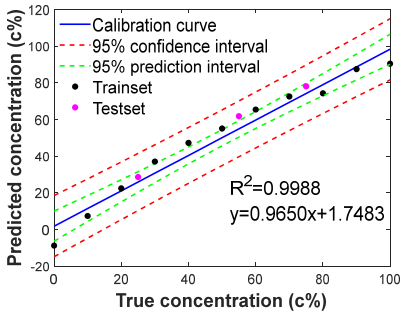

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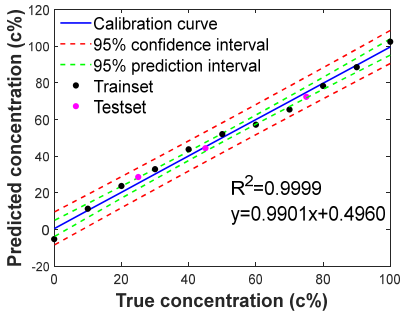

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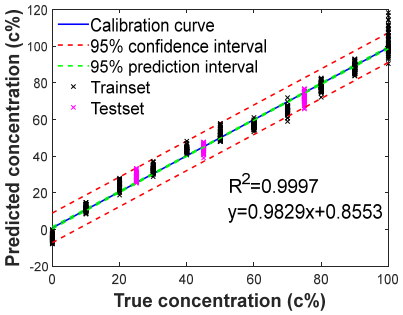

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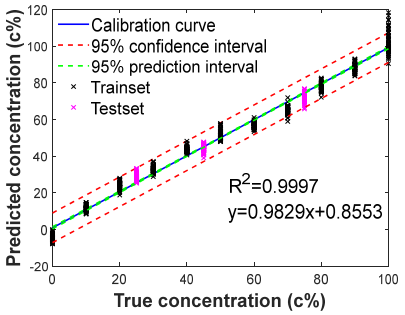

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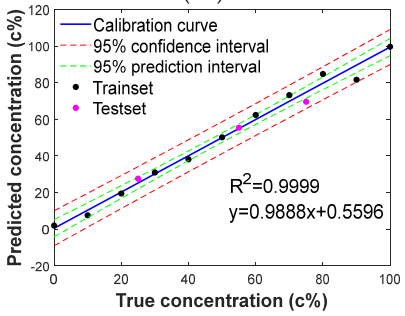

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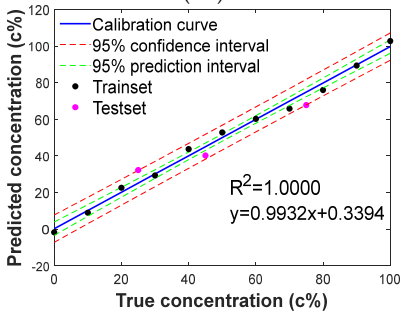

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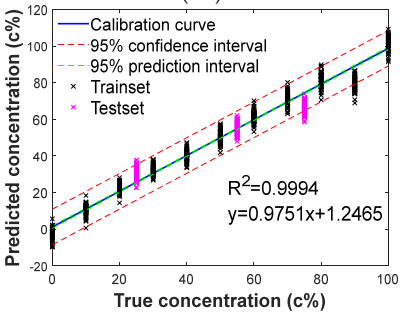

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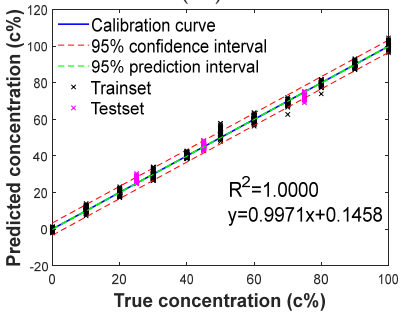

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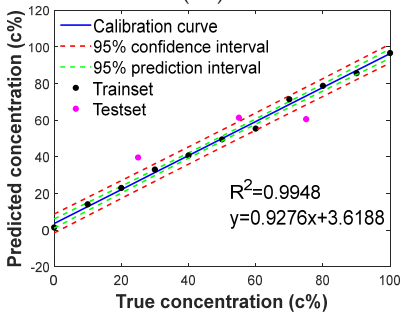

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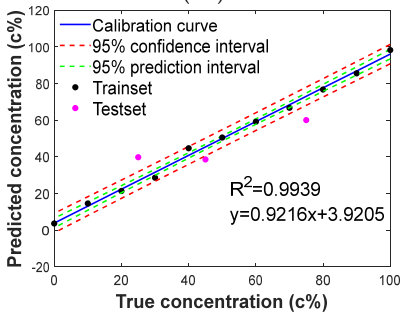

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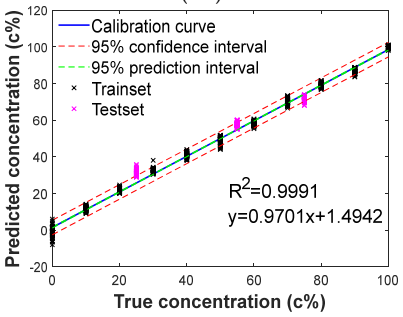

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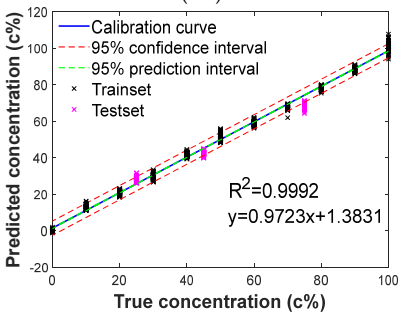

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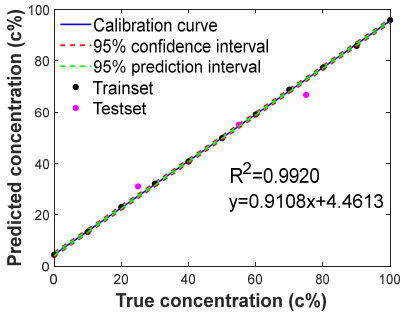

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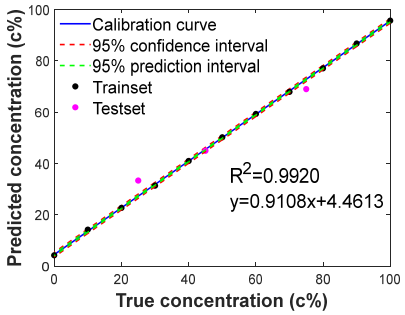

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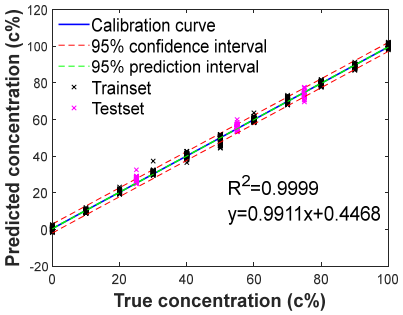

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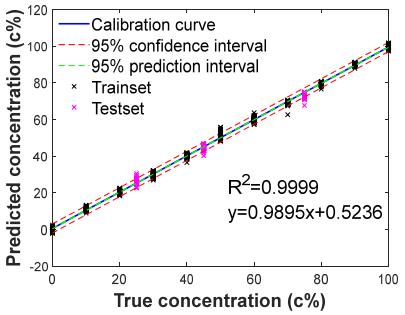

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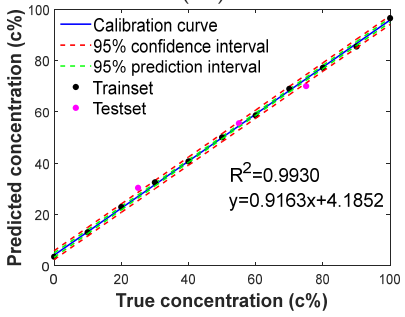

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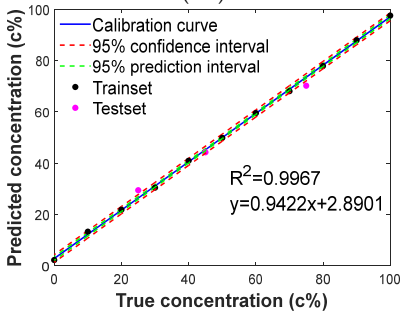

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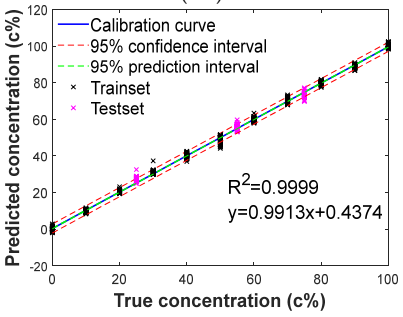

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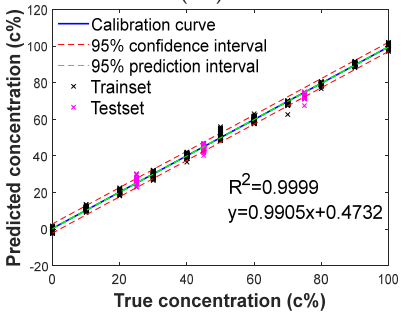

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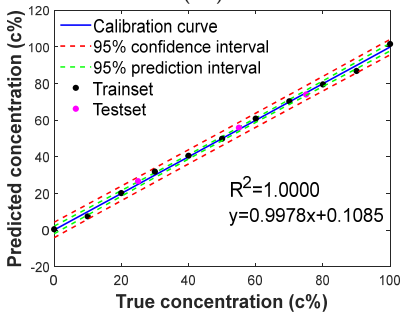

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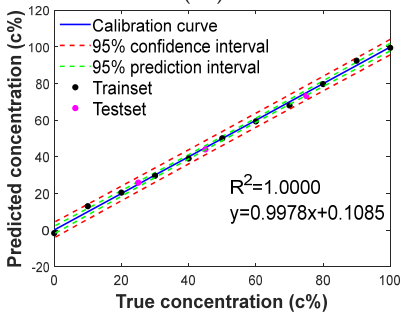

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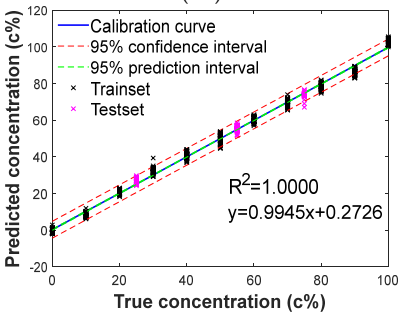

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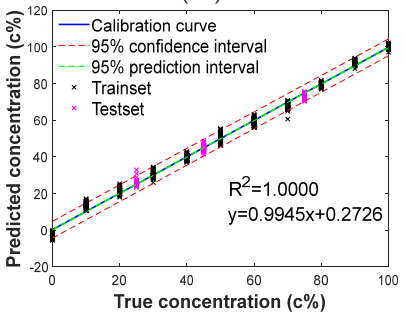

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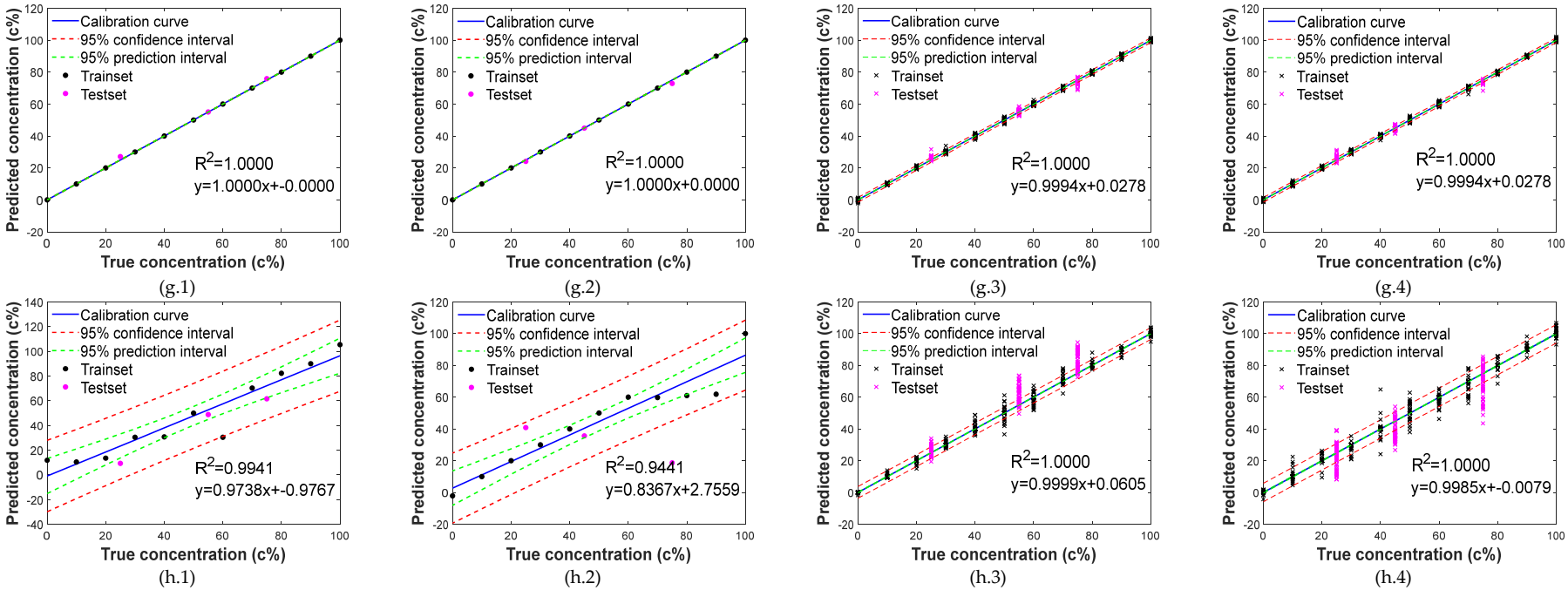

Figure S1. Calibration curve for Fo and Fa with the mean spectrum and the all spectra of the samples analyzed by ULR, ordinary MLR, Ridge, LASSO, Elastic Net, PCR, PLSR and BP. Where the blue lines show the theoretic fitted curve for the samples' contents, the black point show the predicted contents with each spectrum from training samples, and the magenta point show the predicted contents with each spectrum from testing samples. a, b, c, d, e, f, g and h indicate the ULR, ordinary MLR, Ridge, LASSO, Elastic Net, PCR, PLSR and BP, respectively; 1, 2, 3 and 4 indicate mean spectrum for Fo, mean spectrum for Fa, all spectra for Fo and all spectra for Fa, respectively.

Table S1. Predicted content of each sample on calibration and validation analyzed by the mean spectrum.

True content (c%)			Predicted content on calibration (c%)								Predicted content on validation (c%)							
			ULR	MLR	Ridge	LASSO	Elastic Net	PCR	PLSR	BP	ULR	MLR	Ridge	LASSO	Elastic Net	PCR	PLSR	BP
Fo	Train	0	-8.855	2.029	1.734	4.390	3.597	0.493	0.000	11.805	1.748	2.029	3.921	4.461	4.185	0.109	0.000	-0.977
		10	7.305	7.650	14.427	13.288	13.120	7.557	10.000	10.379	11.399	7.650	13.136	13.569	13.348	10.087	10.000	8.761
		20	22.385	19.531	23.270	22.943	22.955	20.260	20.000	13.510	21.049	19.531	22.352	22.677	22.511	20.065	20.000	18.499
		30	36.985	30.999	33.252	32.109	32.543	31.927	30.000	30.413	30.699	30.999	31.568	31.785	31.674	30.043	30.000	28.237
		40	47.190	38.164	40.839	40.742	40.724	40.637	40.000	30.701	40.350	38.164	40.784	40.892	40.837	40.022	40.000	37.975
		50	55.046	50.174	49.453	49.823	50.114	49.896	50.000	49.937	50.000	50.174	50.000	50.000	50.000	50.000	50.000	47.713
		60	65.385	62.381	55.284	59.050	58.662	60.902	60.000	30.413	59.650	62.381	59.216	59.108	59.163	59.978	60.000	57.451
		70	72.507	73.175	71.353	68.689	69.021	70.336	70.000	70.238	69.301	73.175	68.432	68.215	68.326	69.957	70.000	67.189
		80	74.217	84.719	78.608	77.360	77.234	79.548	80.000	82.208	78.951	84.719	77.648	77.323	77.489	79.935	80.000	76.926
		90	87.423	81.594	85.432	85.792	85.496	86.863	90.000	89.931	88.601	81.594	86.864	86.431	86.652	89.913	90.000	86.664
		100	90.411	99.585	96.347	95.814	96.535	101.581	100.000	105.306	98.252	99.585	96.079	95.539	95.815	99.891	100.000	96.402
	Test	25	28.545	27.606	39.949	31.045	30.429	26.762	27.127	9.308	25.874	27.606	26.960	27.231	27.093	25.054	25.000	23.368
		55	61.767	55.414	61.407	55.060	55.578	55.909	55.057	48.781	54.825	55.414	54.608	54.554	54.581	54.989	55.000	52.582
		75	78.048	69.567	60.210	66.703	70.076	74.020	75.888	61.539	74.126	69.567	73.040	72.769	72.907	74.946	75.000	72.057
Fa	Train	100	102.393	102.711	98.266	95.998	97.305	99.506	100.000	100.000	99.504	102.711	96.079	95.935	96.833	99.891	100.000	86.426
		90	88.514	89.320	85.573	86.995	87.708	92.448	90.000	61.849	89.603	89.320	86.864	86.748	87.466	89.913	90.000	78.059
		80	78.255	75.993	76.730	77.334	77.720	79.743	80.000	60.978	79.702	75.993	77.648	77.561	78.100	79.935	80.000	69.692
		70	65.389	65.826	66.748	68.073	67.955	68.070	70.000	59.775	69.802	65.826	68.432	68.374	68.733	69.957	70.000	61.325
		60	57.135	60.229	59.161	59.335	59.507	59.357	60.000	60.000	59.901	60.229	59.216	59.187	59.367	59.978	60.000	52.958
		50	51.980	52.816	50.547	50.165	49.904	50.092	50.000	50.000	50.000	52.816	50.000	50.000	50.000	50.000	50.000	44.591
		40	43.685	43.760	44.716	40.856	41.074	39.098	40.000	40.000	40.099	43.760	40.784	40.813	40.633	40.022	40.000	36.224
		30	32.859	29.321	28.647	31.178	30.600	29.662	30.000	30.000	30.198	29.321	31.568	31.626	31.267	30.043	30.000	27.857
		20	23.718	22.657	21.392	22.420	22.096	20.486	20.000	20.000	20.298	22.657	22.352	22.439	21.900	20.065	20.000	19.490
		10	11.311	9.044	14.568	13.833	13.596	13.122	10.000	10.000	10.397	9.044	13.136	13.252	12.534	10.087	10.000	11.123
		0	-5.239	-1.678	3.653	3.814	2.535	-1.586	0.000	-2.099	0.496	-1.678	3.921	4.065	3.167	0.109	0.000	2.756
	Test	75	72.369	67.736	60.051	69.128	70.115	73.242	72.873	18.662	74.752	67.736	73.040	72.968	73.416	74.946	75.000	65.509
		45	44.332	40.252	38.593	44.902	44.359	44.086	44.943	35.653	45.050	40.252	45.392	45.406	45.317	45.011	45.000	40.408
		25	28.606	32.335	39.790	33.254	29.519	25.958	24.112	40.845	25.248	32.335	26.960	27.032	26.584	25.054	25.000	23.674

Table S2. Predicted content of each sample on calibration and validation analyzed by the all spectra.

True content (c%)			Predicted content on calibration (c%)																Predicted content on validation (c%)											
			ULR		MLR		Ridge		LASSO		Elastic Net		PCR		PLSR		BP		ULR		MLR		Ridge		LASSO		Elastic Net		PCR		PLSR		BP	
			Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.	Avg.	Std.
Fo	Train	0	1.219	-0.043	0.662	-0.047	0.251	1.927	2.2E-15	1.247	4.5E-16	1.494	9.0E-16	0.568	1.1E-16	0.437	3.9E-16	0.273	1.7E-16	0.028	3.8E-17	0.061	5.6E-06	1.219	-0.043	0.662	-0.047	0.251	1.927	2.2E-15	1.247	4.5E-16	1.494	9.0E-16
		10	1.244	10.093	0.469	10.123	0.734	11.542	3.6E-15	10.997	1.8E-15	11.195	1.4E-14	10.454	1.3E-14	10.350	0.0E+00	10.218	1.8E-15	10.022	1.4E-14	10.059	1.4E-14	1.244	10.093	0.469	10.123	0.734	11.542	3.6E-15	10.997	1.8E-15	11.195	1.4E-14
		20	1.164	20.131	0.517	19.874	1.083	21.156	0.0E+00	20.748	1.4E-14	20.897	2.5E-14	20.341	3.6E-15	20.262	1.4E-14	20.164	3.6E-15	20.017	1.8E-14	20.058	7.2E-15	1.164	20.131	0.517	19.874	1.083	21.156	0.0E+00	20.748	1.4E-14	20.897	2.5E-14
		30	1.562	29.941	0.822	30.137	1.278	30.771	3.6E-15	30.499	5.0E-14	30.598	2.9E-14	30.227	1.4E-14	30.175	2.5E-14	30.109	2.1E-14	30.011	1.1E-14	30.057	1.1E-14	1.562	29.941	0.822	30.137	1.278	30.771	3.6E-15	30.499	5.0E-14	30.598	2.9E-14
		40	1.766	39.900	0.902	40.469	2.245	40.385	5.7E-14	40.249	2.9E-14	40.299	1.4E-14	40.114	7.2E-15	40.087	2.1E-14	40.055	2.9E-14	40.006	1.4E-14	40.055	2.9E-14	1.766	39.900	0.902	40.469	2.245	40.385	5.7E-14	40.249	2.9E-14	40.299	1.4E-14
		50	2.481	50.163	1.063	49.861	3.447	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.054	0.0E+00	2.481	50.163	1.063	49.861	3.447	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00
		60	1.354	59.923	0.658	59.623	2.686	59.615	7.9E-14	59.751	8.6E-14	59.701	3.6E-14	59.886	7.2E-14	59.913	2.9E-14	59.945	3.6E-14	59.994	5.0E-14	60.053	5.0E-14	1.354	59.923	0.658	59.623	2.686	59.615	7.9E-14	59.751	8.6E-14	59.701	3.6E-14
		70	1.747	69.973	0.784	70.587	2.374	69.229	1.0E-13	69.501	7.2E-14	69.402	7.2E-14	69.773	4.3E-14	69.825	4.3E-14	69.891	1.4E-14	69.989	1.0E-13	70.052	0.0E+00	1.747	69.973	0.784	70.587	2.374	69.229	1.0E-13	69.501	7.2E-14	69.402	7.2E-14
		80	1.618	79.772	0.654	80.209	1.370	78.844	5.7E-14	79.252	8.6E-14	79.103	2.9E-14	79.659	7.2E-14	79.738	2.9E-14	79.836	5.7E-14	79.983	2.9E-14	80.050	4.3E-14	1.618	79.772	0.654	80.209	1.370	78.844	5.7E-14	79.252	8.6E-14	79.103	2.9E-14
		90	1.735	90.200	0.802	89.736	1.187	88.458	0.0E+00	89.003	1.3E-13	88.805	2.9E-14	89.546	1.4E-14	89.650	2.9E-14	89.782	8.6E-14	89.978	8.6E-14	90.049	1.4E-14	1.735	90.200	0.802	89.736	1.187	88.458	0.0E+00	89.003	1.3E-13	88.805	2.9E-14
		100	1.466	99.948	0.623	100.022	1.327	98.073	1.4E-13	98.753	1.1E-13	98.506	1.6E-13	99.432	4.3E-14	99.563	7.2E-14	99.727	8.6E-14	99.972	1.3E-13	100.048	8.6E-14	1.466	99.948	0.623	100.022	1.327	98.073	1.4E-13	98.753	1.1E-13	98.506	1.6E-13
	Test	25	1.290	26.492	1.098	26.108	3.087	25.963	7.2E-15	25.623	0.0E+00	25.747	3.6E-14	25.284	1.1E-14	25.219	2.5E-14	25.136	3.9E-14	25.014	2.1E-14	25.057	3.6E-15	1.290	26.492	1.098	26.108	3.087	25.963	7.2E-15	25.623	0.0E+00	25.747	3.6E-14
		55	1.361	55.441	1.186	62.333	5.748	54.807	4.3E-14	54.875	7.9E-14	54.851	4.3E-14	54.943	5.0E-14	54.956	5.0E-14	54.973	2.9E-14	54.997	3.6E-14	55.054	1.4E-14	1.361	55.441	1.186	62.333	5.748	54.807	4.3E-14	54.875	7.9E-14	54.851	4.3E-14
		75	1.386	73.320	1.428	83.806	6.049	74.037	4.3E-14	74.377	1.1E-13	74.253	8.6E-14	74.716	2.9E-14	74.781	7.2E-14	74.864	4.3E-14	74.986	7.2E-14	75.051	2.9E-14	1.386	73.320	1.428	83.806	6.049	74.037	4.3E-14	74.377	1.1E-13	74.253	8.6E-14
Fa	Train	100	1.219	100.043	0.662	100.284	2.009	99.145	1.0E-13	99.854	1.1E-13	98.506	1.6E-13	99.476	5.7E-14	99.527	1.1E-13	99.727	8.6E-14	100.043	6.6E-01	99.847	8.6E-14	1.219	100.043	0.662	100.284	2.009	99.145	1.0E-13	99.854	1.1E-13	98.506	1.6E-13
		90	1.244	89.907	0.469	90.335	1.586	89.316	8.6E-14	89.883	1.4E-14	88.805	2.9E-14	89.581	1.4E-14	89.621	1.1E-13	89.782	8.6E-14	89.907	4.7E-01	89.861	1.4E-14	1.244	89.907	0.469	90.335	1.586	89.316	8.6E-14	89.883	1.4E-14	88.805	2.9E-14
		80	1.164	79.869	0.517	80.052	2.466	79.487	7.2E-14	79.913	4.3E-14	79.103	2.9E-14	79.686	5.7E-14	79.716	2.9E-14	79.836	5.7E-14	79.869	5.2E-01	79.876	4.3E-14	1.164	79.869	0.517	80.052	2.466	79.487	7.2E-14	79.913	4.3E-14	79.103	2.9E-14
		70	1.562	70.059	0.822	68.939	4.120	69.658	8.6E-14	69.942	4.3E-14	69.402	7.2E-14	69.791	4.3E-14	69.811	8.6E-14	69.891	1.4E-14	70.059	8.2E-01	69.890	8.6E-14	1.562	70.059	0.822	68.939	4.120	69.658	8.6E-14	69.942	4.3E-14	69.402	7.2E-14
		60	1.766	60.100	0.902	59.034	2.940	59.829	5.0E-14	59.971	3.6E-14	59.701	3.6E-14	59.895	6.4E-14	59.905	5.0E-14	59.945	3.6E-14	60.100	9.0E-01	59.905	4.3E-14	1.766	60.100	0.902	59.034	2.940	59.829	5.0E-14	59.971	3.6E-14	59.701	3.6E-14
		50	2.481	49.837	1.063	50.334	4.084	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00	49.837	1.1E+00	49.919	7.2E-15	2.481	49.837	1.063	50.334	4.084	50.000	0.0E+00	50.000	0.0E+00	50.000	0.0E+00
		40	1.354	40.077	0.658	40.085	4.477	40.171	4.3E-14	40.029	2.1E-14	40.299	1.4E-14	40.105	0.0E+00	40.095	4.3E-14	40.055	2.9E-14	40.077	6.6E-01	39.934	4.3E-14	1.354	40.077	0.658	40.085	4.477	40.171	4.3E-14	40.029	2.1E-14	40.299	1.4E-14
		30	1.747	30.027	0.784	29.299	2.317	30.342	5.0E-14	30.058	2.9E-14	30.598	2.9E-14	30.209	2.9E-14	30.189	4.7E-14	30.109	2.1E-14	30.027	7.8E-01	29.948	2.9E-14	1.747	30.027	0.784	29.299	2.317	30.342	5.0E-14	30.058	2.9E-14	30.598	2.9E-14
		20	1.618	20.228	0.654	20.299	2.401	20.513	1.4E-14	20.087	2.9E-14	20.897	2.5E-14	20.314	0.0E+00	20.284	1.1E-14	20.164	3.6E-15	20.228	6.5E-01	19.963	3.6E-15	1.618	20.228	0.654	20.299	2.401	20.513	1.4E-14	20.087	2.9E-14	20.897	2.5E-14
		10	1.735	9.800	0.802	10.404	2.675	10.684	1.8E-15	10.117	3.6E-15	11.195	1.4E-14	10.419	1.8E-15	10.379	7.2E-15	10.218	1.8E-15	9.800	8.0E-01	9.978	1.1E-14	1.735	9.800	0.802	10.404	2.675	10.684	1.8E-15	10.117	3.6E-15	11.195	1.4E-14
		0	1.466	0.052	0.623	0.046	0.782	0.855	7.8E-16	0.146	1.7E-16	1.494	9.0E-16	0.524	4.5E-16	0.473	3.9E-16	0.273	1.7E-16	0.052	6.2E-01	-0.008	5.2E-18	1.466	0.052	0.623	0.046	0.782	0.855	7.8E-16	0.146	1.7E-16	1.494	9.0E-16
	Test	75	1.290	73.508	1.098	69.119	9.821	74.572	2.9E-14	74.927	8.6E-14	74.253	8.6E-14	74.738	7.2E-14	74.763	2.9E-14	74.864	4.3E-14	73.508	1.1E+00	74.883	7.2E-14	1.290	73.508	1.098	69.119	9.821	74.572	2.9E-14	74.927	8.6E-14	74.253	8.6E-14
		45	1.361	44.559	1.186	39.553	6.271	45.086	2.1E-14	45.015	2.1E-14	45.149	1.4E-14	45.052	4.3E-14	45.047	2.9E-14	45.027	2.1E-14	44.559	1.2E+00	44.927	5.0E-14	1.361	44.559	1.186	39.553	6.271	45.086	2.1E-14	45.015	2.1E-14	45.149	1.4E-14
		25	1.386	26.680	1.428	22.104	8.280	25.428	1.1E-14	25.073	1.1E-14	25.747	3.6E-14	25.262	1.8E-14	25.237	2.1E-14	25.136	3.9E-14	26.680	1.4E+00	24.956	3.6E-15	1.386	26.680	1.428	22.104	8.280	25.428	1.1E-14	25.073	1.1E-14	25.747	3.6E-14