Supplemental material

We provide parameters used for harmonic functions described by Eq. 18 to sample coordinates of fragments Ace, Ala, and Nme. For coordinates histogrammed from a short Langevin simulation we provide names of text files which are attached separately. Additional details regarding the use of the parameters can be found in the main text, Sec. IIG.

I. PARAMETERS FOR FRAGMENT ACE

A. Internal coordinate definitions for fragment Ace

1	CT						
2	C	1	x_1				
3	O	2	x_2	1	x_3		
4	HC	1	x_4	2	x_5	3	x_6
5	HC	1	x_7	2	x_8	3	x_9
6	HC	1	x_{10}	2	x_{11}	3	x_{12}
7	N	2		1	x_{13}	3	x_{14}

B. Parameters for bond lengths

Coordinate	$\bar{x}_i$, Å	σ_i^2, Å^2
x_1	1.5224	9.233×10^{-4}
x_2	1.23	5.436×10^{-4}
x_4	1.0911	9.381×10^{-4}
x_7	1.0911	9.381×10^{-4}
x_{10}	1.0911	9.381×10^{-4}

C. Parameters for bond angles

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_3	120.56	2.955×10^{-3}
x_5	110.44	6.377×10^{-3}
x_8	110.44	6.377×10^{-3}
x_{11}	110.44	6.377×10^{-3}
x_{13}	117.54	2.424×10^{-3}

D. Parameters for dihedrals

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_{14}	180.0	6.872×10^{-3}

E. Parameters for dependent dihedrals

Dependent dihedrals are defined in terms of another diheral which is sampled first. The equilibrium position for a dependent dihedral is described as $\bar{x}_i = x_j + \overline{\Delta x}_{ij}$, where x_j is the actual value of the dihedral on which x_i depends on and $\overline{\Delta x}_{ij}$ is the average

equilibrium difference between dihedrals x_i and x_j. An example of a dependent dihedral can be hydrogen atoms in the methyl group. One of the hydrogens can be sampled first and then the other hydrogen atoms can be sampled based on the position of the first hydrogen.

Coordinate	Depends on coordinate	$\overline{\Delta x}_{ij}$, deg	σ_i^2, deg^2
x_9	x_6	-120.0	1.273×10^{-2}
x_{12}	x_6	120.0	1.273×10^{-2}

F. Coordinates histogrammed from a Langevin simulation

Coordinates for which probability distibutions were directly extracted from a short Langevin simulation are listed along with corresponding files. The file consists of two columns: first column is the coordinate and the second is the corresponding probability.

Coordinate	File
x_6	ace-x6-pdf.dat

II. PARAMETERS FOR FRAGMENT ALA

A. Internal coordinate definitions for fragment Ala.

1	CT						
2	C	1					
3	O	2		1			
4	N	2	x_1	1		3	
5	CT	4	x_2	2	x_3	1	x_4
6	C	5	x_5	4	x_6	2	x_7
7	O	6	x_8	5	x_9	4	x_{10}
8	H	4	x_{11}	2	x_{12}	1	x_{13}
9	HC	5	x_{14}	4	x_{15}	2	x_{16}
10	CT	5	x_{17}	4	x_{18}	2	x_{19}
11	HC	10	x_{20}	5	x_{21}	4	x_{22}
12	HC	10	x_{23}	5	x_{24}	4	x_{25}
13	HC	10	x_{26}	5	x_{27}	4	x_{28}
14	N	6		5	x_{29}	4	x_{30}

B. Parameters for bond lengths

Coordinate	$\bar{x}_i$, Å	σ_i^2, Å^2
x_1	1.337	6.11×10^{-4}
x_2	1.464	8.573×10^{-4}
x_5	1.541	9.02×10^{-4}
x_8	1.234	7.462×10^{-4}
x_{11}	1.012	9.417×10^{-4}
x_{14}	1.093	9.249×10^{-4}
x_{17}	1.542	1.063×10^{-3}
x_{20}	1.092	9.417×10^{-4}
x_{23}	1.092	9.417×10^{-4}
x_{26}	1.092	9.417×10^{-4}

C. Parameters for bond angles

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_3	126.1	3.236×10^{-3}
x_6	110.1	3.731×10^{-3}
x_9	121.2	2.294×10^{-3}
x_{12}	116.9	5.23×10^{-3}
x_{15}	109.7	5.544×10^{-3}
x_{18}	108.9	3.053×10^{-3}
x_{21}	111.4	6.093×10^{-3}
x_{24}	111.4	6.093×10^{-3}
x_{27}	111.4	6.093×10^{-3}
x_{29}	117.5	2.494×10^{-3}

D. Parameters for dihedrals

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_4	180.0	2.256×10^{-2}
x_{13}	0.0	2.504×10^{-2}

E. Parameters for dependent dihedrals

Coordinate	Depends on coordinate	$\overline{\Delta x_{ij}}$, deg	σ_i^2, deg^2
x_{10}	x_{30}	-180.0	1.273×10^{-2}
x_{16}	x_7	119.225	1.273×10^{-2}
x_{19}	x_7	-120.596	1.273×10^{-2}
x_{25}	x_{22}	-120.0	1.273×10^{-2}
x_{28}	x_{22}	120.0	1.273×10^{-2}

F. Coordinates histogrammed from a Langevin simulation.

Coordinate	File
x_{22}	ala-x22-pdf.dat
$x_7,\ x_{30}$	ala-rama-pdf.dat

III. PARAMETERS FOR FRAGMENT NME

A. Internal coordinate definitions for fragment Nme

1	CT						
2	C	1					
3	O	2		1			
4	N	2	x_1	1		3	
5	CT	4	x_2	2	x_3	1	x_4
6	H	4	x_5	2	x_6	1	x_7
7	HC	5	x_8	4	x_9	2	x_{10}
8	HC	5	x_{11}	4	x_{12}	2	x_{13}
9	HC	5	x_{14}	4	x_{15}	2	x_{16}

B. Parameters for bond lengths

Coordinate	$\bar{x}_i$, Å	σ_i^2, Å^2
x_1	1.337	6.415×10^{-4}
x_2	1.46	7.779×10^{-4}
x_5	1.0129	7.434×10^{-4}
x_8	1.0916	9.85×10^{-4}
x_{11}	1.0916	9.85×10^{-4}
x_{14}	1.0916	9.85×10^{-4}

C. Parameters for bond angles

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_3	125.0	3.398×10^{-3}
x_6	116.66	5.141×10^{-3}
x_9	110.5	6.909×10^{-3}
x_{12}	110.5	6.909×10^{-3}
x_{15}	110.5	6.909×10^{-3}

D. Parameters for dihedrals

Coordinate	$\bar{x}_i$, deg	σ_i^2, deg^2
x_4	180.0	2.353×10^{-2}
x_7	0.0	2.462×10^{-2}

E. Parameters for dependent dihedrals

Coordinate	Depends on coordinate	$\overline{\Delta x}_{ij}$, deg	σ_i^2, deg^2
x_{13}	x_{10}	-120.0	1.231×10^{-2}
x_{16}	x_{10}	120.0	1.231×10^{-2}

F. Coordinates histogrammed from a Langevin simulation.

Coordinate	File
x_{10}	nme-x10-pdf.dat