

Supplementary Informations

August 22, 2022

Table 1. Torsional features and corresponding feature indexes used in TICA (Figure 7) and train classifier algorithms (Figure 14)

featureindex	atominds	featuregroup	featurizer	otherinfo	resids	resnames
0	[15, 17, 19, 22]	chi1	Dihedral	sin	[75]	[GLU]
1	[30, 32, 34, 37]	chi1	Dihedral	sin	[76]	[MET]
2	[47, 49, 51, 54]	chi1	Dihedral	sin	[77]	[ASN]
3	[61, 63, 65, 68]	chi1	Dihedral	sin	[78]	[TYR]
4	[82, 84, 86, 88]	chi1	Dihedral	sin	[79]	[VAL]
5	[98, 100, 102, 105]	chi1	Dihedral	sin	[80]	[SER]
6	[116, 118, 120, 126]	chi1	Dihedral	sin	[82]	[THR]
7	[130, 132, 134, 136]	chi1	Dihedral	sin	[83]	[VAL]
8	[146, 148, 150, 153]	chi1	Dihedral	sin	[84]	[SER]
9	[15, 17, 19, 22]	chi1	Dihedral	cos	[75]	[GLU]
10	[30, 32, 34, 37]	chi1	Dihedral	cos	[76]	[MET]
11	[47, 49, 51, 54]	chi1	Dihedral	cos	[77]	[ASN]
12	[61, 63, 65, 68]	chi1	Dihedral	cos	[78]	[TYR]
13	[82, 84, 86, 88]	chi1	Dihedral	cos	[79]	[VAL]
14	[98, 100, 102, 105]	chi1	Dihedral	cos	[80]	[SER]
15	[116, 118, 120, 126]	chi1	Dihedral	cos	[82]	[THR]
16	[130, 132, 134, 136]	chi1	Dihedral	cos	[83]	[VAL]
17	[146, 148, 150, 153]	chi1	Dihedral	cos	[84]	[SER]
18	[17, 19, 22, 25]	chi2	Dihedral	sin	[75]	[GLU]
19	[32, 34, 37, 40]	chi2	Dihedral	sin	[76]	[MET]
20	[49, 51, 54, 55]	chi2	Dihedral	sin	[77]	[ASN]
21	[63, 65, 68, 69]	chi2	Dihedral	sin	[78]	[TYR]
22	[17, 19, 22, 25]	chi2	Dihedral	cos	[75]	[GLU]
23	[32, 34, 37, 40]	chi2	Dihedral	cos	[76]	[MET]
24	[49, 51, 54, 55]	chi2	Dihedral	cos	[77]	[ASN]
25	[63, 65, 68, 69]	chi2	Dihedral	cos	[78]	[TYR]