# of water molecules	Double-precision(dp)				Mixed-precision(mp)				single-precision(sp)				Speedup(mp)	Speedup(sp)	Speedup /iteration (mp)	Speedup /iteration (sp)	mp vs. sp**
	Time/s	Iterations	Time/iteration	Accuracy*	Time /s	Iterations	Time/iteration	Accuracy	Time/s	Iterations	Time/iteration	Accuracy					
1	0.89	17	0.052352941	6	0.84	17	0.049411765	6	0.85	18	0.047222222	5	0.94382022	0.95505618	0.94382022	0.9019975	1.04636678
2	28.99	15	1.932666667	6	22.72	15	1.514666667	6	28.3	16	1.76875	5	0.78371852	0.97619869	0.78371852	0.91518627	0.85634865
3	342.64	16	21.415	6	222.76	16	13.9225	6	232.39	16	14.524375	4	0.65012841	0.67823371	0.65012841	0.67823371	0.95856104
4	1752.63	16	109.539375	6	1121.23	15	74.74866667	6	1152.7	16	72.04375	2	0.63974142	0.65769729	0.68239084	0.65769729	1.03754547
5	6996.3	17	411.5470588	6	4387.18	17	258.0694118	6	4682.54	18	260.1411111	5	0.62707145	0.66928805	0.62707145	0.63210538	0.99203625

Speedup(mp) = time(mp) / time(dp)

Speedup(sp) = time(sp) / time(dp)

*The accuracy is evaluated by comparing the results to the resulyts from PSI4, the number in the table is the number of digits that can match with PSI4

**The comparison of mp vs. sp is the ratio : 'time per iteration(mp) / time per iteration(sp)'