Dynameomics Rotamer Libraries

The Dynameomics database is a research project managed by Dr. Valerie Daggett at the University of Washington. Six rotamer libraries have been compiled from molecular dynamics simulations within the Dynameomics database. Two rotamer libraries were constructed using native state simulations of 807 Dynameomics fold family representative proteins, which cover essentially all of protein fold space. The remaining four were constructed from simulations of end-capped host-guest pentapeptide simulations using both L- (upper case letters) and D- (lower case letters) amino acids. These libraries have been made available to academic users for research purposes.

Dynameomics Backbone Independent (2016) This library contains a backbone independent rotamer library for L-amino acids compiled from simulations of Dynameomics fold family representatives. Details of the construction and analysis of this library are described in:

Towse, C.-L., Rysavy, S.J., Vulovic, I.M., Daggett, V. New Dynamic Rotamer Libraries: Data-Driven Analysis of Side Chain Conformational Propensities. **Structure** *24*: 187-199, 2016.

Scouras A.D. and Daggett V. The Dynameomics rotamer library: Amino acid side chain conformations and dynamics from comprehensive molecular dynamics simulations in water. **Protein Science** *20*:341-352, 2011.

Dynameomics Backbone Dependent (2016) This library contains a backbone dependent rotamer library for L-amino acids compiled from simulations of Dynameomics fold family representatives. Rotamer libraries are provided as a function of the backbone dihedral angles, ϕ and ψ, in $5° \times 5°$ bins. Details of the construction and analysis of this library are described in:

Towse, C.-L., Rysavy, S.J., Vulovic, I.M., Daggett, V. New Dynamic Rotamer Libraries: Data-Driven Analysis of Side Chain Conformational Propensities. **Structure** *24*: 187-199, 2016.

Scouras A.D. and Daggett V. The Dynameomics rotamer library: Amino acid side chain conformations and dynamics from comprehensive molecular dynamics simulations in water. **Protein Science** *20*:341-352, 2011.

AAXAA Backbone Independent (2018) This library contains a backbone independent rotamer library for the guest residues ('X', each of the standard 20 L-amino acids plus the protonated forms of Asp, Glu, and His) within an L-Alanine host pentapeptide. These data are appropriate for use with homochiral, all L-amino acid polypeptide systems. Details of the construction and analysis of this library are described in:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

aaxaa Backbone Independent (2018) This library contains a backbone independent rotamer library for the guest residues ('x', the D-amino acid counterparts to the 20 standard residues plus the protonated forms of D-Asp, D-Glu, and D-His) within a D-Alanine host pentapeptide. These

data are appropriate for use with homochiral, all D-amino acid polypeptide systems. Details of the construction and analysis of this library are described in:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

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Daggett Group Rotamer Library Request Form

Name:	
Research Topic	
Job Title:	
Name of PI:	
Department:	
Institution:	
Address:	
Phone Number:	
Academic Email Address:	

I request access to the following rotamer libraries compiled from the Dynameomics database:

☐	Dynameomics Backbone Independent (2016)
☐	Dynameomics Backbone Dependent (2016)
☐	AAXAA Backbone Independent (2018)
☐	aaxaa Backbone Independent (2018)
☐	AAxAA Backbone Independent (2018)
☐	aaXaa Backbone Independent (2018)

Daggett Group Rotamer Library User Agreement

I understand that if my request is granted, I will be bound by the following terms and conditions:

Access: Rotamer library access is granted for only the user named above and can be limited or terminated at anytime. Should the user change jobs, PI, department, or institution, a new access agreement must be signed and submitted. Other individuals must request access; no sharing of logins is allowed. Access to the database is intended for research purposes only. All materials and services provided on the database are protected by copyright or other intellectual property rights owned and controlled by Dr. Daggett and University of Washington.

Data use: You agree to use these data for internal research purposes only, and not distribute, publish, transfer, or otherwise make available the data to users other than those in your lab. If you are preparing a scientific publication or presentation and would like to publish or disclose the data from our database, you will need to obtain written permission from Dr. Daggett.

Feedback: You agree to provide us feedback on your use of our libraries and we are allowed to use any information you provide in improving our libraries.

Citation: Publications making use of these rotamer libraries must provide appropriate citations.

Publications that utilize the **Dynameomics Backbone Independent (2016)** rotamer library must cite:

Towse, C.-L., Rysavy, S.J., Vulovic, I.M., Daggett, V. New Dynamic Rotamer Libraries: Data-Driven Analysis of Side Chain Conformational Propensities. **Structure** *24*: 187-199, 2016.

Publications that utilize the **Dynameomics Backbone Dependent (2016)** rotamer library must cite:

Towse, C.-L., Rysavy, S.J., Vulovic, I.M., Daggett, V. New Dynamic Rotamer Libraries: Data-Driven Analysis of Side Chain Conformational Propensities. **Structure** *24*: 187-199, 2016.

Publications that utilize the **AAXAA (2018)** pentapeptide-derived rotamer library must cite:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

Publications that utilize the **aaxaa (2018)** pentapeptide-derived rotamer library must cite:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

Publications that utilize the **aaXaa (2018)** pentapeptide-derived rotamer library must cite:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

Publications that utilize the **AAxAA (2018)** pentapeptide-derived rotamer library must cite:

Childers, M.C., Towse, C.-L., Daggett, V. Molecular dynamics-derived libraries for D-amino acids within homochiral and heterochiral polypeptides, **Protein Engineering, Design and Selection**, *31*: 191-204, 2018.

We would also like to promote your publication(s) based on these data on our website, please forward an appropriate reference.

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I AGREE TO THE TERMS AND CONDITIONS

User Signature:

Signature _____

Date _____

Printed Name _____

Principal Investigator Signature:

Signature _____

Date _____

Printed Name _____

Rotamer Library Format & Nomenclature

Rotamer libraries are provided as compressed plain text files. Each rotameric state includes a set of side chain dihedral angles that define the state as well as the fractional population of that specific rotamer.

The following table lists the three letter codes for the amino acids described within these libraries.

Residue	3 Letter Code (L-amino acids)	3 Letter Code (D-amino acid)
Alanine	ALA	DAL
Arginine	ARG	DAR
Asparagine	ASN	DAN
Aspartic Acid (unprotonated)	ASP	DAS
Aspartic Acid (protonated)	ASH	DAH
Cysteine (oxidized)	CYS	DCY
Cysteine (reduced)	CYH	DCP
Glutamic Acid (unprotonated)	GLU	DGL
Glutamic Acid (protonated)	GLH	DGH
Glutamine	GLN	DGN
Glycine	GLY	GLY
Histidine (d-protonated)	HID	DHD
Histidine (e-protonated)	HIE	DHE
Histidine (d,e-protonated)	HIP	DHP
Isoleucine	ILE	DIL
Leucine	LEU	DLE
Lysine	LYS	DLY
Methionine	MET	MED
Phenylalanine	PHE	DPN
Proline	PRO	DPR
Serine	SER	DSN
Threonine	THR	DTH
Tryptophan	TRP	DTR
Tyrosine	TYR	DTY
Valine	VAL	DVA