Table S1. Gay-Berne parameters for the coarse-grained particles defined in dipeptide models.

Index of Gay-Berne Site	L (Å)	D (Å)	d_w	ε_0 (kcal/mol)	ε_E (kcal/mol)	ε_S (kcal/mol)
111	2.475	2.475	0.931	0.363	1.000	1.000
122	3.763	2.462	1.202	0.481	1.479	1.437
152	3.763	2.462	0.942	0.381	1.479	1.437
182	2.475	2.475	0.943	0.363	1.000	1.000
192	2.475	2.475	1.243	0.263	1.000	1.000
202	2.275	2.275	1.243	0.263	1.000	1.000
222	4.257	2.484	0.977	0.496	1.446	0.411
232	2.475	2.475	0.931	0.143	1.000	1.000
242	3.763	2.462	0.942	0.481	1.479	0.437
262	3.722	2.662	0.862	0.732	1.441	0.463
272	2.475	2.475	0.931	0.243	1.000	1.000
281	2.434	2.434	0.897	0.455	1.000	1.000
292	2.475	2.475	1.231	0.243	1.000	1.000
302	2.475	2.475	1.231	0.243	1.000	1.000
312	3.763	2.462	0.902	0.481	1.479	1.437
341	2.434	2.434	0.831	0.113	1.000	1.000
352	2.475	2.475	1.231	0.243	1.000	1.000
372	2.475	2.475	1.231	0.124	1.000	1.000
382	2.475	2.475	0.931	0.243	1.000	1.000
392	2.475	2.475	1.231	0.243	1.000	1.000
402	3.722	2.497	1.261	0.432	1.341	0.763
412	2.475	2.475	1.231	0.243	1.000	1.000
422	2.894	2.461	0.957	0.461	0.957	0.918
432	2.475	2.475	0.983	0.243	1.000	1.000
442	2.475	2.475	1.231	0.243	1.000	1.000
452	3.230	3.230	0.831	0.484	1.000	1.000
462	2.475	2.475	0.943	0.243	1.000	1.000
472	2.789	2.416	0.726	0.693	1.475	0.726
482	2.475	2.475	0.931	0.243	1.000	1.000
492	2.743	4.527	0.588	0.246	1.452	0.692
511	2.475	2.475	1.231	0.010	1.000	1.000
522	2.775	2.775	0.931	0.234	1.000	1.000
532	2.475	2.475	1.231	0.243	1.000	1.000
541	2.073	2.073	1.131	0.115	1.000	1.000
552	2.475	2.475	1.251	0.023	1.000	1.000
561	2.275	2.275	1.231	0.343	1.000	1.000
571	2.075	2.075	0.931	0.145	1.000	1.000

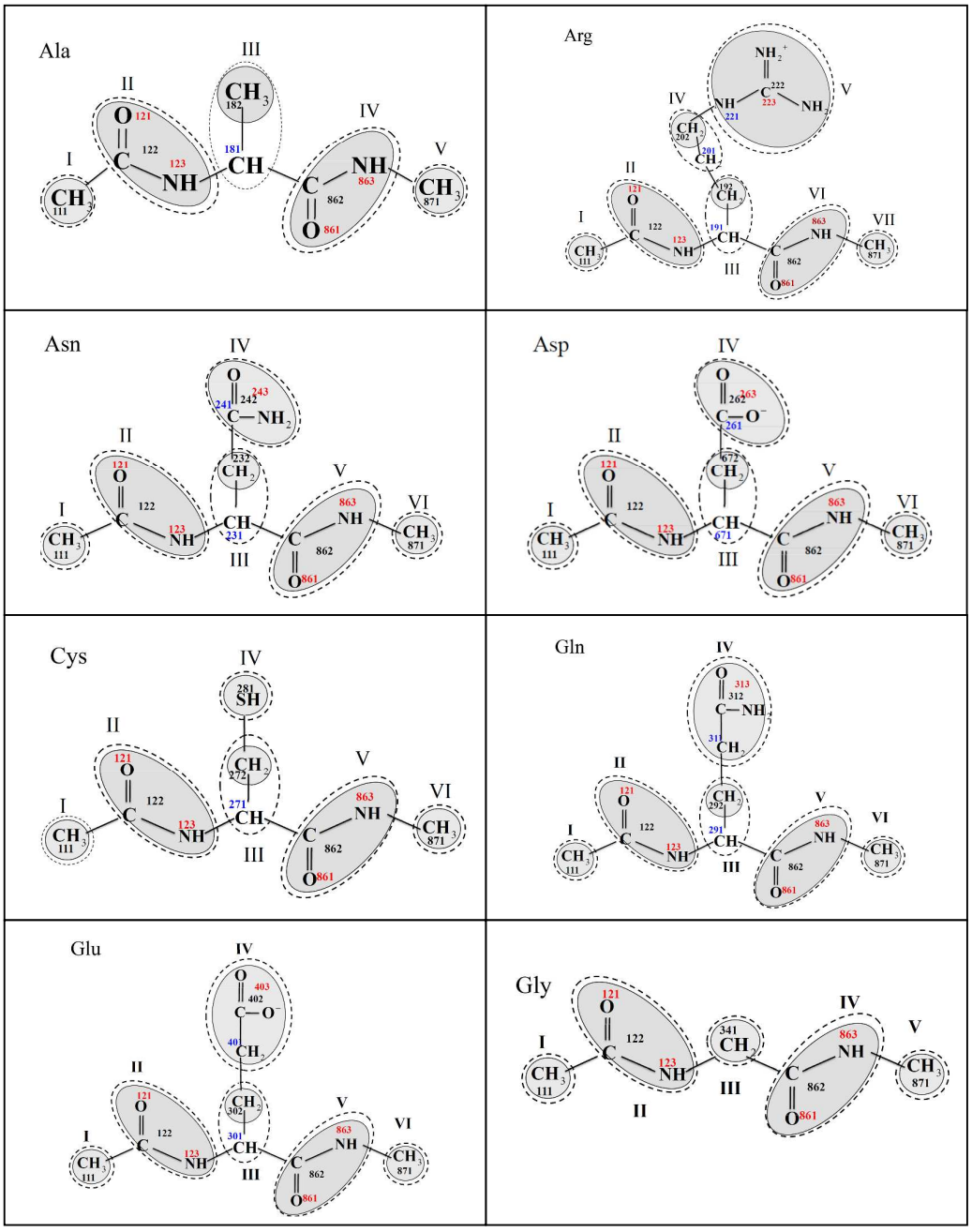
582	2.475	2.475	0.931	0.243	1.000	1.000
592	3.548	6.206	0.668	0.147	1.667	0.322
612	2.475	2.475	0.931	0.243	1.000	1.000
622	2.443	4.645	0.968	0.368	1.000	1.000
632	2.475	2.475	1.231	0.143	1.000	1.000
641	2.275	2.275	1.031	0.243	1.000	1.000
651	2.275	2.275	1.031	0.243	1.000	1.000
662	2.479	3.929	0.921	0.213	1.601	1.228
672	2.475	2.475	0.931	0.243	1.000	1.000
682	3.763	2.462	1.202	0.481	1.479	1.437
742	3.763	2.462	1.202	0.481	1.479	1.437
862	3.763	2.462	1.202	0.481	1.479	1.437
871	2.475	2.475	1.000	0.363	1.000	1.000

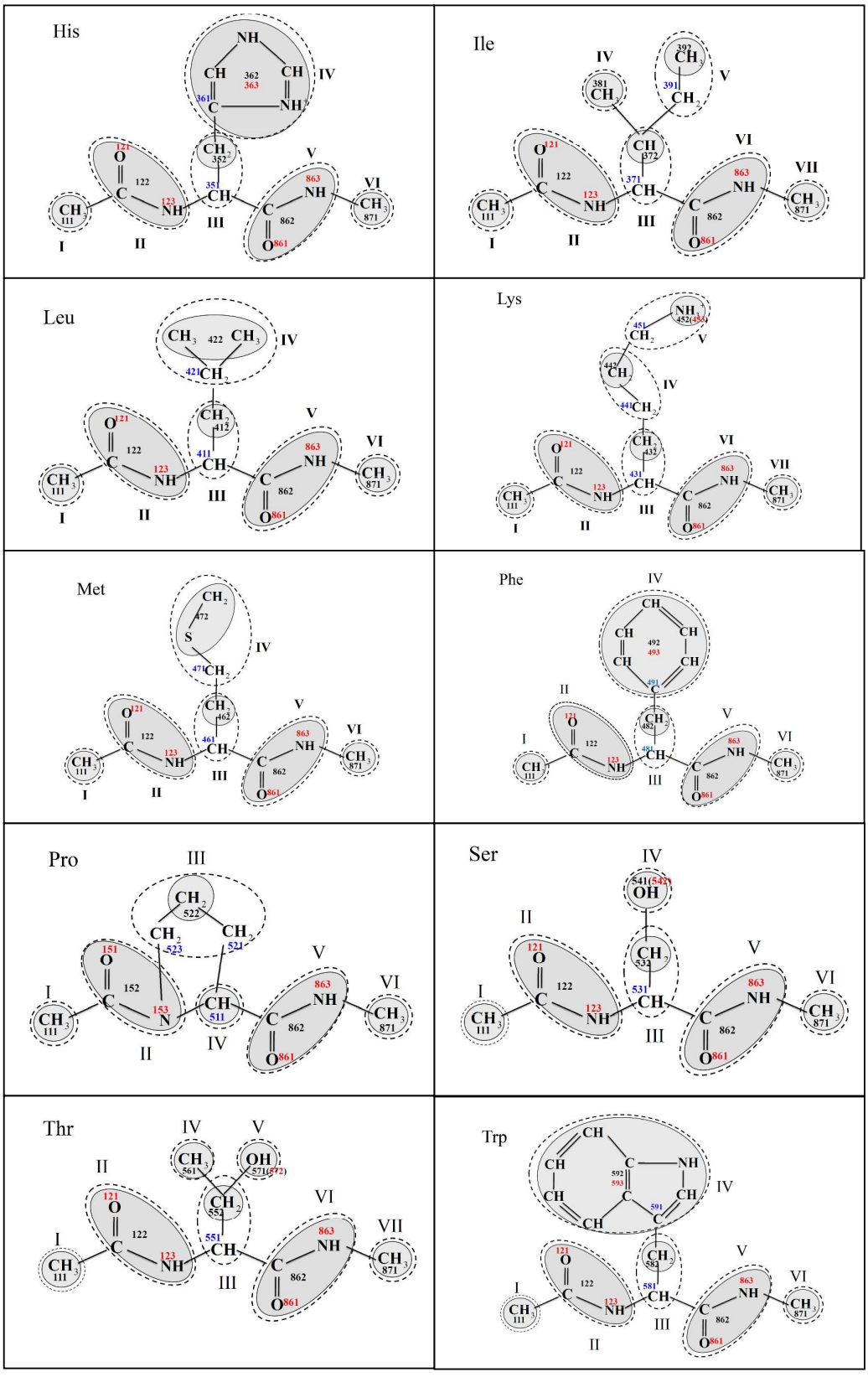
Table S2. EMP parameters for the coarse-grained particles defined in dipeptide models.

Index of EMP site	Charge	dipole	Qudrupole		
121	0.000	-1.463 0.281 -0.003	2.001 -1.148 -0.014	-1.148 -0.927 0.009	-0.014 0.009 -1.074
123	0.000	0.879 -0.437 -0.024	1.067 -1.148 0.138	-1.148 1.258 -0.128	0.138 -0.128 -2.325
151	0.000	-1.463 0.281 -0.003	2.001 -1.148 -0.014	-1.148 -0.927 0.009	-0.014 0.009 -1.074
153	0.000	0.879 -0.437 -0.024	1.067 -1.148 0.138	-1.148 1.258 -0.128	0.138 -0.128 -2.325
223	1.000	-2.743 -0.762 1.818	6.435 -3.860 -0.061	-3.860 2.459 -1.957	-0.061 -1.957 -8.894
243	0.000	-3.653 0.835 -0.086	-0.632 1.318 -0.330	1.318 2.936 0.391	-0.330 0.391 -2.305
263	-1.000	-3.378 0.670 -0.043	-0.632 0.318 -0.230	0.318 1.936 0.491	-0.230 0.491 -1.305
313	0.000	-3.653 0.835 -0.086	-0.632 1.318 -0.330	1.318 2.936 0.391	-0.330 0.391 -2.305
363	1.000	1.241 -1.801 -0.021	-0.605 0.604 -0.501	0.604 -0.700 -0.073	-0.501 -0.073 -1.305
403	0.000	-1.316 5.155 -0.260	3.729 3.893 -0.911	3.893 -13.165 0.044	-0.911 0.044 9.436
453	0.000	-1.316 5.155 -0.260	3.729 3.893 -0.911	3.893 -13.165 0.044	-0.911 0.044 9.436
493	0.000	-1.316 5.155 -0.260	3.729 3.893 -0.911	3.893 -13.165 0.044	-0.911 0.044 9.436
542	0.000	-3.653 0.835 -0.086	-0.632 1.318 -0.330	1.318 2.936 0.391	-0.330 0.391 -2.305

572	0.000	-3.653	-0.632	1.318	-0.330
		0.835	1.318	2.936	0.391
		-0.086	-0.330	0.391	-2.305
593	0.000	-3.653	-0.632	1.318	-0.330
		0.835	1.318	2.936	0.391
		-0.086	-0.330	0.391	-2.305
623	0.000	-3.653	-0.632	1.318	-0.330
		0.835	1.318	2.936	0.391
		-0.086	-0.330	0.391	-2.305
681	0.000	-1.463	2.001	-1.148	-0.014
		0.281	-1.148	-0.927	0.009
		-0.003	-0.014	0.009	-1.074
683	0.000	-0.879	1.067	-1.148	0.138
		-0.437	-1.148	1.258	-0.128
		-0.024	0.138	-0.128	-2.325
863	0.000	0.879	1.067	-1.148	0.138
		-0.437	-1.148	1.258	-0.128
		-0.024	0.138	-0.128	-2.325

Figure S1. GBEMP mapping schemes for amino acid dipeptides. Each rigid body, being enclosed by a dash line, consists of a Gay-Berne particle (represented by shadowed elliposoid, sphere or disk) with a few electric multipoles or without any electric multipole. The indices of rigid bodies, Gay-Berne sites, interacting EMP sites and non-interaction EMP sites (just serve as connecting different rigid bodies), are indicated by Roman numbers and Arabic numbers in black, red and blue, respectively.

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Lys
Met
Phe
Pro
Ser
Thr
Trp

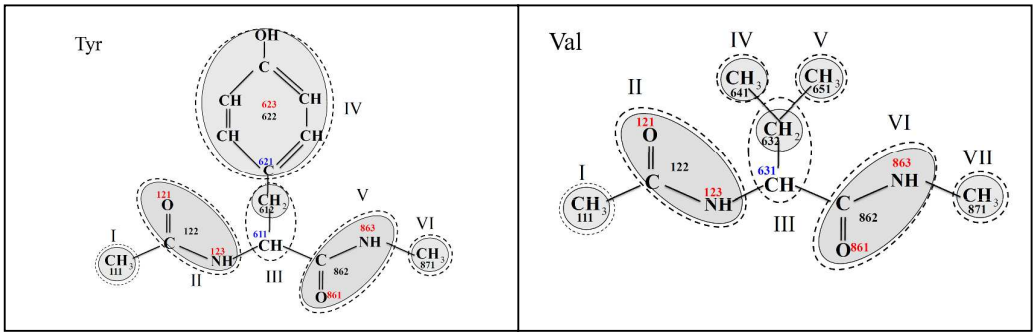
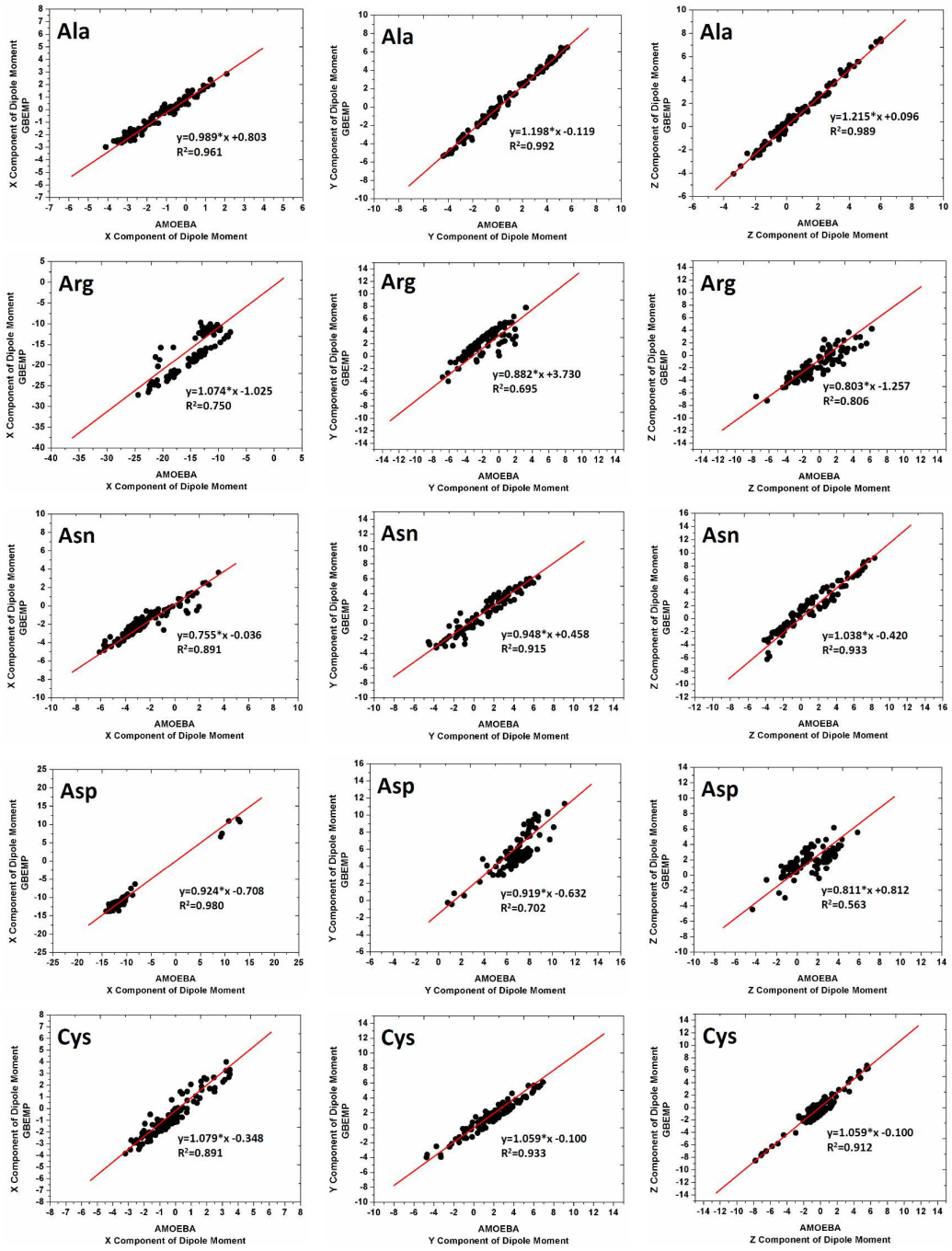
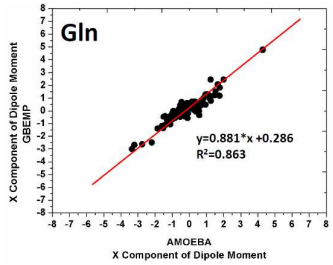
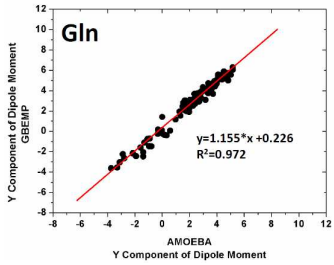
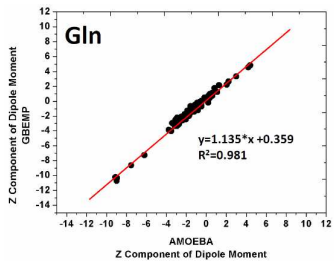

Tyr
OH
C
CH
CH
623
622
CH
CH
IV
621
121
O
CH3
612
V
122
611
863
NH
I
CH3
111
C
123
NH
CH
C
862
VI
CH3
871
II
III
O861
Val
IV
V
CH3
641
CH3
651
II
121
O
CH2
632
VI
122
631
863
NH
VII
I
CH3
111
C
123
NH
CH
C
CH3
871
862
III
O861

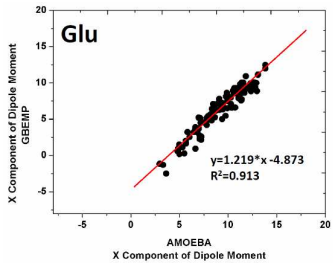
Figure S2. Correlations between GBEMP and AMOEBA results for calculating the x (left panel), y (middle panel) and z (right panel) components of the dipole moment of different dipeptide models (20 kinds of dipeptides in total). For each dipeptide, the conformations were chosen randomly from atomistic structures generated from atomistic MD simulation (AMOEBA force field).

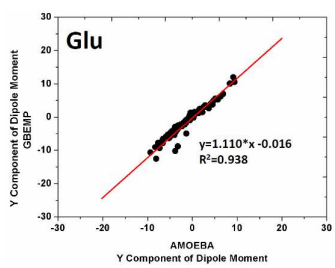


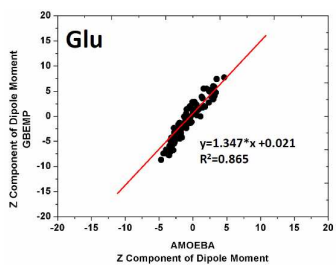

Gln
y=0.881*x +0.286
R²=0.863
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

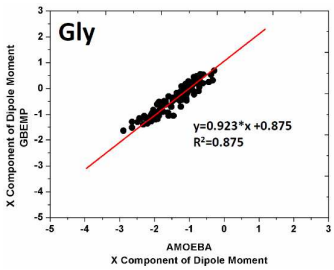

Gln
y=1.155*x +0.226
R²=0.972
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

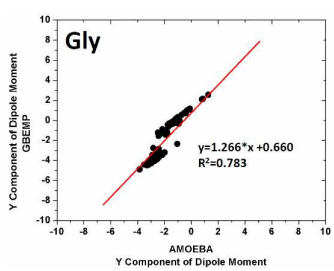

Gln
y=1.135*x +0.359
R²=0.981
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

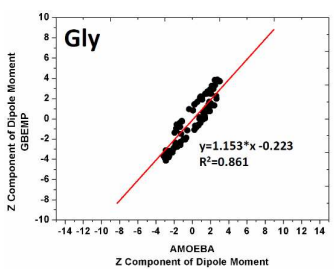

Glu
y=1.219*x -4.873
R²=0.913
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

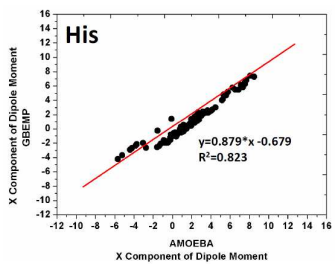

Glu
y=1.110*x -0.016
R²=0.938
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

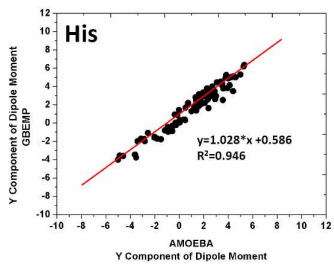

Glu
y=1.347*x +0.021
R²=0.865
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

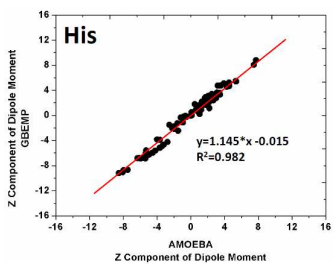

Gly
y=0.923*x +0.875
R²=0.875
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

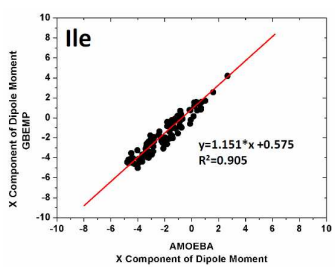

Gly
y=1.266*x +0.660
R²=0.783
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

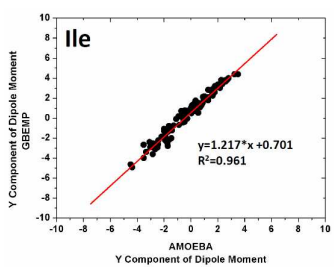

Gly
y=1.153*x -0.223
R²=0.861
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

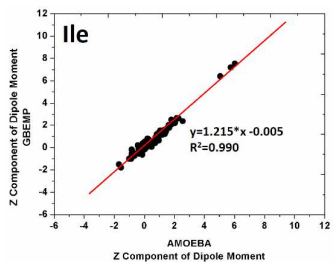

His
y=0.879*x -0.679
R²=0.823
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

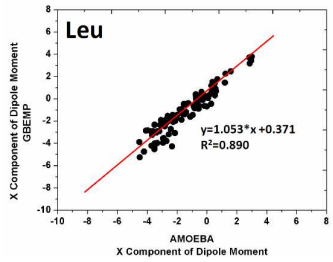

His
y=1.028*x +0.586
R²=0.946
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

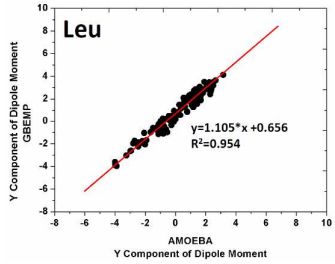

His
y=1.145*x -0.015
R²=0.982
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

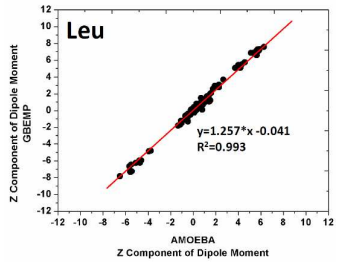

Ile
y=1.151*x +0.575
R²=0.905
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

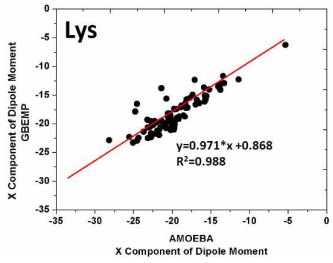

Ile
y=1.217*x +0.701
R²=0.961
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

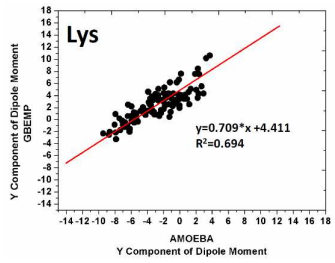

Ile
y=1.215*x -0.005
R²=0.990
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

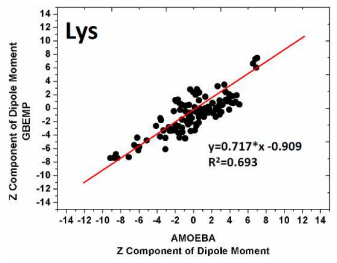

Leu
y=1.053*x +0.371
R²=0.890
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

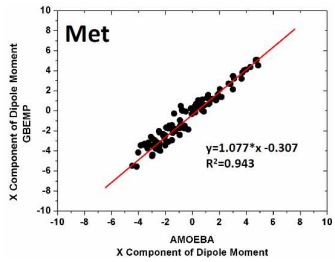

Leu
y=1.105*x +0.656
R²=0.954
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

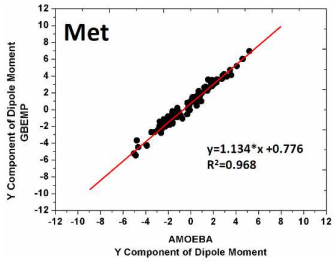

Leu
y=1.257*x -0.041
R²=0.993
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

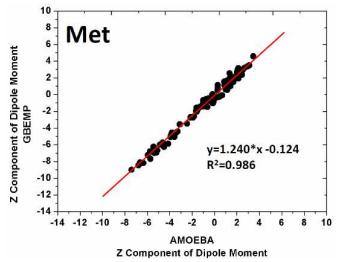

Lys
y=0.971*x +0.868
R²=0.988
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

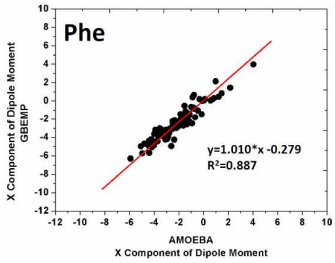

Lys
y=0.709*x +4.411
R²=0.694
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

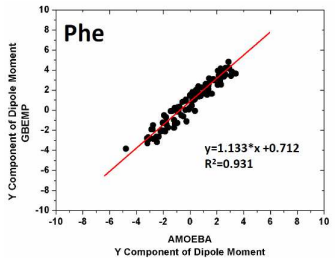

Lys
y=0.717*x -0.909
R²=0.693
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

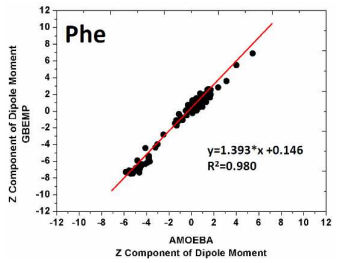

Met
y=1.077*x -0.307
R²=0.943
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment

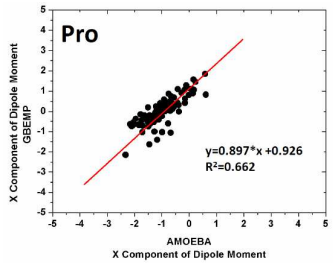

Met
y=1.134*x +0.776
R²=0.968
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment

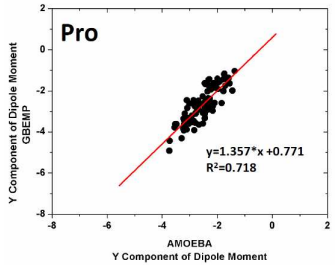

Met
y=1.240*x -0.124
R²=0.986
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

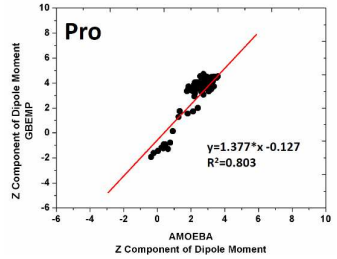

Phe
y=1.010*x -0.279
R²=0.887
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment


Phe
y=1.133*x +0.712
R²=0.931
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment


Phe
y=1.393*x +0.146
R²=0.980
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment


Pro
y=0.897*x +0.926
R²=0.662
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment


Pro
y=1.357*x +0.771
R²=0.718
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment


Pro
y=1.377*x -0.127
R²=0.803
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

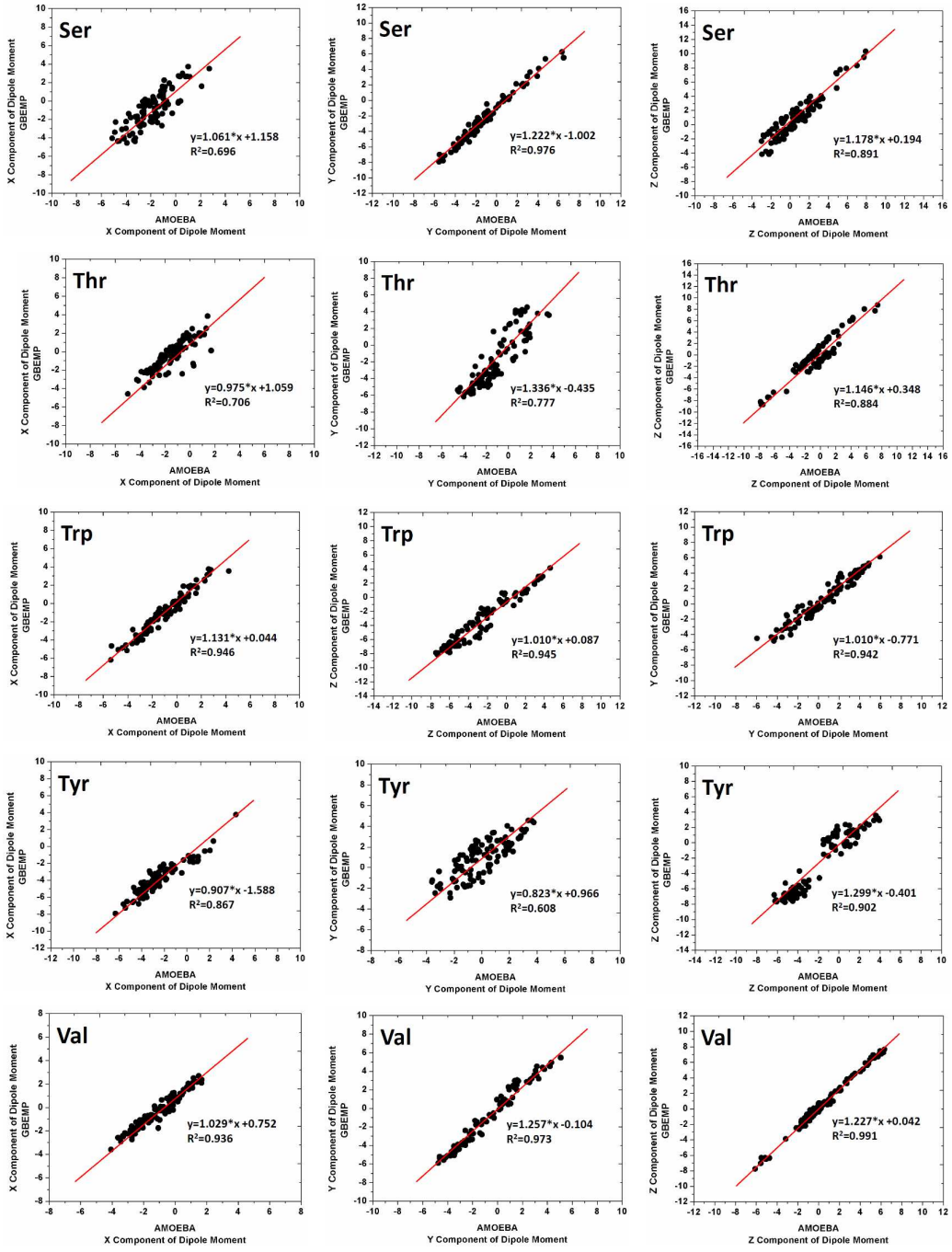
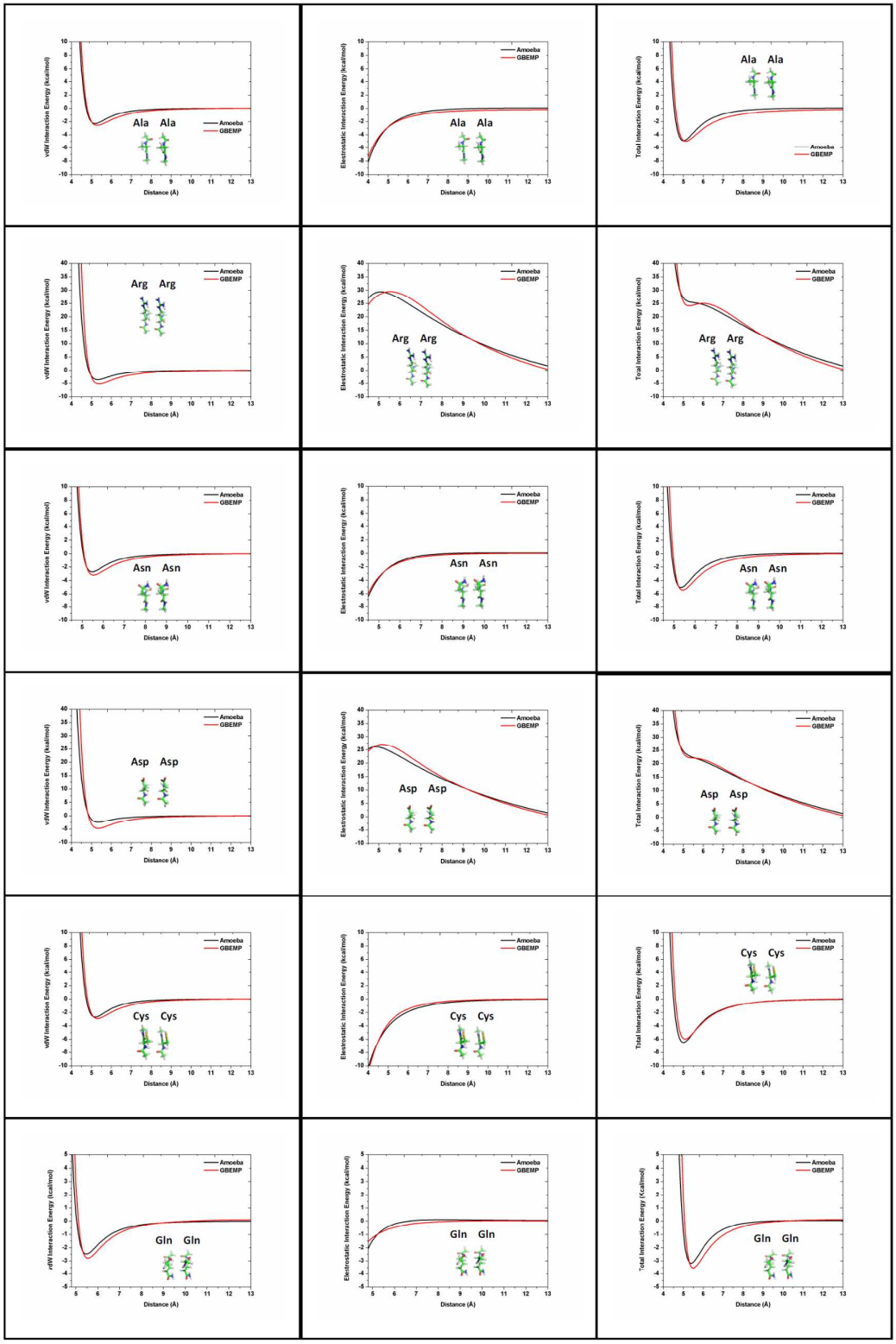
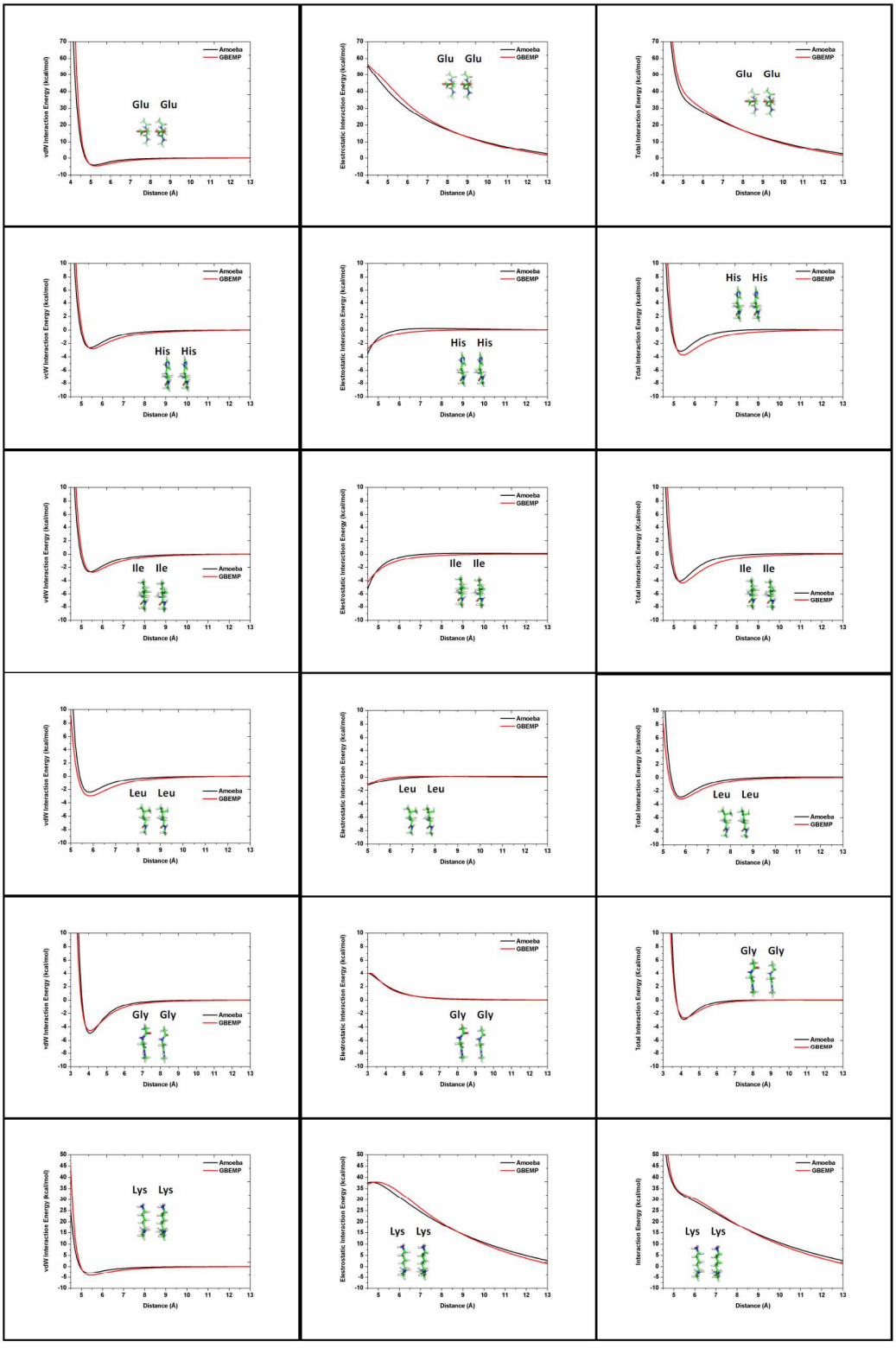
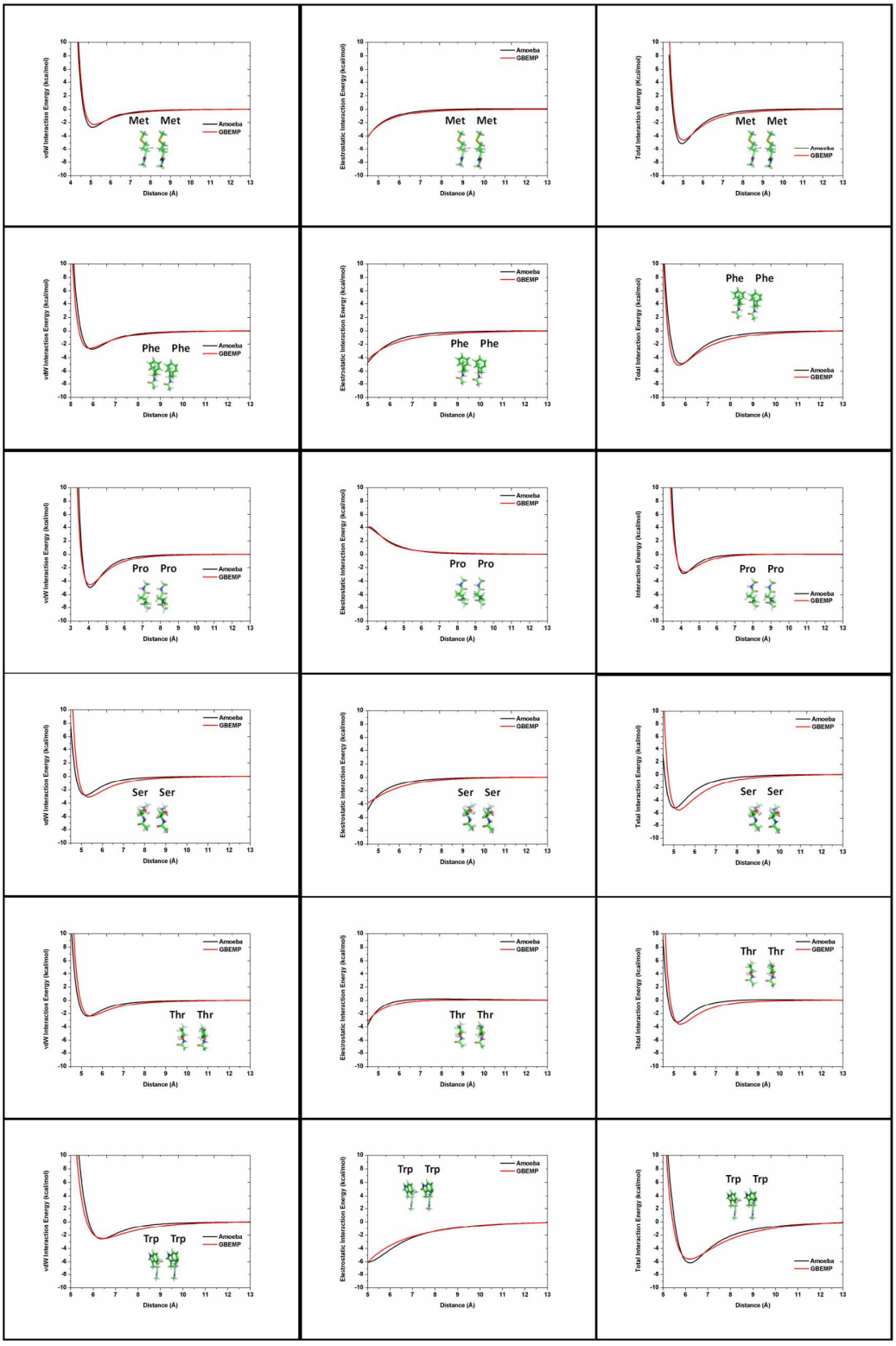

Ser
y=1.061*x +1.158
R²=0.696
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment
Ser
y=1.222*x -1.002
R²=0.976
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment
Ser
y=1.178*x +0.194
R²=0.891
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment
Thr
y=0.975*x +1.059
R²=0.706
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment
Thr
y=1.336*x -0.435
R²=0.777
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment
Thr
y=1.146*x +0.348
R²=0.884
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment
Trp
y=1.131*x +0.044
R²=0.946
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment
Trp
y=1.010*x +0.087
R²=0.945
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment
Trp
y=1.010*x -0.771
R²=0.942
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment
Tyr
y=0.907*x -1.588
R²=0.867
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment
Tyr
y=0.823*x +0.966
R²=0.608
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment
Tyr
y=1.299*x -0.401
R²=0.902
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment
Val
y=1.029*x +0.752
R²=0.936
X Component of Dipole Moment GBEMP
AMOEBA
X Component of Dipole Moment
Val
y=1.257*x -0.104
R²=0.973
Y Component of Dipole Moment GBEMP
AMOEBA
Y Component of Dipole Moment
Val
y=1.227*x +0.042
R²=0.991
Z Component of Dipole Moment GBEMP
AMOEBA
Z Component of Dipole Moment

Figure S3. Intermolecular interaction energies for 20 dipeptide homodimers and 3 dipeptide heterodimers, obtained from AMOEBA atomistic force field (in black) and GBEMP coarse-grained force field (in red). Left, middle and right columns show van der Waals, electrostatic and total interaction energies respectively.




vdW Interaction Energy (kcal/mol)
Electrostatic Interaction Energy (kcal/mol)
Total Interaction Energy (kcal/mol)
Interaction Energy (kcal/mol)
Distance (Å)
Amoeba
GBEMP
Glu Glu
His His
Ile Ile
Leu Leu
Gly Gly
Lys Lys


vdW Interaction Energy (kcal/mol)
Electrostatic Interaction Energy (kcal/mol)
Total Interaction Energy (Kcal/mol)
Interaction Energy (kcal/mol)
Distance (Å)
Amoeba
GBEMP
Met Met
Phe Phe
Pro Pro
Ser Ser
Thr Thr
Trp Trp

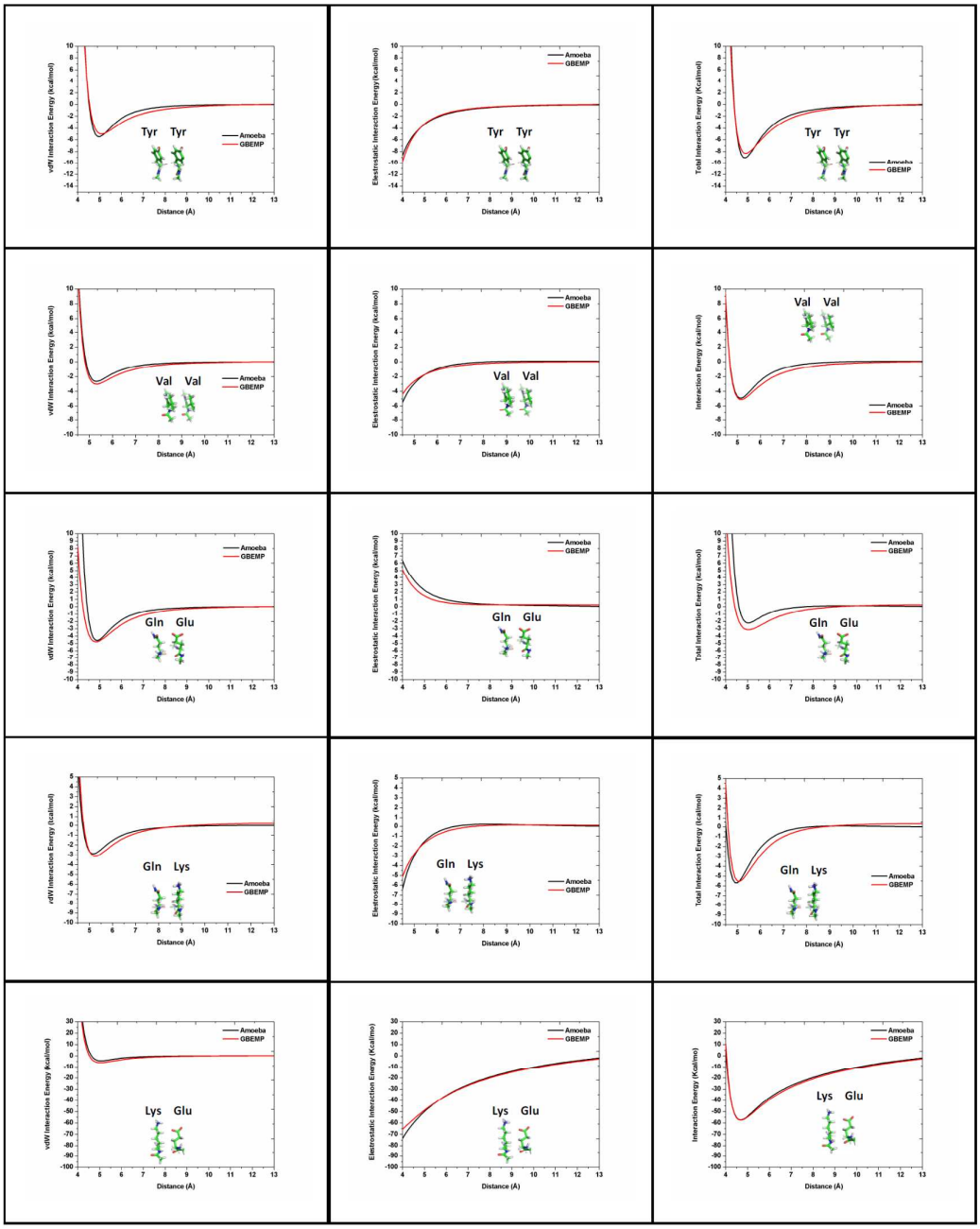
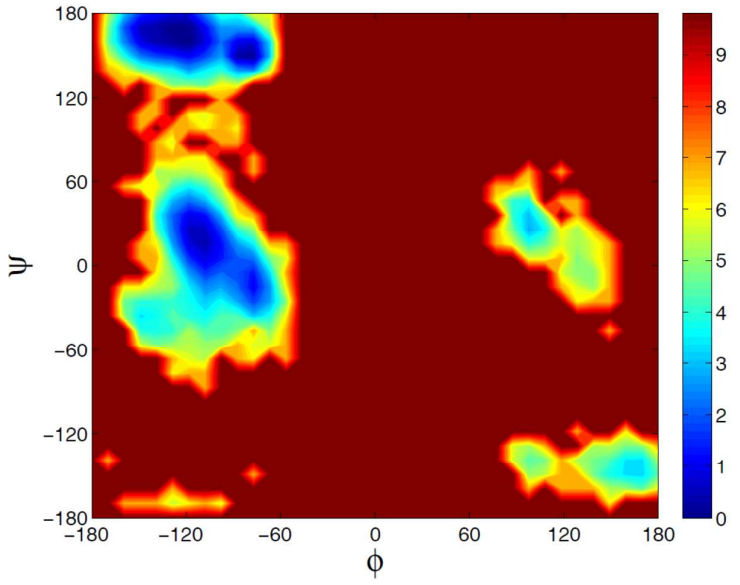
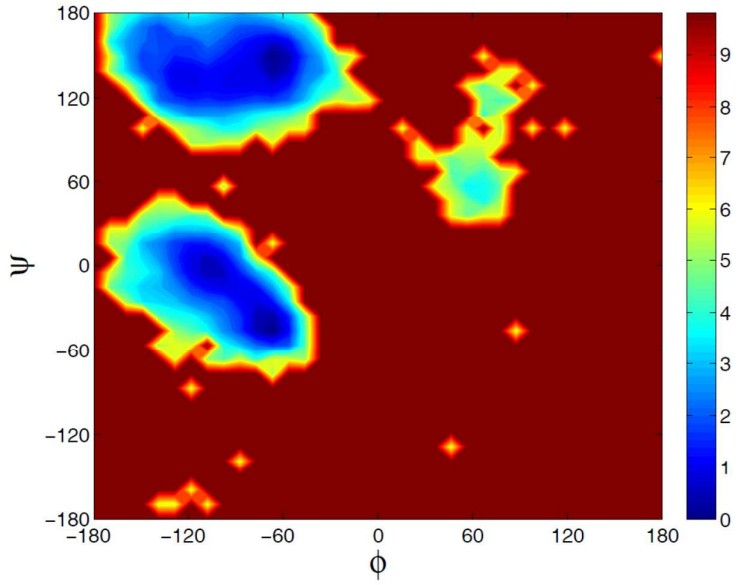

vdW Interaction Energy (kcal/mol)
Electrostatic Interaction Energy (kcal/mol)
Total Interaction Energy (Kcal/mol)
Interaction Energy (Kcal/mol)
Distance (Å)
Amoeba
GBEMP
Tyr Tyr
Val Val
Gln Glu
Gln Lys
Lys Glu

Figure S4. Potentials of mean force (PMFs) for the (ϕ/ψ) distribution for valine (Val), calculated from (A) GBEMP and (B) CHARMM simulations. The color bars represent free energy in the unit of kcal/mol.

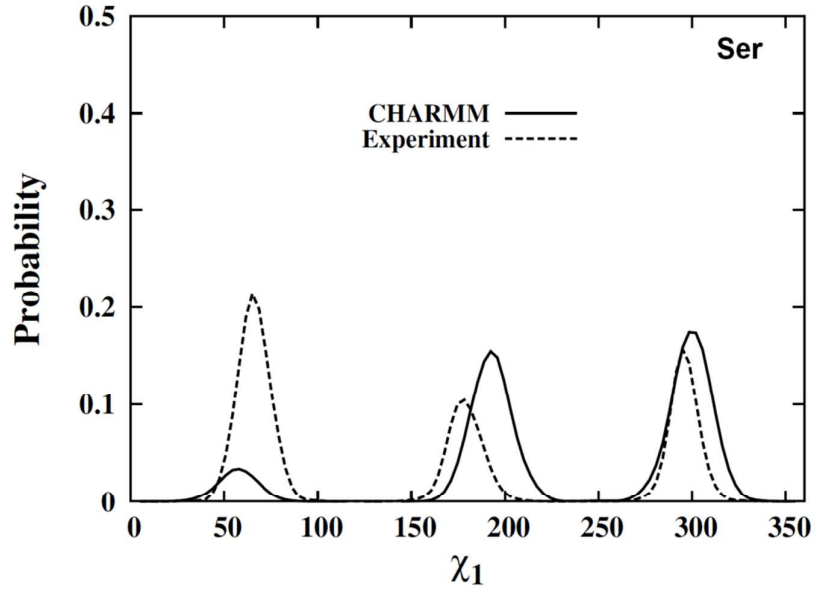


(A)

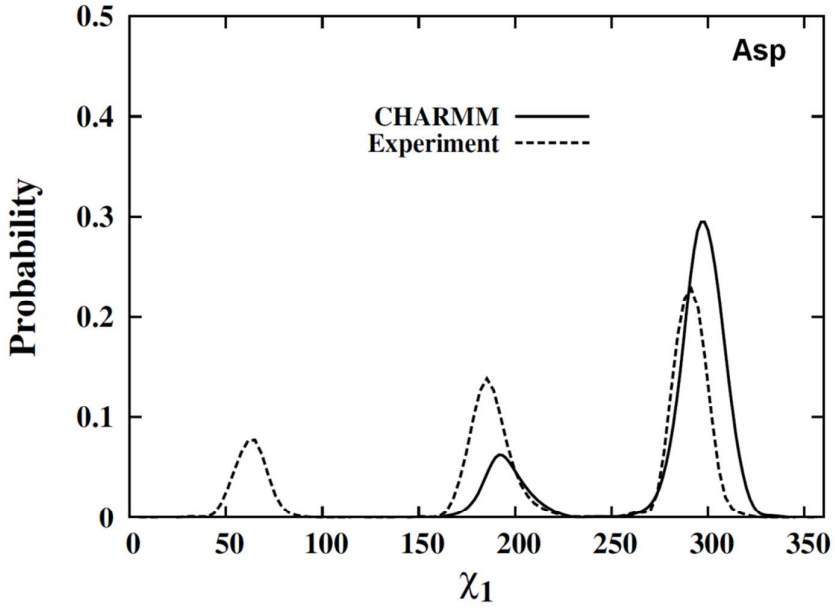


(B)

Figure S5 Distribution of the side chain torsion χ_1 for (A) serine (Ser) and (B) aspartic acid (Asp) from the protein structures (Dunbrack Library) and CHARMM atomistic simulations of dipeptides. Experimental and CHARMM results are represented by the dash and solid lines respectively.



(A)



(B)