40719
C	-1.62697	-1.71095	0.310593	C	-0.88216	-1.18855	1.359651
H	-2.27732	-1.72981	-0.56691	H	-1.58262	-1.42188	0.555067
C	-2.53439	-1.5592	1.567343	C	-1.68682	-0.5258	2.513538
C	-0.69992	-0.49258	0.233203	C	0.167007	-0.19671	0.837745
H	-3.1621	-2.45143	1.63646	H	-2.42038	-1.25333	2.873067
H	-1.91339	-1.5075	2.464449	H	-1.02436	-0.2704	3.341614
C	-3.46078	-0.36537	1.443437	C	-2.43947	0.696311	2.042102
O	0.39062	-0.47924	0.803882	O	1.289497	-0.11969	1.335221
O	-4.22814	-0.26978	0.472486	O	-3.06721	0.728148	0.994666
N	-3.39085	0.577961	2.397113	N	-0.22995	0.60612	-0.17572
H	-3.9474	1.418228	2.30037	H	-1.19279	0.57048	-0.47979
H	-2.73661	0.512051	3.159722	C	0.652535	1.598135	-0.76155
N	-1.19582	0.569675	-0.43752	H	1.60996	1.123116	-0.97505
H	-2.10166	0.503507	-0.8822	C	0.017239	2.146474	-2.05374
C	-0.51083	1.850651	-0.48957	C	0.912797	2.74833	0.209964
H	0.131061	1.920362	0.387178	H	-0.16007	1.289798	-2.71321
C	0.337475	1.974001	-1.77909	H	-0.96176	2.566566	-1.79723
C	-1.55382	2.952227	-0.42697	C	0.841887	3.204736	-2.80642
H	1.004242	1.105047	-1.78652	O	0.059134	3.313091	0.863207
H	-0.33905	1.865827	-2.63353	H	1.019169	4.051468	-2.13147
C	1.172102	3.25637	-1.93227	C	2.203321	2.665653	-3.26753

O	-2.66144	2.863733	-0.91668	C	0.030086	3.72481	-4.00094
H	0.494003	4.117815	-1.91753	H	2.071573	1.789754	-3.91259
C	2.188839	3.427484	-0.79459	H	2.741226	3.426199	-3.84051
C	1.879985	3.241035	-3.29464	H	2.838939	2.376799	-2.42727
H	2.858609	2.561672	-0.74346	H	-0.92944	4.141542	-3.68038
H	2.803374	4.317109	-0.95977	H	0.579257	4.507234	-4.53211
H	1.704186	3.539737	0.178261	H	-0.17337	2.916019	-4.71165
H	1.16275	3.149134	-4.1159	H	-0.84024	-3.04556	2.213536
H	2.452553	4.160698	-3.44585	O	2.196872	3.112597	0.226199
H	2.57672	2.397664	-3.35955	H	2.298508	3.88586	0.806038
H	-1.38368	-3.73129	0.506546	O	-2.31853	1.745638	2.850646
O	-1.10491	4.04554	0.193843	H	-2.64805	2.549629	2.363276
H	-1.78874	4.735004	0.152714	O	-2.71116	3.723703	1.076173
O	-5.16971	2.355097	0.509006	H	-3.16441	3.142051	0.451071
H	-4.9777	1.403628	0.378902	H	-1.76425	3.624136	0.856319
H	-4.44273	2.790338	0.04107				
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.73974	-2.42378	2.702755	N	-1.4161	-3.08335	0.250356
H	-1.82904	-2.5269	3.140038	H	-0.52366	-3.45591	0.562695
C	-2.56671	-1.98527	1.318212	C	-1.55219	-1.69785	0.688368
H	-2.27161	-2.80928	0.650399	H	-2.45814	-1.28264	0.24208
C	-3.92788	-1.41446	0.820914	C	-1.65428	-1.53286	2.225305
C	-1.39448	-0.98404	1.271674	C	-0.32831	-0.9208	0.179268
H	-4.71257	-1.98967	1.313798	H	-2.36354	-2.27191	2.615254
H	-4.03366	-0.37506	1.138334	H	-0.69068	-1.74524	2.698928
C	-4.11861	-1.47131	-0.68387	C	-2.16439	-0.18093	2.671975
O	-0.61743	-0.86315	2.22019	O	0.787115	-1.44239	0.148374
O	-3.56916	-0.65204	-1.44303	O	-2.69433	0.62683	1.934573
N	-4.89111	-2.4539	-1.16296	N	-0.55295	0.356411	-0.18538
H	-5.02439	-2.53806	-2.16014	H	-1.47669	0.753057	-0.07372
H	-5.34354	-3.12264	-0.56061	C	0.519762	1.241777	-0.60446
N	-1.23283	-0.28758	0.128679	H	1.419688	0.996409	-0.03693
H	-1.94264	-0.34697	-0.60028	C	0.815206	1.07311	-2.11523
C	-0.14516	0.658275	-0.01763	C	0.108751	2.668438	-0.28028
H	0.800599	0.166469	0.219752	H	0.948571	-0.00064	-2.27367
C	-0.11488	1.181789	-1.466	H	-0.07275	1.374643	-2.68062
C	-0.3191	1.82144	0.959157	C	2.052179	1.821672	-2.61744
H	-0.04617	0.306777	-2.11963	O	-1.03868	3.049751	-0.21077
H	-1.06808	1.675513	-1.68352	H	1.911408	2.901287	-2.51482
C	1.047454	2.134309	-1.75723	H	2.916548	1.556674	-1.99808
O	-1.38166	2.347611	1.219588	C	2.348992	1.482236	-4.08304
H	0.963332	3.033409	-1.13858	H	2.510142	0.403594	-4.18697
H	1.993486	1.653272	-1.48591	H	1.484277	1.742479	-4.70366
C	1.083144	2.538817	-3.23564	C	3.576677	2.231177	-4.58107
H	1.203953	1.645759	-3.8586	H	3.434674	3.311366	-4.55358
H	0.131911	3.004614	-3.51512	H	4.469564	1.977905	-4.00948
C	2.224728	3.508453	-3.50514	N	3.875745	1.875936	-6.01704

H	2.108964	4.438977	-2.94962	H	3.089813	2.102259	-6.63045
H	3.194265	3.072103	-3.2656	H	4.691739	2.381974	-6.36683
N	2.277808	3.88775	-4.96501	H	4.067599	0.877252	-6.12107
H	1.416531	4.350156	-5.26451	O	1.169859	3.468315	-0.11285
H	3.050751	4.528001	-5.1575	H	0.85584	4.375721	0.035456
H	2.406551	3.06671	-5.56047	H	-2.14767	-3.65669	0.658308
H	-3.19627	-3.32985	2.722323	O	-2.04738	0.118967	3.973637
O	0.84622	2.238129	1.462374	H	-1.61026	-0.58865	4.468823
H	0.686656	3.013533	2.025745	O	-3.34131	3.224602	2.915109
O	-3.6827	2.100079	-0.52276	H	-3.12164	2.322813	2.615609
H	-3.6781	1.192616	-0.86964	H	-3.20315	3.204105	3.868135
H	-2.93508	2.13392	0.097488				
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.35517	-3.57759	0.620545	N	-0.20136	-2.25329	2.850675
H	-1.94655	-3.55291	1.551039	H	0.13454	-1.85448	3.723274
C	-2.8253	-2.24372	0.256186	C	-1.14919	-1.33751	2.226844
H	-3.15583	-2.266	-0.78378	H	-1.39615	-1.7164	1.23287
C	-4.00627	-1.73639	1.121834	C	-2.47792	-1.17222	3.016984
C	-1.64593	-1.27289	0.387052	C	-0.46831	0.030913	2.085334
H	-4.81027	-2.47752	1.063934	H	-2.93722	-2.16059	3.112596
H	-3.70008	-1.6698	2.16889	H	-2.28048	-0.78974	4.019299
C	-4.58342	-0.41943	0.632244	C	-3.45594	-0.27644	2.293401
O	-0.8239	-1.37028	1.29732	O	0.303882	0.463024	2.939308
O	-4.62445	-0.14557	-0.57724	O	-3.65157	-0.33979	1.089264
N	-5.05131	0.42124	1.568235	N	-0.79349	0.743495	0.98152
H	-5.42484	1.316901	1.288804	H	-1.51848	0.39441	0.370272
H	-4.97329	0.220648	2.552123	C	-0.23833	2.059767	0.734089
N	-1.58182	-0.2906	-0.54025	H	0.843057	2.015668	0.873523
H	-2.36559	-0.1705	-1.16748	C	-0.56462	2.49127	-0.70879
C	-0.55306	0.729783	-0.4921	C	-0.79078	3.088192	1.72213
H	0.42153	0.244748	-0.41511	H	-0.19273	1.70457	-1.37109
C	-0.61917	1.579192	-1.77652	H	-1.65172	2.539937	-0.82866
C	-0.72715	1.620177	0.739589	C	0.066703	3.831122	-1.08617
H	-0.52019	0.890473	-2.62033	O	-1.95752	3.186125	2.041197
H	-1.60772	2.04522	-1.84122	H	-0.33228	4.644513	-0.47536
C	0.472955	2.646101	-1.84406	H	1.150722	3.79876	-0.94851
O	-1.79179	2.044391	1.137664	S	-0.28779	4.215767	-2.84423
H	0.357162	3.383172	-1.0458	C	0.547275	5.835986	-2.95577
H	1.46359	2.19315	-1.75115	H	1.612686	5.731912	-2.74226
S	0.381204	3.528787	-3.44949	H	0.416508	6.192432	-3.97834
C	1.741333	4.722035	-3.20195	H	0.093871	6.547971	-2.26361
H	2.687538	4.198237	-3.05416	O	0.157654	3.916739	2.1637
H	1.801597	5.328683	-4.10652	H	-0.24948	4.588399	2.73622
H	1.53253	5.367624	-2.34686	H	-0.65885	-3.13151	3.074771
O	0.443121	1.925347	1.307156	O	-4.05156	0.614055	3.08182
H	0.285558	2.539395	2.04368	H	-4.49443	1.291556	2.50139
H	-3.1358	-4.22631	0.650916	O	-4.58494	2.522451	1.26645

O	-3.99789	2.60926	-0.6817	H	-4.53873	1.90597	0.523196
H	-3.27988	2.484043	-0.04021	H	-3.661	2.810456	1.397409
H	-4.32702	1.703352	-0.82586				
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.22932	-3.02853	1.937892	N	-2.74017	-0.58908	2.510967
H	-0.89088	-2.63254	2.81087	H	-2.73836	-0.12347	3.414454
C	-1.90656	-1.99374	1.161406	C	-2.99765	0.38547	1.454654
H	-2.15672	-2.4041	0.181439	H	-2.89122	-0.11483	0.490191
C	-3.21584	-1.47765	1.811518	C	-4.40854	1.018641	1.518116
C	-0.93382	-0.82246	0.981728	C	-1.94214	1.492658	1.576882
H	-3.87133	-2.33855	1.978812	H	-5.14883	0.220843	1.646078
H	-2.99794	-1.03808	2.787977	H	-4.49458	1.669189	2.393907
C	-3.97742	-0.50606	0.926714	C	-4.80353	1.778111	0.270871
O	-0.17142	-0.46934	1.880412	O	-1.58594	1.917894	2.675107
O	-4.00461	-0.64653	-0.30585	O	-4.21269	1.708189	-0.78814
N	-4.62008	0.498588	1.54289	N	-1.45121	1.98667	0.420145
H	-5.1129	1.185159	0.989791	H	-1.88842	1.708341	-0.44717
H	-4.54981	0.645485	2.536844	C	-0.49715	3.07888	0.411853
N	-0.98781	-0.1857	-0.21018	H	0.364215	2.80656	1.023637
H	-1.73208	-0.42713	-0.85041	C	-0.04203	3.351353	-1.04121
C	-0.17275	0.981133	-0.48571	C	-1.11165	4.34437	1.012835
H	0.869567	0.748812	-0.26342	H	0.382221	2.417205	-1.41943
C	-0.31867	1.367708	-1.97642	H	-0.92524	3.584986	-1.64247
C	-0.58708	2.160013	0.396528	C	0.971293	4.467491	-1.14222
H	-0.01817	0.493686	-2.56036	O	-2.22598	4.754382	0.759077
H	-1.37593	1.558913	-2.18154	C	0.5829	5.750787	-1.54307
C	0.515356	2.568076	-2.35871	C	2.31266	4.241512	-0.80811
O	-1.73647	2.495685	0.595962	H	-0.45215	5.93796	-1.80915
C	-0.06469	3.83723	-2.46549	C	1.513618	6.790317	-1.60457
C	1.891211	2.43344	-2.58433	C	3.245272	5.276948	-0.86815
H	-1.13017	3.95464	-2.29783	H	2.627612	3.249275	-0.50126
C	0.713735	4.951804	-2.78551	H	1.196809	7.778408	-1.91885
C	2.672125	3.544023	-2.90442	C	2.84727	6.556358	-1.26559
H	2.351785	1.453449	-2.51074	H	4.28045	5.085441	-0.60882
H	0.248676	5.927865	-2.86598	H	3.571646	7.361409	-1.31443
C	2.084822	4.808258	-3.00426	O	-0.26262	4.98403	1.81857
H	3.735335	3.422939	-3.07884	H	-0.67634	5.810604	2.118229
H	2.690344	5.671832	-3.25482	H	-3.47488	-1.28942	2.530089
O	0.464109	2.816852	0.890438	O	-5.89228	2.557426	0.352776
H	0.14709	3.591743	1.383637	H	-6.27483	2.54554	1.242185
H	-1.88109	-3.77005	2.175293	O	-3.49369	4.336573	-1.80383
O	-3.89214	2.00257	-1.29225	H	-3.8756	3.45315	-1.68782
H	-4.03396	1.05052	-1.13932	H	-3.10085	4.523328	-0.93499
H	-3.19713	2.228737	-0.65266				
Asn-Pro							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z

N	-0.25582	-2.87655	-0.74939	N	-0.95843	0.419987	-2.42186
H	0.575441	-2.98987	-0.175	H	-0.54182	-0.09661	-3.19169
C	-1.21739	-2.02065	-0.05266	C	-0.07994	0.384278	-1.24746
H	-2.09231	-1.90213	-0.68792	H	-0.61447	0.848593	-0.41549
C	-1.69339	-2.58758	1.308508	C	0.331212	-1.03913	-0.84225
C	-0.52976	-0.67359	0.19056	C	1.169286	1.23065	-1.54764
H	-2.16035	-3.55992	1.127354	H	-0.5746	-1.62026	-0.63801
H	-0.83123	-2.73832	1.961039	H	0.850163	-1.52413	-1.67146
C	-2.73749	-1.69596	1.953394	C	1.179233	-1.10358	0.406395
O	0.52081	-0.63742	0.842977	O	2.265662	0.697447	-1.75656
O	-3.71443	-1.29333	1.305401	O	1.15249	-0.28321	1.300323
N	-2.54691	-1.36003	3.240438	N	1.022246	2.568671	-1.58122
H	-3.20319	-0.74266	3.695643	C	-0.22239	3.342084	-1.39709
H	-1.72132	-1.63662	3.746275	C	2.154417	3.415509	-1.96447
N	-1.10277	0.452269	-0.27778	H	-0.40421	3.489078	-0.32872
C	-2.27462	0.573305	-1.17205	H	-1.06189	2.809334	-1.83798
C	-0.45511	1.745658	-0.03478	C	0.091613	4.662374	-2.10612
H	-3.19412	0.480148	-0.59048	C	1.593268	4.852716	-1.84748
H	-2.25822	-0.20219	-1.93612	H	2.462564	3.190269	-2.98763
C	-2.11372	1.976765	-1.76571	C	3.390528	3.238044	-1.10347
C	-1.44651	2.768682	-0.63318	H	-0.50849	5.488874	-1.72428
H	0.510241	1.784969	-0.5437	H	-0.09737	4.564964	-3.17892
C	-0.17286	2.037226	1.42685	H	1.753698	5.231936	-0.8347
H	-3.06912	2.403341	-2.0721	H	2.081475	5.527389	-2.54947
H	-1.4559	1.941147	-2.63818	O	4.52156	3.320321	-1.52354
H	-2.18968	3.049845	0.117489	O	3.105304	3.068611	0.202843
H	-0.93492	3.670429	-0.96686	H	3.938329	3.0113	0.697275
O	0.802942	2.634723	1.81761	H	-1.84363	-0.03002	-2.21013
O	-1.16618	1.638853	2.246307	O	1.981999	-2.17207	0.545566
H	-0.93294	1.88602	3.155339	H	1.935592	-2.75098	-0.22829
H	-0.65104	-3.80193	-0.88763	O	0.643266	2.464734	1.814002
O	-4.1698	1.407837	1.901728	H	0.71608	1.508169	1.657722
H	-4.14975	0.456035	1.680986	H	1.378393	2.828963	1.302984
H	-3.23616	1.63276	2.008868				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.88541	-3.14099	0.319447	N	-0.80212	-3.20811	0.320665
H	-0.13328	-3.2404	0.995973	H	-0.06016	-3.2733	1.01229
C	-1.30671	-1.74485	0.256165	C	-1.27353	-1.83167	0.233449
H	-2.02415	-1.63613	-0.55925	H	-1.96691	-1.75378	-0.60667
C	-1.98026	-1.23346	1.556021	C	-2.01505	-1.33577	1.507803
C	-0.0721	-0.88735	-0.04678	C	-0.06297	-0.92627	-0.03337
H	-2.82037	-1.89806	1.782643	H	-2.85651	-2.01098	1.689937
H	-1.27781	-1.30016	2.390702	H	-1.35404	-1.37378	2.374733
C	-2.54885	0.169068	1.424715	C	-2.574	0.056583	1.328857
O	1.035055	-1.15571	0.414329	O	1.044123	-1.16465	0.442172
O	-3.04731	0.562426	0.358033	O	-3.13996	0.418856	0.30798
N	-2.49334	0.949625	2.514835	N	-0.3026	0.168706	-0.79635

H	-2.82517	1.902292	2.459425	H	-1.25574	0.375276	-1.06319
H	-2.03909	0.648399	3.361738	C	0.737983	1.130093	-1.09747
N	-0.2888	0.199013	-0.82625	H	1.644848	0.596951	-1.38369
H	-1.2469	0.447634	-1.03626	C	0.277864	2.019027	-2.25801
C	0.770091	1.142589	-1.12041	C	1.065158	2.011263	0.112345
H	1.652052	0.599089	-1.46041	H	0.057532	1.377815	-3.11844
C	0.296328	2.094178	-2.22478	H	-0.63613	2.552538	-1.96939
C	1.156372	1.95482	0.120037	O	1.335249	2.927274	-2.53675
H	0.025671	1.49632	-3.10203	O	0.235743	2.598683	0.776245
H	-0.58993	2.64079	-1.88003	H	1.02942	3.569368	-3.18669
O	1.36982	2.982975	-2.50724	O	2.374087	2.087758	0.347718
O	0.356406	2.502291	0.850422	H	2.526318	2.689673	1.095611
H	1.056257	3.663548	-3.1128	H	-1.55511	-3.81787	0.623803
O	2.476073	2.016927	0.300323	O	-2.47832	3.23762	1.1222
H	2.661753	2.577424	1.072182	H	-1.54524	3.10334	0.866649
H	-1.65471	-3.72382	0.634807	H	-2.98307	2.879511	0.379407
O	-2.37603	3.309797	0.271218	O	-2.35647	0.860938	2.364554
H	-1.44798	3.109114	0.475825	H	-2.56536	1.793629	2.079902
H	-2.77647	2.427068	0.16895				
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	1.692722	-1.80234	-0.45232	N	1.957311	-1.848	-0.24179
H	2.443183	-1.81527	0.233037	H	2.714004	-1.75276	0.429777
C	1.307588	-0.42161	-0.73351	C	1.540569	-0.53158	-0.70675
H	0.609397	-0.42708	-1.57219	H	0.830246	-0.65752	-1.52676
C	0.625686	0.288186	0.463717	C	0.862389	0.342718	0.384916
C	2.565555	0.354752	-1.14076	C	2.774345	0.226154	-1.2087
H	-0.18871	-0.35552	0.814146	H	0.125634	-0.27173	0.914705
H	1.332589	0.3865	1.291842	H	1.598234	0.667445	1.125463
C	-0.01022	1.629373	0.132167	C	0.097859	1.53029	-0.16133
O	3.672368	0.083628	-0.67684	O	3.886609	0.03801	-0.7227
O	-0.46149	1.886498	-0.9947	O	-0.31557	1.614626	-1.29639
N	2.364129	1.359605	-2.02272	N	2.539619	1.157698	-2.16583
H	1.412309	1.64066	-2.22251	H	1.574638	1.366398	-2.39131
C	3.412136	2.283298	-2.38049	C	3.498199	2.209187	-2.41368
H	4.352467	1.735712	-2.46983	H	4.4943	1.775992	-2.52238
C	3.112887	2.949383	-3.73518	C	3.166842	2.966727	-3.70913
C	3.617065	3.334298	-1.28526	C	3.56117	3.161003	-1.21139
H	3.914269	3.669908	-3.92793	H	3.879922	3.791463	-3.79841
C	3.04186	1.942905	-4.87771	C	3.245369	2.076647	-4.94261
O	1.870645	3.643017	-3.55359	O	1.840938	3.497616	-3.52698
O	2.923329	3.465753	-0.30587	O	2.823266	3.116685	-0.25592
H	2.258451	1.203502	-4.69996	H	2.546742	1.241095	-4.86758
H	2.82629	2.462233	-5.81527	H	3.004108	2.657201	-5.83691
H	3.998293	1.425294	-4.98946	H	4.257869	1.682189	-5.05913
H	1.604802	4.033855	-4.39361	H	1.546206	3.898918	-4.3529
H	0.90888	-2.30973	-0.05365	H	1.189053	-2.31863	0.225577
O	4.691891	4.098155	-1.54657	O	4.552869	4.052852	-1.35016

H	4.785561	4.754192	-0.83723	H	4.554524	4.641532	-0.57798
O	-1.4621	0.237754	-3.00138	O	-0.1728	2.533412	0.697782
H	-1.97317	-0.46458	-2.58538	H	0.247995	2.391155	1.557536
H	-1.14501	0.791379	-2.25996	O	0.469953	4.928232	-1.39433
N	-0.10289	2.509719	1.139167	H	0.362431	4.276509	-0.69018
H	-0.53128	3.408041	0.972339	H	0.982707	4.455679	-2.07125
H	0.310695	2.335868	2.040874				
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.65488	-1.82113	3.227358	N	-2.32969	-3.1385	2.023194
H	-4.29966	-1.172	3.670127	H	-2.90382	-2.55275	2.623423
C	-3.59861	-1.55464	1.792782	C	-2.20161	-2.52064	0.708851
H	-2.79684	-2.15632	1.359892	H	-1.47934	-3.09286	0.122917
C	-4.91033	-1.8964	1.041046	C	-3.5322	-2.4607	-0.0875
C	-3.27137	-0.06993	1.590439	C	-1.69145	-1.08687	0.896432
H	-5.19986	-2.91658	1.316469	H	-3.99891	-3.45219	-0.06561
H	-5.71807	-1.2374	1.370803	H	-4.23159	-1.77355	0.397479
C	-4.78898	-1.88062	-0.47428	C	-3.3787	-2.10076	-1.5494
O	-3.64114	0.792498	2.387067	O	-2.0449	-0.39966	1.853261
O	-3.69542	-2.06219	-1.03808	O	-2.33031	-2.17225	-2.16163
N	-5.92257	-1.69807	-1.16655	N	-0.88861	-0.61486	-0.08294
H	-5.88994	-1.69713	-2.17851	H	-0.79327	-1.18169	-0.9149
H	-6.80194	-1.52647	-0.70642	C	-0.59344	0.800819	-0.19512
N	-2.58918	0.229016	0.46269	H	-0.07959	1.140771	0.704597
H	-2.48694	-0.50598	-0.22724	C	0.302208	1.02848	-1.43917
C	-2.3797	1.601981	0.048735	C	-1.8907	1.599034	-0.33107
H	-1.83481	2.137538	0.827227	H	1.18121	0.387753	-1.30989
C	-1.56552	1.613927	-1.26882	H	-0.23813	0.671063	-2.32133
C	-3.71667	2.311834	-0.1654	C	0.717112	2.451364	-1.63619
H	-0.65077	1.042804	-1.07794	O	-2.86739	1.217297	-0.93532
H	-2.13516	1.071865	-2.02989	C	0.288225	3.298958	-2.62909
C	-1.23328	2.987532	-1.758	C	1.621099	3.212001	-0.81216
O	-4.68623	1.801424	-0.67854	H	-0.39477	3.110051	-3.4427
C	-1.77131	3.623004	-2.85113	N	0.868253	4.540135	-2.47205
C	-0.31135	3.917438	-1.15752	C	1.691726	4.520454	-1.36809
H	-2.50003	3.264964	-3.56177	C	2.378062	2.916647	0.334876
N	-1.24185	4.890739	-2.96655	H	0.724359	5.328014	-3.08254
C	-0.34317	5.102858	-1.94465	C	2.490242	5.524576	-0.81186
C	0.538	3.864235	-0.03866	C	3.173128	3.911991	0.891882
H	-1.46729	5.548514	-3.69493	H	2.346005	1.927205	0.777769
C	0.442956	6.219285	-1.64352	H	2.532479	6.515137	-1.2498
C	1.32156	4.971975	0.264861	C	3.22726	5.203662	0.323938
H	0.58467	2.97271	0.577228	H	3.762145	3.696803	1.776393
H	0.405847	7.11311	-2.25545	H	3.855823	5.959718	0.780862
C	1.273149	6.138249	-0.52981	O	-1.80799	2.794969	0.268567
H	1.981341	4.94363	1.124788	H	-2.63215	3.281039	0.102441
H	1.895265	6.986608	-0.26765	H	-2.78685	-4.04167	1.948211
O	-3.67781	3.588723	0.242952	O	-4.48238	-1.72169	-2.20519

H	-4.52757	4.006945	0.028261	H	-5.25371	-1.69016	-1.62092
H	-4.0052	-2.75897	3.395875	O	-1.5901	-0.37127	-4.25343
O	-4.17546	-1.70166	-3.74085	H	-0.74073	-0.6972	-4.56999
H	-4.06808	-2.52007	-4.23745	H	-1.88368	-1.03447	-3.60367
H	-3.83091	-1.89645	-2.84356				
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.79309	-2.25635	1.962016	N	0.771804	-1.86029	1.501316
H	-1.29203	-2.1498	2.840831	H	0.156629	-1.87579	2.310311
C	-1.43476	-1.45072	0.928396	C	0.109673	-1.17773	0.395209
H	-0.79401	-1.44858	0.043785	H	0.833624	-1.03731	-0.4107
C	-2.83037	-1.97383	0.498961	C	-1.10776	-1.94853	-0.1757
C	-1.56523	-0.01042	1.443092	C	-0.37072	0.191405	0.89143
H	-2.74014	-3.04655	0.295612	H	-0.81242	-2.98862	-0.35436
H	-3.54666	-1.86631	1.318243	H	-1.92906	-1.97743	0.544112
C	-3.37226	-1.34418	-0.77423	C	-1.61601	-1.42992	-1.4969
O	-1.6298	0.254327	2.643483	O	-0.76459	0.356453	2.045181
O	-2.61241	-0.85167	-1.62746	O	-0.97573	-0.72813	-2.26035
N	-4.70131	-1.37471	-0.94485	N	-0.38219	1.178288	-0.03057
H	-5.10208	-0.98011	-1.78615	H	-0.1692	0.933644	-0.9873
H	-5.31775	-1.75508	-0.24494	C	-1.04058	2.4394	0.225227
N	-1.64895	0.93725	0.485585	H	-0.65149	2.865086	1.152125
H	-1.68905	0.633053	-0.4791	C	-0.79786	3.430095	-0.93986
C	-1.92991	2.318401	0.801008	C	-2.54435	2.234495	0.402052
H	-1.1605	2.705404	1.472806	H	-1.2669	3.030186	-1.84317
C	-1.95898	3.17161	-0.49211	H	-1.30678	4.362769	-0.68623
C	-3.27811	2.459254	1.504664	C	0.672018	3.672482	-1.19106
H	-2.7973	2.837185	-1.11013	O	-3.17479	1.297798	-0.03034
H	-2.16231	4.204305	-0.19963	C	1.31215	3.105053	-2.29723
C	-0.66799	3.08254	-1.27185	C	1.436366	4.447217	-0.30828
O	-4.22844	1.730197	1.343165	H	0.736657	2.511637	-3.00022
C	-0.57563	2.305665	-2.43052	C	2.676928	3.29759	-2.52028
C	0.482481	3.751422	-0.8319	C	2.797701	4.64813	-0.51674
H	-1.45035	1.780988	-2.80042	H	0.962341	4.902978	0.555166
C	0.62516	2.189708	-3.13273	H	3.157676	2.852469	-3.38527
C	1.687373	3.646113	-1.51981	C	3.42169	4.069611	-1.62659
H	0.437497	4.365105	0.06193	H	3.384421	5.25108	0.166154
H	0.675859	1.5836	-4.03108	O	4.762135	4.300476	-1.78512
C	1.760702	2.86022	-2.67443	H	5.082284	3.857397	-2.58027
H	2.573096	4.16789	-1.1774	O	-3.09609	3.262592	1.067282
O	2.969799	2.791613	-3.31203	H	-4.056	3.124481	1.113405
H	2.902959	2.224318	-4.08978	H	0.974137	-2.82336	1.252387
H	-0.82343	-3.23944	1.71094	O	-2.85051	-1.85956	-1.77145
O	-3.29934	3.549226	2.290389	H	-3.11409	-1.53181	-2.64713
H	-4.18925	3.641942	2.667281	O	-1.54498	1.530566	-3.90514
O	-4.17634	0.349374	-3.56785	H	-1.43903	0.70351	-3.40494
H	-3.50505	0.003333	-2.94206	H	-2.4788	1.751133	-3.81863
H	-4.29481	1.274375	-3.32619				

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.03436	-3.21091	-0.58041	N	-3.4212	-2.6937	-0.65677
H	-2.18243	-3.7653	-0.57115	H	-2.68489	-3.39423	-0.65948
C	-2.85473	-2.0225	0.244421	C	-2.99205	-1.53425	0.112095
H	-3.73119	-1.38329	0.121157	H	-3.72711	-0.73632	-0.02002
C	-2.69246	-2.32982	1.762502	C	-2.85434	-1.79997	1.643241
C	-1.60763	-1.27599	-0.23887	C	-1.63275	-1.06863	-0.42525
H	-3.57602	-2.88555	2.088419	H	-3.80512	-2.20681	1.996581
H	-1.81758	-2.96617	1.913015	H	-2.06693	-2.53095	1.830887
C	-2.62576	-1.06747	2.601638	C	-2.59962	-0.51873	2.401945
O	-0.61128	-1.87828	-0.6401	O	-0.81091	-1.86805	-0.87051
O	-3.52899	-0.2194	2.555786	O	-3.35662	0.438132	2.348095
N	-1.54179	-0.89906	3.375114	N	-1.38516	0.255907	-0.30924
H	-1.45886	-0.06507	3.937647	H	-2.09332	0.865551	0.076034
H	-0.7989	-1.57807	3.409605	C	-0.09318	0.834638	-0.6337
N	-1.66294	0.068067	-0.13322	H	0.656775	0.047873	-0.54007
H	-2.49223	0.509044	0.241511	C	-0.05047	1.373997	-2.09781
C	-0.52017	0.916935	-0.42189	C	0.221127	1.909982	0.390771
H	0.386784	0.383476	-0.13006	H	-0.41649	0.528772	-2.69019
C	-0.42212	1.245592	-1.94531	C	-0.99804	2.560243	-2.3086
C	-0.63853	2.166443	0.433997	C	1.374235	1.696806	-2.5607
H	-0.50848	0.264206	-2.42254	O	-0.62134	2.509537	1.031056
C	-1.58535	2.12132	-2.42423	H	-0.6623	3.440923	-1.75157
C	0.935672	1.840562	-2.33249	H	-1.02839	2.829312	-3.3673
O	-1.67467	2.57585	0.91068	H	-2.01854	2.326979	-1.99409
H	-1.52356	3.130283	-2.00347	H	2.049133	0.851613	-2.39813
H	-1.55997	2.214242	-3.51287	H	1.369851	1.92655	-3.62937
H	-2.55267	1.695283	-2.14563	H	1.782396	2.562224	-2.03303
H	1.761079	1.214666	-1.9809	O	1.528844	2.145546	0.496219
H	1.007447	1.914916	-3.42088	H	1.670509	2.87158	1.126718
H	1.069646	2.842163	-1.91718	H	-4.24236	-3.11414	-0.23347
H	-3.77847	-3.79026	-0.20434	O	-1.46165	-0.51136	3.092485
O	0.538974	2.787761	0.580665	H	-1.32476	0.406541	3.460598
H	0.39802	3.601787	1.091705	O	-1.29084	2.100478	3.765543
O	-5.94269	-0.47421	1.223109	H	-0.94158	2.421752	2.914982
H	-5.09781	-0.42545	1.718605	H	-2.24895	2.190456	3.663233
H	-6.28571	-1.35589	1.403033				

Table S15.B. Succinimide Formation XYZ Coordinates (Implicit solvation + 1 H_2O, $\varepsilon = 80$)

All Reactions			
NH_3			
Product Structure			
Atom	X	Y	Z
N	-1.133326	-0.563263	0.000024
H	-0.744703	-1.50246	-0.000031

H	-0.744689	-0.093642	0.813368
H	-0.7447	-0.093681	-0.813362

Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.80773	-2.89702	0.322781	N	-0.71688	-1.59329	2.364289
H	-0.8935	-2.8566	0.765271	H	-0.99446	-0.82326	2.966158
C	-2.4982	-1.62759	0.512093	C	-1.42881	-1.54866	1.100556
H	-3.41582	-1.63777	-0.0803	H	-1.18551	-2.46301	0.548763
C	-2.89399	-1.33329	1.989232	C	-2.96294	-1.35751	1.104914
C	-1.58617	-0.49828	0.020725	C	-0.93092	-0.40952	0.20298
H	-3.50316	-2.16811	2.345328	H	-3.53081	-2.27731	0.966635
H	-1.99508	-1.27759	2.60751	H	-3.29819	-0.88958	2.035258
C	-3.74049	-0.08017	2.096182	C	-3.24063	-0.39154	-0.02072
O	-0.36607	-0.54394	0.17892	O	0.206047	-0.02921	0.041715
O	-4.79322	0.018047	1.44587	O	-4.32459	-0.06641	-0.47222
N	-3.29073	0.908693	2.885898	N	-2.03569	0.126839	-0.46185
H	-3.79964	1.7833	2.918791	C	-1.91868	1.139117	-1.50862
H	-2.4151	0.835444	3.377462	H	-0.88775	1.500939	-1.44013
N	-2.21562	0.562616	-0.52842	C	-2.1712	0.562861	-2.90012
H	-3.22437	0.567357	-0.60323	C	-2.79272	2.353649	-1.19864
C	-1.50372	1.769975	-0.90598	H	-3.18522	0.171925	-2.98414
H	-0.68459	1.92096	-0.19897	H	-2.03397	1.341214	-3.65079
C	-0.92407	1.686692	-2.33104	H	-1.45966	-0.24171	-3.09134
C	-2.44546	2.954284	-0.78719	O	-3.41287	2.975363	-2.03185
H	-1.72519	1.552601	-3.06165	H	-0.94008	-2.45115	2.857875
H	-0.36707	2.593439	-2.5717	O	-2.7402	2.694113	0.094325
H	-0.25001	0.831005	-2.38509	H	-3.28752	3.484498	0.230719
O	-3.65244	2.870454	-0.69301	O	-5.76503	1.180853	-2.64591
H	-2.32706	-3.64875	0.765413	H	-5.33765	0.718586	-1.90694
O	-1.78502	4.114275	-0.83356	H	-5.17437	1.928603	-2.80346
H	-2.42561	4.843574	-0.79794				
O	-5.5167	2.70548	1.57376				
H	-5.43496	1.734685	1.473014				
H	-4.979	3.044699	0.844549				

Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.58109	-4.21239	-0.25604	N	-2.89653	-4.16913	1.542857
H	-1.75237	-4.48694	0.264381	H	-2.98678	-3.85202	2.504023
C	-3.02324	-2.89574	0.183885	C	-2.88363	-3.04606	0.624019
H	-3.8279	-2.56056	-0.47452	H	-2.90777	-3.44759	-0.39464
C	-3.5645	-2.86043	1.644081	C	-3.96512	-1.94884	0.758229
C	-1.84376	-1.92251	0.08095	C	-1.56821	-2.26199	0.701661
H	-4.37052	-3.59513	1.719168	H	-4.78211	-2.03446	0.042053
H	-2.77277	-3.15091	2.338671	H	-4.39685	-1.94131	1.76332
C	-4.15725	-1.50722	1.985733	C	-3.22978	-0.64537	0.563762
O	-0.68826	-2.2829	0.302176	O	-0.44582	-2.69597	0.821328
O	-5.04757	-1.01849	1.271802	O	-3.70575	0.470053	0.45024

N	-3.66439	-0.86385	3.056292	N	-1.86974	-0.90395	0.572466
H	-3.99544	0.069792	3.265489	C	-0.8408	0.127013	0.467176
H	-2.91333	-1.24867	3.605405	H	0.089695	-0.37256	0.756891
N	-2.17296	-0.64143	-0.19684	C	-0.7142	0.661788	-0.96553
H	-3.13982	-0.39269	-0.35964	C	-1.07085	1.217801	1.515858
C	-1.19361	0.430061	-0.18115	H	-0.78311	-0.19988	-1.63538
H	-0.41897	0.178428	0.545183	H	-1.56099	1.314729	-1.18632
C	-0.54338	0.607341	-1.57429	C	0.607011	1.394723	-1.21658
C	-1.88819	1.704255	0.269473	O	-0.97973	2.405853	1.305794
H	-0.17162	-0.38138	-1.85692	H	0.697758	2.244	-0.53465
H	-1.32452	0.876997	-2.29203	H	1.448569	0.720718	-1.02463
C	0.601135	1.622765	-1.61879	C	0.680482	1.892389	-2.65839
O	-3.06473	1.937338	0.085324	H	0.611897	1.046292	-3.34845
H	0.227618	2.627238	-1.40006	H	-0.15473	2.571688	-2.86107
H	1.347564	1.380435	-0.85548	N	1.952356	2.5832	-2.88642
C	1.26543	1.618999	-2.99418	H	2.471209	2.884024	-2.0742
H	1.687113	0.629958	-3.19572	C	2.427174	2.932481	-4.08125
H	0.522852	1.842516	-3.76796	N	1.703837	2.721699	-5.18519
N	2.343164	2.610846	-3.04085	N	3.644124	3.479816	-4.1829
H	2.363852	3.31405	-2.31665	H	0.720894	2.51119	-5.13527
C	3.223135	2.729264	-4.03478	H	2.07826	2.946446	-6.09286
N	3.160447	1.916484	-5.09324	H	4.275255	3.495287	-3.39828
N	4.182819	3.660222	-3.97043	H	3.98932	3.818576	-5.06607
H	2.365499	1.32052	-5.25184	H	-3.69462	-4.76514	1.35067
H	3.84125	1.979094	-5.83268	O	-1.33254	0.695357	2.719065
H	4.342054	4.183416	-3.12486	H	-1.45315	1.419647	3.354712
H	4.844347	3.778202	-4.72053	O	-3.27977	3.195568	-0.44005
H	-3.30045	-4.90428	-0.07048	H	-3.51131	2.293179	-0.16816
O	-1.04693	2.553898	0.862708	H	-2.43069	3.338939	-0.00226
H	-1.52458	3.37155	1.081958				
O	-5.25826	1.653988	2.032365				
H	-5.34261	0.742645	1.683452				
H	-4.5648	2.037328	1.477253				
Asn-Asn							
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.91832	-3.6156	0.168144	N	-0.72381	-3.12239	2.261567
H	-0.10409	-3.47257	0.759511	H	-1.26269	-2.66373	2.990686
C	-1.80531	-2.46396	0.269113	C	-1.00507	-2.54081	0.962203
H	-2.60376	-2.57206	-0.46831	H	-0.49447	-3.14822	0.207458
C	-2.47287	-2.29451	1.66601	C	-2.47671	-2.33441	0.53088
C	-0.9982	-1.19855	-0.03664	C	-0.38836	-1.14341	0.819588
H	-3.00556	-3.22077	1.896911	H	-2.85265	-3.09405	-0.15423
H	-1.70321	-2.14442	2.426457	H	-3.14182	-2.30478	1.398871
C	-3.497	-1.17657	1.65985	C	-2.5099	-0.97357	-0.12131
O	0.177599	-1.08344	0.307194	O	0.690518	-0.75863	1.207613
O	-4.42125	-1.18344	0.831151	O	-3.42646	-0.44689	-0.72466
N	-3.34254	-0.1853	2.552464	N	-1.29082	-0.35101	0.108916
H	-3.97479	0.604876	2.525598	C	-1.00099	1.00952	-0.32245
H	-2.57075	-0.16975	3.199051	H	-0.06091	1.29064	0.16049

N	-1.67891	-0.20262	-0.64653	C	-0.83282	1.078456	-1.84333
H	-2.65719	-0.3214	-0.87524	C	-2.0561	1.976572	0.218204
C	-1.09147	1.105834	-0.84842	H	-0.04028	0.377392	-2.11815
H	-0.46748	1.356473	0.012974	H	-1.74681	0.76223	-2.34037
C	-0.19006	1.144835	-2.10686	C	-0.38243	2.454725	-2.31342
C	-2.20881	2.131616	-0.94274	O	-2.56489	2.867981	-0.42481
H	0.423892	0.241581	-2.07831	O	0.551278	3.040049	-1.7651
H	-0.7968	1.108336	-3.01381	N	-1.0296	2.939046	-3.39405
C	0.778355	2.321249	-2.09621	H	-0.79802	3.865598	-3.72031
O	-3.3863	1.858325	-1.04046	H	-1.90436	2.531501	-3.69372
O	1.447506	2.582757	-1.09726	H	-0.98844	-4.10166	2.268043
N	0.883161	3.017622	-3.24638	O	-2.30716	1.757459	1.510537
H	1.53907	3.782228	-3.30137	H	-2.96436	2.403333	1.817718
H	0.317202	2.812139	-4.05333	O	-4.00515	1.819502	-2.74452
H	-1.39008	-4.45202	0.4974	H	-3.6508	2.391796	-2.04713
O	-1.73384	3.378267	-0.93373	H	-4.05894	0.959193	-2.3055
H	-2.47312	3.999668	-1.0391				
O	-5.55105	1.360064	0.909186				
H	-5.30502	0.418564	0.797467				
H	-4.96516	1.811705	0.286471				
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.69709	-2.99045	-0.85307	N	-3.79054	-3.91276	-0.7099
H	-3.86947	-3.41083	-0.43862	H	-3.24557	-4.16824	0.108875
C	-4.88767	-1.65224	-0.30794	C	-4.35051	-2.58084	-0.56489
H	-5.69007	-1.16013	-0.86247	H	-5.01856	-2.40633	-1.41483
C	-5.27398	-1.63028	1.201362	C	-5.08907	-2.21392	0.742121
C	-3.5846	-0.86431	-0.48273	C	-3.27366	-1.49535	-0.68348
H	-6.17651	-2.23383	1.325791	H	-6.176	-2.23578	0.664437
H	-4.47358	-2.0829	1.791221	H	-4.79599	-2.87783	1.560607
C	-5.60292	-0.22485	1.664151	C	-4.61543	-0.82173	1.083249
O	-2.48683	-1.40672	-0.34882	O	-2.33953	-1.45675	-1.45175
O	-6.5151	0.413574	1.115869	O	-5.03699	-0.09016	1.96212
N	-4.85491	0.298486	2.649959	N	-3.56457	-0.49498	0.245307
H	-5.00002	1.264049	2.917387	C	-2.82241	0.763626	0.311297
H	-4.08481	-0.20755	3.055854	H	-1.93365	0.619372	-0.30864
N	-3.7287	0.45551	-0.71982	C	-3.60936	1.947531	-0.24553
H	-4.65442	0.855293	-0.79551	C	-2.29762	1.005343	1.723552
C	-2.5951	1.363875	-0.75824	H	-4.08534	1.623387	-1.17637
H	-1.83678	1.017151	-0.0542	H	-4.40197	2.250448	0.437213
C	-1.93807	1.434225	-2.15699	C	-2.7238	3.169208	-0.59569
C	-3.07352	2.736536	-0.32567	O	-2.33462	2.067332	2.302713
H	-1.86318	0.401834	-2.50967	O	-1.50927	2.950438	-0.84226
H	-2.57888	1.981254	-2.85146	O	-3.31801	4.27718	-0.64226
C	-0.50499	2.019695	-2.1516	O	-1.72994	-0.09482	2.238542
O	-4.23888	3.081286	-0.29925	H	-1.39677	0.114769	3.126039
O	0.279622	1.562761	-1.27996	H	-4.537	-4.59485	-0.79322
O	-0.23576	2.869457	-3.0403	O	-5.17744	2.604602	2.998411

O	-2.06248	3.547974	-0.00992	H	-4.24944	2.836454	2.860092
H	-2.42204	4.42449	0.20483	H	-5.21655	1.691202	2.67185
H	-5.48848	-3.58163	-0.61892				
O	-6.17138	3.064268	1.904677				
H	-6.45826	2.186818	1.577593				
H	-5.50505	3.330964	1.255228				
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.69038	-2.56994	-0.53888	N	-2.27658	-2.93749	0.51929
H	-1.82466	-2.83818	-0.07888	H	-1.61049	-2.89934	1.28566
C	-3.11917	-1.26406	-0.05628	C	-2.76614	-1.61239	0.188385
H	-3.97329	-0.93493	-0.65247	H	-3.56481	-1.72655	-0.55219
C	-3.5549	-1.24934	1.439106	C	-3.2612	-0.68557	1.323303
C	-1.96477	-0.27264	-0.23506	C	-1.69763	-0.77103	-0.51975
H	-4.34389	-1.99591	1.563169	H	-4.34494	-0.6469	1.430654
H	-2.71232	-1.53683	2.072253	H	-2.83639	-0.98227	2.286803
C	-4.13936	0.091355	1.839881	C	-2.71731	0.67996	0.982975
O	-0.79064	-0.61667	-0.11773	O	-0.89745	-1.12462	-1.35368
O	-5.07287	0.584889	1.186815	O	-2.97056	1.741437	1.523303
N	-3.59349	0.71793	2.894327	N	-1.81401	0.544587	-0.05871
H	-3.92357	1.642171	3.143348	C	-1.03437	1.646276	-0.61662
H	-2.80922	0.330109	3.392672	H	-0.25746	1.173089	-1.22403
N	-2.3335	1.010897	-0.45908	C	-1.90007	2.547811	-1.50704
H	-3.31338	1.250361	-0.53832	C	-0.30663	2.405289	0.495365
C	-1.36951	2.094134	-0.48396	H	-2.50012	1.910685	-2.15786
H	-0.53218	1.83186	0.163921	H	-2.57228	3.161565	-0.9101
C	-0.85427	2.303818	-1.92541	S	-0.94089	3.613604	-2.65073
C	-2.04383	3.347697	0.057032	O	-0.25725	3.61079	0.588889
H	-0.46517	1.345779	-2.2668	H	-0.43878	4.438673	-1.71529
H	-1.67889	2.610377	-2.57019	H	-3.04524	-3.52611	0.822187
S	0.509461	3.549737	-2.01156	O	0.317322	1.56832	1.328842
O	-3.22897	3.577502	-0.05547	H	0.779071	2.086899	2.008033
H	0.906785	3.214886	-3.25192	O	-3.00485	4.622431	1.219942
H	-3.38622	-3.2734	-0.312	H	-2.0791	4.735595	0.968729
O	-1.1743	4.170837	0.643604	H	-3.06882	3.668072	1.383481
H	-1.63669	4.980612	0.918384				
O	-5.28736	3.230831	2.037697				
H	-5.37338	2.329732	1.663538				
H	-4.64191	3.650636	1.452436				
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.69053	-3.91683	1.184279	N	-1.19847	-4.47956	1.177747
H	-1.36859	-3.71739	2.127681	H	-1.17186	-4.26698	2.170977
C	-2.18243	-2.6886	0.56578	C	-1.64068	-3.32927	0.411198
H	-2.40953	-2.89565	-0.48163	H	-1.76474	-3.64965	-0.62875
C	-3.46325	-2.12271	1.230132	C	-2.90975	-2.56663	0.857491
C	-1.06572	-1.64072	0.640098	C	-0.56773	-2.23529	0.356178

H	-4.22748	-2.90662	1.210512	H	-3.80434	-2.81026	0.284798
H	-3.26474	-1.88623	2.278572	H	-3.12606	-2.74608	1.914716
C	-4.03622	-0.92409	0.494046	C	-2.56659	-1.10538	0.699939
O	-0.33862	-1.53806	1.627688	O	0.627566	-2.36766	0.227821
O	-3.98479	-0.8456	-0.74318	O	-3.31353	-0.14885	0.804647
N	-4.60337	0.033104	1.245364	N	-1.21013	-0.99838	0.445732
H	-4.96045	0.866181	0.799361	C	-0.50404	0.271027	0.288456
H	-4.59145	-0.00384	2.251766	H	0.558178	0.013382	0.359894
N	-0.94874	-0.82302	-0.42979	C	-0.78786	0.911363	-1.07585
H	-1.66464	-0.85886	-1.1425	C	-0.78779	1.188187	1.479882
C	0.026088	0.250141	-0.4631	H	-0.74489	0.118209	-1.82404
H	1.009841	-0.1587	-0.22485	H	-1.80147	1.314814	-1.08964
C	0.043748	0.878403	-1.86751	C	0.222394	1.998217	-1.44398
C	-0.30143	1.312608	0.587402	O	-1.02616	2.371697	1.396849
H	0.235025	0.078223	-2.58485	H	0.185793	2.823738	-0.73126
H	-0.94804	1.286367	-2.0869	H	1.241199	1.593193	-1.40821
C	1.105742	1.966124	-2.03232	C	0.009137	2.522778	-2.85862
O	-1.41605	1.732312	0.818591	O	-0.55498	1.863723	-3.73231
H	0.913642	2.815585	-1.37246	N	0.504897	3.758015	-3.09909
H	2.09191	1.574098	-1.75765	H	0.45727	4.136381	-4.03272
C	1.210061	2.440583	-3.4774	H	0.978479	4.291818	-2.38844
O	0.978283	1.696741	-4.43057	O	-0.68318	0.533349	2.641814
N	1.601347	3.72336	-3.64507	H	-0.85237	1.155955	3.36765
H	1.750821	4.07525	-4.57845	H	-1.8493	-5.24824	1.056125
H	1.799444	4.330429	-2.86645	O	-3.74593	2.647613	0.18052
O	0.796127	1.774514	1.193815	H	-2.88355	2.975974	0.466321
H	0.542538	2.488122	1.80272	H	-3.68928	1.699022	0.377837
H	-2.44275	-4.59472	1.259587				
O	-3.53206	1.912465	-1.18452				
H	-2.83679	1.91967	-0.50679				
H	-3.77344	0.969962	-1.2426				

Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.52678	-2.56927	-1.36222	N	-3.7789	-2.96336	0.831664
H	-2.7765	-3.13144	-0.96928	H	-3.07426	-3.22542	1.515387
C	-3.74056	-1.3907	-0.53204	C	-3.84758	-1.5207	0.684249
H	-4.46022	-0.74197	-1.03542	H	-4.69968	-1.29225	0.035342
C	-4.29768	-1.71444	0.887104	C	-3.92649	-0.63786	1.950333
C	-2.40629	-0.65589	-0.37129	C	-2.62864	-0.96434	-0.06143
H	-5.2467	-2.24198	0.762451	H	-4.92851	-0.28112	2.187746
H	-3.60224	-2.37876	1.404632	H	-3.54099	-1.17016	2.824902
C	-4.58306	-0.45839	1.688056	C	-3.00432	0.525397	1.676065
O	-1.3463	-1.27108	-0.24887	O	-2.05992	-1.4397	-1.01779
O	-5.39851	0.385249	1.287603	O	-2.86625	1.536471	2.341911
N	-3.89633	-0.28687	2.828885	N	-2.27654	0.248772	0.53265
H	-4.03956	0.551523	3.372327	C	-1.2446	1.127888	-0.0184
H	-3.21748	-0.95765	3.15031	H	-0.70766	0.506674	-0.74317
N	-2.49364	0.688009	-0.30295	C	-1.84443	2.346691	-0.73233

H	-3.39323	1.139282	-0.39962	C	-0.21933	1.47656	1.061469
C	-1.34851	1.536508	-0.01376	H	-2.71068	1.994866	-1.29717
H	-0.65067	0.969891	0.604778	H	-2.21499	3.060324	0.003908
C	-0.63633	1.977832	-1.31599	C	-0.86145	3.023277	-1.68719
C	-1.84548	2.736095	0.774715	O	0.239023	2.580018	1.252166
H	-0.43766	1.063787	-1.87901	H	0.01333	3.387825	-1.14289
H	-1.33608	2.5695	-1.91332	H	-0.48452	2.297488	-2.41734
C	0.668165	2.740663	-1.10127	C	-1.44259	4.21512	-2.48062
O	-2.95262	3.2158	0.659039	O	-0.64793	4.765004	-3.29356
H	0.49061	3.689626	-0.58762	O	-2.63738	4.550683	-2.26657
H	1.335157	2.170212	-0.44438	H	-4.6666	-3.31913	1.170401
C	1.456999	3.058133	-2.39296	O	0.162943	0.391374	1.748602
O	2.520942	3.718183	-2.22938	H	0.823349	0.658594	2.408349
O	0.999542	2.645849	-3.49146	O	-1.92922	4.271634	2.411168
H	-4.36286	-3.14498	-1.37782	H	-2.31402	3.380534	2.426972
O	-0.90629	3.230101	1.592204	H	-1.07865	4.125148	1.976975
H	-1.25807	4.026015	2.024294				
O	-6.9967	0.027561	-0.94579				
H	-6.4315	0.168739	-0.15644				
H	-6.77278	0.748968	-1.54314				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.02736	-2.76395	-0.58666	N	-2.24835	-2.81768	0.161468
H	-1.14423	-3.08954	-0.20307	H	-2.2302	-2.87646	1.175658
C	-2.35272	-1.45799	-0.02795	C	-2.36858	-1.43975	-0.27783
H	-3.23076	-1.06605	-0.54615	H	-2.50608	-1.4466	-1.36427
C	-2.67591	-1.48023	1.495442	C	-3.45089	-0.53567	0.359102
C	-1.16427	-0.51825	-0.25875	C	-1.07007	-0.65462	-0.05647
H	-3.48923	-2.19307	1.654873	H	-4.34261	-0.40509	-0.25369
H	-1.80336	-1.82789	2.053139	H	-3.76487	-0.92298	1.332826
C	-3.16132	-0.12769	1.97822	C	-2.76815	0.791927	0.584076
O	-0.00293	-0.92426	-0.21886	O	0.067896	-1.02149	-0.24028
O	-4.1219	0.425142	1.418703	O	-3.27121	1.853344	0.912224
N	-2.49875	0.445528	2.995788	N	-1.41146	0.625494	0.379219
H	-2.75467	1.380923	3.285808	C	-0.44768	1.685713	0.547902
H	-1.69392	0.009691	3.415712	C	-0.27142	2.493573	-0.72853
N	-1.47363	0.783333	-0.44118	H	-0.77222	2.350246	1.349126
H	-2.43891	1.085545	-0.42055	H	0.51414	1.252226	0.825895
C	-0.45034	1.800892	-0.50733	O	-0.82713	2.267443	-1.77633
C	-1.0397	3.169946	-0.26666	O	0.595307	3.495044	-0.52884
H	0.323384	1.615432	0.242854	H	0.696247	3.993334	-1.35621
H	0.053231	1.813319	-1.47996	H	-3.05058	-3.35333	-0.15261
O	-2.21683	3.396626	-0.08144	O	-6.06972	1.999349	1.337044
O	-0.09456	4.112779	-0.29412	H	-5.10465	1.930038	1.208714
H	-0.50791	4.978957	-0.14455	H	-6.30505	1.224262	1.85823
H	-2.73844	-3.44201	-0.3312				
O	-4.0623	3.089198	2.217198				
H	-3.44576	3.433486	1.556301				

H	-4.25218	2.185553	1.890794				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.73845	-3.13342	2.012263	N	-1.47358	-2.95116	2.752778
H	-1.70833	-2.6927	2.927822	H	-1.45285	-2.37272	3.588016
C	-2.3591	-2.22665	1.054478	C	-2.03903	-2.22515	1.630497
H	-2.28966	-2.67134	0.058997	H	-2.14955	-2.9294	0.799227
C	-3.8624	-1.932	1.343849	C	-3.36831	-1.45797	1.821803
C	-1.59525	-0.89772	1.085815	C	-1.0776	-1.15127	1.1071
H	-4.38595	-2.88928	1.394858	H	-4.24437	-1.97405	1.429701
H	-3.95398	-1.43446	2.311813	H	-3.54938	-1.2403	2.878455
C	-4.49974	-1.13367	0.222818	C	-3.17064	-0.14251	1.110328
O	-1.22945	-0.40344	2.149896	O	0.121447	-1.22254	0.971425
O	-4.5956	-1.61422	-0.91516	O	-4.00197	0.720009	0.889777
N	-4.90717	0.114708	0.507276	N	-1.83619	-0.02928	0.759962
H	-5.31598	0.681171	-0.22139	C	-1.26044	1.141976	0.109175
H	-4.83029	0.505964	1.432243	H	-0.17691	1.015105	0.194864
N	-1.41629	-0.30526	-0.11863	C	-1.65038	1.215787	-1.38511
H	-1.77942	-0.74324	-0.96326	C	-1.60104	2.410268	0.893201
C	-0.86733	1.033931	-0.27728	H	-1.64132	0.193225	-1.76621
H	-0.41106	1.322077	0.667999	H	-2.67387	1.586687	-1.47231
C	0.175775	1.059065	-1.41126	C	-0.71416	2.015749	-2.23017
C	-2.03833	1.976865	-0.56816	O	-1.92186	3.463882	0.386533
H	0.966086	0.357499	-1.13883	N	-0.59963	3.38888	-2.18074
H	-0.28912	0.688187	-2.32902	C	0.17535	1.625905	-3.20547
C	0.777957	2.406433	-1.63899	H	-1.09574	3.982602	-1.53098
O	-2.55308	2.103404	-1.66264	C	0.330568	3.76467	-3.09645
N	0.149433	3.409952	-2.35005	N	0.822319	2.721287	-3.74221
C	1.97071	2.960665	-1.23592	H	0.372245	0.621231	-3.54776
H	-0.76155	3.343586	-2.78071	H	0.60809	4.795993	-3.24827
C	0.964084	4.498141	-2.34837	O	-1.45424	2.238046	2.20714
N	2.080468	4.263011	-1.68235	H	-1.66137	3.072151	2.659921
H	2.749794	2.487936	-0.65746	H	-2.04665	-3.76057	2.96607
H	0.698403	5.419504	-2.84239	O	-4.75727	3.042388	-0.64634
O	-2.46247	2.618654	0.52017	H	-4.55858	2.250955	-0.12043
H	-3.23524	3.160836	0.286865	H	-3.96838	3.586441	-0.53325
H	-2.28996	-3.98115	2.10166				
O	-2.75925	-0.63832	-2.7697				
H	-3.54264	-0.95429	-2.27973				
H	-2.80796	0.327322	-2.70915				
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.01329	-3.29598	-1.07912	N	-2.22216	-4.0126	0.610429
H	-2.19508	-3.7476	-0.67933	H	-2.45927	-3.80744	1.576909
C	-3.33099	-2.09468	-0.31731	C	-2.32362	-2.82196	-0.21295
H	-4.1267	-1.55771	-0.83773	H	-2.1736	-3.12346	-1.25543
C	-3.81315	-2.37961	1.136292	C	-3.59041	-1.94562	-0.12282

C	-2.08011	-1.21359	-0.24893	C	-1.19319	-1.82923	0.073247
H	-4.68609	-3.03539	1.078312	H	-4.32019	-2.12628	-0.91139
H	-3.02831	-2.90746	1.682844	H	-4.09223	-2.07978	0.840129
C	-4.25138	-1.11576	1.852165	C	-3.08808	-0.52226	-0.18229
O	-0.95393	-1.70144	-0.1481	O	-0.03572	-2.07624	0.325155
O	-5.13818	-0.38822	1.381614	O	-3.75446	0.487797	-0.32248
N	-3.62487	-0.80865	2.998741	N	-1.71105	-0.53375	-0.03799
H	-3.87933	0.034348	3.492153	C	-0.84979	0.63857	0.081304
H	-2.89048	-1.38421	3.377242	H	0.163506	0.231768	0.067065
N	-2.30982	0.115922	-0.24114	C	-0.98332	1.652635	-1.10918
H	-3.25876	0.46261	-0.28341	C	-1.0139	1.259753	1.463579
C	-1.24689	1.084418	-0.03551	H	-1.52725	1.108715	-1.88748
H	-0.51564	0.649682	0.649088	C	-1.78232	2.919986	-0.76839
C	-0.51698	1.428773	-1.37293	C	0.418532	1.980772	-1.65997
C	-1.85451	2.309336	0.626645	O	-1.87397	0.980135	2.264421
H	-0.29421	0.44488	-1.80077	H	-1.19849	3.593308	-0.13541
C	-1.43707	2.18285	-2.34066	H	-2.03648	3.458759	-1.68291
C	0.822755	2.14558	-1.13558	H	-2.71456	2.675278	-0.25965
O	-3.0306	2.598695	0.586074	H	0.999803	2.478341	-0.87487
H	-1.63147	3.201545	-1.98913	H	0.933801	1.03937	-1.88245
H	-0.98335	2.253533	-3.33067	C	0.403026	2.847855	-2.9224
H	-2.39742	1.673605	-2.45446	H	0.013987	3.849864	-2.72526
H	0.637898	3.162174	-0.775	H	1.41443	2.95924	-3.32267
H	1.362853	1.627745	-0.33471	H	-0.21794	2.393678	-3.70195
C	1.712332	2.195104	-2.3833	O	-0.04482	2.159588	1.691014
H	1.258593	2.78486	-3.18418	H	-0.18296	2.549642	2.569359
H	2.679484	2.64823	-2.14864	H	-2.8794	-4.71447	0.286891
H	1.899268	1.188762	-2.7726	O	-6.56305	0.372895	-0.5513
O	-0.93064	3.056766	1.244241	H	-5.58795	0.390292	-0.49656
H	-1.36397	3.846869	1.606938	H	-6.75712	-0.17197	-1.32142
H	-3.78161	-3.95769	-1.02871				
O	-6.68247	-0.92098	-0.85461				
H	-6.15251	-0.77514	-0.04244				
H	-6.95082	-1.84493	-0.81422				
Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.80945	-2.91742	0.310238	N	-0.63374	-2.91406	1.369969
H	-0.10942	-2.85441	1.044593	H	-0.72955	-2.65963	2.348932
C	-1.62697	-1.71095	0.310593	C	-1.009	-1.81007	0.506543
H	-2.27732	-1.72981	-0.56691	H	-1.01027	-2.17855	-0.52474
C	-2.53439	-1.5592	1.567343	C	-2.33506	-1.06021	0.77451
C	-0.69992	-0.49258	0.233203	C	0.040979	-0.692	0.518717
H	-3.1621	-2.45143	1.63646	H	-3.15641	-1.35619	0.122169
H	-1.91339	-1.5075	2.464449	H	-2.66129	-1.1939	1.810088
C	-3.46078	-0.36537	1.443437	C	-2.00288	0.398767	0.579023
O	0.39062	-0.47924	0.803882	O	1.245784	-0.79946	0.533253
O	-4.22814	-0.26978	0.472486	O	-2.7666	1.350238	0.546643
N	-3.39085	0.577961	2.397113	N	-0.63313	0.529132	0.470025

H	-3.9474	1.418228	2.30037	C	0.050052	1.810898	0.305332
H	-2.73661	0.512051	3.159722	H	1.102427	1.591136	0.505359
N	-1.19582	0.569675	-0.43752	C	-0.11779	2.372691	-1.11431
H	-2.10166	0.503507	-0.8822	C	-0.38337	2.792796	1.395366
C	-0.51083	1.850651	-0.48957	H	-0.09369	1.525703	-1.80809
H	0.131061	1.920362	0.387178	H	-1.10949	2.823837	-1.19102
C	0.337475	1.974001	-1.77909	C	0.962279	3.387828	-1.53292
C	-1.55382	2.952227	-0.42697	O	-0.60395	3.96598	1.213841
H	1.004242	1.105047	-1.78652	H	1.035898	4.149771	-0.7502
H	-0.33905	1.865827	-2.63353	C	2.337586	2.725954	-1.70284
C	1.172102	3.25637	-1.93227	C	0.536334	4.082228	-2.83354
O	-2.66144	2.863733	-0.91668	H	2.302538	1.960466	-2.48623
H	0.494003	4.117815	-1.91753	H	3.088054	3.467561	-1.99117
C	2.188839	3.427484	-0.79459	H	2.689382	2.247511	-0.78443
C	1.879985	3.241035	-3.29464	H	-0.41763	4.604072	-2.71182
H	2.858609	2.561672	-0.74346	H	1.285596	4.813955	-3.14949
H	2.803374	4.317109	-0.95977	H	0.420211	3.35171	-3.64247
H	1.704186	3.539737	0.178261	H	-1.24669	-3.70597	1.207743
H	1.16275	3.149134	-4.1159	O	-0.43019	2.20401	2.601358
H	2.452553	4.160698	-3.44585	H	-0.68558	2.870315	3.259473
H	2.57672	2.397664	-3.35955	O	-5.54796	1.026989	0.953026
H	-1.38368	-3.73129	0.506546	H	-5.83605	0.312008	0.375549
O	-1.10491	4.04554	0.193843	H	-4.58952	1.110689	0.788072
H	-1.78874	4.735004	0.152714				
O	-5.16971	2.355097	0.509006				
H	-4.9777	1.403628	0.378902				
H	-4.44273	2.790338	0.04107				

Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.73974	-2.42378	2.702755	N	-1.44117	-3.27852	2.491056
H	-1.82904	-2.5269	3.140038	H	-0.51738	-3.40401	2.896832
C	-2.56671	-1.98527	1.318212	C	-1.30725	-2.70421	1.155293
H	-2.27161	-2.80928	0.650399	H	-0.74228	-3.34055	0.457683
C	-3.92788	-1.41446	0.820914	C	-2.6404	-2.29888	0.512296
C	-1.39448	-0.98404	1.271674	C	-0.52826	-1.3958	1.229153
H	-4.71257	-1.98967	1.313798	H	-2.96717	-2.94763	-0.29972
H	-4.03366	-0.37506	1.138334	H	-3.43656	-2.25741	1.260898
C	-4.11861	-1.47131	-0.68387	C	-2.41847	-0.89504	-0.00318
O	-0.61743	-0.86315	2.22019	O	0.504369	-1.19853	1.831415
O	-3.56916	-0.65204	-1.44303	O	-3.17511	-0.24348	-0.69874
N	-4.89111	-2.4539	-1.16296	N	-1.19261	-0.44322	0.460792
H	-5.02439	-2.53806	-2.16014	C	-0.65863	0.893512	0.238676
H	-5.34354	-3.12264	-0.56061	H	0.322169	0.892176	0.724387
N	-1.23283	-0.28758	0.128679	C	-0.47283	1.219468	-1.26402
H	-1.94264	-0.34697	-0.60028	C	-1.50261	1.909006	1.009459
C	-0.14516	0.658275	-0.01763	H	-0.33607	0.268175	-1.78491
H	0.800599	0.166469	0.219752	H	-1.38198	1.674178	-1.66042
C	-0.11488	1.181789	-1.466	C	0.735794	2.11936	-1.54062

C	-0.3191	1.82144	0.959157	O	-2.40733	1.627988	1.758742
H	-0.04617	0.306777	-2.11963	H	0.636012	3.059555	-0.99275
H	-1.06808	1.675513	-1.68352	H	1.644469	1.628165	-1.1741
C	1.047454	2.134309	-1.75723	C	0.879433	2.41222	-3.03854
O	-1.38166	2.347611	1.219588	H	0.961642	1.471862	-3.59484
H	0.963332	3.033409	-1.13858	H	-0.01822	2.925998	-3.39991
H	1.993486	1.653272	-1.48591	C	2.104701	3.273496	-3.30959
C	1.083144	2.538817	-3.23564	H	2.040379	4.241465	-2.81274
H	1.203953	1.645759	-3.8586	H	3.026138	2.779343	-3.00193
H	0.131911	3.004614	-3.51512	N	2.247792	3.55968	-4.78469
C	2.224728	3.508453	-3.50514	H	1.426708	4.045318	-5.15246
H	2.108964	4.438977	-2.94962	H	3.061879	4.147393	-4.97506
H	3.194265	3.072103	-3.2656	H	2.360327	2.698109	-5.3234
N	2.277808	3.88775	-4.96501	H	-1.85349	-4.20447	2.423294
H	1.416531	4.350156	-5.26451	O	-1.08568	3.160221	0.777471
H	3.050751	4.528001	-5.1575	H	-1.64195	3.770577	1.287996
H	2.406551	3.06671	-5.56047	O	-3.88324	2.456862	-1.20615
H	-3.19627	-3.32985	2.722323	H	-3.64245	1.528171	-1.04257
O	0.84622	2.238129	1.462374	H	-4.02655	2.508894	-2.15724
H	0.686656	3.013533	2.025745				
O	-3.6827	2.100079	-0.52276				
H	-3.6781	1.192616	-0.86964				
H	-2.93508	2.13392	0.097488				
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.35517	-3.57759	0.620545	N	-1.60105	-4.49862	-1.23635
H	-1.94655	-3.55291	1.551039	H	-0.64329	-4.69008	-0.95589
C	-2.8253	-2.24372	0.256186	C	-2.14748	-3.38073	-0.48878
H	-3.15583	-2.266	-0.78378	H	-3.21024	-3.29861	-0.74015
C	-4.00627	-1.73639	1.121834	C	-1.98906	-3.35431	1.049486
C	-1.64593	-1.27289	0.387052	C	-1.53666	-2.04655	-0.9345
H	-4.81027	-2.47752	1.063934	H	-2.88381	-3.64959	1.597229
H	-3.70008	-1.6698	2.16889	H	-1.16734	-3.99979	1.372907
C	-4.58342	-0.41943	0.632244	C	-1.61582	-1.93091	1.383683
O	-0.8239	-1.37028	1.29732	O	-1.2772	-1.68215	-2.05805
O	-4.62445	-0.14557	-0.57724	O	-1.52188	-1.42413	2.487268
N	-5.05131	0.42124	1.568235	N	-1.34539	-1.25946	0.203679
H	-5.42484	1.316901	1.288804	C	-0.8987	0.129177	0.136909
H	-4.97329	0.220648	2.552123	H	-0.53197	0.258813	-0.88681
N	-1.58182	-0.2906	-0.54025	C	-2.05036	1.111296	0.401537
H	-2.36559	-0.1705	-1.16748	C	0.314834	0.342908	1.044615
C	-0.55306	0.729783	-0.4921	H	-2.92716	0.727161	-0.12619
H	0.42153	0.244748	-0.41511	H	-2.28409	1.119848	1.467697
C	-0.61917	1.579192	-1.77652	C	-1.7356	2.523946	-0.09217
C	-0.72715	1.620177	0.739589	O	0.467578	1.292734	1.778231
H	-0.52019	0.890473	-2.62033	H	-0.86011	2.928838	0.416648
H	-1.60772	2.04522	-1.84122	H	-1.54636	2.519863	-1.16952
C	0.472955	2.646101	-1.84406	S	-3.16016	3.631973	0.240668

O	-1.79179	2.044391	1.137664	C	-2.48014	5.185746	-0.43645
H	0.357162	3.383172	-1.0458	H	-2.26261	5.075917	-1.50054
H	1.46359	2.19315	-1.75115	H	-3.24186	5.954758	-0.30083
S	0.381204	3.528787	-3.44949	H	-1.57562	5.473418	0.102743
C	1.741333	4.722035	-3.20195	O	1.222999	-0.62631	0.886588
H	2.687538	4.198237	-3.05416	H	1.980803	-0.44217	1.465323
H	1.801597	5.328683	-4.10652	H	-2.13907	-5.33783	-1.04791
H	1.53253	5.367624	-2.34686	O	-1.50113	1.036714	4.017748
O	0.443121	1.925347	1.307156	H	-1.55214	0.173785	3.576669
H	0.285558	2.539395	2.04368	H	-0.85223	1.51145	3.48232
H	-3.1358	-4.22631	0.650916				
O	-3.99789	2.60926	-0.6817				
H	-3.27988	2.484043	-0.04021				
H	-4.32702	1.703352	-0.82586				
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.22932	-3.02853	1.937892	N	-1.00788	-3.24399	2.123588
H	-0.89088	-2.63254	2.81087	H	-1.05409	-2.81367	3.042849
C	-1.90656	-1.99374	1.161406	C	-1.48264	-2.33312	1.098689
H	-2.15672	-2.4041	0.181439	H	-1.52639	-2.88641	0.154416
C	-3.21584	-1.47765	1.811518	C	-2.82374	-1.5923	1.30908
C	-0.93382	-0.82246	0.981728	C	-0.48559	-1.19802	0.836848
H	-3.87133	-2.33855	1.978812	H	-3.66786	-2.03313	0.779311
H	-2.99794	-1.03808	2.787977	H	-3.08139	-1.53873	2.370923
C	-3.97742	-0.50606	0.926714	C	-2.57536	-0.18499	0.823884
O	-0.17142	-0.46934	1.880412	O	0.721467	-1.25837	0.79273
O	-4.00461	-0.64653	-0.30585	O	-3.39147	0.705308	0.666673
N	-4.62008	0.498588	1.54289	N	-1.21663	-0.0299	0.607178
H	-5.1129	1.185159	0.989791	C	-0.59358	1.216713	0.172901
H	-4.54981	0.645485	2.536844	H	0.477278	1.070141	0.341112
N	-0.98781	-0.1857	-0.21018	C	-0.84894	1.489761	-1.32158
H	-1.73208	-0.42713	-0.85041	C	-1.00243	2.369696	1.090595
C	-0.17275	0.981133	-0.48571	H	-0.69605	0.537882	-1.83816
H	0.869567	0.748812	-0.26342	H	-1.89177	1.77341	-1.46378
C	-0.31867	1.367708	-1.97642	C	0.073123	2.534209	-1.91276
C	-0.58708	2.160013	0.396528	O	-1.346	3.465886	0.713335
H	-0.01817	0.493686	-2.56036	C	-0.42825	3.746095	-2.39863
H	-1.37593	1.558913	-2.18154	C	1.450056	2.29146	-2.00474
C	0.515356	2.568076	-2.35871	H	-1.49153	3.947138	-2.33205
O	-1.73647	2.495685	0.595962	C	0.424438	4.697538	-2.96134
C	-0.06469	3.83723	-2.46549	C	2.307489	3.241779	-2.56055
C	1.891211	2.43344	-2.58433	H	1.856301	1.350349	-1.64707
H	-1.13017	3.95464	-2.29783	H	0.017373	5.630824	-3.33423
C	0.713735	4.951804	-2.78551	C	1.796337	4.449853	-3.04112
C	2.672125	3.544023	-2.90442	H	3.370266	3.036571	-2.62385
H	2.351785	1.453449	-2.51074	H	2.4602	5.188456	-3.47591
H	0.248676	5.927865	-2.86598	O	-0.87853	2.033686	2.380518
C	2.084822	4.808258	-3.00426	H	-1.13194	2.795428	2.92698

H	3.735335	3.422939	-3.07884	H	-1.59524	-4.07065	2.152401
H	2.690344	5.671832	-3.25482	O	-3.96699	3.235721	-0.64271
O	0.464109	2.816852	0.890438	H	-3.15029	3.671773	-0.36516
H	0.14709	3.591743	1.383637	H	-3.88899	2.361778	-0.22868
H	-1.88109	-3.77005	2.175293				
O	-3.89214	2.00257	-1.29225				
H	-4.03396	1.05052	-1.13932				
H	-3.19713	2.228737	-0.65266				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.88541	-3.14099	0.319447	N	-1.48963	-2.91309	1.292118
H	-0.13328	-3.2404	0.995973	H	-1.23728	-2.55869	2.210433
C	-1.30671	-1.74485	0.256165	C	-1.55414	-1.83734	0.319889
H	-2.02415	-1.63613	-0.55925	H	-1.94505	-2.25469	-0.61396
C	-1.98026	-1.23346	1.556021	C	-2.34444	-0.55405	0.670244
C	-0.0721	-0.88735	-0.04678	C	-0.15761	-1.31279	-0.03753
H	-2.82037	-1.89806	1.782643	H	-3.33057	-0.49727	0.209408
H	-1.27781	-1.30016	2.390702	H	-2.47125	-0.45143	1.751766
C	-2.54885	0.169068	1.424715	C	-1.47396	0.583799	0.197552
O	1.035055	-1.15571	0.414329	O	0.857631	-1.94712	-0.20731
O	-3.04731	0.562426	0.358033	O	-1.741	1.772858	0.147929
N	-2.49334	0.949625	2.514835	N	-0.24499	0.073827	-0.17559
H	-2.82517	1.902292	2.459425	C	0.872773	0.910846	-0.57595
H	-2.03909	0.648399	3.361738	H	1.703764	0.22716	-0.77722
N	-0.2888	0.199013	-0.82625	C	0.588132	1.679799	-1.87972
H	-1.2469	0.447634	-1.03626	C	1.306211	1.768161	0.616597
C	0.770091	1.142589	-1.12041	H	-0.11533	1.08637	-2.47379
H	1.652052	0.599089	-1.46041	H	0.132256	2.648055	-1.66535
C	0.296328	2.094178	-2.22478	O	1.828044	1.825889	-2.56482
C	1.156372	1.95482	0.120037	O	1.085405	1.476383	1.768592
H	0.025671	1.49632	-3.10203	H	1.749106	2.550286	-3.19452
H	-0.58993	2.64079	-1.88003	O	1.989171	2.853208	0.238241
O	1.36982	2.982975	-2.50724	H	2.263716	3.335713	1.035161
O	0.356406	2.502291	0.850422	H	-2.39899	-3.35358	1.383019
H	1.056257	3.663548	-3.1128	O	-4.19874	2.856757	1.047791
O	2.476073	2.016927	0.300323	H	-3.37387	2.445179	0.727873
H	2.661753	2.577424	1.072182	H	-4.87632	2.18447	0.919283
H	-1.65471	-3.72382	0.634807				
O	-2.37603	3.309797	0.271218				
H	-1.44798	3.109114	0.475825				
H	-2.77647	2.427068	0.16895				
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	1.692722	-1.80234	-0.45232	N	-0.91444	-4.17579	0.631642
H	2.443183	-1.81527	0.233037	H	-0.61949	-4.08256	1.599574
C	1.307588	-0.42161	-0.73351	C	-1.58815	-2.97333	0.177121
H	0.609397	-0.42708	-1.57219	H	-1.98793	-3.17228	-0.82291

C	0.625686	0.288186	0.463717	C	-2.70085	-2.35658	1.052887
C	2.565555	0.354752	-1.14076	C	-0.60983	-1.81154	-0.01937
H	-0.18871	-0.35552	0.814146	H	-3.71292	-2.58435	0.718445
H	1.332589	0.3865	1.291842	H	-2.60954	-2.68101	2.093362
C	-0.01022	1.629373	0.132167	C	-2.46182	-0.86629	1.012695
O	3.672368	0.083628	-0.67684	O	0.516839	-1.85029	-0.45635
O	-0.46149	1.886498	-0.9947	O	-3.16448	0.00017	1.499582
N	2.364129	1.359605	-2.02272	N	-1.25353	-0.63292	0.373428
H	1.412309	1.64066	-2.22251	C	-0.64439	0.677962	0.187147
C	3.412136	2.283298	-2.38049	H	0.425326	0.485068	0.049926
H	4.352467	1.735712	-2.46983	C	-1.15276	1.408882	-1.08176
C	3.112887	2.949383	-3.73518	C	-0.72203	1.522938	1.457392
C	3.617065	3.334298	-1.28526	H	-0.73443	2.420869	-1.03294
H	3.914269	3.669908	-3.92793	C	-0.66325	0.718563	-2.34866
C	3.04186	1.942905	-4.87771	O	-2.56682	1.45569	-1.15718
O	1.870645	3.643017	-3.55359	O	-0.96116	2.708927	1.475068
O	2.923329	3.465753	-0.30587	H	-1.07037	-0.29326	-2.42008
H	2.258451	1.203502	-4.69996	H	-1.00207	1.283958	-3.21856
H	2.82629	2.462233	-5.81527	H	0.426767	0.659449	-2.37009
H	3.998293	1.425294	-4.98946	H	-2.93623	2.014602	-0.44804
H	1.604802	4.033855	-4.39361	H	-1.55003	-4.96541	0.590021
H	0.90888	-2.30973	-0.05365	O	-0.4046	0.812124	2.545807
O	4.691891	4.098155	-1.54657	H	-0.43843	1.396552	3.32053
H	4.785561	4.754192	-0.83723	O	-3.89989	2.690265	1.029762
O	-1.4621	0.237754	-3.00138	H	-3.74486	1.797335	1.384469
H	-1.97317	-0.46458	-2.58538	H	-3.20567	3.225561	1.434413
H	-1.14501	0.791379	-2.25996				
N	-0.10289	2.509719	1.139167				
H	-0.53128	3.408041	0.972339				
H	0.310695	2.335868	2.040874				
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.65488	-1.82113	3.227358	N	-1.01798	-2.66136	2.368279
H	-4.29966	-1.172	3.670127	H	-1.6022	-2.4102	3.160839
C	-3.59861	-1.55464	1.792782	C	-1.5658	-2.13586	1.130916
H	-2.79684	-2.15632	1.359892	H	-0.96669	-2.53502	0.305739
C	-4.91033	-1.8964	1.041046	C	-3.06456	-2.35242	0.817417
C	-3.27137	-0.06993	1.590439	C	-1.3979	-0.61449	1.035814
H	-5.19986	-2.91658	1.316469	H	-3.26289	-3.15604	0.108499
H	-5.71807	-1.2374	1.370803	H	-3.63233	-2.55907	1.729263
C	-4.78898	-1.88062	-0.47428	C	-3.545	-1.03331	0.263979
O	-3.64114	0.792498	2.387067	O	-0.44092	0.052402	1.356856
O	-3.69542	-2.06219	-1.03808	O	-4.62439	-0.78802	-0.24635
N	-5.92257	-1.69807	-1.16655	N	-2.55623	-0.08751	0.460669
H	-5.88994	-1.69713	-2.17851	C	-2.68309	1.323457	0.105585
H	-6.80194	-1.52647	-0.70642	H	-1.88584	1.824688	0.661527
N	-2.58918	0.229016	0.46269	C	-2.4836	1.571962	-1.40531
H	-2.48694	-0.50598	-0.22724	C	-3.99386	1.899298	0.643112

C	-2.3797	1.601981	0.048735	H	-1.72995	0.854059	-1.74438
H	-1.83481	2.137538	0.827227	H	-3.40908	1.350029	-1.93748
C	-1.56552	1.613927	-1.26882	C	-2.02087	2.964779	-1.70136
C	-3.71667	2.311834	-0.1654	O	-4.73973	2.614069	0.0205
H	-0.65077	1.042804	-1.07794	C	-2.72429	3.966359	-2.32449
H	-2.13516	1.071865	-2.02989	C	-0.72811	3.514669	-1.37781
C	-1.23328	2.987532	-1.758	H	-3.73142	3.957957	-2.70977
O	-4.68623	1.801424	-0.67854	N	-1.94859	5.103537	-2.41137
C	-1.77131	3.623004	-2.85113	C	-0.71941	4.86129	-1.83888
C	-0.31135	3.917438	-1.15752	C	0.419319	2.999809	-0.74845
H	-2.50003	3.264964	-3.56177	H	-2.24007	5.97262	-2.82814
N	-1.24185	4.890739	-2.96655	C	0.394112	5.693217	-1.68827
C	-0.34317	5.102858	-1.94465	C	1.528351	3.824929	-0.59578
C	0.538	3.864235	-0.03866	H	0.437152	1.978987	-0.38224
H	-1.46729	5.548514	-3.69493	H	0.383025	6.715917	-2.04735
C	0.442956	6.219285	-1.64352	C	1.515462	5.158041	-1.06113
C	1.32156	4.971975	0.264861	H	2.419609	3.441858	-0.11125
H	0.58467	2.97271	0.577228	H	2.3957	5.776825	-0.92748
H	0.405847	7.11311	-2.25545	O	-4.18681	1.555172	1.927768
C	1.273149	6.138249	-0.52981	H	-5.0177	1.95442	2.231869
H	1.981341	4.94363	1.124788	H	-0.98757	-3.67475	2.330982
H	1.895265	6.986608	-0.26765	O	-5.76066	0.44737	-2.5614
O	-3.67781	3.588723	0.242952	H	-5.38479	0.076126	-1.7455
H	-4.52757	4.006945	0.028261	H	-5.88532	-0.31356	-3.13884
H	-4.0052	-2.75897	3.395875				
O	-4.17546	-1.70166	-3.74085				
H	-4.06808	-2.52007	-4.23745				
H	-3.83091	-1.89645	-2.84356				

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.79309	-2.25635	1.962016	N	-0.4981	-2.31032	1.017171
H	-1.29203	-2.1498	2.840831	H	-1.24399	-2.59297	1.646632
C	-1.43476	-1.45072	0.928396	C	-0.91154	-1.1902	0.193179
H	-0.79401	-1.44858	0.043785	H	-0.12147	-1.00614	-0.5431
C	-2.83037	-1.97383	0.498961	C	-2.27109	-1.25129	-0.5396
C	-1.56523	-0.01042	1.443092	C	-0.99899	0.113397	0.994518
H	-2.74014	-3.04655	0.295612	H	-2.20281	-1.54051	-1.5879
H	-3.54666	-1.86631	1.318243	H	-2.95608	-1.94308	-0.04059
C	-3.37226	-1.34418	-0.77423	C	-2.84114	0.140575	-0.41227
O	-1.6298	0.254327	2.643483	O	-0.25828	0.503392	1.867303
O	-2.61241	-0.85167	-1.62746	O	-3.80084	0.615693	-0.99625
N	-4.70131	-1.37471	-0.94485	N	-2.09001	0.840031	0.512957
H	-5.10208	-0.98011	-1.78615	C	-2.35596	2.213921	0.906704
H	-5.31775	-1.75508	-0.24494	H	-1.61065	2.446911	1.673219
N	-1.64895	0.93725	0.485585	C	-2.17359	3.206444	-0.27174
H	-1.68905	0.633053	-0.4791	C	-3.70848	2.300915	1.609422
C	-1.92991	2.318401	0.801008	H	-2.9818	3.05958	-0.98851
H	-1.1605	2.705404	1.472806	H	-2.26928	4.213278	0.136222

C	-1.95898	3.17161	-0.49211	C	-0.83067	3.02205	-0.93798
C	-3.27811	2.459254	1.504664	O	-4.32428	1.355026	2.039977
H	-2.7973	2.837185	-1.11013	C	-0.701	2.240442	-2.09037
H	-2.16231	4.204305	-0.19963	C	0.330273	3.577205	-0.38371
C	-0.66799	3.08254	-1.27185	H	-1.58334	1.800344	-2.54267
O	-4.22844	1.730197	1.343165	C	0.544714	2.009972	-2.67499
C	-0.57563	2.305665	-2.43052	C	1.580651	3.359462	-0.95538
C	0.482481	3.751422	-0.8319	H	0.258836	4.188555	0.510182
H	-1.45035	1.780988	-2.80042	H	0.624581	1.399663	-3.56835
C	0.62516	2.189708	-3.13273	C	1.689706	2.57041	-2.10432
C	1.687373	3.646113	-1.51981	H	2.474777	3.794095	-0.52454
H	0.437497	4.365105	0.06193	O	2.942117	2.386955	-2.62461
H	0.675859	1.5836	-4.03108	H	2.89548	1.835202	-3.41493
C	1.760702	2.86022	-2.67443	H	-0.28415	-3.11091	0.431981
H	2.573096	4.16789	-1.1774	O	-4.10783	3.573783	1.73817
O	2.969799	2.791613	-3.31203	H	-4.94394	3.585804	2.231847
H	2.902959	2.224318	-4.08978	O	-5.1505	-0.88797	-2.97518
H	-0.82343	-3.23944	1.71094	H	-4.50364	-1.00141	-3.67973
O	-3.29934	3.549226	2.290389	H	-4.68454	-0.36885	-2.29198
H	-4.18925	3.641942	2.667281				
O	-4.17634	0.349374	-3.56785				
H	-3.50505	0.003333	-2.94206				
H	-4.29481	1.274375	-3.32619				
Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.03436	-3.21091	-0.58041	N	-1.31355	-4.32451	0.098073
H	-2.18243	-3.7653	-0.57115	H	-0.88688	-4.35281	1.01996
C	-2.85473	-2.0225	0.244421	C	-1.94944	-3.04132	-0.13948
H	-3.73119	-1.38329	0.121157	H	-2.49319	-3.10845	-1.08772
C	-2.69246	-2.32982	1.762502	C	-2.88596	-2.45351	0.939418
C	-1.60763	-1.27599	-0.23887	C	-0.9193	-1.92793	-0.35692
H	-3.57602	-2.88555	2.088419	H	-3.94795	-2.58629	0.734236
H	-1.81758	-2.96617	1.913015	H	-2.67504	-2.88697	1.921462
C	-2.62576	-1.06747	2.601638	C	-2.54488	-0.98403	1.002786
O	-0.61128	-1.87828	-0.6401	O	0.121125	-1.98506	-0.97178
O	-3.52899	-0.2194	2.555786	O	-3.13791	-0.11521	1.614408
N	-1.54179	-0.89906	3.375114	N	-1.39459	-0.76805	0.260687
H	-1.45886	-0.06507	3.937647	C	-0.69613	0.511758	0.117592
H	-0.7989	-1.57807	3.409605	H	0.344175	0.233305	-0.08308
N	-1.66294	0.068067	-0.13322	C	-1.2033	1.319743	-1.09868
H	-2.49223	0.509044	0.241511	C	-0.64229	1.250848	1.453838
C	-0.52017	0.916935	-0.42189	H	-1.16448	0.60035	-1.92496
H	0.386784	0.383476	-0.13006	C	-2.65117	1.808561	-0.97067
C	-0.42212	1.245592	-1.94531	C	-0.2411	2.46489	-1.44658
C	-0.63853	2.166443	0.433997	O	-0.85469	2.43143	1.608804
H	-0.50848	0.264206	-2.42254	H	-2.7576	2.519777	-0.1499
C	-1.58535	2.12132	-2.42423	H	-2.94867	2.30716	-1.89692
C	0.935672	1.840562	-2.33249	H	-3.34523	0.983723	-0.79922

O	-1.67467	2.57585	0.91068	H	0.788296	2.10647	-1.54396
H	-1.52356	3.130283	-2.00347	H	-0.53194	2.910105	-2.40149
H	-1.55997	2.214242	-3.51287	H	-0.26318	3.246207	-0.68509
H	-2.55267	1.695283	-2.14563	H	-2.00649	-5.06495	0.069512
H	1.761079	1.214666	-1.9809	O	-0.24127	0.438013	2.442188
H	1.007447	1.914916	-3.42088	H	-0.19886	0.950476	3.265705
H	1.069646	2.842163	-1.91718	O	-3.67634	2.544943	2.612324
H	-3.77847	-3.79026	-0.20434	H	-3.56502	1.649347	2.256159
O	0.538974	2.787761	0.580665	H	-2.81233	2.946082	2.455766
H	0.39802	3.601787	1.091705				
O	-5.94269	-0.47421	1.223109				
H	-5.09781	-0.42545	1.718605				
H	-6.28571	-1.35589	1.403033				

Table S15.C. Succinimide Hydrolysis into Asp-X XYZ Coordinates (Implicit solvation + 1 H2O, ε = 80)

All Reactions							
H_2O							
Reactant Structure							
Atom	X	Y	Z				
O	-0.999631	0.482902	0				
H	-0.03661	0.526297	0				
H	-1.280189	1.405171	0				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.71688	-1.59329	2.364289	N	-0.59157	-1.64547	0.136553
H	-0.99446	-0.82326	2.966158	H	-0.1567	-2.15966	0.897398
C	-1.42881	-1.54866	1.100556	C	-2.04925	-1.76683	0.225298
H	-1.18551	-2.46301	0.548763	H	-2.40039	-2.79783	0.114037
C	-2.96294	-1.35751	1.104914	C	-2.51337	-1.26851	1.618246
C	-0.93092	-0.40952	0.20298	C	-2.77509	-1.01575	-0.90475
H	-3.53081	-2.27731	0.966635	H	-2.11201	-1.94691	2.372199
H	-3.29819	-0.88958	2.035258	H	-2.12301	-0.26959	1.812327
C	-3.24063	-0.39154	-0.02072	C	-4.02317	-1.28817	1.74477
O	0.206047	-0.02921	0.041715	O	-3.69109	-1.58644	-1.49858
O	-4.32459	-0.06641	-0.47222	O	-4.68554	-0.1836	1.416779
N	-2.03569	0.126839	-0.46185	N	-2.44928	0.263582	-1.21441
C	-1.91868	1.139117	-1.50862	C	-1.43936	1.146074	-0.65649
H	-0.88775	1.500939	-1.44013	H	-0.74196	0.529246	-0.08029
C	-2.1712	0.562861	-2.90012	C	-0.66439	1.849713	-1.77799
C	-2.79272	2.353649	-1.19864	C	-2.06216	2.112959	0.345981
H	-3.18522	0.171925	-2.98414	H	-1.33333	2.458763	-2.3919
H	-2.03397	1.341214	-3.65079	H	0.110789	2.4943	-1.36575
H	-1.45966	-0.24171	-3.09134	H	-0.19725	1.094347	-2.41133
O	-3.41287	2.975363	-2.03185	O	-3.13155	1.943055	0.907418
H	-0.94008	-2.45115	2.857875	H	-0.25851	-2.07015	-0.72421
O	-2.7402	2.694113	0.094325	O	-1.28718	3.162241	0.602797

H	-3.28752	3.484498	0.230719	H	-1.70689	3.705682	1.290638
O	-5.76503	1.180853	-2.64591	O	-4.63638	-2.27837	2.104506
H	-5.33765	0.718586	-1.90694	H	-3.02549	0.653433	-1.95107
H	-5.17437	1.928603	-2.80346	H	-4.08747	0.562781	1.159332
				O	-7.45713	-2.01322	2.097491
				H	-6.4828	-2.09052	2.097059
				H	-7.62443	-1.11616	1.789024
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.89653	-4.16913	1.542857	N	-2.91954	-4.36953	0.887611
H	-2.98678	-3.85202	2.504023	H	-2.30907	-4.60882	1.664343
C	-2.88363	-3.04606	0.624019	C	-3.09341	-2.92019	0.828381
H	-2.90777	-3.44759	-0.39464	H	-3.65954	-2.67852	-0.07359
C	-3.96512	-1.94884	0.758229	C	-3.84335	-2.33145	2.045585
C	-1.56821	-2.26199	0.701661	C	-1.69739	-2.2905	0.736895
H	-4.78211	-2.03446	0.042053	H	-4.74924	-2.92135	2.223737
H	-4.39685	-1.94131	1.76332	H	-3.2413	-2.40669	2.95463
C	-3.22978	-0.64537	0.563762	C	-4.29592	-0.90537	1.862235
O	-0.44582	-2.69597	0.821328	O	-0.75233	-2.72973	1.391009
O	-3.70575	0.470053	0.45024	O	-4.34932	-0.32114	0.795035
N	-1.86974	-0.90395	0.572466	N	-1.56953	-1.22143	-0.07881
C	-0.8408	0.127013	0.467176	C	-0.30376	-0.5254	-0.2082
H	0.089695	-0.37256	0.756891	H	0.471081	-1.24907	-0.4684
C	-0.7142	0.661788	-0.96553	C	-0.41334	0.542301	-1.31197
C	-1.07085	1.217801	1.515858	C	0.096916	0.117599	1.121156
H	-0.78311	-0.19988	-1.63538	H	-0.75011	0.029965	-2.21816
H	-1.56099	1.314729	-1.18632	H	-1.18941	1.262581	-1.03278
C	0.607011	1.394723	-1.21658	C	0.906935	1.264998	-1.59013
O	-0.97973	2.405853	1.305794	O	-0.66706	0.694593	1.866897
H	0.697758	2.244	-0.53465	H	1.235609	1.812421	-0.701
H	1.448569	0.720718	-1.02463	H	1.68823	0.536931	-1.83048
C	0.680482	1.892389	-2.65839	C	0.757762	2.245101	-2.75219
H	0.611897	1.046292	-3.34845	H	0.454236	1.706264	-3.65453
H	-0.15473	2.571688	-2.86107	H	-0.01099	2.989575	-2.51837
N	1.952356	2.5832	-2.88642	N	2.037815	2.910684	-3.00748
H	2.471209	2.884024	-2.0742	H	2.74898	2.842648	-2.29442
C	2.427174	2.932481	-4.08125	C	2.311867	3.658756	-4.07492
N	1.703837	2.721699	-5.18519	N	1.369305	3.904261	-4.98948
N	3.644124	3.479816	-4.1829	N	3.5421	4.16446	-4.23639
H	0.720894	2.51119	-5.13527	H	0.398735	3.712339	-4.80432
H	2.07826	2.946446	-6.09286	H	1.575828	4.467775	-5.7985
H	4.275255	3.495287	-3.39828	H	4.314652	3.819318	-3.68898
H	3.98932	3.818576	-5.06607	H	3.769043	4.711792	-5.05103
H	-3.69462	-4.76514	1.35067	H	-3.81269	-4.82328	1.052361
O	-1.33254	0.695357	2.719065	O	1.40876	0.017156	1.349861
H	-1.45315	1.419647	3.354712	H	1.623077	0.48938	2.171723
O	-3.27977	3.195568	-0.44005	O	-4.6623	-0.3383	3.017463
H	-3.51131	2.293179	-0.16816	H	-4.97863	0.563472	2.842547

H	-2.43069	3.338939	-0.00226	H	-2.4023	-0.81201	-0.47815
				O	-2.89395	2.198075	0.794785
				H	-3.56626	1.509021	0.686891
				H	-2.15437	1.724806	1.210871
Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.72381	-3.12239	2.261567	N	-0.03235	-3.92411	0.047168
H	-1.26269	-2.66373	2.990686	H	0.589377	-3.85616	-0.75354
C	-1.00507	-2.54081	0.962203	C	-1.08783	-2.92286	-0.06691
H	-0.49447	-3.14822	0.207458	H	-1.56771	-3.043	-1.04038
C	-2.47671	-2.33441	0.53088	C	-2.14026	-3.17804	1.027208
C	-0.38836	-1.14341	0.819588	C	-0.54968	-1.47999	0.068873
H	-2.85265	-3.09405	-0.15423	H	-2.34419	-4.25359	1.062493
H	-3.14182	-2.30478	1.398871	H	-1.74792	-2.90193	2.011275
C	-2.5099	-0.97357	-0.12131	C	-3.4647	-2.48692	0.796274
O	0.690518	-0.75863	1.207613	O	0.399948	-1.22621	0.804697
O	-3.42646	-0.44689	-0.72466	O	-4.33568	-2.49309	1.814319
N	-1.29082	-0.35101	0.108916	N	-1.2029	-0.54534	-0.66458
C	-1.00099	1.00952	-0.32245	C	-0.93021	0.882559	-0.57312
H	-0.06091	1.29064	0.16049	H	-0.01842	1.001993	0.007991
C	-0.83282	1.078456	-1.84333	C	-0.77101	1.502046	-1.9581
C	-2.0561	1.976572	0.218204	C	-2.08414	1.520149	0.200321
H	-0.04028	0.377392	-2.11815	H	0.023542	0.973628	-2.49178
H	-1.74681	0.76223	-2.34037	H	-1.6885	1.382127	-2.54045
C	-0.38243	2.454725	-2.31342	C	-0.4153	2.980784	-1.87052
O	-2.56489	2.867981	-0.42481	O	-3.07837	1.984004	-0.31906
O	0.551278	3.040049	-1.7651	O	-0.19765	3.532724	-0.79119
N	-1.0296	2.939046	-3.39405	N	-0.35059	3.634834	-3.04848
H	-0.79802	3.865598	-3.72031	H	-0.10189	4.61215	-3.05902
H	-1.90436	2.531501	-3.69372	H	-0.52749	3.174518	-3.92687
H	-0.98844	-4.10166	2.268043	H	0.540719	-3.71505	0.86181
O	-2.30716	1.757459	1.510537	O	-1.91206	1.432543	1.521986
H	-2.96436	2.403333	1.817718	H	-2.70251	1.781389	1.966444
O	-4.00515	1.819502	-2.74452	O	-3.79268	-1.96132	-0.24929
H	-3.6508	2.391796	-2.04713	H	-2.03662	-0.83827	-1.15745
H	-4.05894	0.959193	-2.3055	H	-3.97045	-2.93072	2.596728
				O	-5.53394	0.349939	-0.2593
				H	-5.05121	-0.49366	-0.2483
				H	-4.83134	1.016222	-0.26552
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.79054	-3.91276	-0.7099	N	-5.81946	-2.82806	-1.88967
H	-3.24557	-4.16824	0.108875	H	-5.17371	-3.39944	-1.35092
C	-4.35051	-2.58084	-0.56489	C	-6.04366	-1.55512	-1.1973
H	-5.01856	-2.40633	-1.41483	H	-6.72451	-0.9575	-1.80387
C	-5.08907	-2.21392	0.742121	C	-6.63869	-1.72332	0.215609
C	-3.27366	-1.49535	-0.68348	C	-4.67517	-0.86722	-1.10688

H	-6.176	-2.23578	0.664437	H	-7.48817	-2.41408	0.165991
H	-4.79599	-2.87783	1.560607	H	-5.89447	-2.18248	0.873454
C	-4.61543	-0.82173	1.083249	C	-7.16385	-0.45088	0.844756
O	-2.33953	-1.45675	-1.45175	O	-3.74882	-1.41396	-0.50062
O	-5.03699	-0.09016	1.96212	O	-7.41247	-0.49288	2.164179
N	-3.56457	-0.49498	0.245307	N	-4.54334	0.314945	-1.73126
C	-2.82241	0.763626	0.311297	C	-3.28762	1.041347	-1.69554
H	-1.93365	0.619372	-0.30864	H	-2.48159	0.392719	-2.0401
C	-3.60936	1.947531	-0.24553	C	-3.35817	2.275485	-2.61256
C	-2.29762	1.005343	1.723552	C	-2.96581	1.477932	-0.26638
H	-4.08534	1.623387	-1.17637	H	-3.77145	1.942422	-3.56969
H	-4.40197	2.250448	0.437213	H	-4.03604	3.019559	-2.18954
C	-2.7238	3.169208	-0.59569	C	-1.97073	2.900352	-2.90301
O	-2.33462	2.067332	2.302713	O	-3.786	1.773771	0.572801
O	-1.50927	2.950438	-0.84226	O	-1.10546	2.124861	-3.38633
O	-3.31801	4.27718	-0.64226	O	-1.83505	4.127621	-2.65891
O	-1.72994	-0.09482	2.238542	O	-1.64047	1.546698	-0.05593
H	-1.39677	0.114769	3.126039	H	-1.49123	1.88751	0.840885
H	-4.537	-4.59485	-0.79322	H	-6.68993	-3.34635	-1.96214
O	-5.17744	2.604602	2.998411	O	-7.40342	0.579057	0.249186
H	-4.24944	2.836454	2.860092	H	-5.36909	0.777454	-2.10924
H	-5.21655	1.691202	2.67185	H	-7.18594	-1.35468	2.541889
				O	-7.07503	1.667857	-2.30868
				H	-7.36116	1.30881	-1.44839
				H	-7.71849	1.348636	-2.95078

Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.27658	-2.93749	0.51929	N	-2.11582	-2.34678	0.581573
H	-1.61049	-2.89934	1.28566	H	-1.3973	-2.51418	1.279772
C	-2.76614	-1.61239	0.188385	C	-2.46881	-0.93372	0.571211
H	-3.56481	-1.72655	-0.55219	H	-3.21875	-0.78063	-0.20881
C	-3.2612	-0.68557	1.323303	C	-3.09752	-0.36839	1.88772
C	-1.69763	-0.77103	-0.51975	C	-1.21199	-0.12415	0.23919
H	-4.34494	-0.6469	1.430654	H	-3.44651	0.650641	1.718316
H	-2.83639	-0.98227	2.286803	H	-3.95502	-0.99731	2.137853
C	-2.71731	0.67996	0.982975	C	-2.14818	-0.34143	3.059511
O	-0.89745	-1.12462	-1.35368	O	-0.12634	-0.41299	0.733
O	-2.97056	1.741437	1.523303	O	-1.87679	-1.55454	3.546189
N	-1.81401	0.544587	-0.05871	N	-1.40093	0.940962	-0.58029
C	-1.03437	1.646276	-0.61662	C	-0.33376	1.861988	-0.94835
H	-0.25746	1.173089	-1.22403	H	0.570036	1.506469	-0.45345
C	-1.90007	2.547811	-1.50704	C	-0.13266	1.887101	-2.46454
C	-0.30663	2.405289	0.495365	C	-0.67709	3.242467	-0.38248
H	-2.50012	1.910685	-2.15786	H	0.043518	0.867237	-2.8085
H	-2.57228	3.161565	-0.9101	H	-1.01581	2.276761	-2.97128
S	-0.94089	3.613604	-2.65073	S	1.341919	2.843808	-2.99836
O	-0.25725	3.61079	0.588889	O	-1.10454	4.169203	-1.03292
H	-0.43878	4.438673	-1.71529	H	0.842517	4.064648	-2.73356

H	-3.04524	-3.52611	0.822187	H	-2.92328	-2.90025	0.851295
O	0.317322	1.56832	1.328842	O	-0.4777	3.289876	0.941478
H	0.779071	2.086899	2.008033	H	-0.75518	4.160988	1.269429
O	-3.00485	4.622431	1.219942	O	-1.67051	0.683622	3.520894
H	-2.0791	4.735595	0.968729	H	-2.31902	1.09732	-0.97163
H	-3.06882	3.668072	1.383481	H	-1.22104	-1.45739	4.285715
				O	-0.16782	-0.74761	5.48788
				H	0.778359	-0.90953	5.390871
				H	-0.33424	0.10804	5.057555
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.19847	-4.47956	1.177747	N	0.392677	-4.6081	-1.02315
H	-1.17186	-4.26698	2.170977	H	0.460218	-4.91439	-0.05643
C	-1.64068	-3.32927	0.411198	C	-0.63195	-3.57791	-1.14331
H	-1.76474	-3.64965	-0.62875	H	-0.59853	-3.16845	-2.15518
C	-2.90975	-2.56663	0.857491	C	-2.07207	-4.09121	-0.87654
C	-0.56773	-2.23529	0.356178	C	-0.32413	-2.46906	-0.13005
H	-3.80434	-2.81026	0.284798	H	-2.22371	-5.01844	-1.44072
H	-3.12606	-2.74608	1.914716	H	-2.19563	-4.34356	0.181088
C	-2.56659	-1.10538	0.699939	C	-3.17246	-3.14778	-1.31041
O	0.627566	-2.36766	0.227821	O	0.165198	-2.7213	0.969575
O	-3.31353	-0.14885	0.804647	O	-4.41152	-3.41749	-0.88141
N	-1.21013	-0.99838	0.445732	N	-0.68235	-1.21879	-0.49959
C	-0.50404	0.271027	0.288456	C	-0.75475	-0.14533	0.473408
H	0.558178	0.013382	0.359894	H	0.227623	0.000525	0.926892
C	-0.78786	0.911363	-1.07585	C	-1.20286	1.144904	-0.23771
C	-0.78779	1.188187	1.479882	C	-1.73451	-0.52352	1.58832
H	-0.74489	0.118209	-1.82404	H	-0.53029	1.300924	-1.08358
H	-1.80147	1.314814	-1.08964	H	-2.20916	0.995824	-0.6432
C	0.222394	1.998217	-1.44398	C	-1.17511	2.386405	0.653933
O	-1.02616	2.371697	1.396849	O	-2.70647	-1.22761	1.441231
H	0.185793	2.823738	-0.73126	H	-1.88351	2.301171	1.480285
H	1.241199	1.593193	-1.40821	H	-0.1829	2.50427	1.105216
C	0.009137	2.522778	-2.85862	C	-1.44746	3.658379	-0.14071
O	-0.55498	1.863723	-3.73231	O	-1.12172	3.779491	-1.32204
N	0.504897	3.758015	-3.09909	N	-2.04594	4.658423	0.544537
H	0.45727	4.136381	-4.03272	H	-2.19244	5.547813	0.091902
H	0.978479	4.291818	-2.38844	H	-2.30491	4.564921	1.513182
O	-0.68318	0.533349	2.641814	O	-1.40559	0.05748	2.753025
H	-0.85237	1.155955	3.36765	H	-2.08067	-0.16763	3.413953
H	-1.8493	-5.24824	1.056125	H	0.15069	-5.41786	-1.58535
O	-3.74593	2.647613	0.18052	O	-3.0047	-2.19321	-2.04531
H	-2.88355	2.975974	0.466321	H	-1.23963	-1.12947	-1.33899
H	-3.68928	1.699022	0.377837	H	-4.43011	-4.19305	-0.3022
				O	-4.46009	0.250159	-1.75199
				H	-4.02713	-0.60837	-1.90593
				H	-4.12933	0.821075	-2.45383
Asn-Glu							

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.7789	-2.96336	0.831664	N	-2.62718	-2.17454	-0.36661
H	-3.07426	-3.22542	1.515387	H	-1.74682	-1.66997	-0.41067
C	-3.84758	-1.5207	0.684249	C	-3.63891	-1.44423	0.408104
H	-4.69968	-1.29225	0.035342	H	-4.48551	-2.11962	0.531451
C	-3.92649	-0.63786	1.950333	C	-3.16613	-1.05264	1.826926
C	-2.62864	-0.96434	-0.06143	C	-4.22964	-0.34596	-0.50268
H	-4.92851	-0.28112	2.187746	H	-3.0117	-1.978	2.391077
H	-3.54099	-1.17016	2.824902	H	-2.19527	-0.55103	1.816683
C	-3.00432	0.525397	1.676065	C	-4.11105	-0.16339	2.600817
O	-2.05992	-1.4397	-1.01779	O	-5.3255	-0.54056	-1.0274
O	-2.86625	1.536471	2.341911	O	-3.84084	0.024662	3.902003
N	-2.27654	0.248772	0.53265	N	-3.5202	0.769419	-0.81624
C	-1.2446	1.127888	-0.0184	C	-2.26498	1.276386	-0.28541
H	-0.70766	0.506674	-0.74317	H	-1.67873	0.459611	0.126722
C	-1.84443	2.346691	-0.73233	C	-1.44686	1.951428	-1.40132
C	-0.21933	1.47656	1.061469	C	-2.55563	2.285729	0.826381
H	-2.71068	1.994866	-1.29717	H	-1.30299	1.211269	-2.19089
H	-2.21499	3.060324	0.003908	H	-2.03886	2.766288	-1.82783
C	-0.86145	3.023277	-1.68719	C	-0.09593	2.478183	-0.92117
O	0.239023	2.580018	1.252166	O	-3.31723	3.220242	0.701512
H	0.01333	3.387825	-1.14289	H	-0.22438	3.240159	-0.14465
H	-0.48452	2.297488	-2.41734	H	0.481867	1.672305	-0.45461
C	-1.44259	4.21512	-2.48062	C	0.788613	3.103461	-2.02548
O	-0.64793	4.765004	-3.29356	O	1.901544	3.553394	-1.63683
O	-2.63738	4.550683	-2.26657	O	0.347268	3.117777	-3.20398
H	-4.6666	-3.31913	1.170401	H	-2.42687	-3.06534	0.07797
O	0.162943	0.391374	1.748602	O	-1.87547	2.025609	1.949802
H	0.823349	0.658594	2.408349	H	-2.07476	2.708665	2.612333
O	-1.92922	4.271634	2.411168	O	-5.06546	0.404265	2.111849
H	-2.31402	3.380534	2.426972	H	-4.02061	1.401842	-1.42877
H	-1.07865	4.125148	1.976975	H	-3.05161	-0.46187	4.180159
				O	-5.53968	3.200877	2.66704
				H	-5.52083	2.230965	2.616454
				H	-4.84057	3.464854	2.051491
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.24835	-2.81768	0.161468	N	-3.57854	3.170227	2.661239
H	-2.2302	-2.87646	1.175658	H	-4.35934	3.530513	2.120902
C	-2.36858	-1.43975	-0.27783	C	-3.21979	1.835993	2.175291
H	-2.50608	-1.4466	-1.36427	H	-2.52379	1.39989	2.897165
C	-3.45089	-0.53567	0.359102	C	-4.38048	0.82972	2.032013
C	-1.07007	-0.65462	-0.05647	C	-2.46706	1.944515	0.835374
H	-4.34261	-0.40509	-0.25369	H	-3.98203	-0.16401	1.819576
H	-3.76487	-0.92298	1.332826	H	-4.90653	0.773994	2.990222
C	-2.76815	0.791927	0.584076	C	-5.40539	1.220437	0.991616
O	0.067896	-1.02149	-0.24028	O	-2.92513	1.440566	-0.19087

O	-3.27121	1.853344	0.912224	O	-5.94576	0.243358	0.247614
N	-1.41146	0.625494	0.379219	N	-1.29269	2.620097	0.820912
C	-0.44768	1.685713	0.547902	C	-0.55372	3.10193	1.962905
C	-0.27142	2.493573	-0.72853	C	0.21246	2.010122	2.694413
H	-0.77222	2.350246	1.349126	H	0.155225	3.864749	1.63752
H	0.51414	1.252226	0.825895	H	-1.2308	3.579629	2.675111
O	-0.82713	2.267443	-1.77633	O	0.110731	0.822802	2.489133
O	0.595307	3.495044	-0.52884	O	1.011012	2.541456	3.634184
H	0.696247	3.993334	-1.35621	H	1.463276	1.821429	4.102946
H	-3.05058	-3.35333	-0.15261	H	-3.88738	3.111725	3.62647
O	-6.06972	1.999349	1.337044	O	-5.81168	2.357322	0.835173
H	-5.10465	1.930038	1.208714	H	-0.81391	2.603799	-0.06936
H	-6.30505	1.224262	1.85823	H	-5.52898	-0.61033	0.429131
				O	-7.71727	2.930637	-1.17495
				H	-7.06146	2.690277	-0.49192
				H	-7.88761	2.109205	-1.64809

Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.47358	-2.95116	2.752778	N	-1.31413	-3.01338	2.061089
H	-1.45285	-2.37272	3.588016	H	-0.8927	-2.62354	2.900371
C	-2.03903	-2.22515	1.630497	C	-2.26516	-2.05311	1.497505
H	-2.14955	-2.9294	0.799227	H	-2.69439	-2.49025	0.593897
C	-3.36831	-1.45797	1.821803	C	-3.40974	-1.68591	2.465096
C	-1.0776	-1.15127	1.1071	C	-1.47216	-0.78665	1.148706
H	-4.24437	-1.97405	1.429701	H	-3.90921	-2.60255	2.796593
H	-3.54938	-1.2403	2.878455	H	-2.99242	-1.20956	3.358287
C	-3.17064	-0.14251	1.110328	C	-4.46318	-0.77586	1.875116
O	0.121447	-1.22254	0.971425	O	-0.88803	-0.16114	2.029991
O	-4.00197	0.720009	0.889777	O	-5.39689	-0.30309	2.715155
N	-1.83619	-0.02928	0.759962	N	-1.45758	-0.43885	-0.15937
C	-1.26044	1.141976	0.109175	C	-0.95864	0.84343	-0.64885
H	-0.17691	1.015105	0.194864	H	-0.37183	1.289485	0.153333
C	-1.65038	1.215787	-1.38511	C	-0.10148	0.651708	-1.9092
C	-1.60104	2.410268	0.893201	C	-2.20972	1.696744	-0.8892
H	-1.64132	0.193225	-1.76621	H	0.701143	-0.04412	-1.65813
H	-2.67387	1.586687	-1.47231	H	-0.71295	0.182014	-2.68578
C	-0.71416	2.015749	-2.23017	C	0.508115	1.915143	-2.42271
O	-1.92186	3.463882	0.386533	O	-2.74446	1.811506	-1.9771
N	-0.59963	3.38888	-2.18074	N	-0.20424	2.889011	-3.09248
C	0.17535	1.625905	-3.20547	C	1.796408	2.396291	-2.37651
H	-1.09574	3.982602	-1.53098	H	-1.19774	2.857031	-3.274
C	0.330568	3.76467	-3.09645	C	0.654841	3.892058	-3.41276
N	0.822319	2.721287	-3.74221	N	1.880921	3.628232	-2.99608
H	0.372245	0.621231	-3.54776	H	2.658858	1.917466	-1.93817
H	0.60809	4.795993	-3.24827	H	0.338601	4.777139	-3.94218
O	-1.45424	2.238046	2.20714	O	-2.68849	2.206083	0.236212
H	-1.66137	3.072151	2.659921	H	-3.65388	2.433103	0.118883
H	-2.04665	-3.76057	2.96607	H	-1.79619	-3.86405	2.336184

O	-4.75727	3.042388	-0.64634	O	-4.51495	-0.45224	0.705144
H	-4.55858	2.250955	-0.12043	H	-2.05232	-0.96364	-0.78524
H	-3.96838	3.586441	-0.53325	H	-5.25514	-0.61196	3.621594
				O	-5.34316	2.188678	0.159163
				H	-5.29556	1.221605	0.299214
				H	-5.75807	2.30694	-0.70335
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.22216	-4.0126	0.610429	N	-1.77598	-4.01945	0.031563
H	-2.45927	-3.80744	1.576909	H	-1.66014	-3.97588	1.040295
C	-2.32362	-2.82196	-0.21295	C	-2.20035	-2.71914	-0.47256
H	-2.1736	-3.12346	-1.25543	H	-2.18594	-2.74614	-1.56426
C	-3.59041	-1.94562	-0.12282	C	-3.62436	-2.30235	-0.01724
C	-1.19319	-1.82923	0.073247	C	-1.2158	-1.65741	0.030776
H	-4.32019	-2.12628	-0.91139	H	-4.30128	-3.15194	-0.16243
H	-4.09223	-2.07978	0.840129	H	-3.63027	-2.07581	1.052831
C	-3.08808	-0.52226	-0.18229	C	-4.228	-1.15288	-0.79318
O	-0.03572	-2.07624	0.325155	O	-0.68897	-1.74593	1.138635
O	-3.75446	0.487797	-0.32248	O	-5.31771	-0.57239	-0.27679
N	-1.71105	-0.53375	-0.03799	N	-1.02298	-0.60024	-0.78901
C	-0.84979	0.63857	0.081304	C	-0.38842	0.612162	-0.30745
H	0.163506	0.231768	0.067065	H	0.584978	0.352611	0.112029
C	-0.98332	1.652635	-1.10918	C	-0.18118	1.613231	-1.479
C	-1.0139	1.259753	1.463579	C	-1.2278	1.212704	0.82361
H	-1.52725	1.108715	-1.88748	H	0.245979	1.003294	-2.28451
C	-1.78232	2.919986	-0.76839	C	-1.50791	2.211761	-1.97223
C	0.418532	1.980772	-1.65997	C	0.85434	2.695366	-1.12352
O	-1.87397	0.980135	2.264421	O	-2.41516	1.03564	0.972942
H	-1.19849	3.593308	-0.13541	H	-1.91173	2.92205	-1.24405
H	-2.03648	3.458759	-1.68291	H	-1.36349	2.74296	-2.91411
H	-2.71456	2.675278	-0.25965	H	-2.27086	1.448809	-2.14217
H	0.999803	2.478341	-0.87487	H	0.446945	3.350388	-0.3471
H	0.933801	1.03937	-1.88245	H	1.734317	2.20929	-0.68804
C	0.403026	2.847855	-2.9224	C	1.295288	3.535527	-2.32729
H	0.013987	3.849864	-2.72526	H	0.472708	4.128479	-2.7353
H	1.41443	2.95924	-3.32267	H	2.089195	4.229778	-2.03887
H	-0.21794	2.393678	-3.70195	H	1.681765	2.89954	-3.13064
O	-0.04482	2.159588	1.691014	O	-0.48874	1.991336	1.629746
H	-0.18296	2.549642	2.569359	H	-1.07159	2.379597	2.302495
H	-2.8794	-4.71447	0.286891	H	-2.47876	-4.72446	-0.16688
O	-6.56305	0.372895	-0.5513	O	-3.81333	-0.76192	-1.86824
H	-5.58795	0.390292	-0.49656	H	-1.62	-0.5347	-1.60176
H	-6.75712	-0.17197	-1.32142	H	-5.55262	-0.94921	0.583439
				O	-5.02163	1.432986	-3.23489
				H	-4.624	0.680667	-2.75888
				H	-4.31364	1.773801	-3.79194
Asn-Leu							
Reactant Structure				Product Structure			

Atom	X	Y	Z	Atom	X	Y	Z
N	-0.63374	-2.91406	1.369969	N	-1.63499	-4.1239	0.738953
H	-0.72955	-2.65963	2.348932	H	-1.82145	-3.95475	1.723678
C	-1.009	-1.81007	0.506543	C	-2.39554	-3.18066	-0.07563
H	-1.01027	-2.17855	-0.52474	H	-2.09761	-3.30688	-1.11826
C	-2.33506	-1.06021	0.77451	C	-3.92914	-3.37155	0.014305
C	0.040979	-0.692	0.518717	C	-2.03482	-1.764	0.391876
H	-3.15641	-1.35619	0.122169	H	-4.16103	-4.43433	-0.11944
H	-2.66129	-1.1939	1.810088	H	-4.29049	-3.09466	1.009565
C	-2.00288	0.398767	0.579023	C	-4.7077	-2.62445	-1.04627
O	1.245784	-0.79946	0.533253	O	-1.88489	-1.50446	1.58578
O	-2.7666	1.350238	0.546643	O	-6.03271	-2.51783	-0.86711
N	-0.63313	0.529132	0.470025	N	-1.92051	-0.82432	-0.56981
C	0.050052	1.810898	0.305332	C	-1.6522	0.564513	-0.24289
H	1.102427	1.591136	0.505359	H	-0.74543	0.611421	0.360516
C	-0.11779	2.372691	-1.11431	C	-1.48051	1.369119	-1.54632
C	-0.38337	2.792796	1.395366	C	-2.79246	1.150608	0.588865
H	-0.09369	1.525703	-1.80809	H	-0.66202	0.901652	-2.10516
H	-1.10949	2.823837	-1.19102	H	-2.39294	1.24596	-2.13981
C	0.962279	3.387828	-1.53292	C	-1.18387	2.868497	-1.37424
O	-0.60395	3.96598	1.213841	O	-3.97246	0.963364	0.373241
H	1.035898	4.149771	-0.7502	H	-2.00166	3.320536	-0.79943
C	2.337586	2.725954	-1.70284	C	0.129419	3.123101	-0.6214
C	0.536334	4.082228	-2.83354	C	-1.15892	3.541027	-2.75402
H	2.302538	1.960466	-2.48623	H	0.969471	2.652107	-1.14416
H	3.088054	3.467561	-1.99117	H	0.332916	4.19588	-0.55851
H	2.689382	2.247511	-0.78443	H	0.102094	2.733513	0.398881
H	-0.41763	4.604072	-2.71182	H	-2.10352	3.394211	-3.28621
H	1.285596	4.813955	-3.14949	H	-0.98689	4.616829	-2.65845
H	0.420211	3.35171	-3.64247	H	-0.35497	3.126397	-3.37247
H	-1.24669	-3.70597	1.207743	H	-1.9204	-5.07628	0.533396
O	-0.43019	2.20401	2.601358	O	-2.34614	1.947694	1.563723
H	-0.68558	2.870315	3.259473	H	-3.10755	2.3439	2.019041
O	-5.54796	1.026989	0.953026	O	-4.21277	-2.14065	-2.04455
H	-5.83605	0.312008	0.375549	H	-2.19864	-1.06111	-1.51188
H	-4.58952	1.110689	0.788072	H	-6.31473	-2.92699	-0.03646
				O	-5.04366	0.639488	-2.30125
				H	-4.8949	-0.30671	-2.45021
				H	-4.72393	0.772482	-1.39358
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.44117	-3.27852	2.491056	N	-3.61221	-0.99219	1.212002
H	-0.51738	-3.40401	2.896832	H	-3.68539	-0.31969	1.96994
C	-1.30725	-2.70421	1.155293	C	-2.50954	-1.92309	1.466896
H	-0.74228	-3.34055	0.457683	H	-2.4677	-2.28223	2.501094
C	-2.6404	-2.29888	0.512296	C	-2.65652	-3.14806	0.537248
C	-0.52826	-1.3958	1.229153	C	-1.15331	-1.25901	1.198585
H	-2.96717	-2.94763	-0.29972	H	-3.64236	-3.58948	0.708966

H	-3.43656	-2.25741	1.260898	H	-2.59066	-2.8393	-0.50651
C	-2.41847	-0.89504	-0.00318	C	-1.64251	-4.22737	0.841295
O	0.504369	-1.19853	1.831415	O	-0.1133	-1.72388	1.668873
O	-3.17511	-0.24348	-0.69874	O	-0.81177	-4.47574	-0.16968
N	-1.19261	-0.44322	0.460792	N	-1.1765	-0.18237	0.391511
C	-0.65863	0.893512	0.238676	C	0.029055	0.53619	0.038562
H	0.322169	0.892176	0.724387	H	0.764389	-0.1682	-0.35714
C	-0.47283	1.219468	-1.26402	C	-0.29884	1.598456	-1.02716
C	-1.50261	1.909006	1.009459	C	0.638911	1.191037	1.280562
H	-0.33607	0.268175	-1.78491	H	-0.77452	1.076162	-1.86325
H	-1.38198	1.674178	-1.66042	H	-1.03881	2.29365	-0.61538
C	0.735794	2.11936	-1.54062	C	0.920811	2.373261	-1.53306
O	-2.40733	1.627988	1.758742	O	0.004935	1.684898	2.183833
H	0.636012	3.059555	-0.99275	H	1.374467	2.938154	-0.71307
H	1.644469	1.628165	-1.1741	H	1.681867	1.669938	-1.88801
C	0.879433	2.41222	-3.03854	C	0.545613	3.337535	-2.66464
H	0.961642	1.471862	-3.59484	H	0.137493	2.774415	-3.51113
H	-0.01822	2.925998	-3.39991	H	-0.23736	4.023149	-2.3222
C	2.104701	3.273496	-3.30959	C	1.760442	4.135426	-3.11732
H	2.040379	4.241465	-2.81274	H	2.163691	4.752848	-2.31473
H	3.026138	2.779343	-3.00193	H	2.552076	3.490993	-3.4989
N	2.247792	3.55968	-4.78469	N	1.401252	5.078441	-4.23901
H	1.426708	4.045318	-5.15246	H	0.689584	5.752222	-3.9483
H	3.061879	4.147393	-4.97506	H	2.214409	5.610093	-4.55622
H	2.360327	2.698109	-5.3234	H	1.031987	4.57442	-5.04806
H	-1.85349	-4.20447	2.423294	H	-4.49697	-1.4887	1.181714
O	-1.08568	3.160221	0.777471	O	1.980817	1.195441	1.225789
H	-1.64195	3.770577	1.287996	H	2.320687	1.669821	2.002113
O	-3.88324	2.456862	-1.20615	O	-1.60559	-4.82576	1.904592
H	-3.64245	1.528171	-1.04257	H	-2.08634	0.15891	0.107699
H	-4.02655	2.508894	-2.15724	H	-0.18471	-5.19478	0.108022
				O	0.673431	-6.36235	1.07902
				H	0.614093	-7.28831	0.81464
				H	-0.00497	-6.23943	1.763671
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.60105	-4.49862	-1.23635	N	-2.19896	-4.6417	-0.93231
H	-0.64329	-4.69008	-0.95589	H	-2.97988	-4.58542	-1.57977
C	-2.14748	-3.38073	-0.48878	C	-2.1365	-3.42022	-0.13689
H	-3.21024	-3.29861	-0.74015	H	-3.11596	-3.25302	0.315822
C	-1.98906	-3.35431	1.049486	C	-1.10381	-3.60771	0.992668
C	-1.53666	-2.04655	-0.9345	C	-1.73262	-2.18388	-0.96482
H	-2.88381	-3.64959	1.597229	H	-1.26216	-4.59486	1.440148
H	-1.16734	-3.99979	1.372907	H	-0.08757	-3.60633	0.586503
C	-1.61582	-1.93091	1.383683	C	-1.20499	-2.59903	2.114261
O	-1.2772	-1.68215	-2.05805	O	-0.18536	-2.54717	2.979146
O	-1.52188	-1.42413	2.487268	O	-2.1626	-1.87144	2.296353
N	-1.34539	-1.25946	0.203679	N	-2.21171	-0.99648	-0.52685

C	-0.8987	0.129177	0.136909	C	-1.65386	0.254205	-1.00432
H	-0.53197	0.258813	-0.88681	H	-1.75731	0.305709	-2.08965
C	-2.05036	1.111296	0.401537	C	-2.41384	1.424366	-0.34652
C	0.314834	0.342908	1.044615	C	-0.15977	0.314303	-0.67218
H	-2.92716	0.727161	-0.12619	H	-3.47588	1.265588	-0.55606
H	-2.28409	1.119848	1.467697	H	-2.27845	1.368378	0.738837
C	-1.7356	2.523946	-0.09217	C	-1.98765	2.798552	-0.86106
O	0.467578	1.292734	1.778231	O	0.354629	-0.21979	0.282907
H	-0.86011	2.928838	0.416648	H	-0.95253	3.019877	-0.59449
H	-1.54636	2.519863	-1.16952	H	-2.08048	2.851987	-1.9491
S	-3.16016	3.631973	0.240668	S	-3.05574	4.094937	-0.121
C	-2.48014	5.185746	-0.43645	C	-2.28026	5.568432	-0.87097
H	-2.26261	5.075917	-1.50054	H	-2.34806	5.523561	-1.95957
H	-3.24186	5.954758	-0.30083	H	-2.83063	6.438447	-0.51028
H	-1.57562	5.473418	0.102743	H	-1.23572	5.648436	-0.56402
O	1.222999	-0.62631	0.886588	O	0.513223	1.065857	-1.55745
H	1.980803	-0.44217	1.465323	H	1.442386	1.116664	-1.27924
H	-2.13907	-5.33783	-1.04791	H	-1.36436	-4.70587	-1.51138
O	-1.50113	1.036714	4.017748	O	-0.98377	-2.27958	-1.93551
H	-1.55214	0.173785	3.576669	H	-2.66091	-0.99161	0.379734
H	-0.85223	1.51145	3.48232	H	0.525382	-3.15729	2.73473
				O	-1.95362	0.812963	3.253034
				H	-2.02792	-0.12839	3.015688
				H	-2.86355	1.122906	3.315697

Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.00788	-3.24399	2.123588	N	-1.61215	-3.00723	1.117422
H	-1.05409	-2.81367	3.042849	H	-1.56474	-2.64156	2.062605
C	-1.48264	-2.33312	1.098689	C	-2.11778	-2.01554	0.181338
H	-1.52639	-2.88641	0.154416	H	-1.98297	-2.40621	-0.82983
C	-2.82374	-1.5923	1.30908	C	-3.63615	-1.65231	0.29263
C	-0.48559	-1.19802	0.836848	C	-1.28689	-0.74283	0.361245
H	-3.66786	-2.03313	0.779311	H	-3.91016	-0.98523	-0.5251
H	-3.08139	-1.53873	2.370923	H	-4.20808	-2.57816	0.185101
C	-2.57536	-0.18499	0.823884	C	-4.02308	-0.96554	1.580807
O	0.721467	-1.25837	0.79273	O	-1.06622	-0.29281	1.484763
O	-3.39147	0.705308	0.666673	O	-4.06104	-1.71017	2.700222
N	-1.21663	-0.0299	0.607178	N	-0.84665	-0.13953	-0.7618
C	-0.59358	1.216713	0.172901	C	-0.11693	1.11367	-0.70905
H	0.477278	1.070141	0.341112	H	0.691366	1.022724	0.017865
C	-0.84894	1.489761	-1.32158	C	0.469544	1.430853	-2.10453
C	-1.00243	2.369696	1.090595	C	-1.03777	2.249142	-0.25652
H	-0.69605	0.537882	-1.83816	H	1.072871	0.567686	-2.39913
H	-1.89177	1.77341	-1.46378	H	-0.35579	1.517551	-2.81725
C	0.073123	2.534209	-1.91276	C	1.311439	2.685601	-2.12311
O	-1.346	3.465886	0.713335	O	-2.18379	2.383751	-0.61814
C	-0.42825	3.746095	-2.39863	C	0.792275	3.890401	-2.60937
C	1.450056	2.29146	-2.00474	C	2.621336	2.666126	-1.62734

H	-1.49153	3.947138	-2.33205	H	-0.21993	3.918653	-2.99927
C	0.424438	4.697538	-2.96134	C	1.56236	5.055417	-2.59575
C	2.307489	3.241779	-2.56055	C	3.393771	3.827472	-1.61151
H	1.856301	1.350349	-1.64707	H	3.038373	1.736542	-1.25315
H	0.017373	5.630824	-3.33423	H	1.145346	5.980659	-2.97718
C	1.796337	4.449853	-3.04112	C	2.864997	5.027348	-2.09506
H	3.370266	3.036571	-2.62385	H	4.406759	3.795541	-1.22638
H	2.4602	5.188456	-3.47591	H	3.464999	5.930168	-2.08508
O	-0.87853	2.033686	2.380518	O	-0.40591	3.107172	0.556191
H	-1.13194	2.795428	2.92698	H	-1.00907	3.84018	0.761747
H	-1.59524	-4.07065	2.152401	H	-2.15676	-3.86216	1.103222
O	-3.96699	3.235721	-0.64271	O	-4.30163	0.213696	1.659172
H	-3.15029	3.671773	-0.36516	H	-1.09843	-0.51881	-1.6624
H	-3.88899	2.361778	-0.22868	H	-3.85833	-2.63864	2.519768
				O	-4.84934	1.31686	4.216188
				H	-4.66086	0.906042	3.35063
				H	-4.74322	0.600807	4.851617
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.48963	-2.91309	1.292118	N	-0.34763	-3.32358	0.852439
H	-1.23728	-2.55869	2.210433	H	0.057352	-2.90635	1.686072
C	-1.55414	-1.83734	0.319889	C	-1.3449	-2.43584	0.245425
H	-1.94505	-2.25469	-0.61396	H	-1.84709	-2.99628	-0.54249
C	-2.34444	-0.55405	0.670244	C	-2.41043	-1.9227	1.234154
C	-0.15761	-1.31279	-0.03753	C	-0.58196	-1.32357	-0.49033
H	-3.33057	-0.49727	0.209408	H	-2.93353	-2.78672	1.658903
H	-2.47125	-0.45143	1.751766	H	-1.95479	-1.40731	2.085589
C	-1.47396	0.583799	0.197552	C	-3.46153	-1.0337	0.601688
O	0.857631	-1.94712	-0.20731	O	-0.34448	-1.39653	-1.69882
O	-1.741	1.772858	0.147929	O	-3.64578	-0.93127	-0.59162
N	-0.24499	0.073827	-0.17559	N	-0.15598	-0.28527	0.256249
C	0.872773	0.910846	-0.57595	C	0.618029	0.803075	-0.30473
H	1.703764	0.22716	-0.77722	H	1.332183	0.414098	-1.03478
C	0.588132	1.679799	-1.87972	C	-0.31035	1.8093	-1.04313
C	1.306211	1.768161	0.616597	C	1.381448	1.47848	0.819152
H	-0.11533	1.08637	-2.47379	H	-0.97214	1.220239	-1.67782
H	0.132256	2.648055	-1.66535	H	-0.92237	2.348871	-0.31029
O	1.828044	1.825889	-2.56482	O	0.391539	2.690827	-1.89938
O	1.085405	1.476383	1.768592	O	1.245596	1.228117	1.994938
H	1.749106	2.550286	-3.19452	H	0.969677	3.252299	-1.36834
O	1.989171	2.853208	0.238241	O	2.206037	2.426474	0.347948
H	2.263716	3.335713	1.035161	H	2.636061	2.872285	1.096512
H	-2.39899	-3.35358	1.383019	H	-0.78486	-4.19316	1.141897
O	-4.19874	2.856757	1.047791	O	-4.24567	-0.33401	1.438924
H	-3.37387	2.445179	0.727873	H	-0.29678	-0.26904	1.256499
H	-4.87632	2.18447	0.919283	H	-4.00525	-0.48277	2.364533
				O	-2.69775	-2.24106	-3.04398
				H	-1.7851	-2.05366	-2.7606

				H	-3.21317	-1.85507	-2.32014
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.91444	-4.17579	0.631642	N	-0.87616	-1.94135	2.014215
H	-0.61949	-4.08256	1.599574	H	-1.47231	-1.88636	2.833214
C	-1.58815	-2.97333	0.177121	C	-1.64954	-2.38011	0.852402
H	-1.98793	-3.17228	-0.82291	H	-0.93094	-2.64051	0.067005
C	-2.70085	-2.35658	1.052887	C	-2.53258	-3.61853	1.069817
C	-0.60983	-1.81154	-0.01937	C	-2.49871	-1.2308	0.27633
H	-3.71292	-2.58435	0.718445	H	-2.97135	-3.94267	0.123494
H	-2.60954	-2.68101	2.093362	H	-1.90781	-4.44149	1.43403
C	-2.46182	-0.86629	1.012695	C	-3.64058	-3.41496	2.080961
O	0.516839	-1.85029	-0.45635	O	-3.68272	-1.39969	-0.01465
O	-3.16448	0.00017	1.499582	O	-3.69302	-2.51183	2.89034
N	-1.25353	-0.63292	0.373428	N	-1.89882	-0.03322	0.078987
C	-0.64439	0.677962	0.187147	C	-0.50857	0.325451	0.226914
H	0.425326	0.485068	0.049926	H	0.140912	-0.52319	0.021395
C	-1.15276	1.408882	-1.08176	C	-0.15509	1.445558	-0.79749
C	-0.72203	1.522938	1.457392	C	-0.19282	0.817143	1.632944
H	-0.73443	2.420869	-1.03294	H	0.850555	1.805447	-0.55762
C	-0.66325	0.718563	-2.34866	C	-0.18779	0.929189	-2.22758
O	-2.56682	1.45569	-1.15718	O	-1.09824	2.51741	-0.71181
O	-0.96116	2.708927	1.475068	O	-0.99612	1.303462	2.402275
H	-1.07037	-0.29326	-2.42008	H	-1.18318	0.560032	-2.48506
H	-1.00207	1.283958	-3.21856	H	0.072256	1.737628	-2.91323
H	0.426767	0.659449	-2.37009	H	0.531036	0.116828	-2.35483
H	-2.93623	2.014602	-0.44804	H	-0.97517	2.997748	0.116107
H	-1.55003	-4.96541	0.590021	H	-0.13881	-2.60762	2.217142
O	-0.4046	0.812124	2.545807	O	1.119709	0.758937	1.884118
H	-0.43843	1.396552	3.32053	H	1.289516	1.143699	2.759241
O	-3.89989	2.690265	1.029762	O	-4.61066	-4.34501	2.098989
H	-3.74486	1.797335	1.384469	H	-2.50955	0.703358	-0.25232
H	-3.20567	3.225561	1.434413	H	-4.47306	-5.01431	1.413568
				O	-3.65579	0.409052	3.071622
				H	-3.66983	-0.55257	2.954718
				H	-2.78823	0.692407	2.738774
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.01798	-2.66136	2.368279	N	-1.80579	-2.77482	2.227179
H	-1.6022	-2.4102	3.160839	H	-1.95531	-2.28155	3.101045
C	-1.5658	-2.13586	1.130916	C	-2.63455	-2.23968	1.158498
H	-0.96669	-2.53502	0.305739	H	-2.2973	-2.67901	0.21683
C	-3.06456	-2.35242	0.817417	C	-4.16735	-2.54542	1.238535
C	-1.3979	-0.61449	1.035814	C	-2.42802	-0.72309	1.125539
H	-3.26289	-3.15604	0.108499	H	-4.65755	-2.18802	0.332614
H	-3.63233	-2.55907	1.729263	H	-4.28594	-3.63153	1.284901
C	-3.545	-1.03331	0.263979	C	-4.87375	-1.9077	2.411372

O	-0.44092	0.052402	1.356856	O	-2.45729	-0.06371	2.163998
O	-4.62439	-0.78802	-0.24635	O	-5.6395	-0.97083	2.308401
N	-2.55623	-0.08751	0.460669	N	-2.24954	-0.16115	-0.08694
C	-2.68309	1.323457	0.105585	C	-2.11867	1.275319	-0.24744
H	-1.88584	1.824688	0.661527	H	-1.35661	1.642083	0.441155
C	-2.4836	1.571962	-1.40531	C	-1.71205	1.597456	-1.70614
C	-3.99386	1.899298	0.643112	C	-3.43639	1.975622	0.085057
H	-1.72995	0.854059	-1.74438	H	-0.79063	1.041213	-1.90854
H	-3.40908	1.350029	-1.93748	H	-2.48504	1.207065	-2.37492
C	-2.02087	2.964779	-1.70136	C	-1.50851	3.058059	-1.95627
O	-4.73973	2.614069	0.0205	O	-4.52579	1.5768	-0.25741
C	-2.72429	3.966359	-2.32449	C	-2.32917	3.889998	-2.6795
C	-0.72811	3.514669	-1.37781	C	-0.43482	3.877144	-1.45498
H	-3.73142	3.957957	-2.70977	H	-3.23951	3.661409	-3.21168
N	-1.94859	5.103537	-2.41137	N	-1.83236	5.175458	-2.65787
C	-0.71941	4.86129	-1.83888	C	-0.67171	5.202359	-1.9166
C	0.419319	2.999809	-0.74845	C	0.701627	3.621486	-0.66823
H	-2.24007	5.97262	-2.82814	H	-2.2477	5.964352	-3.12612
C	0.394112	5.693217	-1.68827	C	0.188487	6.262272	-1.61381
C	1.528351	3.824929	-0.59578	C	1.559778	4.672248	-0.36431
H	0.437152	1.978987	-0.38224	H	0.908618	2.62031	-0.30615
H	0.383025	6.715917	-2.04735	H	-0.00822	7.265009	-1.97513
C	1.515462	5.158041	-1.06113	C	1.304362	5.979918	-0.83207
H	2.419609	3.441858	-0.11125	H	2.440147	4.488623	0.241308
H	2.3957	5.776825	-0.92748	H	1.991332	6.779246	-0.57792
O	-4.18681	1.555172	1.927768	O	-3.23984	3.11381	0.765038
H	-5.0177	1.95442	2.231869	H	-4.09875	3.547972	0.895533
H	-0.98757	-3.67475	2.330982	H	-1.94444	-3.77015	2.361275
O	-5.76066	0.44737	-2.5614	O	-4.63766	-2.41197	3.635566
H	-5.38479	0.076126	-1.7455	H	-2.28242	-0.74009	-0.91289
H	-5.88532	-0.31356	-3.13884	H	-4.04116	-3.17271	3.600464
				O	-6.65351	0.194648	4.691768
				H	-6.29611	-0.2302	3.888563
				H	-6.23331	-0.27515	5.420145

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.4981	-2.31032	1.017171	N	-3.20936	-0.08094	-1.74059
H	-1.24399	-2.59297	1.646632	H	-2.27465	-0.44652	-1.90094
C	-0.91154	-1.1902	0.193179	C	-3.59496	-0.20279	-0.33714
H	-0.12147	-1.00614	-0.5431	H	-4.64198	0.113597	-0.27004
C	-2.27109	-1.25129	-0.5396	C	-3.55707	-1.62785	0.269906
C	-0.99899	0.113397	0.994518	C	-2.8242	0.823804	0.511165
H	-2.20281	-1.54051	-1.5879	H	-3.95925	-1.58625	1.286083
H	-2.95608	-1.94308	-0.04059	H	-4.20612	-2.26445	-0.32984
C	-2.84114	0.140575	-0.41227	C	-2.19483	-2.29551	0.325002
O	-0.25828	0.503392	1.867303	O	-2.42212	0.558136	1.656746
O	-3.80084	0.615693	-0.99625	O	-1.8884	-3.2603	-0.34283
N	-2.09001	0.840031	0.512957	N	-2.657	2.017624	-0.06774

C	-2.35596	2.213921	0.906704	C	-1.85799	3.078747	0.502243
H	-1.61065	2.446911	1.673219	H	-1.63945	2.812716	1.536642
C	-2.17359	3.206444	-0.27174	C	-0.51632	3.26046	-0.26856
C	-3.70848	2.300915	1.609422	C	-2.63844	4.384249	0.494282
H	-2.9818	3.05958	-0.98851	H	-0.73989	3.608524	-1.28104
H	-2.26928	4.213278	0.136222	H	0.048401	4.049876	0.231743
C	-0.83067	3.02205	-0.93798	C	0.279304	1.97913	-0.32207
O	-4.32428	1.355026	2.039977	O	-3.63334	4.596214	-0.15984
C	-0.701	2.240442	-2.09037	C	0.213035	1.137167	-1.43673
C	0.330273	3.577205	-0.38371	C	1.071466	1.579231	0.761722
H	-1.58334	1.800344	-2.54267	H	-0.39029	1.423471	-2.29119
C	0.544714	2.009972	-2.67499	C	0.912777	-0.06953	-1.47794
C	1.580651	3.359462	-0.95538	C	1.777969	0.380322	0.736702
H	0.258836	4.188555	0.510182	H	1.138521	2.212721	1.639974
H	0.624581	1.399663	-3.56835	H	0.850348	-0.71008	-2.35128
C	1.689706	2.57041	-2.10432	C	1.697053	-0.44357	-0.38726
H	2.474777	3.794095	-0.52454	H	2.39136	0.075609	1.575859
O	2.942117	2.386955	-2.62461	O	2.414062	-1.61641	-0.35946
H	2.89548	1.835202	-3.41493	H	2.293812	-2.10091	-1.18573
H	-0.28415	-3.11091	0.431981	H	-3.84561	-0.60625	-2.33067
O	-4.10783	3.573783	1.73817	O	-2.0524	5.2985	1.282403
H	-4.94394	3.585804	2.231847	H	-2.5478	6.131035	1.216401
O	-5.1505	-0.88797	-2.97518	O	-1.31747	-1.77284	1.194089
H	-4.50364	-1.00141	-3.67973	H	-2.96387	2.095686	-1.02986
H	-4.68454	-0.36885	-2.29198	H	-1.68154	-0.92675	1.574339
				O	1.203033	-3.06829	1.880958
				H	1.755869	-2.69272	1.17899
				H	0.330239	-2.6827	1.705297

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.31355	-4.32451	0.098073	N	-2.06971	-1.93083	2.630348
H	-0.88688	-4.35281	1.01996	H	-2.62588	-1.08198	2.620546
C	-1.94944	-3.04132	-0.13948	C	-1.98561	-2.52277	1.29188
H	-2.49319	-3.10845	-1.08772	H	-1.5669	-3.52241	1.409928
C	-2.88596	-2.45351	0.939418	C	-3.33042	-2.71909	0.54814
C	-0.9193	-1.92793	-0.35692	C	-0.92897	-1.79243	0.441915
H	-3.94795	-2.58629	0.734236	H	-3.15454	-3.14968	-0.44427
H	-2.67504	-2.88697	1.921462	H	-3.92385	-3.45806	1.098783
C	-2.54488	-0.98403	1.002786	C	-4.20308	-1.49619	0.380969
O	0.121125	-1.98506	-0.97178	O	0.057138	-2.39124	0.007153
O	-3.13791	-0.11521	1.614408	O	-3.94403	-0.3881	0.816726
N	-1.39459	-0.76805	0.260687	N	-1.13304	-0.48172	0.204562
C	-0.69613	0.511758	0.117592	C	-0.22292	0.300629	-0.60673
H	0.344175	0.233305	-0.08308	H	-0.03231	-0.23498	-1.53977
C	-1.2033	1.319743	-1.09868	C	-0.85972	1.676492	-0.95003
C	-0.64229	1.250848	1.453838	C	1.121387	0.453949	0.104285
H	-1.16448	0.60035	-1.92496	H	-1.85116	1.428463	-1.34647
C	-2.65117	1.808561	-0.97067	C	-1.04302	2.580114	0.277992

C	-0.2411	2.46489	-1.44658	C	-0.08335	2.401895	-2.05552
O	-0.85469	2.43143	1.608804	O	1.277104	0.504714	1.302375
H	-2.7576	2.519777	-0.1499	H	-0.07763	2.889043	0.688434
H	-2.94867	2.30716	-1.89692	H	-1.58525	3.485259	-0.0088
H	-3.34523	0.983723	-0.79922	H	-1.6019	2.093863	1.081978
H	0.788296	2.10647	-1.54396	H	0.03871	1.770194	-2.93944
H	-0.53194	2.910105	-2.40149	H	-0.62416	3.30348	-2.3539
H	-0.26318	3.246207	-0.68509	H	0.910434	2.703401	-1.71469
H	-2.00649	-5.06495	0.069512	H	-2.53425	-2.57743	3.260565
O	-0.24127	0.438013	2.442188	O	2.131244	0.565875	-0.77618
H	-0.19886	0.950476	3.265705	H	2.954446	0.709005	-0.2816
O	-3.67634	2.544943	2.612324	O	-5.34867	-1.66197	-0.28759
H	-3.56502	1.649347	2.256159	H	-1.98191	-0.05563	0.549591
H	-2.81233	2.946082	2.455766	H	-5.45825	-2.57351	-0.59574
				O	-4.65402	2.108488	-0.39257
				H	-4.4874	1.255082	0.044115
				H	-4.01008	2.710043	-0.00375

Table S15.D. Succinimide Hydrolysis into iso-Asp-X XYZ Coordinates (Implicit solvation + 1 H_2O, ε = 80)

All Reactions							
H_2O							
Reactant Structure							
Atom	X	Y	Z				
O	-0.999631	0.482902	0				
H	-0.03661	0.526297	0				
H	-1.280189	1.405171	0				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.71688	-1.59329	2.364289	N	-2.6907	-1.8597	2.324961
H	-0.99446	-0.82326	2.966158	H	-2.32059	-2.61072	2.899466
C	-1.42881	-1.54866	1.100556	C	-1.92692	-1.73945	1.089735
H	-1.18551	-2.46301	0.548763	H	-2.02783	-2.66119	0.515115
C	-2.96294	-1.35751	1.104914	C	-2.50655	-0.58243	0.250515
C	-0.93092	-0.40952	0.20298	C	-0.43036	-1.50262	1.318719
H	-3.53081	-2.27731	0.966635	H	-3.59494	-0.68945	0.278894
H	-3.29819	-0.88958	2.035258	H	-2.26262	0.364866	0.725469
C	-3.24063	-0.39154	-0.02072	C	-2.11152	-0.63893	-1.2172
O	0.206047	-0.02921	0.041715	O	0.325806	-1.991	0.331592
O	-4.32459	-0.06641	-0.47222	O	-2.09295	-1.71687	-1.81358
N	-2.03569	0.126839	-0.46185	N	-1.83766	0.514216	-1.88071
C	-1.91868	1.139117	-1.50862	C	-1.78782	1.891563	-1.41233
H	-0.88775	1.500939	-1.44013	H	-1.47799	2.479941	-2.28048
C	-2.1712	0.562861	-2.90012	C	-3.14438	2.456909	-0.95121
C	-2.79272	2.353649	-1.19864	C	-0.66658	2.107235	-0.39258
H	-3.18522	0.171925	-2.98414	H	-3.50673	1.971831	-0.04477

H	-2.03397	1.341214	-3.65079	H	-3.05517	3.525706	-0.75656
H	-1.45966	-0.24171	-3.09134	H	-3.87716	2.302394	-1.7446
O	-3.41287	2.975363	-2.03185	O	0.0809	1.253005	0.021894
H	-0.94008	-2.45115	2.857875	H	-2.61742	-1.00599	2.873338
O	-2.7402	2.694113	0.094325	O	-0.59619	3.395656	-0.02157
H	-3.28752	3.484498	0.230719	H	0.136096	3.494983	0.608136
O	-5.76503	1.180853	-2.64591	O	0.041926	-0.9377	2.286881
H	-5.33765	0.718586	-1.90694	H	-1.61353	0.367417	-2.85507
H	-5.17437	1.928603	-2.80346	H	1.252249	-1.756	0.505441
				O	-1.57541	0.98744	3.571883
				H	-0.92082	0.395561	3.157137
				H	-1.49133	1.824781	3.103087

Asn-Arg

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.89653	-4.16913	1.542857	N	-3.22569	-4.71601	2.154416
H	-2.98678	-3.85202	2.504023	H	-4.22043	-4.51724	2.091775
C	-2.88363	-3.04606	0.624019	C	-2.44353	-3.51533	1.849012
H	-2.90777	-3.44759	-0.39464	H	-1.39161	-3.80099	1.804258
C	-3.96512	-1.94884	0.758229	C	-2.84044	-2.81716	0.519038
C	-1.56821	-2.26199	0.701661	C	-2.57504	-2.58282	3.04882
H	-4.78211	-2.03446	0.042053	H	-2.81847	-3.56807	-0.27317
H	-4.39685	-1.94131	1.76332	H	-3.85726	-2.42878	0.602282
C	-3.22978	-0.64537	0.563762	C	-1.89704	-1.6647	0.242843
O	-0.44582	-2.69597	0.821328	O	-3.83478	-2.17586	3.229435
O	-3.70575	0.470053	0.45024	O	-1.67338	-2.2736	3.802724
N	-1.86974	-0.90395	0.572466	N	-1.00975	-1.82375	-0.76712
C	-0.8408	0.127013	0.467176	C	0.153623	-0.94802	-0.90563
H	0.089695	-0.37256	0.756891	H	0.842558	-1.47167	-1.57529
C	-0.7142	0.661788	-0.96553	C	-0.19571	0.418007	-1.50975
C	-1.07085	1.217801	1.515858	C	0.878753	-0.83969	0.449545
H	-0.78311	-0.19988	-1.63538	H	-0.92074	0.244351	-2.30995
H	-1.56099	1.314729	-1.18632	H	-0.68805	1.025768	-0.74772
C	0.607011	1.394723	-1.21658	C	1.022725	1.152294	-2.07741
O	-0.97973	2.405853	1.305794	O	1.297888	0.196233	0.922526
H	0.697758	2.244	-0.53465	H	1.768547	1.299111	-1.29217
H	1.448569	0.720718	-1.02463	H	1.483657	0.548477	-2.86749
C	0.680482	1.892389	-2.65839	C	0.619699	2.508044	-2.65141
H	0.611897	1.046292	-3.34845	H	-0.12143	2.371238	-3.44595
H	-0.15473	2.571688	-2.86107	H	0.171857	3.123717	-1.86426
N	1.952356	2.5832	-2.88642	N	1.792919	3.197472	-3.1975
H	2.471209	2.884024	-2.0742	H	2.686003	2.733182	-3.12141
C	2.427174	2.932481	-4.08125	C	1.764175	4.392677	-3.784
N	1.703837	2.721699	-5.18519	N	0.613939	5.062914	-3.89261
N	3.644124	3.479816	-4.1829	N	2.887157	4.925677	-4.2839
H	0.720894	2.51119	-5.13527	H	-0.25151	4.685684	-3.54579
H	2.07826	2.946446	-6.09286	H	0.574745	5.952354	-4.36295
H	4.275255	3.495287	-3.39828	H	3.777622	4.474915	-4.14982
H	3.98932	3.818576	-5.06607	H	2.898989	5.871426	-4.62996

H	-3.69462	-4.76514	1.35067	H	-3.0225	-5.43934	1.471468
O	-1.33254	0.695357	2.719065	O	1.012425	-2.03259	1.0206
H	-1.45315	1.419647	3.354712	H	1.248507	-1.94895	1.986713
O	-3.27977	3.195568	-0.44005	O	-1.89368	-0.66487	0.963792
H	-3.51131	2.293179	-0.16816	H	-0.98894	-2.70729	-1.25172
H	-2.43069	3.338939	-0.00226	H	-3.87806	-1.61822	4.023053
				O	1.116102	-2.12389	3.658059
				H	1.361246	-1.34091	4.164424
				H	0.145537	-2.20937	3.757251
Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.72381	-3.12239	2.261567	N	-1.17316	-4.40467	0.576
H	-1.26269	-2.66373	2.990686	H	-0.86478	-5.1564	-0.03335
C	-1.00507	-2.54081	0.962203	C	-0.62856	-3.1269	0.123466
H	-0.49447	-3.14822	0.207458	H	-1.00489	-2.93841	-0.88488
C	-2.47671	-2.33441	0.53088	C	-1.13584	-2.01279	1.067817
C	-0.38836	-1.14341	0.819588	C	0.897091	-3.07989	0.007782
H	-2.85265	-3.09405	-0.15423	H	-2.17338	-2.25148	1.308527
H	-3.14182	-2.30478	1.398871	H	-0.57331	-2.03106	2.005724
C	-2.5099	-0.97357	-0.12131	C	-1.14181	-0.56377	0.604476
O	0.690518	-0.75863	1.207613	O	1.523782	-3.85989	0.890367
O	-3.42646	-0.44689	-0.72466	O	-1.83779	0.26243	1.200584
N	-1.29082	-0.35101	0.108916	N	-0.37401	-0.20757	-0.44973
C	-1.00099	1.00952	-0.32245	C	-0.30756	1.170513	-0.89675
H	-0.06091	1.29064	0.16049	H	0.497802	1.227948	-1.63482
C	-0.83282	1.078456	-1.84333	C	-1.5998	1.634401	-1.58605
C	-2.0561	1.976572	0.218204	C	0.155152	2.076593	0.247782
H	-0.04028	0.377392	-2.11815	H	-1.94296	0.814966	-2.22436
H	-1.74681	0.76223	-2.34037	H	-2.38144	1.826417	-0.85218
C	-0.38243	2.454725	-2.31342	C	-1.37549	2.830901	-2.50312
O	-2.56489	2.867981	-0.42481	O	0.968149	1.750999	1.088164
O	0.551278	3.040049	-1.7651	O	-0.31353	2.998708	-3.10326
N	-1.0296	2.939046	-3.39405	N	-2.42933	3.660061	-2.65055
H	-0.79802	3.865598	-3.72031	H	-2.3603	4.437826	-3.28907
H	-1.90436	2.531501	-3.69372	H	-3.29142	3.526437	-2.14767
H	-0.98844	-4.10166	2.268043	H	-0.8283	-4.62759	1.505672
O	-2.30716	1.757459	1.510537	O	-0.37354	3.301091	0.188761
H	-2.96436	2.403333	1.817718	H	0.003201	3.8396	0.903664
O	-4.00515	1.819502	-2.74452	O	1.486463	-2.39401	-0.80735
H	-3.6508	2.391796	-2.04713	H	0.294434	-0.86736	-0.83379
H	-4.05894	0.959193	-2.3055	H	2.48017	-3.71793	0.802967
				O	1.789777	-0.82175	2.01272
				H	1.808973	-0.69035	2.966615
				H	1.519542	0.041277	1.650653
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.79054	-3.91276	-0.7099	N	-4.91044	-3.38462	-1.35682

H	-3.24557	-4.16824	0.108875	H	-4.66247	-4.0339	-2.09671
C	-4.35051	-2.58084	-0.56489	C	-5.78786	-2.33888	-1.86987
H	-5.01856	-2.40633	-1.41483	H	-6.71744	-2.81472	-2.1912
C	-5.08907	-2.21392	0.742121	C	-6.19024	-1.33195	-0.76146
C	-3.27366	-1.49535	-0.68348	C	-5.29268	-1.53576	-3.08129
H	-6.176	-2.23578	0.664437	H	-7.09777	-0.81256	-1.07298
H	-4.79599	-2.87783	1.560607	H	-6.44459	-1.90466	0.134576
C	-4.61543	-0.82173	1.083249	C	-5.24219	-0.21279	-0.3227
O	-2.33953	-1.45675	-1.45175	O	-3.98226	-1.62126	-3.29119
O	-5.03699	-0.09016	1.96212	O	-5.6769	0.696234	0.387147
N	-3.56457	-0.49498	0.245307	N	-3.94928	-0.24094	-0.72007
C	-2.82241	0.763626	0.311297	C	-3.06359	0.906663	-0.56484
H	-1.93365	0.619372	-0.30864	H	-2.07124	0.556697	-0.86294
C	-3.60936	1.947531	-0.24553	C	-3.45374	2.074786	-1.4791
C	-2.29762	1.005343	1.723552	C	-2.91786	1.25231	0.918093
H	-4.08534	1.623387	-1.17637	H	-4.43972	2.453324	-1.20724
H	-4.40197	2.250448	0.437213	H	-2.74963	2.89871	-1.33999
C	-2.7238	3.169208	-0.59569	C	-3.4626	1.728075	-2.9788
O	-2.33462	2.067332	2.302713	O	-2.8459	0.428398	1.801306
O	-1.50927	2.950438	-0.84226	O	-2.88047	0.665065	-3.36027
O	-3.31801	4.27718	-0.64226	O	-4.04058	2.546571	-3.73196
O	-1.72994	-0.09482	2.238542	O	-2.793	2.571576	1.137712
H	-1.39677	0.114769	3.126039	H	-2.63996	2.704583	2.087085
H	-4.537	-4.59485	-0.79322	H	-4.03654	-3.00812	-1.00427
O	-5.17744	2.604602	2.998411	O	-6.04379	-0.82712	-3.72814
H	-4.24944	2.836454	2.860092	H	-3.60748	-0.73441	-3.61045
H	-5.21655	1.691202	2.67185	H	-3.64193	-0.92436	-1.39384
				O	-5.31819	1.131676	-5.74609
				H	-5.58938	0.391054	-5.17936
				H	-4.79237	1.685737	-5.12741
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.27658	-2.93749	0.51929	N	-3.91091	-0.91744	2.55036
H	-1.61049	-2.89934	1.28566	H	-4.17394	-1.38499	3.407826
C	-2.76614	-1.61239	0.188385	C	-3.58955	-1.80211	1.444948
H	-3.56481	-1.72655	-0.55219	H	-4.33558	-2.60347	1.435841
C	-3.2612	-0.68557	1.323303	C	-3.69911	-1.07424	0.098814
C	-1.69763	-0.77103	-0.51975	C	-2.24291	-2.55016	1.528196
H	-4.34494	-0.6469	1.430654	H	-3.62173	-1.78201	-0.72929
H	-2.83639	-0.98227	2.286803	H	-4.68165	-0.6013	0.033593
C	-2.71731	0.67996	0.982975	C	-2.61972	-0.01757	-0.06468
O	-0.89745	-1.12462	-1.35368	O	-1.61825	-2.56547	2.707279
O	-2.97056	1.741437	1.523303	O	-1.76116	0.189683	0.795232
N	-1.81401	0.544587	-0.05871	N	-2.63664	0.669049	-1.22971
C	-1.03437	1.646276	-0.61662	C	-1.6993	1.745511	-1.5186
H	-0.25746	1.173089	-1.22403	H	-1.77066	1.941086	-2.59173
C	-1.90007	2.547811	-1.50704	C	-2.04983	3.027807	-0.74759
C	-0.30663	2.405289	0.495365	C	-0.2527	1.303572	-1.27553

H	-2.50012	1.910685	-2.15786	H	-3.12648	3.184324	-0.8212
H	-2.57228	3.161565	-0.9101	H	-1.7864	2.925979	0.303951
S	-0.94089	3.613604	-2.65073	S	-1.30933	4.562156	-1.43152
O	-0.25725	3.61079	0.588889	O	0.589321	1.962275	-0.71487
H	-0.43878	4.438673	-1.71529	H	-0.03509	4.285335	-1.10369
H	-3.04524	-3.52611	0.822187	H	-3.21773	-0.19567	2.706655
O	0.317322	1.56832	1.328842	O	0.007362	0.107237	-1.83723
H	0.779071	2.086899	2.008033	H	0.941329	-0.10751	-1.68105
O	-3.00485	4.622431	1.219942	O	-1.76893	-3.16853	0.595288
H	-2.0791	4.735595	0.968729	H	-3.35379	0.469908	-1.91036
H	-3.06882	3.668072	1.383481	H	-2.09572	-2.00005	3.335527
				O	-1.48536	-2.51482	-2.17252
				H	-1.08285	-1.6372	-2.12819
				H	-1.58325	-2.78482	-1.24365
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.19847	-4.47956	1.177747	N	0.209371	-4.95313	-2.27529
H	-1.17186	-4.26698	2.170977	H	1.15252	-5.3124	-2.38929
C	-1.64068	-3.32927	0.411198	C	0.206319	-3.75779	-1.42714
H	-1.76474	-3.64965	-0.62875	H	0.897745	-3.04208	-1.87211
C	-2.90975	-2.56663	0.857491	C	-1.21453	-3.17506	-1.38618
C	-0.56773	-2.23529	0.356178	C	0.750737	-4.0613	-0.03048
H	-3.80434	-2.81026	0.284798	H	-1.48405	-2.88751	-2.40673
H	-3.12606	-2.74608	1.914716	H	-1.91956	-3.9444	-1.06812
C	-2.56659	-1.10538	0.699939	C	-1.45515	-1.97566	-0.47933
O	0.627566	-2.36766	0.227821	O	-0.07619	-4.83026	0.685967
O	-3.31353	-0.14885	0.804647	O	-2.53805	-1.82799	0.093486
N	-1.21013	-0.99838	0.445732	N	-0.45322	-1.0816	-0.34169
C	-0.50404	0.271027	0.288456	C	-0.58635	0.083764	0.520278
H	0.558178	0.013382	0.359894	H	0.426309	0.487596	0.622438
C	-0.78786	0.911363	-1.07585	C	-1.49094	1.168814	-0.0912
C	-0.78779	1.188187	1.479882	C	-0.95504	-0.38429	1.936243
H	-0.74489	0.118209	-1.82404	H	-1.28656	1.189799	-1.16324
H	-1.80147	1.314814	-1.08964	H	-2.53715	0.886017	0.036468
C	0.222394	1.998217	-1.44398	C	-1.23603	2.572309	0.477821
O	-1.02616	2.371697	1.396849	O	-0.44547	-1.34015	2.475363
H	0.185793	2.823738	-0.73126	H	-1.43528	2.602798	1.548995
H	1.241199	1.593193	-1.40821	H	-0.1854	2.843155	0.32681
C	0.009137	2.522778	-2.85862	C	-2.0634	3.610388	-0.26459
O	-0.55498	1.863723	-3.73231	O	-1.99291	3.737298	-1.48869
N	0.504897	3.758015	-3.09909	N	-2.87696	4.381916	0.490186
H	0.45727	4.136381	-4.03272	H	-3.44112	5.08964	0.044518
H	0.978479	4.291818	-2.38844	H	-2.94084	4.275484	1.489207
O	-0.68318	0.533349	2.641814	O	-1.85284	0.405147	2.544642
H	-0.85237	1.155955	3.36765	H	-1.99067	0.068357	3.44462
H	-1.8493	-5.24824	1.056125	H	-0.34661	-5.69342	-1.85572
O	-3.74593	2.647613	0.18052	O	1.834128	-3.69347	0.385923
H	-2.88355	2.975974	0.466321	H	0.456922	-1.21359	-0.77288

H	-3.68928	1.699022	0.377837	H	0.334539	-5.02708	1.543666
				O	2.428529	-1.20099	-0.78553
				H	2.948228	-1.22813	-1.59648
				H	2.493537	-2.09477	-0.40111
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.7789	-2.96336	0.831664	N	-3.22279	-2.88665	1.812889
H	-3.07426	-3.22542	1.515387	H	-3.04947	-3.45821	0.991395
C	-3.84758	-1.5207	0.684249	C	-3.99324	-1.70259	1.463299
H	-4.69968	-1.29225	0.035342	H	-4.23796	-1.17247	2.389395
C	-3.92649	-0.63786	1.950333	C	-3.23042	-0.7043	0.540592
C	-2.62864	-0.96434	-0.06143	C	-5.32705	-2.13669	0.842857
H	-4.92851	-0.28112	2.187746	H	-2.1863	-0.71756	0.858141
H	-3.54099	-1.17016	2.824902	H	-3.23636	-1.05016	-0.49912
C	-3.00432	0.525397	1.676065	C	-3.75267	0.722332	0.584268
O	-2.05992	-1.4397	-1.01779	O	-5.56266	-3.29057	0.526697
O	-2.86625	1.536471	2.341911	O	-4.90496	0.983614	0.982882
N	-2.27654	0.248772	0.53265	N	-2.94319	1.711378	0.176673
C	-1.2446	1.127888	-0.0184	C	-1.56705	1.597919	-0.28888
H	-0.70766	0.506674	-0.74317	H	-1.45966	0.699518	-0.89725
C	-1.84443	2.346691	-0.73233	C	-1.22386	2.828724	-1.15356
C	-0.21933	1.47656	1.061469	C	-0.60771	1.506427	0.899552
H	-2.71068	1.994866	-1.29717	H	-1.9765	2.885361	-1.94328
H	-2.21499	3.060324	0.003908	H	-1.33165	3.730246	-0.54321
C	-0.86145	3.023277	-1.68719	C	0.170303	2.779913	-1.77457
O	0.239023	2.580018	1.252166	O	-0.73328	2.125829	1.930067
H	0.01333	3.387825	-1.14289	H	0.944816	2.764635	-1.0012
H	-0.48452	2.297488	-2.41734	H	0.301163	1.854326	-2.3451
C	-1.44259	4.21512	-2.48062	C	0.495878	3.962837	-2.71628
O	-0.64793	4.765004	-3.29356	O	-0.35794	4.879791	-2.83852
O	-2.63738	4.550683	-2.26657	O	1.619285	3.905379	-3.28785
H	-4.6666	-3.31913	1.170401	H	-2.32198	-2.61845	2.195826
O	0.162943	0.391374	1.748602	O	0.411692	0.670604	0.648926
H	0.823349	0.658594	2.408349	H	1.020783	0.684925	1.40578
O	-1.92922	4.271634	2.411168	O	-6.22834	-1.18799	0.655101
H	-2.31402	3.380534	2.426972	H	-3.3316	2.642979	0.256564
H	-1.07865	4.125148	1.976975	H	-5.82921	-0.28388	0.867356
				O	-8.09884	-3.71735	-0.64393
				H	-7.22541	-3.55267	-0.23604
				H	-8.52299	-2.8526	-0.65455
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.24835	-2.81768	0.161468	N	-2.45243	0.709196	3.429539
H	-2.2302	-2.87646	1.175658	H	-2.03873	0.194157	4.200086
C	-2.36858	-1.43975	-0.27783	C	-2.6061	-0.1548	2.252618
H	-2.50608	-1.4466	-1.36427	H	-3.17253	-1.0346	2.564009
C	-3.45089	-0.53567	0.359102	C	-3.41139	0.545809	1.137464

C	-1.07007	-0.65462	-0.05647	C	-1.24264	-0.66497	1.786607
H	-4.34261	-0.40509	-0.25369	H	-3.26674	0.013056	0.194286
H	-3.76487	-0.92298	1.332826	H	-4.46616	0.492037	1.402423
C	-2.76815	0.791927	0.584076	C	-3.09749	2.02687	0.955443
O	0.067896	-1.02149	-0.24028	O	-0.81281	-1.67488	2.548553
O	-3.27121	1.853344	0.912224	O	-0.57062	-0.19629	0.882472
N	-1.41146	0.625494	0.379219	N	-1.90078	2.321976	0.390368
C	-0.44768	1.685713	0.547902	C	-1.42858	3.679863	0.33769
C	-0.27142	2.493573	-0.72853	C	-0.94094	4.181645	1.689315
H	-0.77222	2.350246	1.349126	H	-0.59143	3.752432	-0.36019
H	0.51414	1.252226	0.825895	H	-2.21379	4.348502	-0.01702
O	-0.82713	2.267443	-1.77633	O	-0.69714	3.47745	2.648808
O	0.595307	3.495044	-0.52884	O	-0.78205	5.506708	1.689853
H	0.696247	3.993334	-1.35621	H	-0.43021	5.784065	2.551944
H	-3.05058	-3.35333	-0.15261	H	-1.84456	1.501586	3.230677
O	-6.06972	1.999349	1.337044	O	-3.8875	2.903934	1.305362
H	-5.10465	1.930038	1.208714	H	0.085509	-1.92327	2.274065
H	-6.30505	1.224262	1.85823	H	-1.24562	1.560675	0.253956
				O	1.498781	1.538315	2.187389
				H	0.800933	2.166277	2.427319
				H	1.04018	0.876971	1.65139

Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.47358	-2.95116	2.752778	N	-2.03868	-3.43498	2.093509
H	-1.45285	-2.37272	3.588016	H	-2.30846	-3.45471	3.072899
C	-2.03903	-2.22515	1.630497	C	-1.59519	-2.10036	1.703746
H	-2.14955	-2.9294	0.799227	H	-1.38761	-2.11492	0.632053
C	-3.36831	-1.45797	1.821803	C	-2.63609	-0.96143	1.995988
C	-1.0776	-1.15127	1.1071	C	-0.27699	-1.76129	2.381468
H	-4.24437	-1.97405	1.429701	H	-3.62814	-1.40748	1.934695
H	-3.54938	-1.2403	2.878455	H	-2.51265	-0.58343	3.016082
C	-3.17064	-0.14251	1.110328	C	-2.64205	0.208784	1.019806
O	0.121447	-1.22254	0.971425	O	-0.14635	-2.29601	3.590742
O	-4.00197	0.720009	0.889777	O	-3.67586	0.565275	0.451125
N	-1.83619	-0.02928	0.759962	N	-1.46718	0.842156	0.811429
C	-1.26044	1.141976	0.109175	C	-1.31042	1.855078	-0.21783
H	-0.17691	1.015105	0.194864	H	-0.31314	2.276426	-0.06337
C	-1.65038	1.215787	-1.38511	C	-1.39558	1.28525	-1.66283
C	-1.60104	2.410268	0.893201	C	-2.25946	3.038759	-0.01676
H	-1.64132	0.193225	-1.76621	H	-1.27314	0.201741	-1.59337
H	-2.67387	1.586687	-1.47231	H	-2.38405	1.477786	-2.07657
C	-0.71416	2.015749	-2.23017	C	-0.35422	1.847809	-2.57081
O	-1.92186	3.463882	0.386533	O	-2.80579	3.639092	-0.91329
N	-0.59963	3.38888	-2.18074	N	0.963051	1.442535	-2.50374
C	0.17535	1.625905	-3.20547	C	-0.38038	2.812339	-3.55159
H	-1.09574	3.982602	-1.53098	H	1.324791	0.713962	-1.88304
C	0.330568	3.76467	-3.09645	C	1.661153	2.155124	-3.42532
N	0.822319	2.721287	-3.74221	N	0.88197	2.998173	-4.08337

H	0.372245	0.621231	-3.54776	H	-1.23374	3.376651	-3.89511
H	0.60809	4.795993	-3.24827	H	2.720441	2.019888	-3.58001
O	-1.45424	2.238046	2.20714	O	-2.35279	3.396949	1.274014
H	-1.66137	3.072151	2.659921	H	-2.92752	4.177048	1.329955
H	-2.04665	-3.76057	2.96607	H	-2.86172	-3.68637	1.554822
O	-4.75727	3.042388	-0.64634	O	0.563261	-1.01592	1.901561
H	-4.55858	2.250955	-0.12043	H	-0.62532	0.479479	1.237256
H	-3.96838	3.586441	-0.53325	H	0.690419	-1.99555	3.983108
				O	1.715432	-0.73423	-0.73198
				H	2.656052	-0.861	-0.56416
				H	1.289221	-0.82704	0.137444
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.22216	-4.0126	0.610429	N	-3.63455	-2.54298	1.089531
H	-2.45927	-3.80744	1.576909	H	-3.89413	-3.44631	1.473855
C	-2.32362	-2.82196	-0.21295	C	-2.56106	-2.69559	0.113551
H	-2.1736	-3.12346	-1.25543	H	-2.89638	-3.36392	-0.67947
C	-3.59041	-1.94562	-0.12282	C	-2.25663	-1.32228	-0.52327
C	-1.19319	-1.82923	0.073247	C	-1.27258	-3.31821	0.654154
H	-4.32019	-2.12628	-0.91139	H	-3.21778	-0.91908	-0.8505
H	-4.09223	-2.07978	0.840129	H	-1.87122	-0.63754	0.229581
C	-3.08808	-0.52226	-0.18229	C	-1.38423	-1.42924	-1.76631
O	-0.03572	-2.07624	0.325155	O	-0.9835	-2.93212	1.904441
O	-3.75446	0.487797	-0.32248	O	-1.63871	-2.28276	-2.61677
N	-1.71105	-0.53375	-0.03799	N	-0.32811	-0.59025	-1.94454
C	-0.84979	0.63857	0.081304	C	0.117429	0.613361	-1.23736
H	0.163506	0.231768	0.067065	H	1.169995	0.716143	-1.52466
C	-0.98332	1.652635	-1.10918	C	-0.59568	1.907533	-1.70099
C	-1.0139	1.259753	1.463579	C	0.205975	0.414336	0.275441
H	-1.52725	1.108715	-1.88748	H	-0.49091	1.883507	-2.79345
C	-1.78232	2.919986	-0.76839	C	-2.09421	1.934984	-1.37874
C	0.418532	1.980772	-1.65997	C	0.145268	3.167518	-1.20606
O	-1.87397	0.980135	2.264421	O	-0.2054	1.175549	1.116244
H	-1.19849	3.593308	-0.13541	H	-2.26933	1.890839	-0.30171
H	-2.03648	3.458759	-1.68291	H	-2.54545	2.85413	-1.75696
H	-2.71456	2.675278	-0.25965	H	-2.62065	1.106337	-1.85571
H	0.999803	2.478341	-0.87487	H	-0.08262	3.330924	-0.14988
H	0.933801	1.03937	-1.88245	H	1.226338	2.993348	-1.26727
C	0.403026	2.847855	-2.9224	C	-0.19316	4.425427	-2.01413
H	0.013987	3.849864	-2.72526	H	-1.25205	4.686855	-1.93697
H	1.41443	2.95924	-3.32267	H	0.383072	5.2818	-1.65293
H	-0.21794	2.393678	-3.70195	H	0.041101	4.286888	-3.07476
O	-0.04482	2.159588	1.691014	O	0.86847	-0.71985	0.582601
H	-0.18296	2.549642	2.569359	H	0.933285	-0.78616	1.549064
H	-2.8794	-4.71447	0.286891	H	-3.33123	-1.97037	1.872196
O	-6.56305	0.372895	-0.5513	O	-0.56715	-4.0765	0.018381
H	-5.58795	0.390292	-0.49656	H	0.139725	-0.75172	-2.82697
H	-6.75712	-0.17197	-1.32142	H	-0.16444	-3.37179	2.185613

				O	2.072445	-3.14442	-0.79776
				H	1.265747	-3.62348	-0.55274
				H	1.87393	-2.23666	-0.53355
Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.63374	-2.91406	1.369969	N	-2.93628	-4.70942	1.346146
H	-0.72955	-2.65963	2.348932	H	-3.66185	-5.15368	1.900897
C	-1.009	-1.81007	0.506543	C	-3.05555	-3.24717	1.413722
H	-1.01027	-2.17855	-0.52474	H	-3.01908	-2.95437	2.463576
C	-2.33506	-1.06021	0.77451	C	-1.89232	-2.60196	0.662774
C	0.040979	-0.692	0.518717	C	-4.42485	-2.804	0.906791
H	-3.15641	-1.35619	0.122169	H	-0.95685	-2.96279	1.098727
H	-2.66129	-1.1939	1.810088	H	-1.89488	-2.91261	-0.38643
C	-2.00288	0.398767	0.579023	C	-1.93416	-1.08374	0.727493
O	1.245784	-0.79946	0.533253	O	-5.4055	-2.67096	1.616878
O	-2.7666	1.350238	0.546643	O	-2.85538	-0.47274	1.273187
N	-0.63313	0.529132	0.470025	N	-0.89508	-0.44276	0.150216
C	0.050052	1.810898	0.305332	C	-0.80448	1.0112	0.103188
H	1.102427	1.591136	0.505359	H	0.215637	1.230941	-0.22208
C	-0.11779	2.372691	-1.11431	C	-1.80069	1.638933	-0.89115
C	-0.38337	2.792796	1.395366	C	-0.86347	1.557019	1.538421
H	-0.09369	1.525703	-1.80809	H	-1.88808	0.947174	-1.73555
H	-1.10949	2.823837	-1.19102	H	-2.78337	1.686622	-0.41859
C	0.962279	3.387828	-1.53292	C	-1.39931	3.024508	-1.433
O	-0.60395	3.96598	1.213841	O	-0.26921	1.057755	2.467353
H	1.035898	4.149771	-0.7502	H	-1.13767	3.666367	-0.58548
C	2.337586	2.725954	-1.70284	C	-0.18592	2.944584	-2.3715
C	0.536334	4.082228	-2.83354	C	-2.59389	3.661459	-2.15616
H	2.302538	1.960466	-2.48623	H	-0.41428	2.322219	-3.24426
H	3.088054	3.467561	-1.99117	H	0.089455	3.940043	-2.7321
H	2.689382	2.247511	-0.78443	H	0.695767	2.521422	-1.88144
H	-0.41763	4.604072	-2.71182	H	-3.44849	3.779746	-1.48309
H	1.285596	4.813955	-3.14949	H	-2.33378	4.648093	-2.55115
H	0.420211	3.35171	-3.64247	H	-2.91345	3.037541	-2.99898
H	-1.24669	-3.70597	1.207743	H	-3.04612	-5.03781	0.390223
O	-0.43019	2.20401	2.601358	O	-1.58983	2.678056	1.655681
H	-0.68558	2.870315	3.259473	H	-1.53437	2.977468	2.577428
O	-5.54796	1.026989	0.953026	O	-4.48188	-2.67902	-0.42462
H	-5.83605	0.312008	0.375549	H	-0.14965	-0.982	-0.26114
H	-4.58952	1.110689	0.788072	H	-5.39498	-2.47304	-0.68241
				O	-5.17444	-3.00129	4.419667
				H	-5.26969	-2.90138	3.453381
				H	-4.94943	-3.92886	4.549532
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.44117	-3.27852	2.491056	N	-2.31712	-3.67736	2.056476
H	-0.51738	-3.40401	2.896832	H	-1.57147	-3.84507	2.727445

C	-1.30725	-2.70421	1.155293	C	-2.01994	-2.48911	1.260213
H	-0.74228	-3.34055	0.457683	H	-2.766	-2.40283	0.469501
C	-2.6404	-2.29888	0.512296	C	-2.09543	-1.23868	2.160389
C	-0.52826	-1.3958	1.229153	C	-0.63826	-2.57066	0.605705
H	-2.96717	-2.94763	-0.29972	H	-3.10171	-1.19899	2.579312
H	-3.43656	-2.25741	1.260898	H	-1.38197	-1.33808	2.981167
C	-2.41847	-0.89504	-0.00318	C	-1.86441	0.040453	1.37088
O	0.504369	-1.19853	1.831415	O	0.393251	-2.78709	1.214113
O	-3.17511	-0.24348	-0.69874	O	-2.715	0.479043	0.591666
N	-1.19261	-0.44322	0.460792	N	-0.67084	0.639608	1.555234
C	-0.65863	0.893512	0.238676	C	-0.27021	1.808889	0.786741
H	0.322169	0.892176	0.724387	H	0.631749	2.192213	1.275154
C	-0.47283	1.219468	-1.26402	C	0.070063	1.466663	-0.67634
C	-1.50261	1.909006	1.009459	C	-1.31102	2.920365	0.988715
H	-0.33607	0.268175	-1.78491	H	0.557322	0.487739	-0.66761
H	-1.38198	1.674178	-1.66042	H	-0.8537	1.359041	-1.24825
C	0.735794	2.11936	-1.54062	C	1.007183	2.480326	-1.34058
O	-2.40733	1.627988	1.758742	O	-1.77603	3.209649	2.067985
H	0.636012	3.059555	-0.99275	H	0.57896	3.484418	-1.28473
H	1.644469	1.628165	-1.1741	H	1.956088	2.506007	-0.7916
C	0.879433	2.41222	-3.03854	C	1.274335	2.126072	-2.80807
H	0.961642	1.471862	-3.59484	H	1.666699	1.10552	-2.87967
H	-0.01822	2.925998	-3.39991	H	0.33264	2.151581	-3.36754
C	2.104701	3.273496	-3.30959	C	2.266181	3.098661	-3.42913
H	2.040379	4.241465	-2.81274	H	1.907498	4.127244	-3.39011
H	3.026138	2.779343	-3.00193	H	3.24274	3.04698	-2.94778
N	2.247792	3.55968	-4.78469	N	2.494714	2.783823	-4.88818
H	1.426708	4.045318	-5.15246	H	1.631958	2.871936	-5.4294
H	3.061879	4.147393	-4.97506	H	3.181485	3.41585	-5.30427
H	2.360327	2.698109	-5.3234	H	2.840775	1.830338	-5.01577
H	-1.85349	-4.20447	2.423294	H	-2.37111	-4.50048	1.463531
O	-1.08568	3.160221	0.777471	O	-1.61136	3.585005	-0.13702
H	-1.64195	3.770577	1.287996	H	-2.23479	4.294007	0.088641
O	-3.88324	2.456862	-1.20615	O	-0.6739	-2.38887	-0.71766
H	-3.64245	1.528171	-1.04257	H	0.23078	-2.44501	-1.06967
H	-4.02655	2.508894	-2.15724	H	0.006494	0.224471	2.193143
				O	1.166742	-0.94105	3.226957
				H	2.097317	-0.69291	3.188831
				H	1.078266	-1.70772	2.634281

Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.60105	-4.49862	-1.23635	N	-2.22284	-4.26509	-1.47156
H	-0.64329	-4.69008	-0.95589	H	-3.16432	-4.58445	-1.67957
C	-2.14748	-3.38073	-0.48878	C	-2.25024	-2.94307	-0.83328
H	-3.21024	-3.29861	-0.74015	H	-2.87888	-3.00896	0.055773
C	-1.98906	-3.35431	1.049486	C	-0.83356	-2.53231	-0.42124
C	-1.53666	-2.04655	-0.9345	C	-2.87857	-1.92367	-1.78379
H	-2.88381	-3.64959	1.597229	H	-0.42302	-3.33926	0.189282

H	-1.16734	-3.99979	1.372907	H	-0.20276	-2.42049	-1.30525
C	-1.61582	-1.93091	1.383683	C	-0.83514	-1.27229	0.432434
O	-1.2772	-1.68215	-2.05805	O	-4.20797	-1.86202	-1.64725
O	-1.52188	-1.42413	2.487268	O	-1.43718	-1.22598	1.508503
N	-1.34539	-1.25946	0.203679	N	-0.13801	-0.22626	-0.05456
C	-0.8987	0.129177	0.136909	C	-0.12187	1.071982	0.598534
H	-0.53197	0.258813	-0.88681	H	0.643349	1.657143	0.07807
C	-2.05036	1.111296	0.401537	C	-1.46536	1.820722	0.529026
C	0.314834	0.342908	1.044615	C	0.378119	0.985442	2.041336
H	-2.92716	0.727161	-0.12619	H	-2.18028	1.312433	1.179691
H	-2.28409	1.119848	1.467697	H	-1.31749	2.8245	0.932299
C	-1.7356	2.523946	-0.09217	C	-2.07601	1.892146	-0.86912
O	0.467578	1.292734	1.778231	O	-0.04311	1.66224	2.951885
H	-0.86011	2.928838	0.416648	H	-2.27463	0.89423	-1.26421
H	-1.54636	2.519863	-1.16952	H	-3.02219	2.435183	-0.82161
S	-3.16016	3.631973	0.240668	S	-1.00274	2.767965	-2.08473
C	-2.48014	5.185746	-0.43645	C	-2.13808	2.73962	-3.51684
H	-2.26261	5.075917	-1.50054	H	-3.03885	3.313495	-3.29323
H	-3.24186	5.954758	-0.30083	H	-1.61133	3.197608	-4.35458
H	-1.57562	5.473418	0.102743	H	-2.4017	1.711149	-3.76967
O	1.222999	-0.62631	0.886588	O	1.401934	0.127347	2.17588
H	1.980803	-0.44217	1.465323	H	1.695369	0.151449	3.100651
H	-2.13907	-5.33783	-1.04791	H	-1.71598	-4.22925	-2.35241
O	-1.50113	1.036714	4.017748	O	-2.27742	-1.27769	-2.62209
H	-1.55214	0.173785	3.576669	H	-4.5674	-1.26038	-2.3205
H	-0.85223	1.51145	3.48232	H	0.255994	-0.28861	-0.9909
				O	0.338904	-0.15163	-2.9537
				H	0.09672	0.790195	-2.87941
				H	-0.51711	-0.60974	-3.01157

Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.00788	-3.24399	2.123588	N	-2.00024	-4.0473	0.63716
H	-1.05409	-2.81367	3.042849	H	-2.81666	-3.96889	1.237512
C	-1.48264	-2.33312	1.098689	C	-1.31512	-2.75342	0.532769
H	-1.52639	-2.88641	0.154416	H	-0.54258	-2.86161	-0.22749
C	-2.82374	-1.5923	1.30908	C	-2.25544	-1.57866	0.180971
C	-0.48559	-1.19802	0.836848	C	-0.5849	-2.52602	1.851891
H	-3.66786	-2.03313	0.779311	H	-2.68482	-1.78528	-0.80467
H	-3.08139	-1.53873	2.370923	H	-3.08092	-1.54753	0.893701
C	-2.57536	-0.18499	0.823884	C	-1.67422	-0.17029	0.138784
O	0.721467	-1.25837	0.79273	O	0.62304	-2.49397	1.984997
O	-3.39147	0.705308	0.666673	O	-2.36398	0.801588	0.459424
N	-1.21663	-0.0299	0.607178	N	-0.39777	-0.02629	-0.2755
C	-0.59358	1.216713	0.172901	C	0.236019	1.281203	-0.34402
H	0.477278	1.070141	0.341112	H	1.303718	1.084919	-0.47817
C	-0.84894	1.489761	-1.32158	C	-0.26536	2.119267	-1.5437
C	-1.00243	2.369696	1.090595	C	0.146728	1.958461	1.030778
H	-0.69605	0.537882	-1.83816	H	-0.38179	1.415291	-2.3726

H	-1.89177	1.77341	-1.46378	H	-1.25464	2.515328	-1.3153
C	0.073123	2.534209	-1.91276	C	0.675744	3.226394	-1.96791
O	-1.346	3.465886	0.713335	O	0.357403	1.37713	2.071506
C	-0.42825	3.746095	-2.39863	C	0.307968	4.572394	-1.86721
C	1.450056	2.29146	-2.00474	C	1.93647	2.916787	-2.49734
H	-1.49153	3.947138	-2.33205	H	-0.66183	4.828056	-1.45528
C	0.424438	4.697538	-2.96134	C	1.175679	5.585677	-2.27994
C	2.307489	3.241779	-2.56055	C	2.810524	3.924962	-2.90579
H	1.856301	1.350349	-1.64707	H	2.236073	1.878141	-2.59928
H	0.017373	5.630824	-3.33423	H	0.870859	6.622875	-2.19425
C	1.796337	4.449853	-3.04112	C	2.432281	5.265615	-2.79786
H	3.370266	3.036571	-2.62385	H	3.781018	3.664125	-3.31323
H	2.4602	5.188456	-3.47591	H	3.108166	6.050963	-3.11698
O	-0.87853	2.033686	2.380518	O	-0.123	3.268598	0.964602
H	-1.13194	2.795428	2.92698	H	-0.11268	3.625532	1.867322
H	-1.59524	-4.07065	2.152401	H	-2.33215	-4.33122	-0.2796
O	-3.96699	3.235721	-0.64271	O	-1.43121	-2.37571	2.874811
H	-3.15029	3.671773	-0.36516	H	0.195503	-0.82152	-0.49461
H	-3.88899	2.361778	-0.22868	H	-0.92391	-2.25879	3.694775
				O	1.775563	-2.01511	-0.53197
				H	2.62149	-1.55473	-0.56502
				H	1.63907	-2.25184	0.404315
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.48963	-2.91309	1.292118	N	-1.91878	-4.04551	0.547264
H	-1.23728	-2.55869	2.210433	H	-1.06923	-4.5842	0.401875
C	-1.55414	-1.83734	0.319889	C	-1.68265	-2.64432	0.224269
H	-1.94505	-2.25469	-0.61396	H	-2.62245	-2.09516	0.304456
C	-2.34444	-0.55405	0.670244	C	-0.63693	-1.94687	1.148453
C	-0.15761	-1.31279	-0.03753	C	-1.18901	-2.54331	-1.21128
H	-3.33057	-0.49727	0.209408	H	-0.96842	-2.08582	2.179601
H	-2.47125	-0.45143	1.751766	H	0.333033	-2.43693	1.032086
C	-1.47396	0.583799	0.197552	C	-0.55972	-0.45117	0.90626
O	0.857631	-1.94712	-0.20731	O	-0.47746	-3.38355	-1.73396
O	-1.741	1.772858	0.147929	O	-1.56038	-1.41345	-1.80601
N	-0.24499	0.073827	-0.17559	N	0.585823	0.017015	0.354914
C	0.872773	0.910846	-0.57595	C	0.760048	1.419435	0.023093
H	1.703764	0.22716	-0.77722	H	1.815924	1.566658	-0.2209
C	0.588132	1.679799	-1.87972	C	-0.06191	1.821652	-1.21876
C	1.306211	1.768161	0.616597	C	0.518537	2.279794	1.270274
H	-0.11533	1.08637	-2.47379	H	0.11362	1.071662	-1.99048
H	0.132256	2.648055	-1.66535	H	-1.12769	1.82224	-0.97666
O	1.828044	1.825889	-2.56482	O	0.356775	3.066327	-1.76495
O	1.085405	1.476383	1.768592	O	0.920507	2.000541	2.373931
H	1.749106	2.550286	-3.19452	H	0.09377	3.764121	-1.15254
O	1.989171	2.853208	0.238241	O	-0.1365	3.422216	0.993488
H	2.263716	3.335713	1.035161	H	-0.20888	3.945562	1.807925
H	-2.39899	-3.35358	1.383019	H	-2.17143	-4.13939	1.526021

O	-4.19874	2.856757	1.047791	O	-1.49792	0.29655	1.183351
H	-3.37387	2.445179	0.727873	H	1.342402	-0.61884	0.159112
H	-4.87632	2.18447	0.919283	H	-1.10932	-1.35943	-2.69232
				O	-0.15275	-1.67228	-4.08336
				H	0.196956	-2.48705	-3.69024
				H	0.612641	-1.09942	-4.21556
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.91444	-4.17579	0.631642	N	-1.63169	-3.18092	2.057968
H	-0.61949	-4.08256	1.599574	H	-1.10823	-3.8498	2.612537
C	-1.58815	-2.97333	0.177121	C	-1.48967	-3.47607	0.639112
H	-1.98793	-3.17228	-0.82291	H	-1.88974	-4.48275	0.466461
C	-2.70085	-2.35658	1.052887	C	-2.33972	-2.51792	-0.22923
C	-0.60983	-1.81154	-0.01937	C	-0.0513	-3.56815	0.108904
H	-3.71292	-2.58435	0.718445	H	-2.2443	-2.80386	-1.27683
H	-2.60954	-2.68101	2.093362	H	-3.37954	-2.62494	0.075528
C	-2.46182	-0.86629	1.012695	C	-1.94418	-1.06717	-0.01553
O	0.516839	-1.85029	-0.45635	O	0.839514	-3.86457	1.055636
O	-3.16448	0.00017	1.499582	O	0.248658	-3.43977	-1.06428
N	-1.25353	-0.63292	0.373428	N	-0.98649	-0.5879	-0.83836
C	-0.64439	0.677962	0.187147	C	-0.18904	0.615481	-0.63632
H	0.425326	0.485068	0.049926	H	0.38741	0.733945	-1.5547
C	-1.15276	1.408882	-1.08176	C	-0.96967	1.94267	-0.42539
C	-0.72203	1.522938	1.457392	C	0.861406	0.467749	0.464574
H	-0.73443	2.420869	-1.03294	H	-0.22578	2.733077	-0.54941
C	-0.66325	0.718563	-2.34866	C	-2.0753	2.113501	-1.46372
O	-2.56682	1.45569	-1.15718	O	-1.45482	2.082544	0.903281
O	-0.96116	2.708927	1.475068	O	1.748299	1.273869	0.631287
H	-1.07037	-0.29326	-2.42008	H	-2.84776	1.351578	-1.33679
H	-1.00207	1.283958	-3.21856	H	-2.53462	3.096466	-1.34174
H	0.426767	0.659449	-2.37009	H	-1.67604	2.036653	-2.47901
H	-2.93623	2.014602	-0.44804	H	-1.95798	1.261989	1.091459
H	-1.55003	-4.96541	0.590021	H	-1.25736	-2.26061	2.271029
O	-0.4046	0.812124	2.545807	O	0.715204	-0.63639	1.212083
H	-0.43843	1.396552	3.32053	H	1.423946	-0.65574	1.875148
O	-3.89989	2.690265	1.029762	O	-2.46063	-0.40322	0.892544
H	-3.74486	1.797335	1.384469	H	1.71568	-3.9508	0.645513
H	-3.20567	3.225561	1.434413	H	-0.58458	-1.2413	-1.49589
				O	1.682125	-1.38274	-2.35217
				H	2.523446	-1.09171	-1.9838
				H	1.48367	-2.21951	-1.90156
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.01798	-2.66136	2.368279	N	-3.15062	-2.38002	2.859566
H	-1.6022	-2.4102	3.160839	H	-2.91284	-2.65806	3.805863
C	-1.5658	-2.13586	1.130916	C	-2.0646	-2.7035	1.948089
H	-0.96669	-2.53502	0.305739	H	-1.90388	-3.78678	1.97946

C	-3.06456	-2.35242	0.817417	C	-2.43627	-2.36111	0.482997
C	-1.3979	-0.61449	1.035814	C	-0.68421	-2.12555	2.289643
H	-3.26289	-3.15604	0.108499	H	-1.58198	-2.57836	-0.16029
H	-3.63233	-2.55907	1.729263	H	-3.27316	-2.99166	0.18767
C	-3.545	-1.03331	0.263979	C	-2.881	-0.91424	0.333245
O	-0.44092	0.052402	1.356856	O	0.296806	-2.29101	1.587117
O	-4.62439	-0.78802	-0.24635	O	-0.64604	-1.45307	3.44098
N	-2.55623	-0.08751	0.460669	N	-1.89783	0.010438	0.290928
C	-2.68309	1.323457	0.105585	C	-2.1734	1.436601	0.2445
H	-1.88584	1.824688	0.661527	H	-1.23586	1.923883	0.529402
C	-2.4836	1.571962	-1.40531	C	-2.58568	1.944955	-1.15835
C	-3.99386	1.899298	0.643112	C	-3.17558	1.848802	1.324483
H	-1.72995	0.854059	-1.74438	H	-2.08593	1.295294	-1.88318
H	-3.40908	1.350029	-1.93748	H	-3.66012	1.813095	-1.2894
C	-2.02087	2.964779	-1.70136	C	-2.18363	3.366921	-1.40001
O	-4.73973	2.614069	0.0205	O	-4.06957	2.647478	1.171447
C	-2.72429	3.966359	-2.32449	C	-2.98857	4.477443	-1.46844
C	-0.72811	3.514669	-1.37781	C	-0.83236	3.833022	-1.58674
H	-3.73142	3.957957	-2.70977	H	-4.05939	4.554239	-1.36701
N	-1.94859	5.103537	-2.41137	N	-2.22185	5.604211	-1.68912
C	-0.71941	4.86129	-1.83888	C	-0.8948	5.243923	-1.76386
C	0.419319	2.999809	-0.74845	C	0.419459	3.193545	-1.62499
H	-2.24007	5.97262	-2.82814	H	-2.58085	6.540583	-1.77865
C	0.394112	5.693217	-1.68827	C	0.249751	6.019496	-1.97192
C	1.528351	3.824929	-0.59578	C	1.560606	3.961743	-1.82974
H	0.437152	1.978987	-0.38224	H	0.494981	2.11869	-1.49879
H	0.383025	6.715917	-2.04735	H	0.183455	7.093157	-2.1059
C	1.515462	5.158041	-1.06113	C	1.47584	5.360944	-2.00065
H	2.419609	3.441858	-0.11125	H	2.53258	3.482002	-1.86035
H	2.3957	5.776825	-0.92748	H	2.382926	5.93353	-2.15852
O	-4.18681	1.555172	1.927768	O	-2.90032	1.274627	2.511836
H	-5.0177	1.95442	2.231869	H	-3.54451	1.602497	3.159244
H	-0.98757	-3.67475	2.330982	H	-3.31466	-1.37692	2.882647
O	-5.76066	0.44737	-2.5614	O	-4.07314	-0.5969	0.331676
H	-5.38479	0.076126	-1.7455	H	0.263458	-1.14665	3.591765
H	-5.88532	-0.31356	-3.13884	H	-0.92094	-0.25096	0.192295
				O	1.060822	-0.07114	0.027401
				H	1.444304	0.67717	0.49908
				H	1.147066	-0.82442	0.634759

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.4981	-2.31032	1.017171	N	-2.35177	-2.09658	-1.31252
H	-1.24399	-2.59297	1.646632	H	-1.53869	-2.45726	-1.8036
C	-0.91154	-1.1902	0.193179	C	-1.92296	-1.28876	-0.18026
H	-0.12147	-1.00614	-0.5431	H	-1.27716	-0.49556	-0.56711
C	-2.27109	-1.25129	-0.5396	C	-3.15617	-0.63282	0.522196
C	-0.99899	0.113397	0.994518	C	-1.07572	-2.05427	0.837666
H	-2.20281	-1.54051	-1.5879	H	-4.03552	-0.8247	-0.08971

H	-2.95608	-1.94308	-0.04059	H	-3.32817	-1.07546	1.507221
C	-2.84114	0.140575	-0.41227	C	-3.0397	0.879084	0.669294
O	-0.25828	0.503392	1.867303	O	-0.87075	-3.25214	0.800442
O	-3.80084	0.615693	-0.99625	O	-0.57593	-1.2546	1.786463
N	-2.09001	0.840031	0.512957	N	-2.01112	1.312194	1.433875
C	-2.35596	2.213921	0.906704	C	-1.61068	2.702655	1.499186
H	-1.61065	2.446911	1.673219	H	-0.7252	2.731113	2.141297
C	-2.17359	3.206444	-0.27174	C	-1.21918	3.305204	0.119184
C	-3.70848	2.300915	1.609422	C	-2.65135	3.535503	2.248989
H	-2.9818	3.05958	-0.98851	H	-2.12558	3.552421	-0.43236
H	-2.26928	4.213278	0.136222	H	-0.68391	4.2383	0.307241
C	-0.83067	3.02205	-0.93798	C	-0.37294	2.351791	-0.69199
O	-4.32428	1.355026	2.039977	O	-3.48094	3.094362	3.009191
C	-0.701	2.240442	-2.09037	C	-0.84675	1.820897	-1.89482
C	0.330273	3.577205	-0.38371	C	0.887044	1.93254	-0.242
H	-1.58334	1.800344	-2.54267	H	-1.8236	2.116394	-2.26114
C	0.544714	2.009972	-2.67499	C	-0.09935	0.897583	-2.62969
C	1.580651	3.359462	-0.95538	C	1.641323	1.006272	-0.95576
H	0.258836	4.188555	0.510182	H	1.285325	2.325478	0.687831
H	0.624581	1.399663	-3.56835	H	-0.4897	0.493736	-3.55791
C	1.689706	2.57041	-2.10432	C	1.145614	0.483	-2.15426
H	2.474777	3.794095	-0.52454	H	2.61056	0.680929	-0.59693
O	2.942117	2.386955	-2.62461	O	1.924887	-0.43049	-2.81195
H	2.89548	1.835202	-3.41493	H	1.479848	-0.72746	-3.61495
H	-0.28415	-3.11091	0.431981	H	-2.86276	-2.9122	-0.98386
O	-4.10783	3.573783	1.73817	O	-2.49893	4.850424	2.011528
H	-4.94394	3.585804	2.231847	H	-3.14577	5.332718	2.551277
O	-5.1505	-0.88797	-2.97518	O	-3.82149	1.652779	0.115368
H	-4.50364	-1.00141	-3.67973	H	-1.37863	0.619914	1.811195
H	-4.68454	-0.36885	-2.29198	H	-0.05488	-1.80376	2.436725
				O	0.767984	-3.03676	3.249337
				H	0.483529	-3.23732	4.149518
				H	0.397867	-3.74023	2.69496

Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.31355	-4.32451	0.098073	N	-3.71715	-3.58328	0.936455
H	-0.88688	-4.35281	1.01996	H	-3.85292	-4.4126	0.366451
C	-1.94944	-3.04132	-0.13948	C	-2.49345	-2.89119	0.549011
H	-2.49319	-3.10845	-1.08772	H	-2.59448	-2.58728	-0.49573
C	-2.88596	-2.45351	0.939418	C	-2.33554	-1.63093	1.431442
C	-0.9193	-1.92793	-0.35692	C	-1.21584	-3.72783	0.616091
H	-3.94795	-2.58629	0.734236	H	-3.33151	-1.19194	1.525432
H	-2.67504	-2.88697	1.921462	H	-2.0302	-1.91415	2.443652
C	-2.54488	-0.98403	1.002786	C	-1.42821	-0.48091	1.00657
O	0.121125	-1.98506	-0.97178	O	-0.24771	-3.52363	-0.09838
O	-3.13791	-0.11521	1.614408	O	-1.24036	-4.67441	1.551735
N	-1.39459	-0.76805	0.260687	N	-0.63823	-0.63167	-0.0783
C	-0.69613	0.511758	0.117592	C	0.261051	0.411272	-0.56703

H	0.344175	0.233305	-0.08308	H	1.073099	-0.12315	-1.07152
C	-1.2033	1.319743	-1.09868	C	-0.40358	1.313549	-1.63617
C	-0.64229	1.250848	1.453838	C	0.978552	1.056027	0.626528
H	-1.16448	0.60035	-1.92496	H	-0.80175	0.589941	-2.35804
C	-2.65117	1.808561	-0.97067	C	-1.58616	2.148369	-1.13036
C	-0.2411	2.46489	-1.44658	C	0.626784	2.172843	-2.38455
O	-0.85469	2.43143	1.608804	O	1.588631	0.39677	1.446718
H	-2.7576	2.519777	-0.1499	H	-1.26276	2.89845	-0.40671
H	-2.94867	2.30716	-1.89692	H	-2.05258	2.664894	-1.97418
H	-3.34523	0.983723	-0.79922	H	-2.34509	1.523937	-0.65629
H	0.788296	2.10647	-1.54396	H	1.463181	1.56839	-2.7498
H	-0.53194	2.910105	-2.40149	H	0.153194	2.643318	-3.25032
H	-0.26318	3.246207	-0.68509	H	1.028996	2.964129	-1.74941
H	-2.00649	-5.06495	0.069512	H	-3.66134	-3.89827	1.900906
O	-0.24127	0.438013	2.442188	O	0.967555	2.388083	0.644477
H	-0.19886	0.950476	3.265705	H	1.498516	2.687416	1.400768
O	-3.67634	2.544943	2.612324	O	-1.44991	0.56435	1.658603
H	-3.56502	1.649347	2.256159	H	-0.54011	-1.54813	-0.49534
H	-2.81233	2.946082	2.455766	H	-0.38522	-5.13555	1.56184
				O	2.191968	-2.38897	1.182274
				H	1.915887	-1.45839	1.262259
				H	1.454876	-2.8324	0.739817

Table S15.E. Isoimide Formation XYZ Coordinates (Implicit solvation + 1 H_2O, ε = 80)

All Reactions							
NH_3							
Product Structure							
Atom	X	Y	Z				
N	-1.133326	-0.563263	0.000024				
H	-0.744703	-1.50246	-0.000031				
H	-0.744689	-0.093642	0.813368				
H	-0.7447	-0.093681	-0.813362				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.80773	-2.89702	0.322781	N	-1.59506	-2.42318	-0.79937
H	-0.8935	-2.8566	0.765271	H	-0.95848	-3.13224	-0.44522
C	-2.4982	-1.62759	0.512093	C	-2.08098	-1.58885	0.23944
H	-3.41582	-1.63777	-0.0803	C	-2.93084	-1.97335	1.42576
C	-2.89399	-1.33329	1.989232	C	-1.81663	-0.27884	0.331431
C	-1.58617	-0.49828	0.020725	H	-3.91306	-2.38077	1.163305
H	-3.50316	-2.16811	2.345328	H	-2.45939	-2.68718	2.111499
H	-1.99508	-1.27759	2.60751	C	-3.10796	-0.64757	2.129439
C	-3.74049	-0.08017	2.096182	O	-2.41963	0.317388	1.451599
O	-0.36607	-0.54394	0.17892	O	-3.72811	-0.37035	3.128785
O	-4.79322	0.018047	1.44587	N	-1.00642	0.562908	-0.39535
N	-3.29073	0.908693	2.885898	H	-0.6233	0.064601	-1.19257

H	-3.79964	1.7833	2.918791	C	-1.49723	1.895088	-0.74088
H	-2.4151	0.835444	3.377462	H	-1.85624	2.376866	0.169618
N	-2.21562	0.562616	-0.52842	C	-0.36036	2.733926	-1.33962
H	-3.22437	0.567357	-0.60323	C	-2.66291	1.841144	-1.72959
C	-1.50372	1.769975	-0.90598	H	0.027514	2.264058	-2.24774
H	-0.68459	1.92096	-0.19897	H	-0.71539	3.734376	-1.59035
C	-0.92407	1.686692	-2.33104	H	0.450256	2.815643	-0.61394
C	-2.44546	2.954284	-0.78719	O	-2.90247	0.91199	-2.46664
H	-1.72519	1.552601	-3.06165	H	-2.35193	-2.91362	-1.2677
H	-0.36707	2.593439	-2.5717	O	-3.38417	2.974843	-1.70367
H	-0.25001	0.831005	-2.38509	H	-4.0832	2.91509	-2.37519
O	-3.65244	2.870454	-0.69301	O	-3.60779	2.436444	3.75507
H	-2.32706	-3.64875	0.765413	H	-3.65513	1.482857	3.560919
O	-1.78502	4.114275	-0.83356	H	-3.05576	2.79436	3.051258
H	-2.42561	4.843574	-0.79794				
O	-5.5167	2.70548	1.57376				
H	-5.43496	1.734685	1.473014				
H	-4.979	3.044699	0.844549				
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.58109	-4.21239	-0.25604	N	-4.07733	-3.31817	-0.66602
H	-1.75237	-4.48694	0.264381	H	-3.99186	-4.27284	-0.32701
C	-3.02324	-2.89574	0.183885	C	-4.00562	-2.37834	0.394791
H	-3.8279	-2.56056	-0.47452	C	-4.93919	-2.2221	1.568764
C	-3.5645	-2.86043	1.644081	C	-3.02722	-1.47238	0.526184
C	-1.84376	-1.92251	0.08095	H	-5.96889	-1.96992	1.293225
H	-4.37052	-3.59513	1.719168	H	-4.98756	-3.09512	2.230106
H	-2.77277	-3.15091	2.338671	C	-4.32017	-1.05939	2.318086
C	-4.15725	-1.50722	1.985733	O	-3.18164	-0.66129	1.658228
O	-0.68826	-2.2829	0.302176	O	-4.67491	-0.50301	3.32382
O	-5.04757	-1.01849	1.271802	N	-1.8677	-1.25348	-0.18612
N	-3.66439	-0.86385	3.056292	H	-1.84494	-1.87615	-0.98839
H	-3.99544	0.069792	3.265489	C	-1.52025	0.124395	-0.54088
H	-2.91333	-1.24867	3.605405	H	-1.55407	0.734551	0.360834
N	-2.17296	-0.64143	-0.19684	C	-0.08601	0.154655	-1.09623
H	-3.13982	-0.39269	-0.35964	C	-2.50113	0.69402	-1.56603
C	-1.19361	0.430061	-0.18115	H	0.551074	-0.2919	-0.32823
H	-0.41897	0.178428	0.545183	H	-0.03046	-0.48868	-1.98148
C	-0.54338	0.607341	-1.57429	C	0.41435	1.560999	-1.43494
C	-1.88819	1.704255	0.269473	O	-3.00664	0.050076	-2.45804
H	-0.17162	-0.38138	-1.85692	H	-0.16563	1.985576	-2.2601
H	-1.32452	0.876997	-2.29203	H	0.280812	2.212942	-0.56646
C	0.601135	1.622765	-1.61879	C	1.890054	1.533802	-1.8249
O	-3.06473	1.937338	0.085324	H	2.486559	1.156302	-0.98786
H	0.227618	2.627238	-1.40006	H	2.038638	0.869744	-2.68305
H	1.347564	1.380435	-0.85548	N	2.341374	2.88506	-2.17036
C	1.26543	1.618999	-2.99418	H	1.656184	3.625973	-2.15213
H	1.687113	0.629958	-3.19572	C	3.579544	3.200427	-2.54661

H	0.522852	1.842516	-3.76796	N	4.529542	2.263222	-2.5972
N	2.343164	2.610846	-3.04085	N	3.877773	4.460908	-2.88698
H	2.363852	3.31405	-2.31665	H	4.334101	1.301014	-2.37942
C	3.223135	2.729264	-4.03478	H	5.463732	2.488777	-2.89799
N	3.160447	1.916484	-5.09324	H	3.19881	5.198324	-2.79048
N	4.182819	3.660222	-3.97043	H	4.82725	4.731697	-3.08533
H	2.365499	1.32052	-5.25184	H	-4.96583	-3.25899	-1.15576
H	3.84125	1.979094	-5.83268	O	-2.72756	2.004845	-1.37834
H	4.342054	4.183416	-3.12486	H	-3.32106	2.321983	-2.07931
H	4.844347	3.778202	-4.72053	O	0.14238	1.465139	2.045154
H	-3.30045	-4.90428	-0.07048	H	1.076499	1.246602	1.949518
O	-1.04693	2.553898	0.862708	H	0.135755	2.407574	2.248106
H	-1.52458	3.37155	1.081958				
O	-5.25826	1.653988	2.032365				
H	-5.34261	0.742645	1.683452				
H	-4.5648	2.037328	1.477253				
Asn-Asn							
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.91832	-3.6156	0.168144	N	-1.9847	-3.12832	-0.60326
H	-0.10409	-3.47257	0.759511	H	-1.64181	-3.9264	-0.07516
C	-1.80531	-2.46396	0.269113	C	-2.53154	-2.1346	0.247582
H	-2.60376	-2.57206	-0.46831	C	-3.72366	-2.24387	1.165528
C	-2.47287	-2.29451	1.66601	C	-2.02098	-0.90435	0.386267
C	-0.9982	-1.19855	-0.03664	H	-4.66834	-2.45602	0.653432
H	-3.00556	-3.22077	1.896911	H	-3.6166	-2.98783	1.963776
H	-1.70321	-2.14442	2.426457	C	-3.78053	-0.86067	1.774786
C	-3.497	-1.17657	1.65985	O	-2.74778	-0.11276	1.29099
O	0.177599	-1.08344	0.307194	O	-4.56072	-0.38884	2.567724
O	-4.42125	-1.18344	0.831151	N	-0.88049	-0.30987	-0.10722
N	-3.34254	-0.1853	2.552464	H	-0.42473	-0.94483	-0.75567
H	-3.97479	0.604876	2.525598	C	-0.9729	1.053173	-0.62255
H	-2.57075	-0.16975	3.199051	H	-1.497	1.671001	0.106732
N	-1.67891	-0.20262	-0.64653	C	0.443055	1.632198	-0.81062
H	-2.65719	-0.3214	-0.87524	C	-1.73886	1.108356	-1.94761
C	-1.09147	1.105834	-0.84842	H	1.013292	1.381906	0.087576
H	-0.46748	1.356473	0.012974	H	0.941033	1.1605	-1.66104
C	-0.19006	1.144835	-2.10686	C	0.440983	3.153668	-0.91355
C	-2.20881	2.131616	-0.94274	O	-1.90014	0.163339	-2.68473
H	0.423892	0.241581	-2.07831	O	-0.1442	3.84346	-0.07997
H	-0.7968	1.108336	-3.01381	N	1.141385	3.683574	-1.93682
C	0.778355	2.321249	-2.09621	H	1.200675	4.686755	-2.02624
O	-3.3863	1.858325	-1.04046	H	1.606664	3.11282	-2.62342
O	1.447506	2.582757	-1.09726	H	-2.67875	-3.48236	-1.25569
N	0.883161	3.017622	-3.24638	O	-2.18684	2.345369	-2.21162
H	1.53907	3.782228	-3.30137	H	-2.61935	2.341943	-3.08149
H	0.317202	2.812139	-4.05333	O	-6.69448	-2.00737	3.549043
H	-1.39008	-4.45202	0.4974	H	-5.95077	-1.4689	3.222013
O	-1.73384	3.378267	-0.93373	H	-6.31128	-2.87315	3.726545
H	-2.47312	3.999668	-1.0391				

O	-5.55105	1.360064	0.909186				
H	-5.30502	0.418564	0.797467				
H	-4.96516	1.811705	0.286471				
Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.69709	-2.99045	-0.85307	N	-4.92788	-2.2107	-1.3455
H	-3.86947	-3.41083	-0.43862	H	-4.67287	-3.19225	-1.2743
C	-4.88767	-1.65224	-0.30794	C	-4.80587	-1.54034	-0.10191
H	-5.69007	-1.16013	-0.86247	C	-5.63034	-1.73068	1.149579
C	-5.27398	-1.63028	1.201362	C	-3.88067	-0.60598	0.15685
C	-3.5846	-0.86431	-0.48273	H	-6.69995	-1.53347	1.022159
H	-6.17651	-2.23383	1.325791	H	-5.5384	-2.7234	1.60668
H	-4.47358	-2.0829	1.791221	C	-5.03706	-0.69612	2.079271
C	-5.60292	-0.22485	1.664151	O	-3.97821	-0.09273	1.457216
O	-2.48683	-1.40672	-0.34882	O	-5.35992	-0.35431	3.190864
O	-6.5151	0.413574	1.115869	N	-2.83368	-0.08887	-0.56884
N	-4.85491	0.298486	2.649959	H	-2.90514	-0.36651	-1.54176
H	-5.00002	1.264049	2.917387	C	-2.48323	1.322967	-0.37967
H	-4.08481	-0.20755	3.055854	H	-2.11817	1.463219	0.636263
N	-3.7287	0.45551	-0.71982	C	-1.37141	1.718528	-1.35978
H	-4.65442	0.855293	-0.79551	C	-3.69924	2.225971	-0.59296
C	-2.5951	1.363875	-0.75824	H	-0.58272	0.965345	-1.26962
H	-1.83678	1.017151	-0.0542	H	-1.75237	1.696985	-2.38328
C	-1.93807	1.434225	-2.15699	C	-0.74501	3.100821	-1.04486
C	-3.07352	2.736536	-0.32567	O	-4.5003	2.096303	-1.48951
H	-1.86318	0.401834	-2.50967	O	-0.33646	3.268677	0.133293
H	-2.57888	1.981254	-2.85146	O	-0.67934	3.924191	-1.99429
C	-0.50499	2.019695	-2.1516	O	-3.78967	3.199617	0.33697
O	-4.23888	3.081286	-0.29925	H	-4.55521	3.758849	0.122972
O	0.279622	1.562761	-1.27996	H	-5.88104	-2.17681	-1.69552
O	-0.23576	2.869457	-3.0403	O	-4.32606	2.456462	3.349269
O	-2.06248	3.547974	-0.00992	H	-4.62306	1.533519	3.388516
H	-2.42204	4.42449	0.20483	H	-4.08078	2.591689	2.42441
H	-5.48848	-3.58163	-0.61892				
O	-6.17138	3.064268	1.904677				
H	-6.45826	2.186818	1.577593				
H	-5.50505	3.330964	1.255228				
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.69038	-2.56994	-0.53888	N	-3.10512	-1.35953	-1.65889
H	-1.82466	-2.83818	-0.07888	H	-2.81299	-2.31681	-1.83753
C	-3.11917	-1.26406	-0.05628	C	-2.94551	-1.00889	-0.29474
H	-3.97329	-0.93493	-0.65247	C	-3.64976	-1.58464	0.909648
C	-3.5549	-1.24934	1.439106	C	-2.07743	-0.08776	0.142413
C	-1.96477	-0.27264	-0.23506	H	-4.73619	-1.44779	0.902134
H	-4.34389	-1.99591	1.563169	H	-3.45985	-2.65068	1.080329
H	-2.71232	-1.53683	2.072253	C	-3.0478	-0.78151	2.040383

C	-4.13936	0.091355	1.839881	O	-2.11213	0.075961	1.535127
O	-0.79064	-0.61667	-0.11773	O	-3.27676	-0.80944	3.226027
O	-5.07287	0.584889	1.186815	N	-1.10689	0.648813	-0.49718
N	-3.59349	0.71793	2.894327	H	-1.09944	0.433474	-1.48952
H	-3.92357	1.642171	3.143348	C	-0.98457	2.090732	-0.20885
H	-2.80922	0.330109	3.392672	H	-1.07332	2.223071	0.868921
N	-2.3335	1.010897	-0.45908	C	0.37966	2.580908	-0.6851
H	-3.31338	1.250361	-0.53832	C	-2.13548	2.833011	-0.89071
C	-1.36951	2.094134	-0.48396	H	1.153901	1.990031	-0.19488
H	-0.53218	1.83186	0.163921	H	0.482279	2.460771	-1.76404
C	-0.85427	2.303818	-1.92541	S	0.730781	4.32673	-0.23736
C	-2.04383	3.347697	0.057032	O	-2.07294	3.360019	-1.97968
H	-0.46517	1.345779	-2.2668	H	-0.11426	4.890696	-1.11961
H	-1.67889	2.610377	-2.57019	H	-4.07611	-1.28828	-1.94968
S	0.509461	3.549737	-2.01156	O	-3.26074	2.759027	-0.16349
O	-3.22897	3.577502	-0.05547	H	-3.98664	3.16512	-0.66551
H	0.906785	3.214886	-3.25192	O	-1.7927	1.203549	4.661026
H	-3.38622	-3.2734	-0.312	H	-2.29669	0.510707	4.197631
O	-1.1743	4.170837	0.643604	H	-1.28669	1.634386	3.963415
H	-1.63669	4.980612	0.918384				
O	-5.28736	3.230831	2.037697				
H	-5.37338	2.329732	1.663538				
H	-4.64191	3.650636	1.452436				

Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.69053	-3.91683	1.184279	N	-2.59196	-3.28762	-1.05246
H	-1.36859	-3.71739	2.127681	H	-2.41859	-4.19452	-0.62698
C	-2.18243	-2.6886	0.56578	C	-2.95238	-2.31613	-0.08469
H	-2.40953	-2.89565	-0.48163	C	-4.17033	-2.2923	0.806463
C	-3.46325	-2.12271	1.230132	C	-2.20446	-1.24621	0.215211
C	-1.06572	-1.64072	0.640098	H	-5.12201	-2.24192	0.266905
H	-4.22748	-2.90662	1.210512	H	-4.23928	-3.13571	1.503417
H	-3.26474	-1.88623	2.278572	C	-3.96544	-1.01396	1.586459
C	-4.03622	-0.92409	0.494046	O	-2.7835	-0.44208	1.210759
O	-0.33862	-1.53806	1.627688	O	-4.66095	-0.49016	2.424054
O	-3.98479	-0.8456	-0.74318	N	-0.95381	-0.8385	-0.19201
N	-4.60337	0.033104	1.245364	H	-0.61243	-1.46602	-0.91411
H	-4.96045	0.866181	0.799361	C	-0.75844	0.570783	-0.54009
H	-4.59145	-0.00384	2.251766	H	-1.12995	1.184381	0.281416
N	-0.94874	-0.82302	-0.42979	C	0.744976	0.834862	-0.73147
H	-1.66464	-0.85886	-1.1425	C	-1.53162	0.93936	-1.80836
C	0.026088	0.250141	-0.4631	H	1.248818	0.505302	0.178357
H	1.009841	-0.1587	-0.22485	H	1.113969	0.21146	-1.55299
C	0.043748	0.878403	-1.86751	C	1.087028	2.303472	-0.99608
C	-0.30143	1.312608	0.587402	O	-1.69184	0.192523	-2.74707
H	0.235025	0.078223	-2.58485	H	0.662695	2.649185	-1.94088
H	-0.94804	1.286367	-2.0869	H	0.657105	2.932981	-0.20852
C	1.105742	1.966124	-2.03232	C	2.591669	2.542638	-0.96716

O	-1.41605	1.732312	0.818591	O	3.325275	1.98393	-0.15087
H	0.913642	2.815585	-1.37246	N	3.066626	3.42614	-1.87274
H	2.09191	1.574098	-1.75765	H	4.047434	3.661837	-1.86506
C	1.210061	2.440583	-3.4774	H	2.468834	3.882692	-2.542
O	0.978283	1.696741	-4.43057	O	-1.99503	2.199031	-1.77207
N	1.601347	3.72336	-3.64507	H	-2.43593	2.394539	-2.61566
H	1.750821	4.07525	-4.57845	H	-3.32889	-3.41994	-1.7394
H	1.799444	4.330429	-2.86645	O	-3.59433	2.03798	3.299436
O	0.796127	1.774514	1.193815	H	-3.96741	1.181602	3.022889
H	0.542538	2.488122	1.80272	H	-2.78225	2.11857	2.787316
H	-2.44275	-4.59472	1.259587				
O	-3.53206	1.912465	-1.18452				
H	-2.83679	1.91967	-0.50679				
H	-3.77344	0.969962	-1.2426				
Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.52678	-2.56927	-1.36222	N	-4.22623	-1.33545	-1.41117
H	-2.7765	-3.13144	-0.96928	H	-4.30556	-2.34368	-1.30773
C	-3.74056	-1.3907	-0.53204	C	-4.06036	-0.68687	-0.16114
H	-4.46022	-0.74197	-1.03542	C	-5.05422	-0.56451	0.970012
C	-4.29768	-1.71444	0.887104	C	-2.93024	-0.07626	0.220818
C	-2.40629	-0.65589	-0.37129	H	-5.98423	-0.05141	0.703692
H	-5.2467	-2.24198	0.762451	H	-5.33419	-1.51897	1.432163
H	-3.60224	-2.37876	1.404632	C	-4.29065	0.270398	1.973024
C	-4.58306	-0.45839	1.688056	O	-3.02661	0.492611	1.497822
O	-1.3463	-1.27108	-0.24887	O	-4.62866	0.737094	3.033474
O	-5.39851	0.385249	1.287603	N	-1.69069	0.059394	-0.35775
N	-3.89633	-0.28687	2.828885	H	-1.71737	-0.22562	-1.3307
H	-4.03956	0.551523	3.372327	C	-0.93529	1.293588	-0.1231
H	-3.21748	-0.95765	3.15031	H	-0.69251	1.350514	0.938643
N	-2.49364	0.688009	-0.30295	C	0.363124	1.261677	-0.94502
H	-3.39323	1.139282	-0.39962	C	-1.75994	2.526808	-0.4916
C	-1.34851	1.536508	-0.01376	H	0.877169	0.329269	-0.70113
H	-0.65067	0.969891	0.604778	H	0.108434	1.217145	-2.00839
C	-0.63633	1.977832	-1.31599	C	1.28573	2.449094	-0.676
C	-1.84548	2.736095	0.774715	O	-2.41449	2.637114	-1.5019
H	-0.43766	1.063787	-1.87901	H	0.800382	3.393022	-0.94701
H	-1.33608	2.5695	-1.91332	H	1.503712	2.525098	0.394925
C	0.668165	2.740663	-1.10127	C	2.638078	2.406082	-1.42469
O	-2.95262	3.2158	0.659039	O	3.422529	3.364751	-1.18241
H	0.49061	3.689626	-0.58762	O	2.856727	1.443766	-2.20635
H	1.335157	2.170212	-0.44438	H	-5.06656	-1.01947	-1.88684
C	1.456999	3.058133	-2.39296	O	-1.67831	3.498135	0.442551
O	2.520942	3.718183	-2.22938	H	-2.18518	4.267879	0.133863
O	0.999542	2.645849	-3.49146	O	-2.80033	3.083376	3.353092
H	-4.36286	-3.14498	-1.37782	H	-3.37716	2.302985	3.347638
O	-0.90629	3.230101	1.592204	H	-2.41345	3.102031	2.467856
H	-1.25807	4.026015	2.024294				

O	-6.9967	0.027561	-0.94579				
H	-6.4315	0.168739	-0.15644				
H	-6.77278	0.748968	-1.54314				
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.02736	-2.76395	-0.58666	N	-1.38995	-1.86371	-1.67232
H	-1.14423	-3.08954	-0.20307	H	-0.6958	-2.59721	-1.56078
C	-2.35272	-1.45799	-0.02795	C	-1.62747	-1.18331	-0.45097
H	-3.23076	-1.06605	-0.54615	C	-2.00919	-1.77091	0.885715
C	-2.67591	-1.48023	1.495442	C	-1.58544	0.149143	-0.31577
C	-1.16427	-0.51825	-0.25875	H	-2.97233	-2.29486	0.892272
H	-3.48923	-2.19307	1.654873	H	-1.26668	-2.45747	1.306007
H	-1.80336	-1.82789	2.053139	C	-2.10612	-0.53893	1.756044
C	-3.16132	-0.12769	1.97822	O	-1.86339	0.56913	0.996638
O	-0.00293	-0.92426	-0.21886	O	-2.35145	-0.43336	2.934672
O	-4.1219	0.425142	1.418703	N	-1.41802	1.173158	-1.21522
N	-2.49875	0.445528	2.995788	H	-1.23646	0.810667	-2.14521
H	-2.75467	1.380923	3.285808	C	-0.52224	2.263478	-0.8473
H	-1.69392	0.009691	3.415712	C	-0.37714	3.230408	-1.99918
N	-1.47363	0.783333	-0.44118	H	-0.91542	2.798875	0.018182
H	-2.43891	1.085545	-0.42055	H	0.490192	1.923339	-0.58436
C	-0.45034	1.800892	-0.50733	O	-0.74825	3.023301	-3.13225
C	-1.0397	3.169946	-0.26666	O	0.255216	4.34859	-1.61181
H	0.323384	1.615432	0.242854	H	0.370193	4.924464	-2.38503
H	0.053231	1.813319	-1.47996	H	-2.23356	-2.30731	-2.02607
O	-2.21683	3.396626	-0.08144	O	-2.23278	2.307585	3.810023
O	-0.09456	4.112779	-0.29412	H	-2.28526	1.373531	3.538003
H	-0.50791	4.978957	-0.14455	H	-2.01364	2.777335	2.99781
H	-2.73844	-3.44201	-0.3312				
O	-4.0623	3.089198	2.217198				
H	-3.44576	3.433486	1.556301				
H	-4.25218	2.185553	1.890794				
Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.73845	-3.13342	2.012263	N	-0.46866	-2.34514	0.84412
H	-1.70833	-2.6927	2.927822	H	-0.51674	-2.73949	1.779893
C	-2.3591	-2.22665	1.054478	C	-1.42808	-1.31827	0.657513
H	-2.28966	-2.67134	0.058997	C	-2.93324	-1.42586	0.681668
C	-3.8624	-1.932	1.343849	C	-1.11427	-0.03346	0.446945
C	-1.59525	-0.89772	1.085815	H	-3.34792	-2.08913	-0.08469
H	-4.38595	-2.88928	1.394858	H	-3.35142	-1.74353	1.644011
H	-3.95398	-1.43446	2.311813	C	-3.35522	-0.00181	0.398823
C	-4.49974	-1.13367	0.222818	O	-2.24333	0.783491	0.287291
O	-1.22945	-0.40344	2.149896	O	-4.45772	0.475937	0.274424
O	-4.5956	-1.61422	-0.91516	N	0.084242	0.640626	0.450851
N	-4.90717	0.114708	0.507276	H	0.849706	-0.00181	0.630543
H	-5.31598	0.681171	-0.22139	C	0.377454	1.618045	-0.61325

H	-4.83029	0.505964	1.432243	H	-0.51207	2.232524	-0.75324
N	-1.41629	-0.30526	-0.11863	C	1.559348	2.498015	-0.18248
H	-1.77942	-0.74324	-0.96326	C	0.652927	0.864758	-1.91642
C	-0.86733	1.033931	-0.27728	H	1.313882	2.906638	0.799092
H	-0.41106	1.322077	0.667999	H	2.446575	1.868142	-0.06372
C	0.175775	1.059065	-1.41126	C	1.846617	3.63382	-1.10941
C	-2.03833	1.976865	-0.56816	O	1.754693	0.615551	-2.35976
H	0.966086	0.357499	-1.13883	N	2.476962	3.490781	-2.32861
H	-0.28912	0.688187	-2.32902	C	1.593115	4.982314	-1.00503
C	0.777957	2.406433	-1.63899	H	2.77711	2.612095	-2.72644
O	-2.55308	2.103404	-1.66264	C	2.573979	4.720836	-2.89778
N	0.149433	3.409952	-2.35005	N	2.049448	5.653757	-2.12251
C	1.97071	2.960665	-1.23592	H	1.11581	5.49703	-0.18496
H	-0.76155	3.343586	-2.78071	H	3.029395	4.876858	-3.86312
C	0.964084	4.498141	-2.34837	O	-0.4839	0.440332	-2.48452
N	2.080468	4.263011	-1.68235	H	-0.26561	-0.09981	-3.26208
H	2.749794	2.487936	-0.65746	H	-0.61286	-3.11189	0.192989
H	0.698403	5.419504	-2.84239	O	-4.33583	3.280715	-0.38548
O	-2.46247	2.618654	0.52017	H	-4.40215	2.336205	-0.15681
H	-3.23524	3.160836	0.286865	H	-3.3891	3.459579	-0.37781
H	-2.28996	-3.98115	2.10166				
O	-2.75925	-0.63832	-2.7697				
H	-3.54264	-0.95429	-2.27973				
H	-2.80796	0.327322	-2.70915				
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.01329	-3.29598	-1.07912	N	-3.22113	-3.01255	-1.57672
H	-2.19508	-3.7476	-0.67933	H	-2.86327	-3.95966	-1.48507
C	-3.33099	-2.09468	-0.31731	C	-3.33499	-2.37221	-0.31662
H	-4.1267	-1.55771	-0.83773	C	-4.21028	-2.75833	0.850598
C	-3.81315	-2.37961	1.136292	C	-2.61498	-1.30196	0.045823
C	-2.08011	-1.21359	-0.24893	H	-5.28424	-2.72956	0.637808
H	-4.68609	-3.03539	1.078312	H	-3.99233	-3.74567	1.274427
H	-3.02831	-2.90746	1.682844	C	-3.86979	-1.69163	1.865848
C	-4.25138	-1.11576	1.852165	O	-2.91399	-0.86606	1.347972
O	-0.95393	-1.70144	-0.1481	O	-4.30496	-1.50442	2.977553
O	-5.13818	-0.38822	1.381614	N	-1.5865	-0.62118	-0.56538
N	-3.62487	-0.80865	2.998741	H	-1.44549	-1.00482	-1.4944
H	-3.87933	0.034348	3.492153	C	-1.62475	0.844937	-0.5638
H	-2.89048	-1.38421	3.377242	H	-1.9069	1.171809	0.437033
N	-2.30982	0.115922	-0.24114	C	-0.21671	1.425547	-0.87449
H	-3.25876	0.46261	-0.28341	C	-2.68119	1.35841	-1.54235
C	-1.24689	1.084418	-0.03551	H	0.436052	0.93517	-0.14282
H	-0.51564	0.649682	0.649088	C	0.27475	1.058699	-2.28183
C	-0.51698	1.428773	-1.37293	C	-0.16167	2.942514	-0.61233
C	-1.85451	2.309336	0.626645	O	-2.99909	0.790753	-2.56384
H	-0.29421	0.44488	-1.80077	H	-0.33947	1.533826	-3.05254
C	-1.43707	2.18285	-2.34066	H	1.305266	1.388682	-2.42354

C	0.822755	2.14558	-1.13558	H	0.261538	-0.02035	-2.45517
O	-3.0306	2.598695	0.586074	H	-0.73621	3.470133	-1.38109
H	-1.63147	3.201545	-1.98913	H	-0.65869	3.154443	0.340739
H	-0.98335	2.253533	-3.33067	C	1.264041	3.503297	-0.56212
H	-2.39742	1.673605	-2.45446	H	1.775643	3.408848	-1.52338
H	0.637898	3.162174	-0.775	H	1.249447	4.565019	-0.30106
H	1.362853	1.627745	-0.33471	H	1.864355	2.981357	0.190389
C	1.712332	2.195104	-2.3833	O	-3.21484	2.526808	-1.15054
H	1.258593	2.78486	-3.18418	H	-3.84661	2.821245	-1.82734
H	2.679484	2.64823	-2.14864	H	-4.12153	-3.08112	-2.04266
H	1.899268	1.188762	-2.7726	O	-3.16521	0.849011	4.186694
O	-0.93064	3.056766	1.244241	H	-3.56111	0.046268	3.802018
H	-1.36397	3.846869	1.606938	H	-2.55682	1.160412	3.507569
H	-3.78161	-3.95769	-1.02871				
O	-6.68247	-0.92098	-0.85461				
H	-6.15251	-0.77514	-0.04244				
H	-6.95082	-1.84493	-0.81422				
Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.80945	-2.91742	0.310238	N	-2.1808	-1.95039	-0.95349
H	-0.10942	-2.85441	1.044593	H	-1.97056	-2.89694	-0.64792
C	-1.62697	-1.71095	0.310593	C	-2.2011	-1.04164	0.134872
H	-2.27732	-1.72981	-0.56691	C	-3.13261	-1.02816	1.3224
C	-2.53439	-1.5592	1.567343	C	-1.3286	-0.03649	0.286468
C	-0.69992	-0.49258	0.233203	H	-4.18836	-0.89164	1.065337
H	-3.1621	-2.45143	1.63646	H	-3.06867	-1.91799	1.95964
H	-1.91339	-1.5075	2.464449	C	-2.64242	0.175709	2.093812
C	-3.46078	-0.36537	1.443437	O	-1.56704	0.715901	1.449086
O	0.39062	-0.47924	0.803882	O	-3.05405	0.66812	3.117611
O	-4.22814	-0.26978	0.472486	N	-0.20681	0.341111	-0.41615
N	-3.39085	0.577961	2.397113	H	-0.1046	-0.24959	-1.23591
H	-3.9474	1.418228	2.30037	C	-0.02243	1.762492	-0.72521
H	-2.73661	0.512051	3.159722	H	-0.12946	2.325937	0.200347
N	-1.19582	0.569675	-0.43752	C	1.387155	1.969556	-1.30987
H	-2.10166	0.503507	-0.8822	C	-1.07834	2.250695	-1.71724
C	-0.51083	1.850651	-0.48957	H	2.09384	1.567038	-0.57636
H	0.131061	1.920362	0.387178	H	1.472549	1.350525	-2.21058
C	0.337475	1.974001	-1.77909	C	1.77395	3.41925	-1.64974
C	-1.55382	2.952227	-0.42697	O	-1.49124	1.594382	-2.64717
H	1.004242	1.105047	-1.78652	H	1.053946	3.81125	-2.37846
H	-0.33905	1.865827	-2.63353	C	1.750173	4.331904	-0.4153
C	1.172102	3.25637	-1.93227	C	3.160237	3.434996	-2.3091
O	-2.66144	2.863733	-0.91668	H	2.426053	3.950181	0.358309
H	0.494003	4.117815	-1.91753	H	2.07842	5.341621	-0.67823
C	2.188839	3.427484	-0.79459	H	0.750249	4.413985	0.017212
C	1.879985	3.241035	-3.29464	H	3.181237	2.812853	-3.20902
H	2.858609	2.561672	-0.74346	H	3.444394	4.452173	-2.59362
H	2.803374	4.317109	-0.95977	H	3.921598	3.054899	-1.61863

H	1.704186	3.539737	0.178261	H	-3.08021	-1.98577	-1.4251
H	1.16275	3.149134	-4.1159	O	-1.48658	3.502632	-1.45441
H	2.452553	4.160698	-3.44585	H	-2.12147	3.773156	-2.13838
H	2.57672	2.397664	-3.35955	O	-1.64057	3.090995	3.781599
H	-1.38368	-3.73129	0.506546	H	-2.12496	2.269508	3.582803
O	-1.10491	4.04554	0.193843	H	-0.99607	3.16346	3.069115
H	-1.78874	4.735004	0.152714				
O	-5.16971	2.355097	0.509006				
H	-4.9777	1.403628	0.378902				
H	-4.44273	2.790338	0.04107				
Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.73974	-2.42378	2.702755	N	-1.85452	0.429406	3.795251
H	-1.82904	-2.5269	3.140038	H	-1.04975	0.093067	3.275795
C	-2.56671	-1.98527	1.318212	C	-2.79915	1.049702	2.983591
H	-2.27161	-2.80928	0.650399	C	-4.24392	1.192751	3.367583
C	-3.92788	-1.41446	0.820914	C	-2.60108	1.706346	1.831796
C	-1.39448	-0.98404	1.271674	H	-4.77323	0.238883	3.4516
H	-4.71257	-1.98967	1.313798	H	-4.39883	1.736024	4.305475
H	-4.03366	-0.37506	1.138334	C	-4.80843	1.993135	2.211654
C	-4.11861	-1.47131	-0.68387	O	-3.82363	2.285219	1.343693
O	-0.61743	-0.86315	2.22019	O	-5.95246	2.353384	2.026463
O	-3.56916	-0.65204	-1.44303	N	-1.47776	2.03449	1.08779
N	-4.89111	-2.4539	-1.16296	H	-0.65648	2.141243	1.67256
H	-5.02439	-2.53806	-2.16014	C	-1.20311	1.228073	-0.10265
H	-5.34354	-3.12264	-0.56061	H	-2.10115	1.222498	-0.72425
N	-1.23283	-0.28758	0.128679	C	-0.04117	1.857563	-0.89405
H	-1.94264	-0.34697	-0.60028	C	-0.87266	-0.21854	0.270661
C	-0.14516	0.658275	-0.01763	H	-0.30964	2.905738	-1.05424
H	0.800599	0.166469	0.219752	H	0.857278	1.849271	-0.26579
C	-0.11488	1.181789	-1.466	C	0.256962	1.188403	-2.23879
C	-0.3191	1.82144	0.959157	O	-0.29115	-0.54705	1.282879
H	-0.04617	0.306777	-2.11963	H	0.555736	0.146831	-2.08845
H	-1.06808	1.675513	-1.68352	H	-0.65401	1.169065	-2.84722
C	1.047454	2.134309	-1.75723	C	1.36606	1.927351	-2.99739
O	-1.38166	2.347611	1.219588	H	1.069156	2.968431	-3.16466
H	0.963332	3.033409	-1.13858	H	2.278404	1.942292	-2.39125
H	1.993486	1.653272	-1.48591	C	1.65072	1.255922	-4.33341
C	1.083144	2.538817	-3.23564	H	1.989896	0.227568	-4.20925
H	1.203953	1.645759	-3.8586	H	0.777956	1.263202	-4.98586
H	0.131911	3.004614	-3.51512	N	2.74636	1.977288	-5.08006
C	2.224728	3.508453	-3.50514	H	3.621735	1.98163	-4.55153
H	2.108964	4.438977	-2.94962	H	2.937859	1.535923	-5.98157
H	3.194265	3.072103	-3.2656	H	2.496406	2.951316	-5.2646
N	2.277808	3.88775	-4.96501	H	-2.24211	-0.31719	4.358318
H	1.416531	4.350156	-5.26451	O	-1.27174	-1.09274	-0.66382
H	3.050751	4.528001	-5.1575	H	-0.99465	-1.98521	-0.39734
H	2.406551	3.06671	-5.56047	O	-6.3413	3.849874	-0.36897

H	-3.19627	-3.32985	2.722323	H	-5.46393	3.905337	-0.76283
O	0.84622	2.238129	1.462374	H	-6.20649	3.337076	0.45038
H	0.686656	3.013533	2.025745				
O	-3.6827	2.100079	-0.52276				
H	-3.6781	1.192616	-0.86964				
H	-2.93508	2.13392	0.097488				
Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.35517	-3.57759	0.620545	N	-3.33616	-2.64987	-0.73451
H	-1.94655	-3.55291	1.551039	H	-3.29648	-3.55607	-0.27544
C	-2.8253	-2.24372	0.256186	C	-3.56347	-1.6031	0.194374
H	-3.15583	-2.266	-0.78378	C	-4.77094	-1.37903	1.071815
C	-4.00627	-1.73639	1.121834	C	-2.67737	-0.63528	0.462427
C	-1.64593	-1.27289	0.387052	H	-5.70372	-1.21933	0.52068
H	-4.81027	-2.47752	1.063934	H	-4.95845	-2.1783	1.798232
H	-3.70008	-1.6698	2.16889	C	-4.39669	-0.11203	1.80626
C	-4.58342	-0.41943	0.632244	O	-3.14587	0.278474	1.420991
O	-0.8239	-1.37028	1.29732	O	-5.01748	0.532701	2.617724
O	-4.62445	-0.14557	-0.57724	N	-1.38031	-0.4181	0.052471
N	-5.05131	0.42124	1.568235	H	-1.12165	-1.12166	-0.63302
H	-5.42484	1.316901	1.288804	C	-1.00318	0.933242	-0.36845
H	-4.97329	0.220648	2.552123	H	-1.29802	1.633483	0.413529
N	-1.58182	-0.2906	-0.54025	C	0.52494	0.990333	-0.55619
H	-2.36559	-0.1705	-1.16748	C	-1.71202	1.326342	-1.66653
C	-0.55306	0.729783	-0.4921	H	0.969297	0.653017	0.383839
H	0.42153	0.244748	-0.41511	H	0.813045	0.272669	-1.33173
C	-0.61917	1.579192	-1.77652	C	1.041324	2.384332	-0.91259
C	-0.72715	1.620177	0.739589	O	-1.93732	0.559275	-2.57492
H	-0.52019	0.890473	-2.62033	H	0.663081	2.713701	-1.88292
H	-1.60772	2.04522	-1.84122	H	0.732396	3.114484	-0.15962
C	0.472955	2.646101	-1.84406	S	2.874389	2.370471	-0.99289
O	-1.79179	2.044391	1.137664	C	3.155286	4.112394	-1.46404
H	0.357162	3.383172	-1.0458	H	2.763898	4.78345	-0.69715
H	1.46359	2.19315	-1.75115	H	4.233951	4.250859	-1.54899
S	0.381204	3.528787	-3.44949	H	2.685999	4.328494	-2.42567
C	1.741333	4.722035	-3.20195	O	-2.0386	2.628065	-1.69191
H	2.687538	4.198237	-3.05416	H	-2.44389	2.832498	-2.55115
H	1.801597	5.328683	-4.10652	H	-4.07954	-2.70158	-1.42538
H	1.53253	5.367624	-2.34686	O	-3.58182	2.893677	3.434016
O	0.443121	1.925347	1.307156	H	-4.08544	2.099799	3.178931
H	0.285558	2.539395	2.04368	H	-2.75994	2.821182	2.936436
H	-3.1358	-4.22631	0.650916				
O	-3.99789	2.60926	-0.6817				
H	-3.27988	2.484043	-0.04021				
H	-4.32702	1.703352	-0.82586				
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z

N	-1.22932	-3.02853	1.937892	N	-2.36261	-2.69594	-0.79508
H	-0.89088	-2.63254	2.81087	H	-2.2562	-3.56939	-0.28592
C	-1.90656	-1.99374	1.161406	C	-2.71248	-1.62733	0.068716
H	-2.15672	-2.4041	0.181439	C	-3.95178	-1.47893	0.916876
C	-3.21584	-1.47765	1.811518	C	-1.93591	-0.55873	0.288982
C	-0.93382	-0.82246	0.981728	H	-4.88536	-1.44751	0.345333
H	-3.87133	-2.33855	1.978812	H	-4.07056	-2.25058	1.686321
H	-2.99794	-1.03808	2.787977	C	-3.7215	-0.13998	1.58048
C	-3.97742	-0.50606	0.926714	O	-2.51282	0.35602	1.186129
O	-0.17142	-0.46934	1.880412	O	-4.42093	0.477502	2.347989
O	-4.00461	-0.64653	-0.30585	N	-0.66122	-0.23186	-0.11981
N	-4.62008	0.498588	1.54289	H	-0.31168	-0.95494	-0.7421
H	-5.1129	1.185159	0.989791	C	-0.43211	1.113219	-0.6551
H	-4.54981	0.645485	2.536844	H	-0.83322	1.840614	0.049937
N	-0.98781	-0.1857	-0.21018	C	1.086834	1.340807	-0.82082
H	-1.73208	-0.42713	-0.85041	C	-1.13139	1.295188	-2.00423
C	-0.17275	0.981133	-0.48571	H	1.537464	1.169304	0.15984
H	0.869567	0.748812	-0.26342	H	1.477169	0.578522	-1.50174
C	-0.31867	1.367708	-1.97642	C	1.427652	2.722521	-1.32954
C	-0.58708	2.160013	0.396528	O	-1.1202	0.462872	-2.88364
H	-0.01817	0.493686	-2.56036	C	1.734851	2.937623	-2.67788
H	-1.37593	1.558913	-2.18154	C	1.409196	3.82062	-0.45962
C	0.515356	2.568076	-2.35871	H	1.755968	2.096012	-3.36246
O	-1.73647	2.495685	0.595962	C	2.013056	4.222215	-3.15042
C	-0.06469	3.83723	-2.46549	C	1.686352	5.105274	-0.92709
C	1.891211	2.43344	-2.58433	H	1.177959	3.667366	0.589731
H	-1.13017	3.95464	-2.29783	H	2.250545	4.370671	-4.19785
C	0.713735	4.951804	-2.78551	C	1.988004	5.310151	-2.27627
C	2.672125	3.544023	-2.90442	H	1.670393	5.943851	-0.23998
H	2.351785	1.453449	-2.51074	H	2.205413	6.307762	-2.6406
H	0.248676	5.927865	-2.86598	O	-1.74647	2.481677	-2.10978
C	2.084822	4.808258	-3.00426	H	-2.13348	2.554679	-2.99825
H	3.735335	3.422939	-3.07884	H	-3.07633	-2.85181	-1.50147
H	2.690344	5.671832	-3.25482	O	-3.51063	3.035442	3.268508
O	0.464109	2.816852	0.890438	H	-3.82417	2.163905	2.965154
H	0.14709	3.591743	1.383637	H	-4.20757	3.359583	3.849036
H	-1.88109	-3.77005	2.175293				
O	-3.89214	2.00257	-1.29225				
H	-4.03396	1.05052	-1.13932				
H	-3.19713	2.228737	-0.65266				
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.88541	-3.14099	0.319447	N	-1.37895	-2.06951	-1.02515
H	-0.13328	-3.2404	0.995973	H	-1.19964	-3.05114	-0.83103
C	-1.30671	-1.74485	0.256165	C	-1.01246	-1.23996	0.064098
H	-2.02415	-1.63613	-0.55925	C	-1.65537	-1.14002	1.427503
C	-1.98026	-1.23346	1.556021	C	0.029761	-0.39922	0.044293
C	-0.0721	-0.88735	-0.04678	H	-2.7073	-0.83691	1.410978

H	-2.82037	-1.89806	1.782643	H	-1.59319	-2.0578	2.024446
H	-1.27781	-1.30016	2.390702	C	-0.83159	-0.05668	2.086953
C	-2.54885	0.169068	1.424715	O	0.182052	0.309785	1.241036
O	1.035055	-1.15571	0.414329	O	-0.95493	0.490474	3.154759
O	-3.04731	0.562426	0.358033	N	1.003822	-0.14067	-0.89621
N	-2.49334	0.949625	2.514835	H	0.756149	-0.57912	-1.77811
H	-2.82517	1.902292	2.459425	C	1.471951	1.237832	-1.04101
H	-2.03909	0.648399	3.361738	H	1.879544	1.57305	-0.08809
N	-0.2888	0.199013	-0.82625	C	2.578041	1.275615	-2.09511
H	-1.2469	0.447634	-1.03626	C	0.333483	2.177146	-1.45301
C	0.770091	1.142589	-1.12041	H	3.378085	0.597078	-1.78159
H	1.652052	0.599089	-1.46041	H	2.177802	0.933285	-3.05717
C	0.296328	2.094178	-2.22478	O	3.031416	2.622687	-2.1786
C	1.156372	1.95482	0.120037	O	-0.38226	1.991363	-2.40861
H	0.025671	1.49632	-3.10203	H	3.657395	2.694401	-2.90733
H	-0.58993	2.64079	-1.88003	O	0.196825	3.221662	-0.61455
O	1.36982	2.982975	-2.50724	H	-0.53797	3.77804	-0.92349
O	0.356406	2.502291	0.850422	H	-2.36781	-1.98545	-1.24191
H	1.056257	3.663548	-3.1128	O	0.135728	3.227612	2.520261
O	2.476073	2.016927	0.300323	H	-0.15462	2.357618	2.834877
H	2.661753	2.577424	1.072182	H	0.2042	3.126121	1.561788
H	-1.65471	-3.72382	0.634807				
O	-2.37603	3.309797	0.271218				
H	-1.44798	3.109114	0.475825				
H	-2.77647	2.427068	0.16895				

Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	1.692722	-1.80234	-0.45232	N	-3.85744	0.363921	-1.59599
H	2.443183	-1.81527	0.233037	H	-4.43732	-0.41654	-1.89261
C	1.307588	-0.42161	-0.73351	C	-3.35989	0.179066	-0.28054
H	0.609397	-0.42708	-1.57219	C	-4.13865	0.084002	1.00833
C	0.625686	0.288186	0.463717	C	-2.0609	0.033301	0.013782
C	2.565555	0.354752	-1.14076	H	-4.71984	0.980177	1.251617
H	-0.18871	-0.35552	0.814146	H	-4.82495	-0.76921	1.065774
H	1.332589	0.3865	1.291842	C	-3.03803	-0.09243	2.029262
C	-0.01022	1.629373	0.132167	O	-1.83263	-0.12957	1.390499
O	3.672368	0.083628	-0.67684	O	-3.10107	-0.19595	3.231555
O	-0.46149	1.886498	-0.9947	N	-0.93734	-0.07864	-0.76647
N	2.364129	1.359605	-2.02272	H	-1.16003	0.072232	-1.744
H	1.412309	1.64066	-2.22251	C	0.292049	0.582538	-0.35969
C	3.412136	2.283298	-2.38049	H	0.499358	0.342523	0.68441
H	4.352467	1.735712	-2.46983	C	1.480327	0.072525	-1.19715
C	3.112887	2.949383	-3.73518	C	0.193179	2.108289	-0.46469
C	3.617065	3.334298	-1.28526	H	2.367596	0.625917	-0.8709
H	3.914269	3.669908	-3.92793	C	1.719588	-1.42259	-1.02892
C	3.04186	1.942905	-4.87771	O	1.169044	0.41819	-2.55406
O	1.870645	3.643017	-3.55359	O	-0.70564	2.710832	-1.00296
O	2.923329	3.465753	-0.30587	H	0.840917	-1.99256	-1.33505

H	2.258451	1.203502	-4.69996	H	2.572733	-1.73118	-1.63936
H	2.82629	2.462233	-5.81527	H	1.948381	-1.65663	0.014367
H	3.998293	1.425294	-4.98946	H	1.860821	0.074575	-3.13043
H	1.604802	4.033855	-4.39361	H	-4.43112	1.200009	-1.66352
H	0.90888	-2.30973	-0.05365	O	1.240061	2.706666	0.129479
O	4.691891	4.098155	-1.54657	H	1.148348	3.667945	0.027459
H	4.785561	4.754192	-0.83723	O	-0.64809	-0.41905	4.695176
O	-1.4621	0.237754	-3.00138	H	-0.90028	-0.43054	5.624705
H	-1.97317	-0.46458	-2.58538	H	-1.48982	-0.34759	4.208859
H	-1.14501	0.791379	-2.25996				
N	-0.10289	2.509719	1.139167				
H	-0.53128	3.408041	0.972339				
H	0.310695	2.335868	2.040874				
Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.65488	-1.82113	3.227358	N	-2.26251	-3.19384	-0.03518
H	-4.29966	-1.172	3.670127	H	-1.67106	-3.92057	0.359352
C	-3.59861	-1.55464	1.792782	C	-2.62095	-2.22602	0.937097
H	-2.79684	-2.15632	1.359892	C	-3.44647	-2.41841	2.186415
C	-4.91033	-1.8964	1.041046	C	-2.22501	-0.94692	0.900778
C	-3.27137	-0.06993	1.590439	H	-4.47394	-2.74849	2.000518
H	-5.19986	-2.91658	1.316469	H	-3.01134	-3.11303	2.914482
H	-5.71807	-1.2374	1.370803	C	-3.46329	-1.02428	2.771151
C	-4.78898	-1.88062	-0.47428	O	-2.71453	-0.198	1.984046
O	-3.64114	0.792498	2.387067	O	-4.01139	-0.59702	3.759539
O	-3.69542	-2.06219	-1.03808	N	-1.37144	-0.25331	0.072161
N	-5.92257	-1.69807	-1.16655	H	-1.05074	-0.8607	-0.67626
H	-5.88994	-1.69713	-2.17851	C	-1.80186	1.058279	-0.41924
H	-6.80194	-1.52647	-0.70642	H	-2.17089	1.637754	0.425384
N	-2.58918	0.229016	0.46269	C	-0.60184	1.791027	-1.06081
H	-2.48694	-0.50598	-0.22724	C	-2.92524	0.920343	-1.44741
C	-2.3797	1.601981	0.048735	H	0.191688	1.806265	-0.30725
H	-1.83481	2.137538	0.827227	H	-0.23958	1.19541	-1.90408
C	-1.56552	1.613927	-1.26882	C	-0.939	3.177783	-1.51143
C	-3.71667	2.311834	-0.1654	O	-2.91694	0.108117	-2.34602
H	-0.65077	1.042804	-1.07794	C	-1.06781	3.620504	-2.80605
H	-2.13516	1.071865	-2.02989	C	-1.24619	4.301673	-0.66353
C	-1.23328	2.987532	-1.758	H	-0.92584	3.083792	-3.73125
O	-4.68623	1.801424	-0.67854	N	-1.43538	4.949604	-2.8149
C	-1.77131	3.623004	-2.85113	C	-1.55383	5.39749	-1.51786
C	-0.31135	3.917438	-1.15752	C	-1.28721	4.489712	0.729054
H	-2.50003	3.264964	-3.56177	H	-1.5798	5.505212	-3.64219
N	-1.24185	4.890739	-2.96655	C	-1.8997	6.657341	-1.01923
C	-0.34317	5.102858	-1.94465	C	-1.63093	5.74034	1.229708
C	0.538	3.864235	-0.03866	H	-1.0488	3.674747	1.403814
H	-1.46729	5.548514	-3.69493	H	-2.13091	7.480286	-1.6856
C	0.442956	6.219285	-1.64352	C	-1.93567	6.812849	0.363093
C	1.32156	4.971975	0.264861	H	-1.66593	5.898456	2.301755

H	0.58467	2.97271	0.577228	H	-2.20139	7.77652	0.782832
H	0.405847	7.11311	-2.25545	O	-3.91731	1.800844	-1.25129
C	1.273149	6.138249	-0.52981	H	-4.57843	1.686807	-1.95435
H	1.981341	4.94363	1.124788	H	-3.08168	-3.6566	-0.41897
H	1.895265	6.986608	-0.26765	O	-3.70439	2.267877	4.011264
O	-3.67781	3.588723	0.242952	H	-3.79796	1.30181	3.932505
H	-4.52757	4.006945	0.028261	H	-3.18754	2.522226	3.239081
H	-4.0052	-2.75897	3.395875				
O	-4.17546	-1.70166	-3.74085				
H	-4.06808	-2.52007	-4.23745				
H	-3.83091	-1.89645	-2.84356				
Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.79309	-2.25635	1.962016	N	-0.83484	-1.29185	-0.26955
H	-1.29203	-2.1498	2.840831	H	-0.42338	-1.53691	0.626633
C	-1.43476	-1.45072	0.928396	C	-2.18787	-0.89073	-0.12944
H	-0.79401	-1.44858	0.043785	C	-3.32795	-1.64028	0.516332
C	-2.83037	-1.97383	0.498961	C	-2.67417	0.265959	-0.59915
C	-1.56523	-0.01042	1.443092	H	-3.58527	-2.58704	0.026933
H	-2.74014	-3.04655	0.295612	H	-3.18072	-1.85761	1.579591
H	-3.54666	-1.86631	1.318243	C	-4.4755	-0.66874	0.35627
C	-3.37226	-1.34418	-0.77423	O	-4.04011	0.432835	-0.32292
O	-1.6298	0.254327	2.643483	O	-5.62334	-0.74952	0.724088
O	-2.61241	-0.85167	-1.62746	N	-2.1164	1.276456	-1.34495
N	-4.70131	-1.37471	-0.94485	H	-1.1227	1.107542	-1.45985
H	-5.10208	-0.98011	-1.78615	C	-2.41854	2.656208	-0.97035
H	-5.31775	-1.75508	-0.24494	H	-2.49896	2.76741	0.116491
N	-1.64895	0.93725	0.485585	C	-1.29995	3.602695	-1.47736
H	-1.68905	0.633053	-0.4791	C	-3.73865	3.113879	-1.58355
C	-1.92991	2.318401	0.801008	H	-1.2593	3.539274	-2.56811
H	-1.1605	2.705404	1.472806	H	-1.58831	4.623748	-1.21657
C	-1.95898	3.17161	-0.49211	C	0.045457	3.260422	-0.88007
C	-3.27811	2.459254	1.504664	O	-4.20363	2.732099	-2.63123
H	-2.7973	2.837185	-1.11013	C	1.038628	2.636312	-1.64114
H	-2.16231	4.204305	-0.19963	C	0.316669	3.523855	0.470642
C	-0.66799	3.08254	-1.27185	H	0.860531	2.427322	-2.69092
O	-4.22844	1.730197	1.343165	C	2.266026	2.277598	-1.07963
C	-0.57563	2.305665	-2.43052	C	1.533238	3.172359	1.045093
C	0.482481	3.751422	-0.8319	H	-0.43453	4.011212	1.083551
H	-1.45035	1.780988	-2.80042	H	3.024704	1.795821	-1.68727
C	0.62516	2.189708	-3.13273	C	2.5124	2.543705	0.268016
C	1.687373	3.646113	-1.51981	H	1.738717	3.380134	2.088417
H	0.437497	4.365105	0.06193	O	3.689293	2.218841	0.884907
H	0.675859	1.5836	-4.03108	H	4.285431	1.79084	0.258315
C	1.760702	2.86022	-2.67443	H	-0.74258	-2.10673	-0.87024
H	2.573096	4.16789	-1.1774	O	-4.3068	4.067398	-0.82349
O	2.969799	2.791613	-3.31203	H	-5.10768	4.382842	-1.27239
H	2.902959	2.224318	-4.08978	O	-7.28292	1.525614	0.13626

H	-0.82343	-3.23944	1.71094	H	-6.73806	0.743855	0.339696
O	-3.29934	3.549226	2.290389	H	-8.15781	1.311929	0.477858
H	-4.18925	3.641942	2.667281				
O	-4.17634	0.349374	-3.56785				
H	-3.50505	0.003333	-2.94206				
H	-4.29481	1.274375	-3.32619				
Asn-Val							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.03436	-3.21091	-0.58041	N	-3.04427	-2.82682	-0.89639
H	-2.18243	-3.7653	-0.57115	H	-2.7109	-3.78639	-0.93554
C	-2.85473	-2.0225	0.244421	C	-2.61621	-2.16467	0.282083
H	-3.73119	-1.38329	0.121157	C	-3.02971	-2.43006	1.710828
C	-2.69246	-2.32982	1.762502	C	-1.72596	-1.16352	0.294316
C	-1.60763	-1.27599	-0.23887	H	-4.10199	-2.31596	1.901367
H	-3.57602	-2.88555	2.088419	H	-2.73821	-3.41651	2.091603
H	-1.81758	-2.96617	1.913015	C	-2.27009	-1.36086	2.463425
C	-2.62576	-1.06747	2.601638	O	-1.47921	-0.67303	1.582925
O	-0.61128	-1.87828	-0.6401	O	-2.28396	-1.0525	3.629964
O	-3.52899	-0.2194	2.555786	N	-0.97703	-0.55845	-0.68801
N	-1.54179	-0.89906	3.375114	H	-1.32265	-0.82314	-1.60297
H	-1.45886	-0.06507	3.937647	C	-0.66853	0.865193	-0.54575
H	-0.7989	-1.57807	3.409605	H	-0.0651	0.986845	0.354163
N	-1.66294	0.068067	-0.13322	C	0.17633	1.363875	-1.74748
H	-2.49223	0.509044	0.241511	C	-1.93944	1.694796	-0.3622
C	-0.52017	0.916935	-0.42189	H	1.02039	0.666734	-1.7901
H	0.386784	0.383476	-0.13006	C	-0.56645	1.306645	-3.08958
C	-0.42212	1.245592	-1.94531	C	0.729726	2.771406	-1.48767
C	-0.63853	2.166443	0.433997	O	-2.98576	1.493394	-0.93232
H	-0.50848	0.264206	-2.42254	H	-1.42471	1.983898	-3.0983
C	-1.58535	2.12132	-2.42423	H	0.110024	1.608863	-3.89298
C	0.935672	1.840562	-2.33249	H	-0.92686	0.303639	-3.33343
O	-1.67467	2.57585	0.91068	H	1.271164	2.821373	-0.53913
H	-1.52356	3.130283	-2.00347	H	1.4189	3.051597	-2.28792
H	-1.55997	2.214242	-3.51287	H	-0.06955	3.517722	-1.4604
H	-2.55267	1.695283	-2.14563	H	-4.05775	-2.86242	-0.95721
H	1.761079	1.214666	-1.9809	O	-1.76692	2.693919	0.530116
H	1.007447	1.914916	-3.42088	H	-2.58753	3.212642	0.575459
H	1.069646	2.842163	-1.91718	O	-1.43392	1.827079	3.586311
H	-3.77847	-3.79026	-0.20434	H	-1.65057	0.884333	3.663876
O	0.538974	2.787761	0.580665	H	-1.46258	2.005358	2.637456
H	0.39802	3.601787	1.091705				
O	-5.94269	-0.47421	1.223109				
H	-5.09781	-0.42545	1.718605				
H	-6.28571	-1.35589	1.403033				

Table S15.F. Isoimide Hydrolysis into Asp-X XYZ Coordinates (Implicit solvation + 1 H_2O, ε = 80)

All Reactions							
H_2O							
Reactant Structure							
Atom	X	Y	Z				
O	-0.999631	0.482902	0				
H	-0.03661	0.526297	0				
H	-1.280189	1.405171	0				
Asn-Ala							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.59506	-2.42318	-0.79937	N	-2.67529	-1.38008	-0.18077
H	-0.95848	-3.13224	-0.44522	H	-1.96061	-1.49576	0.533373
C	-2.08098	-1.58885	0.23944	C	-3.52385	-0.22392	0.117596
C	-2.93084	-1.97335	1.42576	C	-3.98012	-0.11393	1.577347
C	-1.81663	-0.27884	0.331431	C	-2.87181	1.093221	-0.32814
H	-3.91306	-2.38077	1.163305	H	-3.12198	-0.0947	2.255838
H	-2.45939	-2.68718	2.111499	H	-4.52081	0.823739	1.736898
C	-3.10796	-0.64757	2.129439	C	-4.89614	-1.24039	1.986757
O	-2.41963	0.317388	1.451599	O	-3.33667	2.187551	-0.00225
O	-3.72811	-0.37035	3.128785	O	-5.10284	-1.27691	3.303522
N	-1.00642	0.562908	-0.39535	N	-1.7882	0.964339	-1.1183
H	-0.6233	0.064601	-1.19257	H	-1.54125	0.023244	-1.3982
C	-1.49723	1.895088	-0.74088	C	-1.1303	2.107124	-1.7075
H	-1.85624	2.376866	0.169618	H	-0.96943	2.85953	-0.93212
C	-0.36036	2.733926	-1.33962	C	0.21744	1.698743	-2.3171
C	-2.66291	1.841144	-1.72959	C	-2.00737	2.754153	-2.78061
H	0.027514	2.264058	-2.24774	H	0.076709	0.9541	-3.10521
H	-0.71539	3.734376	-1.59035	H	0.7172	2.56854	-2.74433
H	0.450256	2.815643	-0.61394	H	0.856156	1.273199	-1.54094
O	-2.90247	0.91199	-2.46664	O	-2.89537	2.204832	-3.38964
H	-2.35193	-2.91362	-1.2677	H	-3.23974	-2.22289	-0.16881
O	-3.38417	2.974843	-1.70367	O	-1.63558	4.027868	-2.99804
H	-4.0832	2.91509	-2.37519	H	-2.17806	4.390561	-3.7168
O	-3.60779	2.436444	3.75507	O	-5.41039	-2.02876	1.208159
H	-3.65513	1.482857	3.560919	H	-5.72579	-2.02408	3.505173
H	-3.05576	2.79436	3.051258	H	-4.41695	-0.31394	-0.50962
				O	-6.84548	-3.34772	3.333491
				H	-6.58327	-4.20071	3.700404
				H	-6.61898	-3.38675	2.390018
Asn-Arg							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.07733	-3.31817	-0.66602	N	-3.91504	-1.82667	-0.34493
H	-3.99186	-4.27284	-0.32701	H	-3.38926	-2.65543	-0.60648
C	-4.00562	-2.37834	0.394791	C	-3.66035	-1.44899	1.041258
C	-4.93919	-2.2221	1.568764	C	-3.50995	-2.63458	2.031511
C	-3.02722	-1.47238	0.526184	C	-2.41858	-0.54707	1.173299
H	-5.96889	-1.96992	1.293225	H	-2.69616	-3.2821	1.702445

H	-4.98756	-3.09512	2.230106	H	-3.26785	-2.2444	3.022459
C	-4.32017	-1.05939	2.318086	C	-4.76625	-3.46475	2.081571
O	-3.18164	-0.66129	1.658228	O	-1.95805	-0.24303	2.274135
O	-4.67491	-0.50301	3.32382	O	-5.80976	-2.97614	2.774924
N	-1.8677	-1.25348	-0.18612	N	-1.90247	-0.10424	0.012818
H	-1.84494	-1.87615	-0.98839	H	-2.40953	-0.34326	-0.83056
C	-1.52025	0.124395	-0.54088	C	-0.78118	0.80887	-0.02027
H	-1.55407	0.734551	0.360834	H	0.024893	0.404438	0.596211
C	-0.08601	0.154655	-1.09623	C	-0.29311	0.969381	-1.47204
C	-2.50113	0.69402	-1.56603	C	-1.17886	2.163933	0.571733
H	0.551074	-0.2919	-0.32823	H	-0.10989	-0.0376	-1.85913
H	-0.03046	-0.48868	-1.98148	H	-1.09926	1.406255	-2.07111
C	0.41435	1.560999	-1.43494	C	0.979712	1.808841	-1.60633
O	-3.00664	0.050076	-2.45804	O	-2.27032	2.671828	0.464335
H	-0.16563	1.985576	-2.2601	H	0.800252	2.83296	-1.26704
H	0.280812	2.212942	-0.56646	H	1.767525	1.389755	-0.97169
C	1.890054	1.533802	-1.8249	C	1.461786	1.84009	-3.05521
H	2.486559	1.156302	-0.98786	H	1.671976	0.822569	-3.40008
H	2.038638	0.869744	-2.68305	H	0.685291	2.269728	-3.69667
N	2.341374	2.88506	-2.17036	N	2.680028	2.647999	-3.1548
H	1.656184	3.625973	-2.15213	H	3.022333	3.082667	-2.31101
C	3.579544	3.200427	-2.54661	C	3.377813	2.842699	-4.27286
N	4.529542	2.263222	-2.5972	N	2.968663	2.307822	-5.42597
N	3.877773	4.460908	-2.88698	N	4.5032	3.567157	-4.24099
H	4.334101	1.301014	-2.37942	H	2.125769	1.762039	-5.48468
H	5.463732	2.488777	-2.89799	H	3.495947	2.434796	-6.27466
H	3.19881	5.198324	-2.79048	H	4.80742	4.017965	-3.39333
H	4.82725	4.731697	-3.08533	H	4.999357	3.794025	-5.08716
H	-4.96583	-3.25899	-1.15576	H	-4.89577	-2.03027	-0.49835
O	-2.72756	2.004845	-1.37834	O	-0.14347	2.749105	1.195368
H	-3.32106	2.321983	-2.07931	H	-0.42349	3.625624	1.506184
O	0.14238	1.465139	2.045154	O	-4.8998	-4.52386	1.501978
H	1.076499	1.246602	1.949518	H	-4.49152	-0.81501	1.367679
H	0.135755	2.407574	2.248106	H	-5.5894	-2.15023	3.228213
				O	-7.42744	-5.82604	1.66315
				H	-6.57109	-5.35924	1.627375
				H	-7.99102	-5.25577	2.196997

Asn-Asn							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.9847	-3.12832	-0.60326	N	-2.61878	-2.67386	-0.53811
H	-1.64181	-3.9264	-0.07516	H	-1.8033	-3.22334	-0.28832
C	-2.53154	-2.1346	0.247582	C	-3.17687	-1.96998	0.613966
C	-3.72366	-2.24387	1.165528	C	-2.97732	-2.66827	1.96685
C	-2.02098	-0.90435	0.386267	C	-2.64876	-0.52593	0.72369
H	-4.66834	-2.45602	0.653432	H	-1.91893	-2.90867	2.112479
H	-3.6166	-2.98783	1.963776	H	-3.25601	-1.98687	2.777789
C	-3.78053	-0.86067	1.774786	C	-3.80444	-3.92008	2.144828
O	-2.74778	-0.11276	1.29099	O	-2.94409	0.194734	1.678434

O	-4.56072	-0.38884	2.567724	O	-4.74436	-4.24794	1.451085
N	-0.88049	-0.30987	-0.10722	N	-1.87006	-0.12765	-0.29994
H	-0.42473	-0.94483	-0.75567	H	-1.79307	-0.78577	-1.06795
C	-0.9729	1.053173	-0.62255	C	-1.38857	1.225191	-0.42058
H	-1.497	1.671001	0.106732	H	-1.14128	1.5969	0.576131
C	0.443055	1.632198	-0.81062	C	-0.11531	1.272785	-1.28731
C	-1.73886	1.108356	-1.94761	C	-2.47587	2.143823	-0.98698
H	1.013292	1.381906	0.087576	H	0.509159	0.422294	-0.9992
H	0.941033	1.1605	-1.66104	H	-0.35881	1.156255	-2.3457
C	0.440983	3.153668	-0.91355	C	0.725413	2.519175	-1.02595
O	-1.90014	0.163339	-2.68473	O	-3.53064	1.777883	-1.44825
O	-0.1442	3.84346	-0.07997	O	0.967687	2.89485	0.119689
N	1.141385	3.683574	-1.93682	N	1.220005	3.138834	-2.11652
H	1.200675	4.686755	-2.02624	H	1.821822	3.939664	-1.99735
H	1.606664	3.11282	-2.62342	H	1.004905	2.835852	-3.05226
H	-2.67875	-3.48236	-1.25569	H	-3.3103	-3.29046	-0.95213
O	-2.18684	2.345369	-2.21162	O	-2.0998	3.431395	-0.91947
H	-2.61935	2.341943	-3.08149	H	-2.79713	3.980527	-1.31309
O	-6.69448	-2.00737	3.549043	O	-3.4793	-4.70473	3.186263
H	-5.95077	-1.4689	3.222013	H	-4.25148	-1.85235	0.444354
H	-6.31128	-2.87315	3.726545	H	-2.72392	-4.35139	3.677677
				O	-5.44993	-3.79452	-1.2297
				H	-5.31701	-3.99187	-0.28497
				H	-5.60048	-4.64978	-1.64652

Asn-Asp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.92788	-2.2107	-1.3455	N	-6.0064	0.384602	0.50954
H	-4.67287	-3.19225	-1.2743	H	-6.23335	-0.47797	0.025785
C	-4.80587	-1.54034	-0.10191	C	-5.02842	0.168612	1.574338
C	-5.63034	-1.73068	1.149579	C	-5.09525	-1.20572	2.253456
C	-3.88067	-0.60598	0.15685	C	-3.58556	0.418446	1.095845
H	-6.69995	-1.53347	1.022159	H	-5.04072	-2.0099	1.514333
H	-5.5384	-2.7234	1.60668	H	-4.23156	-1.33562	2.913995
C	-5.03706	-0.69612	2.079271	C	-6.32009	-1.40927	3.104609
O	-3.97821	-0.09273	1.457216	O	-2.61682	0.191532	1.826048
O	-5.35992	-0.35431	3.190864	O	-7.04823	-0.53551	3.536722
N	-2.83368	-0.08887	-0.56884	N	-3.47093	0.92353	-0.14352
H	-2.90514	-0.36651	-1.54176	H	-4.34069	1.144542	-0.6139
C	-2.48323	1.322967	-0.37967	C	-2.19389	1.309974	-0.70526
H	-2.11817	1.463219	0.636263	H	-1.49444	0.476307	-0.63163
C	-1.37141	1.718528	-1.35978	C	-2.36032	1.693686	-2.18629
C	-3.69924	2.225971	-0.59296	C	-1.60909	2.489248	0.073436
H	-0.58272	0.965345	-1.26962	H	-2.92098	0.885345	-2.66587
H	-1.75237	1.696985	-2.38328	H	-2.94473	2.612834	-2.26872
C	-0.74501	3.100821	-1.04486	C	-1.01402	1.835147	-2.93921
O	-4.5003	2.096303	-1.48951	O	-2.25845	3.362665	0.602765
O	-0.33646	3.268677	0.133293	O	-0.26052	0.827493	-2.91997
O	-0.67934	3.924191	-1.99429	O	-0.80007	2.929409	-3.52307

O	-3.78967	3.199617	0.33697	O	-0.26607	2.472597	0.065402
H	-4.55521	3.758849	0.122972	H	0.052326	3.270531	0.517863
H	-5.88104	-2.17681	-1.69552	H	-6.86314	0.779947	0.883185
O	-4.32606	2.456462	3.349269	O	-6.5205	-2.70442	3.386755
H	-4.62306	1.533519	3.388516	H	-7.29587	-2.77984	3.967005
H	-4.08078	2.591689	2.42441	H	-5.19505	0.935936	2.336871
				O	-7.99957	1.882971	2.455853
				H	-7.64247	1.131273	2.961505
				H	-7.51691	2.653685	2.773854
Asn-Cys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.10512	-1.35953	-1.65889	N	-3.72959	-0.71654	0.08453
H	-2.81299	-2.31681	-1.83753	H	-3.43672	-1.51222	-0.47462
C	-2.94551	-1.00889	-0.29474	C	-2.80553	-0.46718	1.186247
C	-3.64976	-1.58464	0.909648	C	-2.21833	-1.73732	1.853529
C	-2.07743	-0.08776	0.142413	C	-1.63836	0.45155	0.764963
H	-4.73619	-1.44779	0.902134	H	-1.6918	-2.33256	1.106607
H	-3.45985	-2.65068	1.080329	H	-1.50699	-1.44008	2.626909
C	-3.0478	-0.78151	2.040383	C	-3.30642	-2.59743	2.443335
O	-2.11213	0.075961	1.535127	O	-0.65826	0.611391	1.488322
O	-3.27676	-0.80944	3.226027	O	-3.87164	-2.18719	3.592215
N	-1.10689	0.648813	-0.49718	N	-1.81831	1.069874	-0.42161
H	-1.09944	0.433474	-1.48952	H	-2.67976	0.845596	-0.90882
C	-0.98457	2.090732	-0.20885	C	-0.8596	1.996582	-0.9983
H	-1.07332	2.223071	0.868921	H	-0.02004	2.059191	-0.30493
C	0.37966	2.580908	-0.6851	C	-0.38329	1.502574	-2.36609
C	-2.13548	2.833011	-0.89071	C	-1.51829	3.376458	-1.07837
H	1.153901	1.990031	-0.19488	H	0.012905	0.492857	-2.25185
H	0.482279	2.460771	-1.76404	H	-1.20755	1.473884	-3.0792
S	0.730781	4.32673	-0.23736	S	0.995224	2.490325	-3.07257
O	-2.07294	3.360019	-1.97968	O	-1.95519	3.876548	-2.09018
H	-0.11426	4.890696	-1.11961	H	0.269204	3.581799	-3.37486
H	-4.07611	-1.28828	-1.94968	H	-4.66531	-0.91017	0.421563
O	-3.26074	2.759027	-0.16349	O	-1.58661	3.956446	0.128025
H	-3.98664	3.16512	-0.66551	H	-2.05359	4.803687	0.041476
O	-1.7927	1.203549	4.661026	O	-3.71957	-3.6137	1.922174
H	-2.29669	0.510707	4.197631	H	-3.34463	0.116299	1.940135
H	-1.28669	1.634386	3.963415	H	-3.44839	-1.39	3.941281
				O	-5.82944	-5.10717	3.114025
				H	-5.94073	-5.87324	2.540923
				H	-5.10501	-4.59406	2.708468
Asn-Gln							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.59196	-3.28762	-1.05246	N	-3.0566	-2.10577	-1.24801
H	-2.41859	-4.19452	-0.62698	H	-2.32447	-2.80179	-1.13168
C	-2.95238	-2.31613	-0.08469	C	-3.33348	-1.42905	0.021189
C	-4.17033	-2.2923	0.806463	C	-3.44358	-2.35411	1.239227

C	-2.20446	-1.24621	0.215211	C	-2.32012	-0.3109	0.302769
H	-5.12201	-2.24192	0.266905	H	-2.53774	-2.95651	1.356819
H	-4.23928	-3.13571	1.503417	H	-3.54465	-1.76543	2.155933
C	-3.96544	-1.01396	1.586459	C	-4.63266	-3.27906	1.160503
O	-2.7835	-0.44208	1.210759	O	-2.26662	0.25652	1.39602
O	-4.66095	-0.49016	2.424054	O	-5.53802	-3.1708	0.347732
N	-0.95381	-0.8385	-0.19201	N	-1.52726	0.026977	-0.73205
H	-0.61243	-1.46602	-0.91411	H	-1.70649	-0.43822	-1.61326
C	-0.75844	0.570783	-0.54009	C	-0.59005	1.125267	-0.64747
H	-1.12995	1.184381	0.281416	H	0.047268	0.986196	0.229068
C	0.744976	0.834862	-0.73147	C	0.27609	1.154803	-1.91938
C	-1.53162	0.93936	-1.80836	C	-1.33536	2.450432	-0.46912
H	1.248818	0.505302	0.178357	H	0.720906	0.164597	-2.03723
H	1.113969	0.21146	-1.55299	H	-0.36981	1.327912	-2.78636
C	1.087028	2.303472	-0.99608	C	1.393255	2.199507	-1.88201
O	-1.69184	0.192523	-2.74707	O	-2.40285	2.71741	-0.96979
H	0.662695	2.649185	-1.94088	H	0.990444	3.213283	-1.83885
H	0.657105	2.932981	-0.20852	H	2.000501	2.063307	-0.97981
C	2.591669	2.542638	-0.96716	C	2.338795	2.050991	-3.06805
O	3.325275	1.98393	-0.15087	O	2.650738	0.949055	-3.52089
N	3.066626	3.42614	-1.87274	N	2.835653	3.201767	-3.57292
H	4.047434	3.661837	-1.86506	H	3.510365	3.16153	-4.32173
H	2.468834	3.882692	-2.542	H	2.58295	4.103452	-3.20301
O	-1.99503	2.199031	-1.77207	O	-0.63025	3.313713	0.280884
H	-2.43593	2.394539	-2.61566	H	-1.11237	4.155904	0.318885
H	-3.32889	-3.41994	-1.7394	H	-3.88711	-2.60277	-1.55176
O	-3.59433	2.03798	3.299436	O	-4.60069	-4.23112	2.093466
H	-3.96741	1.181602	3.022889	H	-5.41464	-4.79302	1.999806
H	-2.78225	2.11857	2.787316	H	-4.29019	-0.9094	-0.09622
				O	-6.96221	-5.40781	1.488963
				H	-6.94292	-4.78096	0.747681
				H	-6.97733	-6.28543	1.088248

Asn-Glu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-4.22623	-1.33545	-1.41117	N	-2.55212	-3.20346	-1.59456
H	-4.30556	-2.34368	-1.30773	H	-2.16034	-3.71332	-0.80816
C	-4.06036	-0.68687	-0.16114	C	-3.19739	-1.9875	-1.11251
C	-5.05422	-0.56451	0.970012	H	-3.59674	-1.45426	-1.9787
C	-2.93024	-0.07626	0.220818	C	-4.40262	-2.18245	-0.13753
H	-5.98423	-0.05141	0.703692	C	-2.1351	-1.12602	-0.4271
H	-5.33419	-1.51897	1.432163	H	-4.87165	-1.21795	0.06021
C	-4.29065	0.270398	1.973024	H	-5.12861	-2.82759	-0.63897
O	-3.02661	0.492611	1.497822	C	-4.04633	-2.8017	1.191447
O	-4.62866	0.737094	3.033474	O	-1.36849	-1.61081	0.40588
N	-1.69069	0.059394	-0.35775	O	-4.098	-2.20425	2.255391
H	-1.71737	-0.22562	-1.3307	N	-2.11039	0.181001	-0.75841
C	-0.93529	1.293588	-0.1231	C	-1.20356	1.118875	-0.11915
H	-0.69251	1.350514	0.938643	H	-0.18519	0.730425	-0.18678

C	0.363124	1.261677	-0.94502	C	-1.29352	2.483808	-0.82746
C	-1.75994	2.526808	-0.4916	C	-1.55391	1.26166	1.361854
H	0.877169	0.329269	-0.70113	H	-1.09963	2.314743	-1.88942
H	0.108434	1.217145	-2.00839	H	-2.31966	2.855843	-0.7463
C	1.28573	2.449094	-0.676	C	-0.31572	3.528429	-0.29449
O	-2.41449	2.637114	-1.5019	O	-2.67973	1.299351	1.803051
H	0.800382	3.393022	-0.94701	H	-0.51841	3.759736	0.755318
H	1.503712	2.525098	0.394925	H	0.707546	3.13669	-0.31994
C	2.638078	2.406082	-1.42469	C	-0.31674	4.866566	-1.06996
O	3.422529	3.364751	-1.18241	O	0.423355	5.770583	-0.59233
O	2.856727	1.443766	-2.20635	O	-1.03261	4.95784	-2.10155
H	-5.06656	-1.01947	-1.88684	H	-3.24352	-3.81252	-2.02167
O	-1.67831	3.498135	0.442551	O	-0.45564	1.392611	2.123574
H	-2.18518	4.267879	0.133863	H	-0.73434	1.540772	3.041984
O	-2.80033	3.083376	3.353092	O	-3.68133	-4.08311	1.095457
H	-3.37716	2.302985	3.347638	H	-2.79002	0.540282	-1.4117
H	-2.41345	3.102031	2.467856	H	-3.44731	-4.41207	2.002028
				O	-3.10529	-4.43712	3.723809
				H	-3.67983	-4.97989	4.277012
				H	-3.48361	-3.54158	3.749509
Asn-Gly							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.38995	-1.86371	-1.67232	N	-3.65014	-0.87495	0.390522
H	-0.6958	-2.59721	-1.56078	H	-3.37245	-1.5182	-0.34369
C	-1.62747	-1.18331	-0.45097	C	-2.55797	-0.62034	1.324588
C	-2.00919	-1.77091	0.885715	C	-1.56573	-1.80494	1.495482
C	-1.58544	0.149143	-0.31577	C	-1.77503	0.653946	0.973209
H	-2.97233	-2.29486	0.892272	H	-1.39495	-2.277	0.527672
H	-1.26668	-2.45747	1.306007	H	-0.60878	-1.43965	1.871081
C	-2.10612	-0.53893	1.756044	C	-2.11175	-2.84316	2.454765
O	-1.86339	0.56913	0.996638	O	-0.84081	1.040131	1.6929
O	-2.35145	-0.43336	2.934672	O	-2.58639	-3.90376	2.099494
N	-1.41802	1.173158	-1.21522	N	-2.17345	1.308241	-0.12275
H	-1.23646	0.810667	-2.14521	H	-3.01821	0.958511	-0.55952
C	-0.52224	2.263478	-0.8473	C	-1.60862	2.571733	-0.51724
C	-0.37714	3.230408	-1.99918	C	-2.18373	3.74674	0.261648
H	-0.91542	2.798875	0.018182	H	-0.52727	2.56306	-0.36664
H	0.490192	1.923339	-0.58436	H	-1.79138	2.741336	-1.57964
O	-0.74825	3.023301	-3.13225	O	-3.05869	3.680594	1.091624
O	0.255216	4.34859	-1.61181	O	-1.58184	4.889623	-0.10587
H	0.370193	4.924464	-2.38503	H	-1.9707	5.622925	0.397776
H	-2.23356	-2.30731	-2.02607	H	-4.45012	-1.28141	0.859968
O	-2.23278	2.307585	3.810023	O	-2.07613	-2.51979	3.750864
H	-2.28526	1.373531	3.538003	H	-2.99863	-0.3845	2.297888
H	-2.01364	2.777335	2.99781	H	-1.63083	-1.64123	3.909444
				O	-0.83423	-0.17045	4.137886
				H	-0.79192	0.356179	3.303112
				H	-1.24203	0.403048	4.796564

Asn-His							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.46866	-2.34514	0.84412	N	-2.10458	-2.61751	0.125297
H	-0.51674	-2.73949	1.779893	H	-1.17075	-2.83977	0.45937
C	-1.42808	-1.31827	0.657513	C	-2.78701	-1.70559	1.043104
C	-2.93324	-1.42586	0.681668	H	-3.85193	-1.72753	0.79271
C	-1.11427	-0.03346	0.446945	C	-2.63136	-2.07246	2.533585
H	-3.34792	-2.08913	-0.08469	C	-2.35614	-0.24851	0.805291
H	-3.35142	-1.74353	1.644011	H	-2.90708	-3.12622	2.643905
C	-3.35522	-0.00181	0.398823	H	-1.59478	-1.96235	2.85457
O	-2.24333	0.783491	0.287291	C	-3.50415	-1.29891	3.491147
O	-4.45772	0.475937	0.274424	O	-2.55053	0.619263	1.655212
N	0.084242	0.640626	0.450851	O	-3.11588	-0.86613	4.565747
H	0.849706	-0.00181	0.630543	N	-1.79591	-0.01506	-0.401
C	0.377454	1.618045	-0.61325	C	-1.33809	1.290298	-0.83879
H	-0.51207	2.232524	-0.75324	H	-1.48021	1.973133	0.001298
C	1.559348	2.498015	-0.18248	C	0.148462	1.248568	-1.24169
C	0.652927	0.864758	-1.91642	C	-2.24554	1.766783	-1.97675
H	1.313882	2.906638	0.799092	H	0.683302	0.753684	-0.42902
H	2.446575	1.868142	-0.06372	H	0.258343	0.624677	-2.13402
C	1.846617	3.63382	-1.10941	C	0.772075	2.589203	-1.45625
O	1.754693	0.615551	-2.35976	O	-1.90485	1.897148	-3.13304
N	2.476962	3.490781	-2.32861	N	0.545177	3.378926	-2.56422
C	1.593115	4.982314	-1.00503	C	1.657305	3.31222	-0.68933
H	2.77711	2.612095	-2.72644	H	-0.08982	3.148386	-3.31536
C	2.573979	4.720836	-2.89778	C	1.276022	4.515927	-2.42648
N	2.049448	5.653757	-2.12251	N	1.967781	4.511472	-1.3002
H	1.11581	5.49703	-0.18496	H	2.086815	3.026467	0.25893
H	3.029395	4.876858	-3.86312	H	1.267222	5.301838	-3.16538
O	-0.4839	0.440332	-2.48452	O	-3.48947	2.006809	-1.5451
H	-0.26561	-0.09981	-3.26208	H	-4.03736	2.273307	-2.3015
H	-0.61286	-3.11189	0.192989	H	-2.61056	-3.49315	0.051585
O	-4.33583	3.280715	-0.38548	O	-4.77142	-1.20138	3.082689
H	-4.40215	2.336205	-0.15681	H	-5.28602	-0.70459	3.768715
H	-3.3891	3.459579	-0.37781	H	-1.67091	-0.82799	-0.99432
				O	-5.67818	0.121407	5.277207
				H	-4.72423	0.06573	5.462325
				H	-5.87936	1.063024	5.21876
Asn-Ile							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.22113	-3.01255	-1.57672	N	-3.46016	-2.17764	-0.98773
H	-2.86327	-3.95966	-1.48507	H	-2.70157	-2.78294	-0.68568
C	-3.33499	-2.37221	-0.31662	C	-3.99569	-1.40894	0.135457
C	-4.21028	-2.75833	0.850598	C	-4.25006	-2.22495	1.417557
C	-2.61498	-1.30196	0.045823	C	-3.1055	-0.19828	0.452599
H	-5.28424	-2.72956	0.637808	H	-4.78342	-3.13851	1.136228
H	-3.99233	-3.74567	1.274427	H	-3.31176	-2.51883	1.890342

C	-3.86979	-1.69163	1.865848	C	-5.13319	-1.51183	2.412468
O	-2.91399	-0.86606	1.347972	O	-3.16899	0.379588	1.540358
O	-4.30496	-1.50442	2.977553	O	-4.75183	-1.68233	3.678959
N	-1.5865	-0.62118	-0.56538	N	-2.28909	0.196831	-0.54029
H	-1.44549	-1.00482	-1.4944	H	-2.32091	-0.34588	-1.39344
C	-1.62475	0.844937	-0.5638	C	-1.42831	1.353081	-0.41212
H	-1.9069	1.171809	0.437033	H	-0.85488	1.260663	0.513324
C	-0.21671	1.425547	-0.87449	C	-0.43441	1.425703	-1.60549
C	-2.68119	1.35841	-1.54235	C	-2.26958	2.624619	-0.29058
H	0.436052	0.93517	-0.14282	H	0.001444	0.419966	-1.65796
C	0.27475	1.058699	-2.28183	C	-1.13812	1.72166	-2.93872
C	-0.16167	2.942514	-0.61233	C	0.715442	2.408913	-1.3194
O	-2.99909	0.790753	-2.56384	O	-3.35622	2.795023	-0.79289
H	-0.33947	1.533826	-3.05254	H	-1.50467	2.752121	-2.9675
H	1.305266	1.388682	-2.42354	H	-0.44816	1.586128	-3.77301
H	0.261538	-0.02035	-2.45517	H	-1.9922	1.062417	-3.11251
H	-0.73621	3.470133	-1.38109	H	0.326924	3.432405	-1.30668
H	-0.65869	3.154443	0.340739	H	1.102764	2.213721	-0.31348
C	1.264041	3.503297	-0.56212	C	1.868776	2.309305	-2.32393
H	1.775643	3.408848	-1.52338	H	1.560568	2.601507	-3.33101
H	1.249447	4.565019	-0.30106	H	2.691102	2.966429	-2.02828
H	1.864355	2.981357	0.190389	H	2.258413	1.287169	-2.375
O	-3.21484	2.526808	-1.15054	O	-1.6328	3.566578	0.426783
H	-3.84661	2.821245	-1.82734	H	-2.18087	4.368008	0.435673
H	-4.12153	-3.08112	-2.04266	H	-4.17775	-2.7755	-1.38285
O	-3.16521	0.849011	4.186694	O	-6.13634	-0.88936	2.095737
H	-3.56111	0.046268	3.802018	H	-5.40045	-1.21682	4.266966
H	-2.55682	1.160412	3.507569	H	-4.95186	-0.98277	-0.18544
				O	-6.82528	-0.30677	4.78487
				H	-6.98071	-0.1629	3.834949
				H	-6.6681	0.568021	5.159945

Asn-Leu							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.1808	-1.95039	-0.95349	N	-1.46888	-2.18097	-0.05149
H	-1.97056	-2.89694	-0.64792	H	-1.31857	-3.14497	0.224929
C	-2.2011	-1.04164	0.134872	C	-1.96684	-1.39408	1.074783
C	-3.13261	-1.02816	1.3224	C	-3.44155	-1.66589	1.437675
C	-1.3286	-0.03649	0.286468	C	-1.75534	0.108202	0.838501
H	-4.18836	-0.89164	1.065337	H	-4.10357	-1.33536	0.636394
H	-3.06867	-1.91799	1.95964	H	-3.56599	-2.74691	1.553311
C	-2.64242	0.175709	2.093812	C	-3.86874	-1.05196	2.746153
O	-1.56704	0.715901	1.449086	O	-2.41383	0.953091	1.449562
O	-3.05405	0.66812	3.117611	O	-3.24148	-1.12716	3.788391
N	-0.20681	0.341111	-0.41615	N	-0.78764	0.428056	-0.03891
H	-0.1046	-0.24959	-1.23591	H	-0.36944	-0.3365	-0.55357
C	-0.02243	1.762492	-0.72521	C	-0.45761	1.803021	-0.35068
H	-0.12946	2.325937	0.200347	H	-0.26899	2.339648	0.580259
C	1.387155	1.969556	-1.30987	C	0.792306	1.832015	-1.25281

C	-1.07834	2.250695	-1.71724	C	-1.63373	2.486961	-1.04923
H	2.09384	1.567038	-0.57636	H	1.582146	1.289279	-0.72099
H	1.472549	1.350525	-2.21058	H	0.565205	1.261728	-2.16067
C	1.77395	3.41925	-1.64974	C	1.317001	3.22395	-1.64378
O	-1.49124	1.594382	-2.64717	O	-2.37241	1.953767	-1.84468
H	1.053946	3.81125	-2.37846	H	0.518658	3.762041	-2.16839
C	1.750173	4.331904	-0.4153	C	1.732671	4.055314	-0.42209
C	3.160237	3.434996	-2.3091	C	2.493386	3.066478	-2.61774
H	2.426053	3.950181	0.358309	H	2.501179	3.530692	0.156865
H	2.07842	5.341621	-0.67823	H	2.148677	5.01672	-0.73677
H	0.750249	4.413985	0.017212	H	0.889483	4.262874	0.240665
H	3.181237	2.812853	-3.20902	H	2.201579	2.502119	-3.50863
H	3.444394	4.452173	-2.59362	H	2.862779	4.043662	-2.94158
H	3.921598	3.054899	-1.61863	H	3.324264	2.535775	-2.1393
H	-3.08021	-1.98577	-1.4251	H	-2.13771	-2.18937	-0.81658
O	-1.48658	3.502632	-1.45441	O	-1.72466	3.783126	-0.708
H	-2.12147	3.773156	-2.13838	H	-2.44507	4.186753	-1.21895
O	-1.64057	3.090995	3.781599	O	-5.06915	-0.46222	2.682303
H	-2.12496	2.269508	3.582803	H	-5.29653	-0.13027	3.566401
H	-0.99607	3.16346	3.069115	O	-0.82312	-2.49528	4.270166
				H	-1.65704	-2.00719	4.132983
				H	-0.191	-1.82798	4.558224
				H	-1.34608	-1.64159	1.941327

Asn-Lys							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.85452	0.429406	3.795251	N	-4.34669	-0.44445	0.593934
H	-1.04975	0.093067	3.275795	H	-4.63137	-0.0597	1.488926
C	-2.79915	1.049702	2.983591	C	-3.3147	-1.46749	0.775729
C	-4.24392	1.192751	3.367583	H	-3.46886	-2.08583	1.667225
C	-2.60108	1.706346	1.831796	C	-3.28752	-2.43656	-0.43027
H	-4.77323	0.238883	3.4516	C	-1.91748	-0.84522	0.94875
H	-4.39883	1.736024	4.305475	H	-2.46716	-3.1399	-0.28855
C	-4.80843	1.993135	2.211654	H	-4.2288	-2.98629	-0.46689
O	-3.82363	2.285219	1.343693	C	-3.06209	-1.70352	-1.73266
O	-5.95246	2.353384	2.026463	O	-0.97311	-1.52984	1.340129
N	-1.47776	2.03449	1.08779	O	-4.17906	-1.49946	-2.43059
H	-0.65648	2.141243	1.67256	N	-1.83247	0.46015	0.622228
C	-1.20311	1.228073	-0.10265	C	-0.57498	1.182384	0.510588
H	-2.10115	1.222498	-0.72425	H	0.207809	0.501415	0.84903
C	-0.04117	1.857563	-0.89405	C	-0.31562	1.627499	-0.93087
C	-0.87266	-0.21854	0.270661	C	-0.63453	2.359696	1.48646
H	-0.30964	2.905738	-1.05424	H	-0.43961	0.746931	-1.56679
H	0.857278	1.849271	-0.26579	H	-1.08209	2.352275	-1.22385
C	0.256962	1.188403	-2.23879	C	1.078194	2.229735	-1.12768
O	-0.29115	-0.54705	1.282879	O	-0.94272	3.491721	1.189225
H	0.555736	0.146831	-2.08845	H	1.204123	3.100129	-0.47532
H	-0.65401	1.169065	-2.84722	H	1.836906	1.496204	-0.83124
C	1.36606	1.927351	-2.99739	C	1.316371	2.650117	-2.58248

H	1.069156	2.968431	-3.16466	H	1.189999	1.785117	-3.24303
H	2.278404	1.942292	-2.39125	H	0.569876	3.396	-2.87726
C	1.65072	1.255922	-4.33341	C	2.713614	3.226861	-2.75844
H	1.989896	0.227568	-4.20925	H	2.867305	4.116343	-2.14776
H	0.777956	1.263202	-4.98586	H	3.487611	2.497448	-2.52044
N	2.74636	1.977288	-5.08006	N	2.950247	3.645806	-4.18923
H	3.621735	1.98163	-4.55153	H	2.282242	4.360999	-4.48475
H	2.937859	1.535923	-5.98157	H	3.888338	4.030866	-4.31671
H	2.496406	2.951316	-5.2646	H	2.854062	2.854892	-4.82987
H	-2.24211	-0.31719	4.358318	H	-5.17649	-0.83836	0.163469
O	-1.27174	-1.09274	-0.66382	O	-0.33909	1.978896	2.739891
H	-0.99465	-1.98521	-0.39734	H	-0.44386	2.743373	3.329815
O	-6.3413	3.849874	-0.36897	O	-1.9635	-1.31451	-2.09732
H	-5.46393	3.905337	-0.76283	H	-2.68233	0.874784	0.2544
H	-6.20649	3.337076	0.45038	H	-3.95337	-0.95914	-3.233
				O	-3.02634	-0.04522	-4.4113
				H	-2.25842	-0.171	-3.82826
				H	-3.18155	0.906698	-4.43699

Asn-Met							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.33616	-2.64987	-0.73451	N	-4.32482	-1.30321	-1.28482
H	-3.29648	-3.55607	-0.27544	H	-3.79927	-2.12755	-1.56158
C	-3.56347	-1.6031	0.194374	C	-4.20036	-1.05687	0.149735
C	-4.77094	-1.37903	1.071815	C	-4.22266	-2.32243	1.044355
C	-2.67737	-0.63528	0.462427	C	-2.93761	-0.23912	0.47943
H	-5.70372	-1.21933	0.52068	H	-3.42472	-2.99976	0.737
H	-4.95845	-2.1783	1.798232	H	-4.0499	-2.03471	2.081894
C	-4.39669	-0.11203	1.80626	C	-5.53259	-3.05986	0.908189
O	-3.14587	0.278474	1.420991	O	-2.56229	-0.06677	1.639825
O	-5.01748	0.532701	2.617724	O	-5.70903	-4.00358	0.171899
N	-1.38031	-0.4181	0.052471	N	-2.30418	0.29292	-0.58195
H	-1.12165	-1.12166	-0.63302	H	-2.74302	0.159679	-1.48484
C	-1.00318	0.933242	-0.36845	C	-1.15373	1.155815	-0.42796
H	-1.29802	1.633483	0.413529	H	-0.40587	0.649873	0.186926
C	0.52494	0.990333	-0.55619	C	-0.56169	1.466745	-1.81729
C	-1.71202	1.326342	-1.66653	C	-1.54724	2.447815	0.292821
H	0.969297	0.653017	0.383839	H	-0.36906	0.505972	-2.30377
H	0.813045	0.272669	-1.33173	H	-1.31409	1.992711	-2.41385
C	1.041324	2.384332	-0.91259	C	0.729537	2.282341	-1.75925
O	-1.93732	0.559275	-2.57492	O	-2.60676	3.015543	0.166107
H	0.663081	2.713701	-1.88292	H	0.554028	3.276285	-1.34292
H	0.732396	3.114484	-0.15962	H	1.476449	1.778604	-1.13999
S	2.874389	2.370471	-0.99289	S	1.412916	2.484622	-3.45034
C	3.155286	4.112394	-1.46404	C	2.870194	3.510833	-3.05252
H	2.763898	4.78345	-0.69715	H	3.541777	2.9762	-2.37821
H	4.233951	4.250859	-1.54899	H	3.385997	3.710404	-3.99278
H	2.685999	4.328494	-2.42567	H	2.560999	4.455855	-2.60202
O	-2.0386	2.628065	-1.69191	O	-0.54359	2.907298	1.057777

H	-2.44389	2.832498	-2.55115	H	-0.81428	3.754386	1.448191
H	-4.07954	-2.70158	-1.42538	H	-5.29079	-1.46709	-1.54386
O	-3.58182	2.893677	3.434016	O	-6.58127	-2.57545	1.610101
H	-4.08544	2.099799	3.178931	H	-5.02856	-0.40178	0.441461
H	-2.75994	2.821182	2.936436	H	-6.31004	-1.86305	2.205058
				O	-4.51135	-4.52363	3.434992
				H	-4.29907	-3.93805	4.170833
				H	-3.65465	-4.83785	3.12381
Asn-Phe							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.36261	-2.69594	-0.79508	N	-3.02631	-1.50468	0.316844
H	-2.2562	-3.56939	-0.28592	H	-2.69427	-1.97834	-0.51894
C	-2.71248	-1.62733	0.068716	C	-1.94584	-1.34022	1.289188
C	-3.95178	-1.47893	0.916876	H	-2.40593	-1.09225	2.250338
C	-1.93591	-0.55873	0.288982	C	-1.07047	-2.59693	1.479966
H	-4.88536	-1.44751	0.345333	C	-1.06309	-0.13016	0.94282
H	-4.07056	-2.25058	1.686321	H	-1.74032	-3.4387	1.683156
C	-3.7215	-0.13998	1.58048	H	-0.51424	-2.82279	0.569189
O	-2.51282	0.35602	1.186129	C	-0.09119	-2.54195	2.626409
O	-4.42093	0.477502	2.347989	O	0.063711	-0.00369	1.427044
N	-0.66122	-0.23186	-0.11981	O	1.062475	-2.93823	2.554654
H	-0.31168	-0.95494	-0.7421	N	-1.62451	0.77432	0.120085
C	-0.43211	1.113219	-0.6551	C	-0.93378	1.971187	-0.30929
H	-0.83322	1.840614	0.049937	H	-0.31746	2.337659	0.512186
C	1.086834	1.340807	-0.82082	C	-0.01715	1.67473	-1.53532
C	-1.13139	1.295188	-2.00423	C	-1.97035	3.022268	-0.66717
H	1.537464	1.169304	0.15984	H	0.613658	0.835221	-1.23339
H	1.477169	0.578522	-1.50174	H	-0.65083	1.332821	-2.35773
C	1.427652	2.722521	-1.32954	C	0.836795	2.842814	-1.96327
O	-1.1202	0.462872	-2.88364	O	-3.05973	2.769825	-1.13362
C	1.734851	2.937623	-2.67788	C	0.503234	3.606003	-3.08773
C	1.409196	3.82062	-0.45962	C	1.972583	3.196512	-1.22271
H	1.755968	2.096012	-3.36246	H	-0.37231	3.342146	-3.67212
C	2.013056	4.222215	-3.15042	C	1.282989	4.70156	-3.46445
C	1.686352	5.105274	-0.92709	C	2.753412	4.291276	-1.59376
H	1.177959	3.667366	0.589731	H	2.247293	2.609299	-0.35212
H	2.250545	4.370671	-4.19785	H	1.011021	5.280469	-4.33999
C	1.988004	5.310151	-2.27627	C	2.409784	5.048695	-2.71693
H	1.670393	5.943851	-0.23998	H	3.630315	4.550169	-1.01089
H	2.205413	6.307762	-2.6406	H	3.017316	5.898049	-3.00814
O	-1.74647	2.481677	-2.10978	O	-1.52494	4.264325	-0.44518
H	-2.13348	2.554679	-2.99825	H	-2.19503	4.895684	-0.75555
H	-3.07633	-2.85181	-1.50147	H	-3.77028	-2.07432	0.704604
O	-3.51063	3.035442	3.268508	O	-0.63515	-2.08883	3.758598
H	-3.82417	2.163905	2.965154	H	0.054493	-2.11005	4.469589
H	-4.20757	3.359583	3.849036	H	-2.53509	0.552411	-0.26505
				O	1.628235	-2.29683	5.253702
				H	1.704208	-2.98487	5.925484

				H	1.899769	-2.71274	4.416331
Asn-Ser							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-1.37895	-2.06951	-1.02515	N	-1.33069	-1.57802	-0.82451
H	-1.19964	-3.05114	-0.83103	H	-0.53344	-2.20227	-0.73893
C	-1.01246	-1.23996	0.064098	C	-1.38578	-0.63599	0.28972
C	-1.65537	-1.14002	1.427503	C	-1.15942	-1.25969	1.682231
C	0.029761	-0.39922	0.044293	C	-0.40832	0.529504	0.072307
H	-2.7073	-0.83691	1.410978	H	-1.77233	-2.16316	1.751608
H	-1.59319	-2.0578	2.024446	H	-0.11576	-1.55892	1.801093
C	-0.83159	-0.05668	2.086953	C	-1.61699	-0.3559	2.809015
O	0.182052	0.309785	1.241036	O	-0.01159	1.222485	1.014707
O	-0.95493	0.490474	3.154759	O	-0.84036	-0.29397	3.91406
N	1.003822	-0.14067	-0.89621	N	-0.05396	0.74808	-1.20306
H	0.756149	-0.57912	-1.77811	H	-0.39078	0.087795	-1.89509
C	1.471951	1.237832	-1.04101	C	0.83357	1.819942	-1.60479
H	1.879544	1.57305	-0.08809	H	0.724725	2.655474	-0.9137
C	2.578041	1.275615	-2.09511	C	2.292768	1.328884	-1.57472
C	0.333483	2.177146	-1.45301	C	0.452052	2.260492	-3.01157
H	3.378085	0.597078	-1.78159	H	2.493871	0.960368	-0.56315
H	2.177802	0.933285	-3.05717	H	2.405364	0.49888	-2.28235
O	3.031416	2.622687	-2.1786	O	3.137696	2.421406	-1.91228
O	-0.38226	1.991363	-2.40861	O	0.093174	1.492448	-3.87666
H	3.657395	2.694401	-2.90733	H	4.050962	2.114328	-1.92036
O	0.196825	3.221662	-0.61455	O	0.577219	3.579503	-3.18629
H	-0.53797	3.77804	-0.92349	H	0.363648	3.793106	-4.10998
H	-2.36781	-1.98545	-1.24191	H	-2.16378	-2.15546	-0.84625
O	0.135728	3.227612	2.520261	O	-2.65269	0.267165	2.788847
H	-0.15462	2.357618	2.834877	H	-0.02911	-0.80902	3.804487
H	0.2042	3.126121	1.561788	H	-2.38099	-0.17984	0.288188
				O	-0.04884	2.66856	3.440468
				H	-0.34182	1.992976	4.063163
				H	-0.05176	2.201869	2.586671
Asn-Thr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.85744	0.363921	-1.59599	N	-3.10944	-2.27022	-1.48213
H	-4.43732	-0.41654	-1.89261	H	-2.40971	-2.97753	-1.275
C	-3.35989	0.179066	-0.28054	C	-3.40975	-1.46858	-0.29669
C	-4.13865	0.084002	1.00833	C	-3.64047	-2.28033	0.992753
C	-2.0609	0.033301	0.013782	C	-2.32959	-0.40185	-0.05653
H	-4.71984	0.980177	1.251617	H	-4.32572	-3.10087	0.757168
H	-4.82495	-0.76921	1.065774	H	-2.70866	-2.71758	1.354254
C	-3.03803	-0.09243	2.029262	C	-4.30205	-1.48271	2.090125
O	-1.83263	-0.12957	1.390499	O	-2.20676	0.145037	1.041063
O	-3.10107	-0.19595	3.231555	O	-3.81389	-1.7425	3.303779
N	-0.93734	-0.07864	-0.76647	N	-1.56766	-0.10924	-1.12687
H	-1.16003	0.072232	-1.744	H	-1.77818	-0.59814	-1.9879

C	0.292049	0.582538	-0.35969	C	-0.55714	0.91488	-1.12354
H	0.499358	0.342523	0.68441	H	-0.20971	1.059848	-0.09799
C	1.480327	0.072525	-1.19715	C	0.648911	0.503097	-1.98841
C	0.193179	2.108289	-0.46469	C	-1.13191	2.25687	-1.58644
H	2.367596	0.625917	-0.8709	H	1.358801	1.336412	-1.97997
C	1.719588	-1.42259	-1.02892	C	1.33067	-0.75808	-1.47145
O	1.169044	0.41819	-2.55406	O	0.124881	0.32591	-3.31189
O	-0.70564	2.710832	-1.00296	O	-2.25566	2.436215	-1.99181
H	0.840917	-1.99256	-1.33505	H	0.635021	-1.59955	-1.45475
H	2.572733	-1.73118	-1.63936	H	2.174474	-1.01465	-2.1174
H	1.948381	-1.65663	0.014367	H	1.714932	-0.59641	-0.46074
H	1.860821	0.074575	-3.13043	H	0.832264	0.018806	-3.89005
H	-4.43112	1.200009	-1.66352	H	-3.93978	-2.75772	-1.80046
O	1.240061	2.706666	0.129479	O	-0.2188	3.236272	-1.46962
H	1.148348	3.667945	0.027459	H	-0.61556	4.067752	-1.77551
O	-0.64809	-0.41905	4.695176	O	-5.23672	-0.71915	1.896338
H	-0.90028	-0.43054	5.624705	H	-4.32949	-1.21731	3.968012
H	-1.48982	-0.34759	4.208859	H	-4.32474	-0.90465	-0.50555
				O	-5.47382	-0.04568	4.639181
				H	-5.82256	0.010707	3.732208
				H	-6.19496	-0.39495	5.176328

Asn-Trp							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-2.26251	-3.19384	-0.03518	N	-3.53785	-2.40347	-0.219
H	-1.67106	-3.92057	0.359352	H	-3.00511	-2.64383	0.610383
C	-2.62095	-2.22602	0.937097	C	-4.63426	-1.48624	0.086989
C	-3.44647	-2.41841	2.186415	C	-5.23461	-1.63094	1.491554
C	-2.22501	-0.94692	0.900778	C	-4.23426	-0.01536	-0.13264
H	-4.47394	-2.74849	2.000518	H	-4.45572	-1.57116	2.257067
H	-3.01134	-3.11303	2.914482	H	-5.92353	-0.80287	1.688221
C	-3.46329	-1.02428	2.771151	C	-6.01992	-2.89917	1.694305
O	-2.71453	-0.198	1.984046	O	-4.99046	0.912471	0.16536
O	-4.01139	-0.59702	3.759539	O	-6.45607	-3.62236	0.818574
N	-1.37144	-0.25331	0.072161	N	-3.02916	0.173532	-0.69684
H	-1.05074	-0.8607	-0.67626	H	-2.52707	-0.66597	-0.96275
C	-1.80186	1.058279	-0.41924	C	-2.53552	1.488837	-1.03763
H	-2.17089	1.637754	0.425384	H	-2.56372	2.128513	-0.15364
C	-0.60184	1.791027	-1.06081	C	-1.08072	1.372216	-1.55564
C	-2.92524	0.920343	-1.44741	C	-3.41333	2.135367	-2.10959
H	0.191688	1.806265	-0.30725	H	-0.51075	0.854121	-0.77701
H	-0.23958	1.19541	-1.90408	H	-1.08103	0.729908	-2.44131
C	-0.939	3.177783	-1.51143	C	-0.45007	2.690353	-1.8744
O	-2.91694	0.108117	-2.34602	O	-3.87286	1.551135	-3.06448
C	-1.06781	3.620504	-2.80605	C	-0.16555	3.186354	-3.12395
C	-1.24619	4.301673	-0.66353	C	-0.05323	3.704991	-0.93194
H	-0.92584	3.083792	-3.73125	H	-0.31486	2.73316	-4.09169
N	-1.43538	4.949604	-2.8149	N	0.382267	4.447016	-3.01622
C	-1.55383	5.39749	-1.51786	C	0.465939	4.79451	-1.68617

C	-1.28721	4.489712	0.729054	C	-0.08116	3.797949	0.47038
H	-1.5798	5.505212	-3.64219	H	0.687975	5.013674	-3.79037
C	-1.8997	6.657341	-1.01923	C	0.950679	5.957504	-1.07982
C	-1.63093	5.74034	1.229708	C	0.399636	4.952389	1.077991
H	-1.0488	3.674747	1.403814	H	-0.46858	2.981393	1.069953
H	-2.13091	7.480286	-1.6856	H	1.343253	6.7767	-1.67117
C	-1.93567	6.812849	0.363093	C	0.909412	6.021857	0.309546
H	-1.66593	5.898456	2.301755	H	0.384287	5.036714	2.158843
H	-2.20139	7.77652	0.782832	H	1.276442	6.909856	0.811753
O	-3.91731	1.800844	-1.25129	O	-3.57908	3.448933	-1.89432
H	-4.57843	1.686807	-1.95435	H	-4.08747	3.820044	-2.63381
H	-3.08168	-3.6566	-0.41897	H	-3.89066	-3.25921	-0.63534
O	-3.70439	2.267877	4.011264	O	-6.23592	-3.1473	2.993776
H	-3.79796	1.30181	3.932505	H	-6.77736	-3.95003	3.071428
H	-3.18754	2.522226	3.239081	H	-5.42843	-1.66234	-0.64535
				O	-5.44928	-4.44469	-1.67848
				H	-5.93652	-4.13868	-0.89285
				H	-5.84001	-3.96925	-2.41967

Asn-Tyr							
Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-0.83484	-1.29185	-0.26955	N	-0.36231	-1.25228	-2.7954
H	-0.42338	-1.53691	0.626633	H	0.290148	-1.18501	-2.02003
C	-2.18787	-0.89073	-0.12944	C	-1.7319	-1.38574	-2.30115
C	-3.32795	-1.64028	0.516332	C	-1.95592	-2.44436	-1.20856
C	-2.67417	0.265959	-0.59915	C	-2.3057	-0.02893	-1.85639
H	-3.58527	-2.58704	0.026933	H	-3.02143	-2.52873	-0.97831
H	-3.18072	-1.85761	1.579591	H	-1.62873	-3.42175	-1.57707
C	-4.4755	-0.66874	0.35627	C	-1.21806	-2.15612	0.077759
O	-4.04011	0.432835	-0.32292	O	-3.30258	0.04188	-1.13598
O	-5.62334	-0.74952	0.724088	O	-0.46414	-1.21815	0.243299
N	-2.1164	1.276456	-1.34495	N	-1.6605	1.045113	-2.34769
H	-1.1227	1.107542	-1.45985	H	-0.84977	0.850537	-2.92197
C	-2.41854	2.656208	-0.97035	C	-2.02209	2.399472	-2.01806
H	-2.49896	2.76741	0.116491	H	-2.50585	2.392992	-1.03855
C	-1.29995	3.602695	-1.47736	C	-0.76547	3.306245	-1.95243
C	-3.73865	3.113879	-1.58355	C	-3.03421	2.969723	-3.00884
H	-1.2593	3.539274	-2.56811	H	-0.31891	3.367724	-2.94926
H	-1.58831	4.623748	-1.21657	H	-1.09346	4.311641	-1.68114
C	0.045457	3.260422	-0.88007	C	0.24235	2.779786	-0.95813
O	-4.20363	2.732099	-2.63123	O	-3.3092	2.497705	-4.08721
C	1.038628	2.636312	-1.64114	C	1.394972	2.1123	-1.3809
C	0.316669	3.523855	0.470642	C	0.013645	2.898123	0.419156
H	0.860531	2.427322	-2.69092	H	1.599033	2.007918	-2.44122
C	2.266026	2.277598	-1.07963	C	2.294182	1.565186	-0.46428
C	1.533238	3.172359	1.045093	C	0.89931	2.358591	1.347046
H	-0.43453	4.011212	1.083551	H	-0.87225	3.41434	0.774415
H	3.024704	1.795821	-1.68727	H	3.17875	1.041883	-0.81082
C	2.5124	2.543705	0.268016	C	2.038543	1.685735	0.900766

H	1.738717	3.380134	2.088417	H	0.717706	2.447768	2.411275
O	3.689293	2.218841	0.884907	O	2.860514	1.141297	1.860994
H	4.285431	1.79084	0.258315	H	3.641258	0.749933	1.449131
H	-0.74258	-2.10673	-0.87024	H	-0.10195	-2.05906	-3.3513
O	-4.3068	4.067398	-0.82349	O	-3.5814	4.101844	-2.53245
H	-5.10768	4.382842	-1.27239	H	-4.19473	4.453772	-3.19757
O	-7.28292	1.525614	0.13626	O	-1.41458	-3.0119	1.093723
H	-6.73806	0.743855	0.339696	H	-2.35472	-1.68137	-3.1521
H	-8.15781	1.311929	0.477858	H	-2.03719	-3.71344	0.854604
				O	1.04929	-1.07513	2.700065
				H	1.701062	-0.37743	2.539295
				H	0.523905	-1.11389	1.881279

Asn-Val

Reactant Structure				Product Structure			
Atom	X	Y	Z	Atom	X	Y	Z
N	-3.04427	-2.82682	-0.89639	N	-3.83242	-1.46151	-0.34872
H	-2.7109	-3.78639	-0.93554	H	-3.32405	-2.25508	-0.72996
C	-2.61621	-2.16467	0.282083	C	-3.29574	-1.07425	0.955659
C	-3.02971	-2.43006	1.710828	C	-3.02777	-2.23533	1.924135
C	-1.72596	-1.16352	0.294316	C	-2.0302	-0.21253	0.818792
H	-4.10199	-2.31596	1.901367	H	-2.35149	-2.96672	1.468105
H	-2.73821	-3.41651	2.091603	H	-2.52778	-1.86619	2.825366
C	-2.27009	-1.36086	2.463425	C	-4.29465	-2.93497	2.352379
O	-1.47921	-0.67303	1.582925	O	-1.31282	0.041301	1.788884
O	-2.28396	-1.0525	3.629964	O	-5.41594	-2.54279	2.097066
N	-0.97703	-0.55845	-0.68801	N	-1.79216	0.265417	-0.41566
H	-1.32265	-0.82314	-1.60297	H	-2.48238	0.046705	-1.12257
C	-0.66853	0.865193	-0.54575	C	-0.68637	1.155895	-0.69417
H	-0.0651	0.986845	0.354163	H	0.225501	0.716897	-0.28291
C	0.17633	1.363875	-1.74748	C	-0.50375	1.328755	-2.22803
C	-1.93944	1.694796	-0.3622	C	-0.8958	2.496289	0.012346
H	1.02039	0.666734	-1.7901	H	-0.49566	0.304214	-2.61757
C	-0.56645	1.306645	-3.08958	C	-1.66233	2.089568	-2.88868
C	0.729726	2.771406	-1.48767	C	0.845461	1.970505	-2.57359
O	-2.98576	1.493394	-0.93232	O	-1.96919	2.995097	0.260047
H	-1.42471	1.983898	-3.0983	H	-1.68634	3.132823	-2.56045
H	0.110024	1.608863	-3.89298	H	-1.53635	2.082165	-3.97409
H	-0.92686	0.303639	-3.33343	H	-2.63781	1.649285	-2.66614
H	1.271164	2.821373	-0.53913	H	1.676339	1.424797	-2.11829
H	1.4189	3.051597	-2.28792	H	0.988235	1.965297	-3.65712
H	-0.06955	3.517722	-1.4604	H	0.894578	3.007826	-2.23315
H	-4.05775	-2.86242	-0.95721	H	-4.79932	-1.75023	-0.24761
O	-1.76692	2.693919	0.530116	O	0.276596	3.085845	0.303298
H	-2.58753	3.212642	0.575459	H	0.093921	3.95089	0.704815
O	-1.43392	1.827079	3.586311	O	-4.15488	-4.05748	3.075878
H	-1.65057	0.884333	3.663876	H	-4.03218	-0.41134	1.421505
H	-1.46258	2.005358	2.637456	H	-3.22329	-4.27448	3.224577
				O	-7.66746	-4.00997	3.034425
				H	-6.87155	-3.5329	2.732512

				H	-7.32668	-4.7517	3.545773