

S22-2005 data set: Results with infinite non-bonded cut-offs

	MM2*	MM2* (LP)	MM3*	AMBER*	AMBER+1012	OPLS*	OPLSAA	MMFF94	MMFF94s	DFT (Lit)
<b>H-bonding</b>										
ME	-7.32	-6.89	-9.18	-3.63	-3.81	-3.33	-3.97	-3.16	-3.08	4.79
MUE	7.32	6.89	9.78	4.64	4.84	4.12	4.45	3.61	3.53	4.79
RMSE	8.41	8.42	11.22	5.66	5.82	5.08	5.19	4.33	4.23	5.18
<b>Stacking</b>										
ME	-0.76	-0.77	-1.74	-0.11	-0.12	-0.92	-0.63	0.02	0.02	-0.13
MUE	1.29	1.30	1.84	0.98	0.99	1.20	1.07	0.73	0.72	0.70
RMSE	2.37	2.37	2.87	1.19	1.20	1.53	1.44	0.93	0.93	0.78
<b>Mixed</b>										
ME	-2.16	-2.03	-1.67	0.66	0.67	0.20	-0.10	-0.37	-0.37	1.07
MUE	2.16	2.03	1.67	0.89	0.88	0.73	0.56	0.60	0.60	1.07
RMSE	2.40	2.27	2.13	1.14	1.14	0.91	0.62	0.68	0.68	1.25
<b>Total</b>										
MUE	<b>3.49</b>	<b>3.31</b>	<b>4.31</b>	<b>2.12</b>	<b>2.18</b>	<b>1.98</b>	<b>1.98</b>	<b>1.61</b>	<b>1.58</b>	<b>2.10</b>
RMSE	<b>5.14</b>	<b>5.12</b>	<b>6.67</b>	<b>3.33</b>	<b>3.42</b>	<b>3.05</b>	<b>3.07</b>	<b>2.54</b>	<b>2.48</b>	<b>3.04</b>

S22-2005 data set: Results with default (vdW 7 Å, electrostatic 12 Å) non-bonded cut-offs

	MM2*	MM2* (LP)	MM3*	AMBER*	AMBER+1012	OPLS*	OPLSAA	MMFF94	MMFF94s	DFT (Lit)
<b>H-bonding</b>										
ME	-7.32	-6.89	-9.18	-3.63	-3.70	-3.33	-3.97	-3.16	-3.08	4.79
MUE	7.32	6.89	9.78	4.64	4.73	4.12	4.45	3.61	3.53	4.79
RMSE	8.41	8.42	11.22	5.66	5.70	5.08	5.19	4.33	4.23	5.18
<b>Stacking</b>										
ME	-0.76	-0.77	-1.74	-0.11	-0.13	-0.92	-0.63	0.02	0.02	-0.13
MUE	1.29	1.30	1.84	0.98	0.99	1.20	1.07	0.73	0.72	0.70
RMSE	2.37	2.37	2.87	1.19	1.20	1.53	1.44	0.93	0.93	0.78
<b>Mixed</b>										
ME	-2.16	-2.03	-1.67	0.66	0.65	0.20	-0.10	-0.37	-0.37	1.07
MUE	2.16	2.03	1.67	0.89	0.88	0.73	0.56	0.60	0.60	1.07
RMSE	2.40	2.27	2.13	1.14	1.13	0.91	0.62	0.68	0.68	1.25
<b>Total</b>										
MUE	<b>3.49</b>	<b>3.31</b>	<b>4.31</b>	<b>2.12</b>	<b>2.14</b>	<b>1.98</b>	<b>1.98</b>	<b>1.61</b>	<b>1.58</b>	<b>2.10</b>
RMSE	<b>5.14</b>	<b>5.12</b>	<b>6.67</b>	<b>3.33</b>	<b>3.35</b>	<b>3.05</b>	<b>3.07</b>	<b>2.54</b>	<b>2.48</b>	<b>3.04</b>

JSCH-2005 data set: Results with default bond dipole cut-offs

	MM2*	MM2* (LP)	MM3*	AMBER*	AMBER+1012	OPLS*	OPLSAA	MMFF94	MMFF94s	DFT (Lit)
<b>H-bonding</b>										
ME	-7.34	-6.89	-9.21	-3.66	-3.84	-3.36	-4.00	-3.16	-3.08	4.79
MUE	7.34	6.89	9.80	4.67	4.87	4.15	4.48	3.61	3.54	4.79
RMSE	8.45	8.42	11.26	5.69	5.85	5.12	5.23	4.34	4.23	5.18
<b>Stacking</b>										
ME	-0.77	-0.77	-1.75	-0.12	-0.13	-0.93	-0.64	0.02	0.02	-0.13
MUE	1.30	1.30	1.84	0.98	0.99	1.20	1.07	0.73	0.72	0.70
RMSE	2.37	2.37	2.87	1.19	1.20	1.53	1.44	0.93	0.92	0.78
<b>Mixed</b>										
ME	-2.17	-2.03	-1.68	0.64	0.65	0.18	-0.12	-0.37	-0.37	1.07
MUE	2.17	2.03	1.68	0.89	0.88	0.72	0.55	0.60	0.60	1.07
RMSE	2.41	2.27	2.15	1.14	1.13	0.89	0.62	0.68	0.68	1.25
<b>Total</b>										
MUE	<b>3.50</b>	<b>3.31</b>	<b>4.32</b>	<b>2.13</b>	<b>2.19</b>	<b>1.99</b>	<b>1.99</b>	<b>1.61</b>	<b>1.58</b>	<b>2.10</b>
RMSE	<b>5.16</b>	<b>5.12</b>	<b>6.69</b>	<b>3.35</b>	<b>3.44</b>	<b>3.08</b>	<b>3.10</b>	<b>2.54</b>	<b>2.48</b>	<b>3.04</b>