	ExaMiniMD			SWFFT			NEKbone		
	base	norm	poly	base	norm	poly	base	norm	poly
	(1562, 21)	(1562, 21)	(1562, 253)	(1618, 7)	(1618, 7)	(1618, 36)	(1579, 12)	(1579, 12)	(1579, 91)
Random Forest Regressor	**4764.0635**	**4344.310531**	6216.032985	**1984.463122**	2934.427639	**1950.449106**	**3.044853225**	**5.567193378**	**3.601639548**
Bayesian Ridge	7730.456744	7335.208279	6482.042066	4108.664267	4133.159498	3823.764683	13.91073033	12.77640106	7.500978111
SVR RBF	10120.01668	10119.17998	10148.71726	4368.249249	4368.669888	4366.061623	15.45483292	16.06738243	22.67029422
SVR poly 1	10078.91811	10076.3341	10150.29825	4364.522991	4369.286557	4342.563724	15.38666495	14.3280767	19.73967553
SVR poly 2	10157.10917	10152.80042	10151.30319	4329.654969	4363.462208	4244.064148	26.14556249	26.07264023	23.54561252
SVR poly 3	10091.59019	10090.78828	10153.04162	4269.752789	4368.340657	4032.488027	19.39532429	18.08152828	25.25771899
SVR sigmoid	10093.92853	10091.83707	10152.72053	4371.166088	4369.697273	4365.703857	16.08637268	14.70008479	20.07135868
Linear SGD Regressor	7927.628557	7488.17857	1.88807E+11	4112.130851	4131.58221	3876.717579	13.91938001	12.77738418	7.492680585
1NN Regressor	7468.294059	7705.558648	7280.469043	4613.103499	4896.980068	4749.619263	15.57436879	15.8905247	15.58813591
2NN Regressor	5948.171084	6482.735557	6044.297695	3832.246768	4235.656757	3690.293745	12.99773857	13.36825479	13.76908096
3NN Regressor	5458.098362	5841.793638	5675.6854	3670.077754	4054.454614	3540.377414	12.14990148	12.13905918	12.74128691
4NN Regressor	5208.57866	5552.29751	5431.693803	3719.987708	4003.825544	3661.034185	11.63936022	11.47894145	12.47266208
5NN Regressor	5152.027705	5379.906484	5467.067627	3640.755414	3909.405461	3458.508781	11.63953895	11.39414831	12.40888042
6NN Regressor	5127.556554	5284.267226	5431.507417	3628.158765	3764.559547	3552.046522	11.48507653	11.31048168	12.47938819
7NN Regressor	5179.451219	5249.574956	5465.172992	3615.848061	3777.844413	3544.018091	11.2424553	11.14222375	12.62152581
1 PLS Regression	8284.079663	8261.872841	8850.901526	4105.025942	4126.412677	3955.213893	15.63751258	13.89744037	15.75137981
2 PLS Regression	7508.58113	7472.08404	8496.058787	4108.507607	4126.257046	3836.64187	14.28339654	12.9111078	10.35366502
3 PLS Regression	7834.019319	7422.996532	7833.375707	4109.298424	4126.262593	3841.813525	13.93152899	12.7809775	8.255324176
4 PLS Regression	7977.663264	7526.007376	7403.047017	4109.25824	4126.263668	3842.33465	13.9110034	12.77649626	7.667895026
Decision Tree Regressor	6624.213927	6001.071861	8435.889115	**2320.195573**	3887.837932	**2122.509291**	**3.639024101**	7.557621643	**4.116250758**
1 MLP Regressor relu	7620.639923	9318.766969	6949.325099	4066.161382	4233.700716	3806.6849	6.607609646	7.476429498	6.802067508
1 MLP Regressor identity	8653.227927	9175.145963	7322.207498	4107.017751	4234.959925	3822.219383	13.91681649	12.77341891	7.502869386
1 MLP Regressor logistic	10842.08469	10821.93386	10853.70541	4338.270046	4339.042088	4337.601266	10.42096377	10.76678111	6.239098649
1 MLP Regressor tanh	10862.99289	10808.74715	10827.17304	4338.045305	4336.549787	4338.335149	**5.58313105**	7.902744896	7.409365629
2 MLP Regressor relu	5354.910336	5869.897705	6988.295187	3506.686653	3827.847763	2941.955442	6.381990634	6.892106524	7.807019547
2 MLP Regressor identity	8141.459571	7381.462806	6885.83083	4107.910929	4126.647308	3837.446434	13.92643386	12.76628715	7.542652368
2 MLP Regressor logistic	10850.70998	10841.5804	10860.48521	4340.435522	4339.866395	4343.986237	6.370689002	8.683666747	8.094524548
2 MLP Regressor tanh	10842.89539	10825.08915	10827.32742	4340.838193	4337.747468	4345.534466	**5.622828168**	**5.464777967**	7.951266986
3 MLP Regressor relu	5363.516327	**4723.886702**	6876.83982	**2705.189722**	3789.370489	2969.813025	6.952794781	7.449227394	8.022188246
3 MLP Regressor identity	8053.537416	7360.482815	6811.765731	4105.268507	4127.732332	3834.984429	13.95566632	12.79138106	7.692975548
3 MLP Regressor logistic	10869.42044	10869.34228	10867.4922	4348.238244	4348.209766	4347.516253	**5.774487471**	8.756217346	8.63026788
3 MLP Regressor tanh	10835.02308	10827.05044	10826.89322	4344.438815	4342.764441	4342.192106	6.555705236	**5.626514635**	7.901808663
4 MLP Regressor relu	5232.735121	**4732.432145**	6794.991558	**2681.016954**	3968.28712	2897.018906	7.435002378	7.610236295	7.99134921
4 MLP Regressor identity	7959.269829	7357.028798	6840.169282	4110.732405	4125.746512	3841.219239	13.95944308	12.76953866	7.579606692
4 MLP Regressor logistic	10872.74207	10872.73636	10863.14535	4350.246699	4350.242039	4348.738555	14.72643685	28.1411383	8.011969165
4 MLP Regressor tanh	10860.92201	10827.12487	10827.50273	4346.600734	4339.422125	4345.103987	6.65522009	6.264609967	7.645729265
5 MLP Regressor relu	5215.688006	4992.889247	6742.728684	**2620.119918**	3914.893174	3115.139606	7.387467066	7.663536281	7.983688085
5 MLP Regressor identity	7973.701989	7345.685686	6890.874314	4107.354789	4126.852924	3851.163037	13.97752331	12.80318731	7.543686137
5 MLP Regressor logistic	10871.56673	10871.56454	10862.6004	4348.638784	4348.638628	4348.195261	28.13648566	28.13648885	28.14040896
5 MLP Regressor tanh	10863.63122	10827.27362	10827.57146	4343.751542	4343.761025	4343.204459	6.416864475	6.504703309	7.649365095
6 MLP Regressor relu	5388.342481	5109.840875	6938.095456	**2409.364742**	3771.556276	2938.101031	7.343932148	7.664252551	8.113798167
6 MLP Regressor identity	7788.520727	7358.112557	6940.477783	4117.932656	4129.955645	3837.050683	13.94166818	12.88769125	7.72646213
6 MLP Regressor logistic	10872.82066	10872.82048	10870.01951	4348.653288	4348.653286	4348.174469	28.13634664	28.13634686	28.13806817
6 MLP Regressor tanh	10840.03763	10826.62143	10827.07469	4343.756518	4343.762599	4343.714501	6.780900385	28.1388945	7.411563135
7 MLP Regressor relu	**4779.591288**	**4831.015113**	6216.042166	**2321.53799**	4017.298189	3015.966069	7.292516691	7.684824171	8.204169949
7 MLP Regressor identity	7786.528762	7366.829509	6607.891996	4108.059277	4124.055217	3857.326368	14.11469274	12.78228204	7.830427656
7 MLP Regressor logistic	10872.37906	10872.37905	10873.76037	4349.153497	4349.153496	4348.492411	28.14075616	28.14075618	28.13942279
7 MLP Regressor tanh	10855.32458	10827.17614	10827.20895	4343.777717	4343.784931	4343.805887	6.666939314	28.13969762	7.534844913
8 MLP Regressor relu	5432.26437	**4967.139186**	6358.503543	2833.495348	3885.64122	2934.864033	7.194507264	7.917560365	8.108161572
8 MLP Regressor identity	7867.600593	7380.998025	6860.340604	4106.444333	4132.172416	3840.613251	14.06935825	12.8952392	7.704947334
8 MLP Regressor logistic	10873.48925	10873.48925	10866.8069	4348.872151	4348.872151	4349.290924	28.13550591	28.13550592	28.13931057
8 MLP Regressor tanh	10840.17295	10827.81361	10827.05284	4343.674138	4343.676436	4343.68271	6.788920068	28.14051234	7.314400007
9 MLP Regressor relu	**4951.77647**	5042.253521	6529.845995	2818.068644	3767.071421	3210.409634	7.216739822	7.411463759	7.965710543
9 MLP Regressor identity	7862.061538	7331.874215	6759.100495	4112.415417	4134.810681	3824.733924	14.12241519	13.16915458	8.030733945
9 MLP Regressor logistic	10867.4133	10867.41329	10880.54318	4349.548795	4349.548795	4348.029646	28.13997793	28.13997793	28.13733572
9 MLP Regressor tanh	10827.55505	10827.5601	10827.06958	4343.76029	4343.765419	4343.853388	6.844997652	28.14047022	15.35213705
10 MLP Regressor relu	**4982.965002**	**4804.556992**	6576.40138	**2445.247125**	4007.414082	3053.139028	7.217723945	7.487983314	8.083747214
10 MLP Regressor identity	7865.473031	7327.436524	6879.293441	4116.437759	4138.081036	3844.324224	14.18818844	13.27826937	7.769067759
10 MLP Regressor logistic	10863.8445	10863.8445	10873.00779	4349.81699	4349.81699	4349.520785	28.13993313	28.13993313	28.13938126
10 MLP Regressor tanh	10843.52706	10827.02851	10827.37766	4343.839795	4343.844507	4343.719106	6.962819567	28.13776351	19.61608228