SUPPORTING INFORMATION

SI.1 Datasets used for nested-ANOVA for the quantification of sub-sampling uncertainty for TG-DTG of SRF

Table SI.1-1. Analytical results of critical TG-DTG points of SRF used for the calculation of sub-sampling uncertainty emerging from the 1st to 4th stage of sub-sampling through four level nested-ANOVA (*Gross_nested*: from the sample mass of nearly 850 g to the sub-sample of 53 g) .

No	TG-DTG critical points											Sub-sampling stages			
	$T_{10\%}$	$T_{20\%}$	$T_{30\%}$	$T_{50\%}$	$T_{75\%}$	Res.MC	Res.MC_Inf.T	Res.MC_Mid.T	1st_ML	1st_Inf.T*	1st_Mid.T	1st	2nd	3rd	4th
1	256.78	281.7	296.48	332.12	416.31	2.3884	44.4	57.17	7.6865	239.15	241.7	A	A1	A11	A111
2	256.71	282.12	296.94	332.24	418.71	2.5204	42.42	57.76	7.7828	239.56	241.66	A	A1	A11	A111
3	256.65	281.83	296.64	335.29	418.43	2.3996	50.98	57.08	7.6574	235.99	239.12	A	A1	A11	A111
4	258	282.85	298.53	336.44	423.78	2.8676	41.75	55.62	7.484	243.02	243.52	A	A1	A11	A112
5	259.25	283.78	299.36	341.38	427.82	2.6069	41.29	55.45	7.1847	241.95	242.61	A	A1	A11	A112
6	259.66	283.84	299.61	340.58	427.52	2.5006	59.95	55.01	7.0574	241.17	243.38	A	A1	A11	A112
7	257.24	282.23	297.01	333.8	420.12	2.4716	42.2	57.17	7.7956	239.3	241.55	A	A1	A12	A121
8	257.9	282.66	297.53	334.51	419.49	2.4493	42	56.78	7.5233	239.41	241.53	A	A1	A12	A121
9	257.28	282.38	297.18	331.93	417.82	2.5535	42.05	56.96	7.7742	239.76	241.42	A	A1	A12	A121
10	256.5	281.51	296.45	335.85	420.41	2.3561	42.25	56.84	7.9392	237.21	240.58	A	A1	A12	A122
11	256.4	281.45	296.37	334.48	419.57	2.2359	42.47	56.99	7.9995	237.52	241.03	A	A1	A12	A122
12	255.33	280.91	296.14	332.94	417.89	2.2965	42.29	56.96	8.4076	237.47	241.05	A	A1	A12	A122
13	257.32	282.37	297.67	330.84	418.36	2.7526	43.78	56.76	7.6268	240.38	241.93	A	A2	A21	A211
14	257.31	281.92	296.75	331.48	417.28	2.7049	42.21	56.75	7.655	240.53	242.2	A	A2	A21	A211
15	257.25	282.3	297.39	332.65	419.68	2.6755	42.4	56.32	7.6788	239.47	241.74	A	A2	A21	A211
16	258.73	283.86	299.12	334.63	420.65	2.53	42.06	57.24	7.4481	239.91	242.13	A	A2	A21	A212

17	258.58	283.4	298.3	334.02	418.81	2.5378	42.09	57.03	7.4712	239.83	241.7	A	A2	A21	A212
18	258.34	283.32	298.05	332.09	417.03	2.6264	42.15	57.09	7.4159	239.74	241.53	A	A2	A21	A212
19	256.11	282.11	296.73	331.9	416.37	2.4629	42.06	57.02	7.7486	237.11	240.7	A	A2	A22	A221
20	257.37	281.56	296.25	332.8	419.61	2.4615	49.21	56.85	7.7782	240.22	242.55	A	A2	A22	A221
21	257.6	281.21	295.86	331.45	419.11	2.5004	42.1	57.07	7.6446	243.06	243.72	A	A2	A22	A221
22	257.39	281.78	296.83	333.86	420.25	2.6512	43.52	56.61	7.7038	242.25	243.2	A	A2	A22	A222
23	256.72	281.56	296.59	332.28	418.1	2.6095	41.72	56.6	7.8656	240.41	242.35	A	A2	A22	A222
24	258.71	283	297.83	335.67	421.89	2.64	41.97	56.6	7.3455	241.6	243.1	A	A2	A22	A222
25	256.58	282.71	297.01	333.4	418.24	2.7605	42.23	56.35	7.8169	233.6	238.15	B	B1	B11	B111
26	257.31	282.59	296.74	334.66	418.61	2.6228	41.83	56.39	7.6009	235.92	238.28	B	B1	B11	B111
27	256.5	282.28	296.64	332.72	417.23	2.702	42.22	56.55	7.7744	234.5	238.12	B	B1	B11	B111
28	258	284.3	300.42	344.16	428.41	2.3506	42.12	56.49	7.6046	236.92	240.05	B	B1	B11	B112
29	258.05	283.71	299.71	342.1	427.8	2.4568	42.26	55.29	7.5745	238.67	240.93	B	B1	B11	B112
30	257.58	283.33	298.98	340.43	425.13	2.4637	42.24	55.12	7.5939	236.5	239.74	B	B1	B11	B112
31	253.65	280.64	296.23	335.73	419.94	2.4602	41.58	55.6	8.4085	233.07	237.63	B	B1	B12	B121
32	253.38	280.95	296.71	338.24	422.6	2.4722	44.17	56.69	8.4688	236.29	238.37	B	B1	B12	B121
33	254.53	281.12	296.5	336.75	421.73	2.3583	46.25	56.69	8.1954	232.91	238.08	B	B1	B12	B121
34	258.36	281.56	295.89	332.9	419.08	2.4287	41.94	56.91	7.2341	242.29	234.15	B	B1	B12	B122
35	258.38	283.6	298	335.92	418.23	2.6145	42.11	57.55	7.1994	235.55	238.75	B	B1	B12	B122
36	257.55	283.01	298.28	339.53	424.52	2.4173	42.04	56.28	7.4911	236.06	239.64	B	B1	B12	B122
37	251.32	279.25	294.56	328.62	415.2	3.6262	39.82	56.36	8.6082	230.72	235	B	B2	B21	B211
38	254.47	280.78	295.73	328.63	415.49	2.959	43.82	57.51	8.4031	233.21	237.91	B	B2	B21	B211
39	257.02	282.3	296.68	331.57	415.88	2.8166	43.97	57.3	7.6998	234.1	237.66	B	B2	B21	B211

40	255.35	282.07	297.64	333.11	419.57	2.5037	42.09	57.12	8.0708	236	239.05	B	B2	B21	B212
41	257.26	282.74	297.94	335.73	421.6	2.4917	41.91	56.94	7.6655	237.4	239.3	B	B2	B21	B212
42	257.86	283.37	298.52	336.16	421.58	2.5078	42.22	57.02	7.5215	233.88	238.67	B	B2	B21	B212
43	256.83	282.73	297.65	334.37	417.74	3.3456	48.2	55.01	7.5328	234.43	238.43	B	B2	B22	B221
44	256.15	282.07	296.73	332.04	415.03	2.7992	43.7	56.82	7.8849	235.41	238.41	B	B2	B22	B221
45	257.31	282.32	296.72	333.54	416.62	2.6766	42.24	57.21	7.6186	233.53	238.11	B	B2	B22	B221
46	255.8	282.41	297.37	333.34	418.02	2.8387	42.24	57	7.8606	234.06	237.93	B	B2	B22	B222
47	255.85	282.62	297.78	333.57	418.96	2.7303	44.09	56.21	7.963	233.17	238.02	B	B2	B22	B222
48	256.06	282.98	298.09	334.47	419.14	2.6186	42.01	56.28	7.8376	233.26	237.76	B	B2	B22	B222

Table SI.1-1. *Contin.*

No	TG-DTG critical points										Sub-sampling stages			
	2nd_ML	2nd_Inf.T*	2nd_Mid.T	3rd_ML	3rd_Inf.T*	3rd_Mid.T	4th_ML	4th_Inf.T*	4th_Mid.T	Res.	1st	2nd	3rd	4th
1	44.15	298.82	304.22	29.032	432.07	424.7	2.8226	637.97	627.33	12.5628	A	A1	A11	A111
2	44.6708	299.52	304.55	29.2985	428.81	427.03	3.0765	637.97	629.53	11.1427	A	A1	A11	A111
3	43.4067	297	304.04	29.393	428.07	426.21	3.1732	638.02	628.07	13.97	A	A1	A11	A111
4	43.9522	299.24	305.11	30.7661	431.5	430.05	3.3149	634.51	628.63	10.4865	A	A1	A11	A112
5	43.0665	299.05	304.77	31.9489	436.81	432.47	3.6815	638.07	630.77	10.2709	A	A1	A11	A112
6	43.4629	297.2	305.17	31.8081	436	433.07	3.3266	637.42	630.15	10.8395	A	A1	A11	A112
7	44.875	298.3	304.13	30.5101	428.36	427.7	2.932	638.13	626.57	10.7511	A	A1	A12	A121
8	44.3019	298.56	304.45	30.3454	430.63	427.02	2.8377	638.14	626.68	10.9558	A	A1	A12	A121

9	45.4927	298.71	304.78	29.5669	425.23	425.56	2.9381	638.2	626.26	11.193	A	A1	A12	A121
10	43.9511	295.56	303.89	30.4256	429.47	427.99	3.0046	638.3	628.51	11.5451	A	A1	A12	A122
11	44.6151	295.91	304.4	29.6725	431.56	428.03	3.0217	638.22	629.25	11.5883	A	A1	A12	A122
12	44.898	298.12	304.55	29.6202	423.87	424.82	3.0165	638.28	629.46	11.1523	A	A1	A12	A122
13	45.1123	302.1	305.59	28.6486	425.41	426.14	3.0377	638.13	627.99	11.3993	A	A2	A21	A211
14	44.9884	299.68	304.6	28.9037	424.45	424.7	2.9965	638.29	626.37	11.6808	A	A2	A21	A211
15	44.6026	298.91	304.91	29.4191	433.45	427.77	3.1343	638.1	628.72	11.2272	A	A2	A21	A211
16	45.2193	301.99	305.93	30.484	427.71	427.47	3.1919	638.11	627.58	10.8482	A	A2	A21	A212
17	45.4678	299.53	305.51	29.9548	426.16	425.87	3.1654	638.13	629.37	11.2572	A	A2	A21	A212
18	45.2434	300.22	305.44	28.9739	423.7	423.92	3.1938	638.29	629.41	11.5278	A	A2	A21	A212
19	44.7359	299.06	304.42	29.016	422.96	423.3	3.1137	638.22	631.14	10.8496	A	A2	A22	A221
20	45.0604	296.4	303.43	30.4399	432.59	427.69	3.0387	638.14	627.09	11.2222	A	A2	A22	A221
21	45.6955	298.2	303.36	29.6836	429.68	428.02	3.1343	638.02	627.36	11.3431	A	A2	A22	A221
22	44.9602	298.18	304.2	29.9718	429.53	428.34	3.3057	642.46	629.36	11.151	A	A2	A22	A222
23	45.223	298.55	304.29	29.6249	423.79	424.64	3.159	638.31	628.73	11.0536	A	A2	A22	A222
24	44.7323	298.25	304.5	30.2041	431.84	429.56	3.4824	642.50	630.95	11.2586	A	A2	A22	A222
25	43.9737	296.75	304.21	29.1709	429.23	425.8	3.4733	638.53	631.13	11.8521	B	B1	B11	B111
26	43.4982	296.65	303.53	29.4773	433.49	425.7	3.4091	637.94	630.86	12.4721	B	B1	B11	B111
27	44.0167	299.46	304.11	28.69002	426.38	425.31	3.419	638.15	630.9	12.4836	B	B1	B11	B111
28	42.177	298.88	306.05	32.7398	440.21	433.15	3.1961	638.04	627.2	11.6917	B	B1	B11	B112
29	42.6926	299.55	305.8	31.9101	437.54	433.31	3.297	638.12	628.47	11.553	B	B1	B11	B112
30	42.7005	298.16	305.51	31.0496	436.54	430.96	3.2972	638.09	628.85	11.5461	B	B1	B11	B112
31	42.6357	299.05	304.21	29.7737	429.76	427.21	3.2845	648.22	631.6	12.1824	B	B1	B12	B121

32	41.7571	295.52	304.21	30.516	431.59	428.76	3.3953	633.21	632.31	11.8189	B	B1	B12	B121
33	42.6216	296.48	304.2	29.6758	433.73	428.76	3.5137	638.26	632.58	12.683	B	B1	B12	B121
34	44.1249	295.94	302.91	29.339	429.27	427.29	3.0093	638.07	627.61	13.8646	B	B1	B12	B122
35	42.9039	299.48	304.66	29.2221	428.58	425.22	3.1103	638.05	626.55	13.8623	B	B1	B12	B122
36	42.0792	298.48	304.54	30.7427	437.83	430.56	3.2265	751.70	627.14	13.4893	B	B1	B12	B122
37	44.4619	297.57	302.55	29.4056	423.51	422.37	3.6133	637.83	634.61	10.0946	B	B2	B21	B211
38	45.8913	296.69	304.53	28.1322	427.54	426.43	3.3384	637.86	626.32	11.1373	B	B2	B21	B211
39	45.061	298.12	304.22	29.0894	429.23	424.77	3.19	638.03	627.59	11.929	B	B2	B21	B211
40	43.7399	299.87	305.31	29.3881	426.49	426.49	3.2822	637.98	627.43	12.0094	B	B2	B21	B212
41	43.6396	298.58	304.85	30.1997	435.93	428.76	3.3516	645.08	628.08	11.5075	B	B2	B21	B212
42	43.7739	299.71	305.36	30.151	434.38	428.73	3.3221	638.46	628.12	11.6742	B	B2	B21	B212
43	43.7695	297.34	304.98	29.2632	429.86	425.65	3.1303	638.23	626.25	12.0877	B	B2	B22	B221
44	44.5586	297.15	304.52	28.77	421.17	421.66	3.33	638.41	628.56	12.1943	B	B2	B22	B221
45	44.368	296.33	304.12	29.1254	427.12	424.69	3.3346	638.31	627.93	12.4078	B	B2	B22	B221
46	43.6857	298.95	304.91	29.1516	427.56	425.71	3.3646	638.29	630.05	12.2019	B	B2	B22	B222
47	43.8904	298.91	305.44	29.0443	427.1	426.4	3.4201	647.60	629.88	11.9334	B	B2	B22	B222
48	43.1872	298.82	305.47	29.2419	426.41	425.91	3.2589	645.00	628.66	12.8898	B	B2	B22	B222

Table SI.1-1. *Contin.*

No	TG-DTG critical points								Sub-sampling stages			
	1st_RML	1st_ On.T	1st_Peak.T	1st_End.T	2nd_RML	2nd_On.T	2nd_Peak.T	2nd_End.T	1st	2nd	3rd	4th

1	3.46	227.01	240.05	243.97	6.52	282.03	297.97	343.07	A	A1	A11	A111
2	3.48	227.03	240.28	245.57	6.66	282.82	298.65	343.93	A	A1	A11	A111
3	2.93	222.52	236.17	240.76	6.14	282.04	296.66	344.09	A	A1	A11	A111
4	3.64	229.73	243.2	247.08	6.2	282.67	301.13	347.48	A	A1	A11	A112
5	3.25	228.22	242.48	246.3	6.01	283.17	298.18	346.54	A	A1	A11	A112
6	3.38	229.22	243.16	248.07	5.99	281.44	299.27	349.89	A	A1	A11	A112
7	3.41	226.58	239.66	244.57	6.62	282.78	297.79	343.74	A	A1	A12	A121
8	3.31	226.65	239.93	244.67	6.52	282.54	298.39	346.06	A	A1	A12	A121
9	3.27	226.17	239.76	244.59	6.73	282.80	299.22	345.26	A	A1	A12	A121
10	3.27	224.85	237.74	243.99	6.26	281.92	295.9	343.37	A	A1	A12	A122
11	3.32	225.34	238.41	244.21	6.34	282.29	296.24	344.34	A	A1	A12	A122
12	3.36	224.81	238.18	244.28	6.44	282.47	297.27	345.54	A	A1	A12	A122
13	3.29	227.04	240.73	244.96	6.58	286.18	301.58	351.06	A	A2	A21	A211
14	3.4	227.59	241.06	245.28	6.51	282.41	298.99	347.83	A	A2	A21	A211
15	3.38	227.23	240.02	244.64	6.47	283.06	299.08	350.02	A	A2	A21	A211
16	3.33	227.96	240.81	245.11	6.47	284.52	301.63	350.06	A	A2	A21	A212
17	3.24	227.14	240.18	244.61	6.48	282.63	299.7	349.2	A	A2	A21	A212
18	3.33	227.13	240.11	244.64	6.65	282.52	300.74	347.16	A	A2	A21	A212
19	3.37	226.24	238.38	242.92	6.55	281.61	298.19	344.34	A	A2	A22	A221
20	3.61	229.00	241.13	245.8	6.43	282.40	297.41	345.43	A	A2	A22	A221
21	3.73	230.10	243.78	248.42	6.57	282.35	297.51	345.83	A	A2	A22	A221
22	3.7	229.41	242.6	246.92	6.42	282.14	298	345.97	A	A2	A22	A222
23	3.54	227.84	241.31	246.26	6.58	282.72	298.38	345.11	A	A2	A22	A222

24	3.5	229.74	242.32	247.39	6.42	282.48	298.08	345.09	A	A2	A22	A222
25	2.81	221.24	234.48	240.93	6.69	282.62	297.78	341.29	B	B1	B11	B111
26	2.8	221.38	234.88	239.43	6.66	281.91	296.65	340.55	B	B1	B11	B111
27	2.78	220.99	234.33	241.29	6.61	281.73	297.58	341.81	B	B1	B11	B111
28	2.9	223.09	237.6	243.26	5.79	283.51	298.71	349.35	B	B1	B11	B112
29	3.06	224.19	239.19	244.2	5.83	282.10	298.69	350.46	B	B1	B11	B112
30	2.86	222.85	237.02	242.15	5.92	281.73	298	349.22	B	B1	B11	B112
31	2.95	219.46	232.73	240.12	6.19	280.17	296.82	343.02	B	B1	B12	B121
32	3.06	220.04	234.58	239.49	6.12	281.55	296.36	341.28	B	B1	B12	B121
33	2.96	219.88	234.14	239.74	6.11	281.24	296.32	343.23	B	B1	B12	B121
34	3.22	229.82	242.64	247.18	5.91	281.42	296.29	344.59	B	B1	B12	B122
35	2.72	221.79	236.26	241.66	6.42	282.61	298.44	341.85	B	B1	B12	B122
36	2.93	223.05	237.11	242.88	5.96	282.29	297.63	346.28	B	B1	B12	B122
37	2.73	216.43	230.2	239.11	6.92	281.40	297.75	339.51	B	B2	B21	B211
38	2.76	218.96	234.43	241.05	6.94	283.39	298.6	342.04	B	B2	B21	B211
39	2.57	219.26	233.59	239.99	6.76	282.69	298.12	342.42	B	B2	B21	B211
40	2.92	221.61	235.83	242.58	6.42	286.32	300.74	346.42	B	B2	B21	B212
41	2.92	222.45	236.53	241.21	6.33	282.37	298.92	348.86	B	B2	B21	B212
42	2.68	221.35	235.46	243.73	6.24	284.35	299.37	349.24	B	B2	B21	B212
43	2.79	221.98	234.96	240.82	6.45	283.27	298.38	344.78	B	B2	B22	B221
44	2.93	221.44	234.54	239.66	6.64	282.22	298.01	344.16	B	B2	B22	B221
45	2.82	221.02	234.25	240.13	6.52	282.18	296.83	344.3	B	B2	B22	B221
46	2.88	220.67	234.23	240.36	6.52	282.66	299.46	345.27	B	B2	B22	B222

47	2.78	219.84	234.39	241.12	6.42	285.15	299.6	346.67	B	B2	B22	B222
48	2.77	220.03	233.6	239.69	6.34	282.27	300.01	346.93	B	B2	B22	B222

Table SI.1-1. *Contin.*

No	TG-DTG critical points								S	Sub-sampling stages			
	3rd_RML	3rd_On.T	3rd_Peak.T	3rd_End.T	4th_RML	4th_On.T	4th_Peak.T	4th_End.T		1st	2nd	3rd	4th
1	10.4	415.93	431.21	437.97	0.458	660.94	645.19	663.55	2.70E-07	A	A1	A11	A111
2	9.64	416.96	431.13	440.88	0.46	592.73	637.32	650.16	2.60E-07	A	A1	A11	A111
3	8.4	416.64	429.6	440.02	0.458	604.36	637.03	657.22	2.30E-07	A	A1	A11	A111
4	9.16	419.59	432.82	441.25	0.469	591.57	637.45	662.12	2.30E-07	A	A1	A11	A112
5	6.01	420.94	436.98	451.32	0.541	663.24	636.59	666.89	1.50E-07	A	A1	A11	A112
6	6.38	422.20	435.64	447.95	0.517	590.72	645.96	663.08	1.60E-07	A	A1	A11	A112
7	8.85	417.09	430.42	441.29	0.429	600.78	639.76	663.34	2.30E-07	A	A1	A12	A121
8	9.93	418.42	433.23	441.74	0.425	609.12	637.33	661.33	2.60E-07	A	A1	A12	A121
9	8.66	414.28	425.74	434.26	0.434	614.27	639.99	662.86	2.20E-07	A	A1	A12	A121
10	8.86	417.79	431.95	443.1	0.463	630.49	639.77	644.1	2.40E-07	A	A1	A12	A122
11	9.46	418.51	433.97	442.63	0.462	604.82	637.4	643.75	2.60E-07	A	A1	A12	A122
12	10.4	412.75	426.83	438.8	0.445	551.15	639.91	643.88	2.80E-07	A	A1	A12	A122
13	8.61	414.52	426.56	441.1	0.47	612.13	644.84	696	2.10E-07	A	A2	A21	A211
14	9.24	413.48	425.48	435.05	0.454	589.42	639.91	660.77	2.40E-07	A	A2	A21	A211
15	8.4	419.37	433.86	441.66	0.466	620.89	644.8	663.27	2.20E-07	A	A2	A21	A211

16	8.24	416.43	428.2	440.83	0.482	597.32	644.85	696.03	2.00E-07	A	A2	A21	A212
17	10.8	415.55	428.91	439.25	0.475	590.77	645.18	662.34	2.80E-07	A	A2	A21	A212
18	10.3	412.60	425.66	437.36	0.472	588.36	645.18	662.36	2.70E-07	A	A2	A21	A212
19	10.2	411.98	425.2	435.83	0.455	592.02	645.25	663.82	2.70E-07	A	A2	A22	A221
20	7.7	419.82	433.06	441.43	0.437	588.71	639.95	661.11	2.00E-07	A	A2	A22	A221
21	8.24	418.56	429.91	437.69	0.452	589.34	639.51	657.38	2.10E-07	A	A2	A22	A221
22	7.3	417.63	430.62	443.28	0.503	593.16	644.27	657.32	1.90E-07	A	A2	A22	A222
23	10	413.31	425.33	434.75	0.474	592.60	637.82	661.75	2.60E-07	A	A2	A22	A222
24	7.3	420.07	432.05	440.46	0.51	634.00	644.31	656.16	1.90E-07	A	A2	A22	A222
25	9.99	418.26	431.69	440.07	0.52	588.93	645.24	662.81	2.70E-07	B	B1	B11	B111
26	9.36	420.95	435.23	441.73	0.523	609.08	639.74	662.6	2.50E-07	B	B1	B11	B111
27	9.58	415.77	429.03	438.4	0.516	641.06	645.03	696.01	2.50E-07	B	B1	B11	B111
28	6.47	425.52	440.06	452.05	0.471	593.64	645.11	695.98	1.60E-07	B	B1	B11	B112
29	6.12	423.29	437.37	449.26	0.485	572.28	639.93	643.48	1.70E-07	B	B1	B11	B112
30	7.8	423.33	437.19	445.82	0.487	582.91	645.16	662.23	2.10E-07	B	B1	B11	B112
31	10	419.09	432.53	441.61	0.521	585.68	647.41	663.46	2.80E-07	B	B1	B12	B121
32	9.47	420.46	433.04	441.18	0.531	623.57	641.58	663.48	2.50E-07	B	B1	B12	B121
33	7.59	422.34	433.73	442.14	0.56	596.41	644.48	664.77	2.10E-07	B	B1	B12	B121
34	7.43	417.63	429.75	437.76	0.399	634.49	637.08	680.97	1.80E-07	B	B1	B12	B122
35	7.68	416.01	429.02	437.83	0.469	581.39	637.06	661.23	2.10E-07	B	B1	B12	B122
36	5.28	405.02	438.75	458.09	0.483	588.17	637.24	660.19	1.60E-07	B	B1	B12	B122
37	12.9	413.74	426.37	433.14	0.533	608.72	644.23	695.69	3.40E-07	B	B2	B21	B211
38	7.13	416.65	427.54	434.99	0.492	591.04	636.73	659.07	2.00E-07	B	B2	B21	B211

39	8.76	417.76	430.88	438.81	0.468	584.75	637.05	660.58	2.40E-07	B	B2	B21	B211
40	7.88	415.63	426.74	435.17	0.492	594.32	640.11	643.31	2.20E-07	B	B2	B21	B212
41	5.16	402.64	435.93	454.02	0.499	643.85	644.59	661.31	1.70E-07	B	B2	B21	B212
42	7.93	422.81	434.86	442.93	0.499	657.91	640.1	661.87	2.20E-07	B	B2	B21	B212
43	9.73	418.78	432.65	439.99	0.516	603.06	640.02	696.04	2.50E-07	B	B2	B22	B221
44	10.3	410.66	423.64	434.3	0.511	584.15	640.36	661.78	2.80E-07	B	B2	B22	B221
45	9.05	416.45	429.35	438.53	0.507	548.66	637.16	643.98	2.50E-07	B	B2	B22	B221
46	9.78	416.45	429.74	437.58	0.51	590.84	645.17	663.07	2.70E-07	B	B2	B22	B222
47	9.68	416.31	428.81	436.04	0.517	583.93	645.63	663.32	2.70E-07	B	B2	B22	B222
48	10	415.67	429	437.72	0.494	583.71	639.92	662.77	2.70E-07	B	B2	B22	B222

Table SI.1-1. Analytical results of critical TG-DTG points of SRF used for the calculation of sub-sampling uncertainty emerging from the 5th to 7th stage of sub-sampling through three level nested-ANOVA (*Intra_nested*: from the sample mass of nearly 53 g to the sub-sample of 6-7 g) .

No.	TG-DTG critical points											Sub-sampling stages		
	T10%	T20%	T30%	T50%	T75%	Res.MC	Res.MC_Inf.T	Res.MC_Mid.T	1st_ML	1st_Inf.T*	1st_Mid.T	5th	6th	7th
1	257.1	281.76	297.67	343.69	424.35	2.288	42.41	54.05	7.4518	239.68	241.36	a	a1	a11
2	255.67	280.49	296.3	340.12	422.35	2.3551	42.77	54.12	7.8918	239.59	241.25	a	a1	a11
3	256.12	281.15	296.6	339.95	420.86	2.4485	42.05	54.71	7.92	238.12	240.84	a	a1	a11
4	254.44	279.99	295.32	337.06	419.51	2.6919	41.87	56.56	8.1023	239.86	241.38	a	a1	a12
5	255.33	280.75	296.2	340.07	418.74	2.329	42.27	54.61	7.5555	237.38	238.65	a	a1	a12
6	255.29	280.29	295.53	339.27	418.77	2.391	45.86	54.69	7.7753	236.96	240.1	a	a1	a12
7	256.91	281.93	297.94	336.97	423.02	2.4148	42.05	55.83	7.5693	240.44	241.96	a	a2	a21

8	257.56	283.33	300	340.9	426.07	2.4282	42.16	56.41	7.2961	240.1	241.7	a	a2	a21
9	257.24	282.83	299.13	341.62	424.15	2.4745	41.96	54.39	7.4822	239.67	241.28	a	a2	a21
10	259.85	284.04	298.91	342.19	423.07	2.5737	42.97	55.27	6.9933	239.47	240.59	a	a2	a22
11	258.18	282.45	297.15	338.5	421.28	2.4804	41.93	55.13	7.0494	240.29	240.97	a	a2	a22
12	258.69	282.88	297.73	340.92	422.06	2.5647	44.61	55.38	7.167	239.69	241.12	a	a2	a22
13	258.7	283.37	297.96	333.82	419.03	2.6223	42.26	57.15	7.2237	241.68	242.22	b	b1	b11
14	259.22	283.9	298.77	335.15	420.63	2.6552	44.26	56.89	7.0695	241.75	242.32	b	b1	b11
15	257.98	282.4	297.34	332.99	419.08	2.7776	42.17	56.72	7.4766	241.7	242.52	b	b1	b11
16	259.64	283.54	298.4	340.68	423.37	2.6118	42.63	55.24	6.9445	239.9	241.52	b	b1	b12
17	257.93	282.35	297.41	338.69	422.1	2.5331	42.09	54.93	7.3055	240.14	240.84	b	b1	b12
18	257.6	282.68	297.93	337.69	422.71	2.689	42.27	55.01	7.5452	240.16	240.86	b	b1	b12
19	256.13	281.28	296.89	334.98	419.25	2.5408	42.04	54.38	7.7196	239.62	241.5	b	b2	b21
20	257.91	282.42	297.74	338.63	421.3	2.4608	42.08	54.45	7.1655	240.29	241.79	b	b2	b21
21	258.31	282.58	297.78	340.97	423.69	2.4571	42.04	54.33	7.1876	239.71	241.6	b	b2	b21
22	256.85	281.73	296.42	335.29	418.49	2.6881	42.26	55.03	7.5448	237.12	240.57	b	b2	b22
23	256.14	281.24	296.4	335.06	420.25	2.6624	42.03	55.29	7.9544	240.25	241.41	b	b2	b22
24	256.89	281.62	296.41	335.08	418.99	2.7091	42.38	55.63	7.7784	239.68	240.85	b	b2	b22

Table SI.1-2. *Contin.*

No.	TG-DTG critical points										Sub-sampling stages		
	2nd_ML	2nd_Inf.T*	2nd_Mid.T	3rd_ML	3rd_Inf.T*	3rd_Mid.T	4th_ML	4th_Inf.T*	4th_Mid.T	Res.	5th	6th	7th

1	40.4814	292.91	304.23	31.5001	435.1	430.14	2.5304	638.19	625.27	14.5223	a	a1	a11
2	41.3015	293.54	303.89	30.7426	434.85	429.06	2.6727	639.06	625.63	14.4455	a	a1	a11
3	42.1748	293.43	304.01	31.1786	427.59	426.76	2.7292	638.22	628.06	12.4977	a	a1	a11
4	41.2372	291.3	303.81	29.2746	425.62	425.9	2.9611	637.45	627.57	14.8235	a	a1	a12
5	39.1853	291.98	303.79	29.3866	426.15	424.94	2.4431	636.73	625.97	18.1721	a	a1	a12
6	40.4514	288.9	303.23	29.9603	424.85	424.54	2.6175	637.22	626.18	15.9201	a	a1	a12
7	42.7941	298.54	305.47	29.8019	436.11	431.09	3.0702	638.22	627.7	13.14	a	a2	a21
8	41.1727	300.1	306.57	30.4842	435.36	432.26	3.0018	637.75	627.53	14.8458	a	a2	a21
9	41.2642	298.14	305.39	31.434	430.52	429.48	2.908	638.22	627.96	13.272	a	a2	a21
10	41.9603	295.66	304.29	31.8013	432.97	428.24	3.0072	638.11	630	13.2094	a	a2	a22
11	40.9952	294.92	303.56	29.7087	429.74	428.16	2.8309	638.73	627.7	15.7014	a	a2	a22
12	41.4855	293.87	303.5	31.2313	429.02	427.49	2.9716	638.29	628.08	14.3273	a	a2	a22
13	43.9647	298.85	304.68	29.7281	427.85	426.84	2.9479	638.18	626.87	12.7479	b	b1	b11
14	43.6601	299.78	305.11	30.1601	432.78	427.99	2.9346	638.35	627.09	12.2644	b	b1	b11
15	44.9063	299.32	304.62	29.7465	431.48	427.81	3.0067	638.18	627.78	11.522	b	b1	b11
16	42.2103	293.42	304.26	31.0776	431.51	429.48	2.961	637.88	628.03	12.9527	b	b1	b12
17	42.0292	296.13	303.99	30.5452	433.86	429.06	2.8321	638.20	626.67	13.6386	b	b1	b12
18	42.8603	296.07	304.66	30.7337	435.42	429.84	2.9746	638.24	627.72	12.2631	b	b1	b12
19	42.4893	298.19	304.78	29.3449	425.85	426.17	2.6982	638.41	626.46	13.7075	b	b2	b21
20	41.3319	293.82	304.55	30.0687	432.83	428.73	2.4677	638.17	622.78	15.9746	b	b2	b21
21	41.3614	294.28	303.83	31.2627	437.58	430.04	2.6669	638.21	625.11	13.9525	b	b2	b21
22	42.3001	296.01	303.45	29.8476	427.11	425.8	2.7036	638.53	626.29	13.5867	b	b2	b22
23	43.2932	295.68	303.64	30.6586	427.67	427.09	2.8878	638.38	626.33	11.5196	b	b2	b22

24	43.7752	295.74	303.65	30.4328	425.65	425.59	2.9029	638.93	625.87	11.2868	b	b2	b22

Table SI.1-2. *Contin.*

No.	TG-DTG critical points								Sub-sampling stages		
	1st_RML	1st_ On.T	1st_Peak.T	1st_End.T	2nd_RML	2nd_On.T	2nd_Peak.T	2nd_End.T	5th	6th	7th
1	3.073967	226.19	239.86	244.55	5.379443	280.60	292.74	349.44	a	a1	a11
2	3.225806	225.85	239.77	244.56	5.571848	281.06	292.86	350.7	a	a1	a11
3	3.185328	225.42	238.81	244.48	5.791506	279.43	292.92	345.9	a	a1	a11
4	3.438395	226.51	239.69	244.35	5.730659	279.94	291.8	347.96	a	a1	a12
5	2.972196	223.95	236.69	243.1	5.369128	279.80	291.47	345.92	a	a1	a12
6	3.106796	224.05	238.18	243.69	5.631068	280.77	290.84	346.84	a	a1	a12
7	3.210117	226.97	241.48	245.94	5.642023	281.96	297.53	358.17	a	a2	a21
8	2.898551	226.29	241.48	245.87	5.31401	282.18	299.93	361.86	a	a2	a21
9	2.969349	225.89	240.2	244.98	5.45977	282.77	297.46	356.06	a	a2	a21
10	2.810078	225.62	239.47	244.67	5.910853	281.86	295.14	348.95	a	a2	a22
11	2.890173	255.73	240.29	244.81	5.876686	281.65	294.06	345.96	a	a2	a22
12	2.95858	225.78	240.55	244.59	5.91716	282.04	293.87	346.96	a	a2	a22
13	3.197674	228.27	242.38	246.64	6.395349	282.66	298.85	347.73	b	b1	b11
14	3.210117	228.93	242.28	246.37	6.322957	282.51	299.95	349.68	b	b1	b11
15	3.398058	228.95	241.88	245.75	6.407767	282.80	298.64	349.31	b	b1	b11
16	2.837573	226.98	241.47	246.41	5.870841	281.86	294.95	349.62	b	b1	b12

17	2.895753	224.98	240.14	244.52	5.888031	280.81	295.1	350.12	b	b1	b12
18	2.904163	224.63	240.33	244.97	6.001936	282.47	296.75	351.09	b	b1	b12
19	3.188406	226.27	240.14	244.72	5.797101	281.48	297.17	354.06	b	b2	b21
20	3.021442	227.39	240.46	244.88	5.653021	281.74	295.34	353.48	b	b2	b21
21	3.039216	226.96	240.41	244.23	5.784314	281.53	294.1	350.24	b	b2	b21
22	3.00679	225.45	238.86	244.52	6.110572	281.23	295.33	346.98	b	b2	b22
23	3.257651	226.52	240.94	245.73	6.120434	282.27	296.53	347.62	b	b2	b22
24	3.100775	225.69	239.51	244.45	6.29845	281.59	295.23	347.46	b	b2	b22

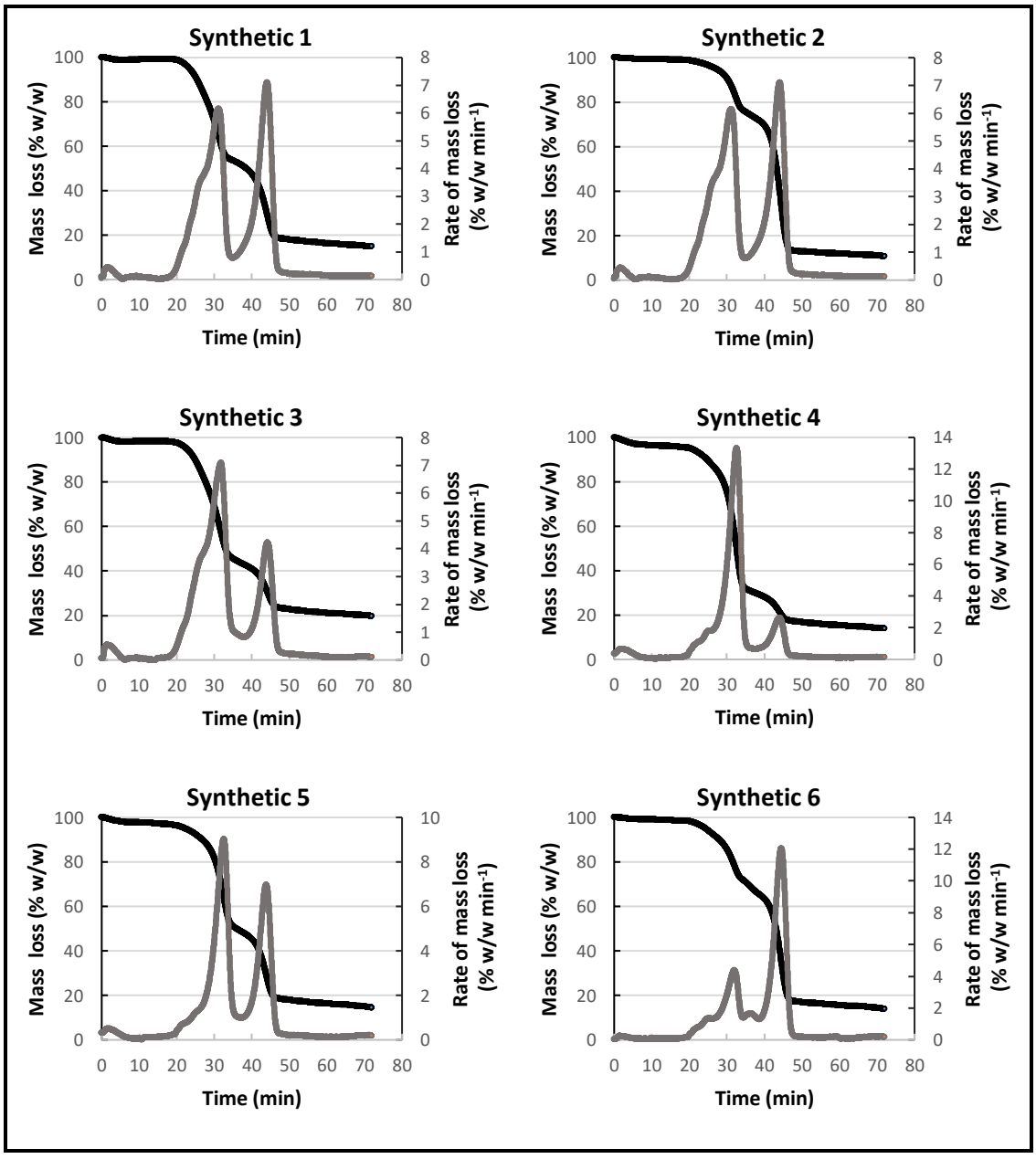
Table SI.1-2. *Contin.*

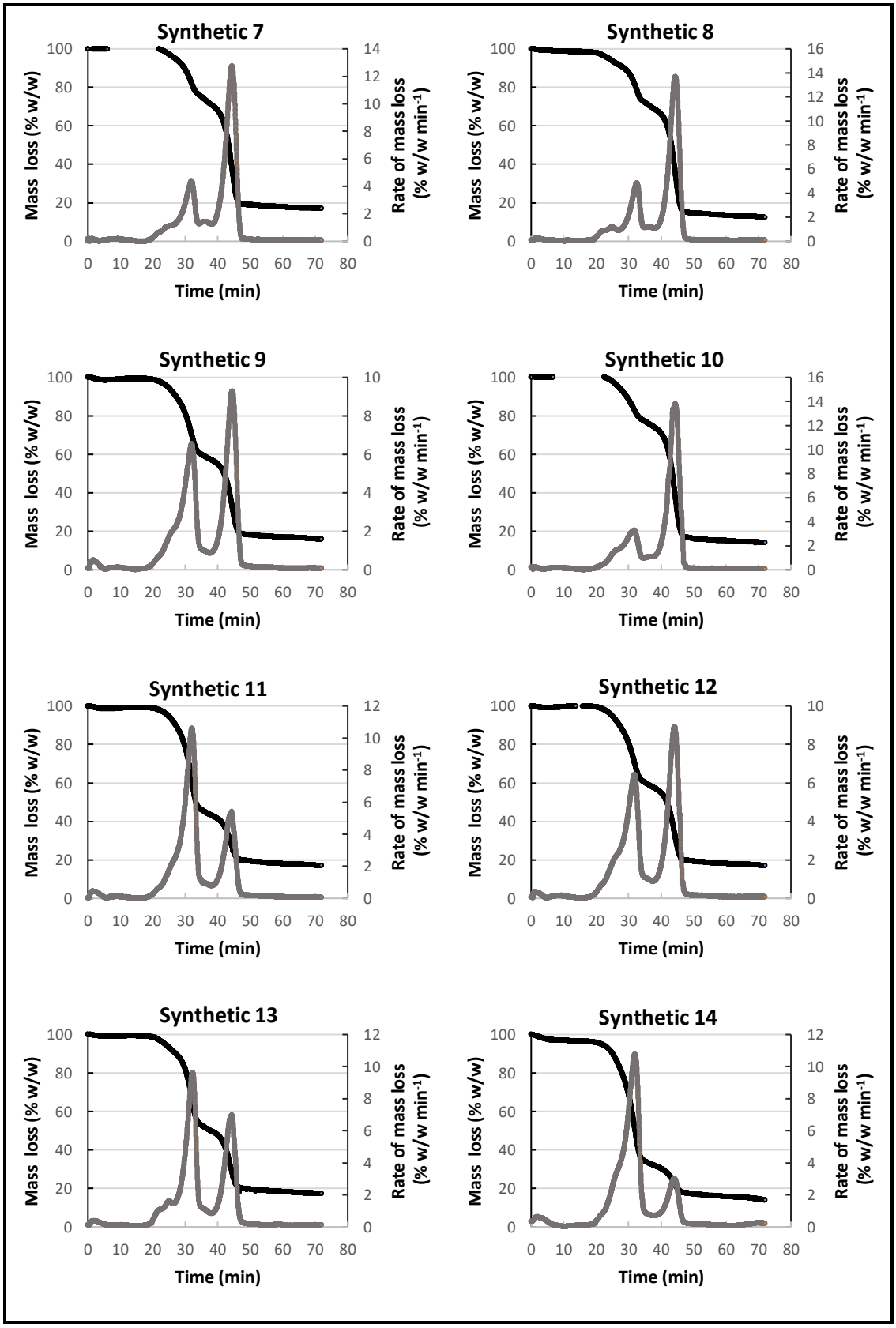
No.	TG-DTG critical points									Sub-sampling stages		
	3rd_RML	3rd_On.T	3rd_Peak.T	3rd_End.T	4th_RML	4th_On.T	4th_Peak.T	4th_End.T	S	5th	6th	7th
1	8.069164	423.17	435.98	444.55	0.394909	5.92E+02	637.05	656.28	2.07E-07	a	a1	a11
2	7.624633	421.18	435.23	444.72	0.404399	5.92E+02	637.43	661.90	1.94E-07	a	a1	a11
3	10.32819	416.81	430.06	441.75	0.410907	5.92E+02	637.40	660.40	2.67E-07	a	a1	a11
4	7.831901	415.22	426.59	434.97	0.429226	5.88E+02	636.14	656.04	2.01E-07	a	a1	a12
5	9.87536	415.62	429.51	438.15	0.394247	6.58E+02	636.24	663.67	2.56E-07	a	a1	a12
6	10	414.87	426.95	438.67	0.413398	5.93E+02	635.42	656.97	2.63E-07	a	a1	a12
7	5.544747	420.52	435.79	449.43	0.473833	5.90E+02	644.58	695.73	1.36E-07	a	a2	a21
8	6.956522	424.17	435.36	443.31	0.458454	5.90E+02	639.87	660.01	1.77E-07	a	a2	a21
9	7.854406	419.40	431.02	439.62	0.450383	4.67E+02	639.69	661.27	2.00E-07	a	a2	a21

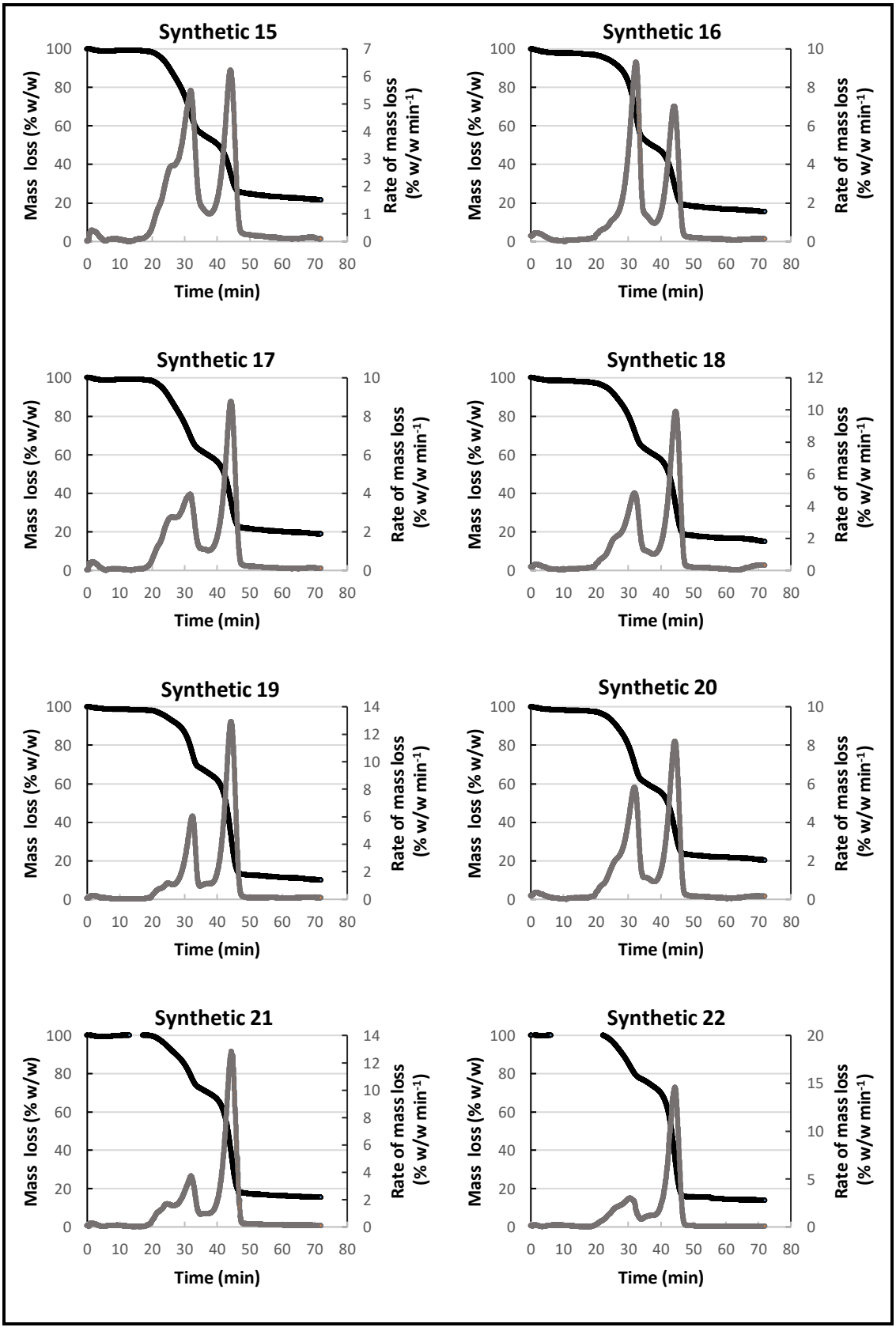
10	9.496124	422.08	435.92	444.41	0.465795	5.90E+02	639.75	655.16	2.45E-07	a	a2	a22
11	8.766859	419.63	431.38	438.13	0.455395	5.95E+02	638.08	658.96	2.23E-07	a	a2	a22
12	9.171598	418.88	430.06	436.74	0.455128	6.49E+02	633.65	673.39	2.30E-07	a	a2	a22
13	8.333333	417.57	428.38	435	0.454167	5.87E+02	637.37	663.76	2.08E-07	b	b1	b11
14	7.198444	420.95	433.01	441.39	0.459339	6.38E+02	637.54	654.25	1.82E-07	b	b1	b11
15	9.029126	420.39	433.44	440.42	0.470097	5.88E+02	640.14	659.16	2.27E-07	b	b1	b11
16	9.393346	421.30	433.65	441.12	0.459295	5.89E+02	636.56	659.62	2.40E-07	b	b1	b12
17	6.563707	421.04	434.05	444.31	0.443243	5.91E+02	636.72	685.36	1.61E-07	b	b1	b12
18	6.96999	423.20	435.42	444.37	0.459729	5.93E+02	637.42	663.97	1.76E-07	b	b1	b12
19	9.275362	415.93	427.37	434.91	0.41913	5.91E+02	637.27	659.66	2.37E-07	b	b2	b21
20	8.479532	421.88	433.34	441	0.404873	5.91E+02	637.03	656.12	2.17E-07	b	b2	b21
21	5.294118	409.12	437.58	456.05	0.406667	5.89E+02	637.23	657.69	1.48E-07	b	b2	b21
22	8.923375	416.40	429.35	439.24	0.424248	5.94E+02	639.84	695.88	2.21E-07	b	b2	b22
23	9.970385	417.27	430.06	437.81	0.443337	5.90E+02	637.25	656.82	2.55E-07	b	b2	b22
24	9.496124	415.67	426.68	433.23	0.452229	5.94E+02	637.46	657.15	2.44E-07	b	b2	b22

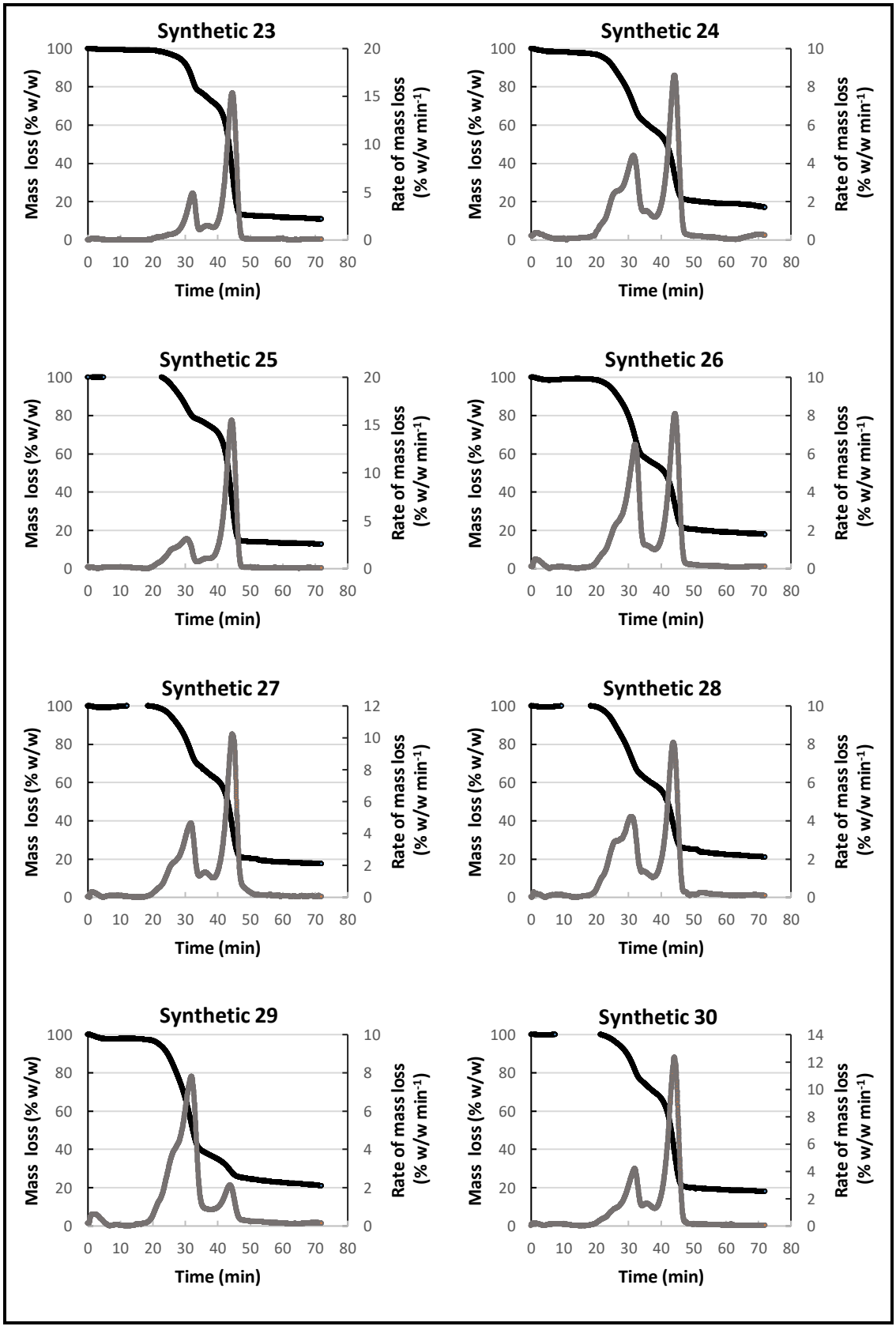
SI.2 Analytical results of ML model datasets

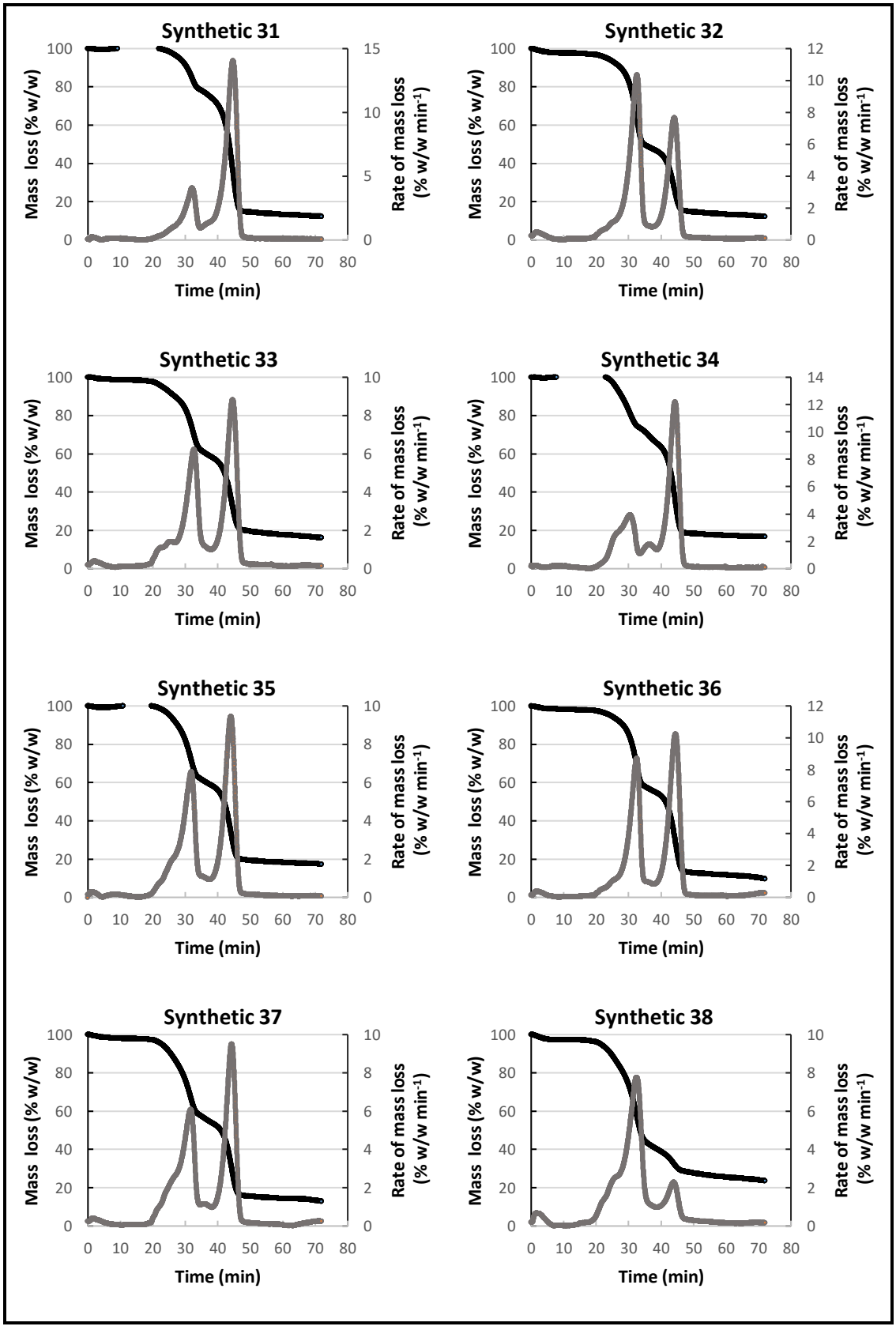
I. TG-DTG and FTIR profiles of training set (synthetic mixtures)

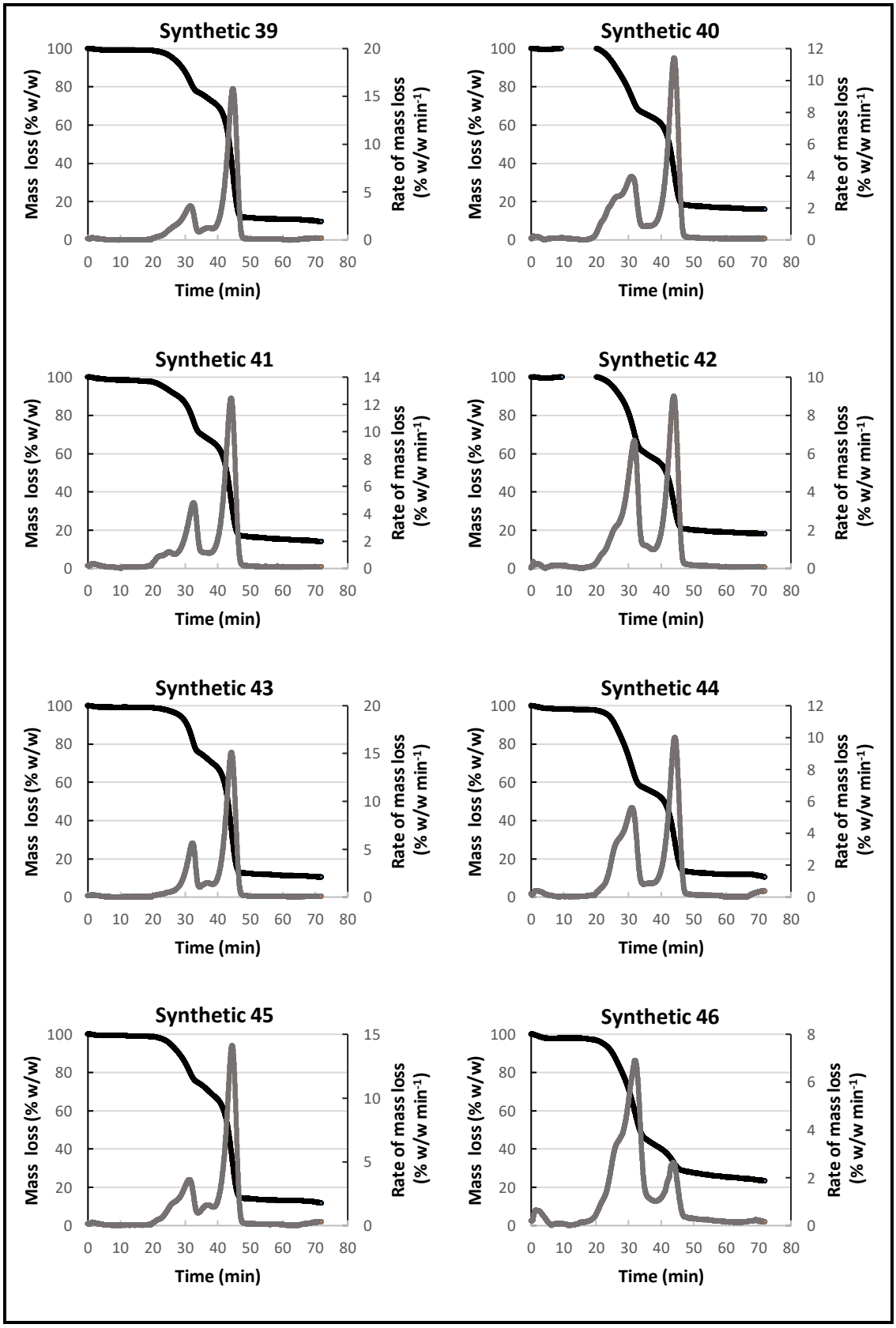



Synthetic 7
Synthetic 8
Synthetic 9
Synthetic 10
Synthetic 11
Synthetic 12
Synthetic 13
Synthetic 14
Mass loss (% w/w)
Rate of mass loss (% w/w min-1)
Time (min)


Synthetic 15
Synthetic 16
Synthetic 17
Synthetic 18
Synthetic 19
Synthetic 20
Synthetic 21
Synthetic 22
Mass loss (% w/w)
Rate of mass loss (% w/w min-1)
Time (min)


Synthetic 23
Synthetic 24
Synthetic 25
Synthetic 26
Synthetic 27
Synthetic 28
Synthetic 29
Synthetic 30
Mass loss (% w/w)
Rate of mass loss (% w/w min-1)
Time (min)


Synthetic 31
Synthetic 32
Synthetic 33
Synthetic 34
Synthetic 35
Synthetic 36
Synthetic 37
Synthetic 38
Mass loss (% w/w)
Rate of mass loss (% w/w min-1)
Time (min)


Synthetic 39
Synthetic 40
Synthetic 41
Synthetic 42
Synthetic 43
Synthetic 44
Synthetic 45
Synthetic 46
Mass loss (% w/w)
Rate of mass loss (% w/w min-1)
Time (min)

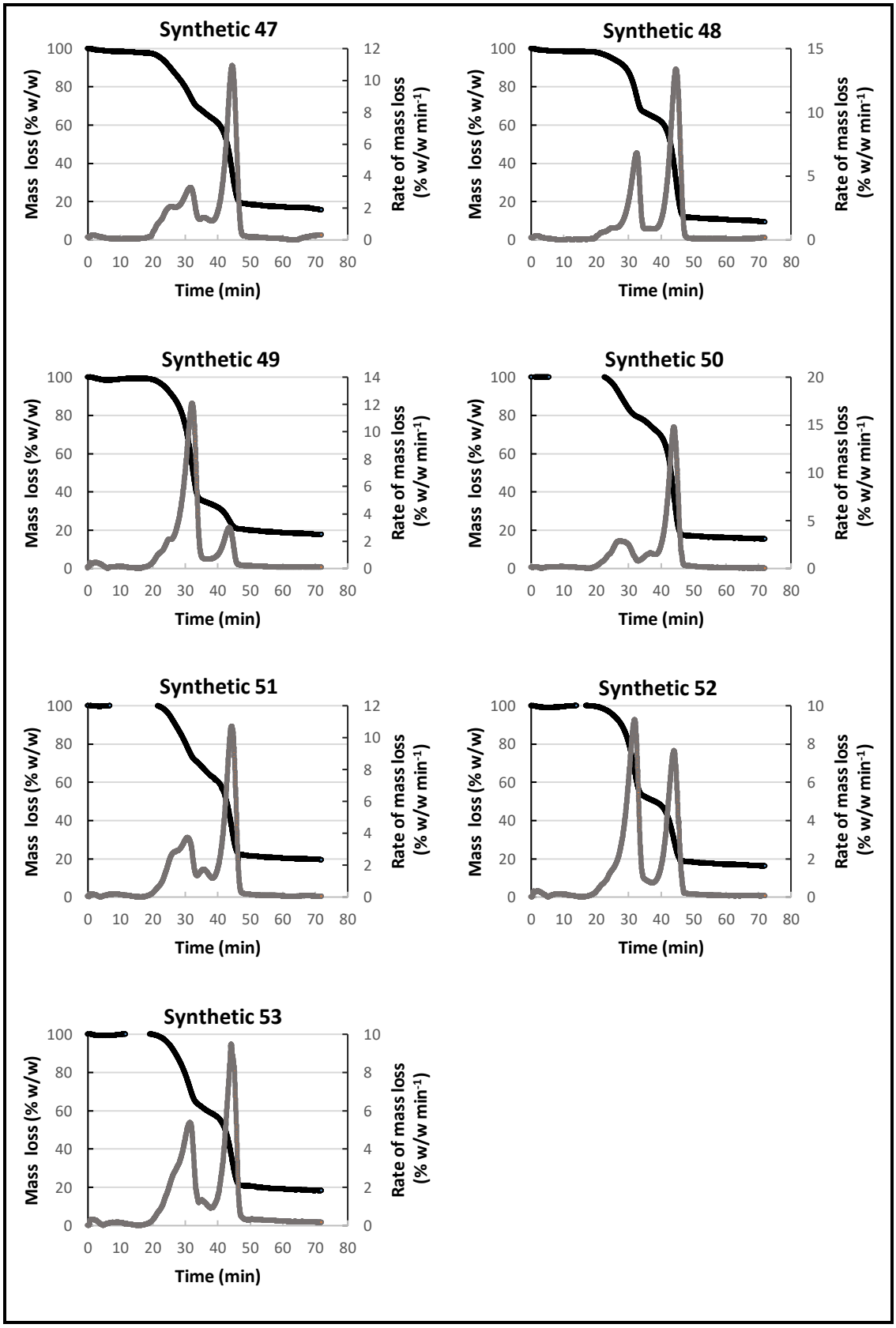
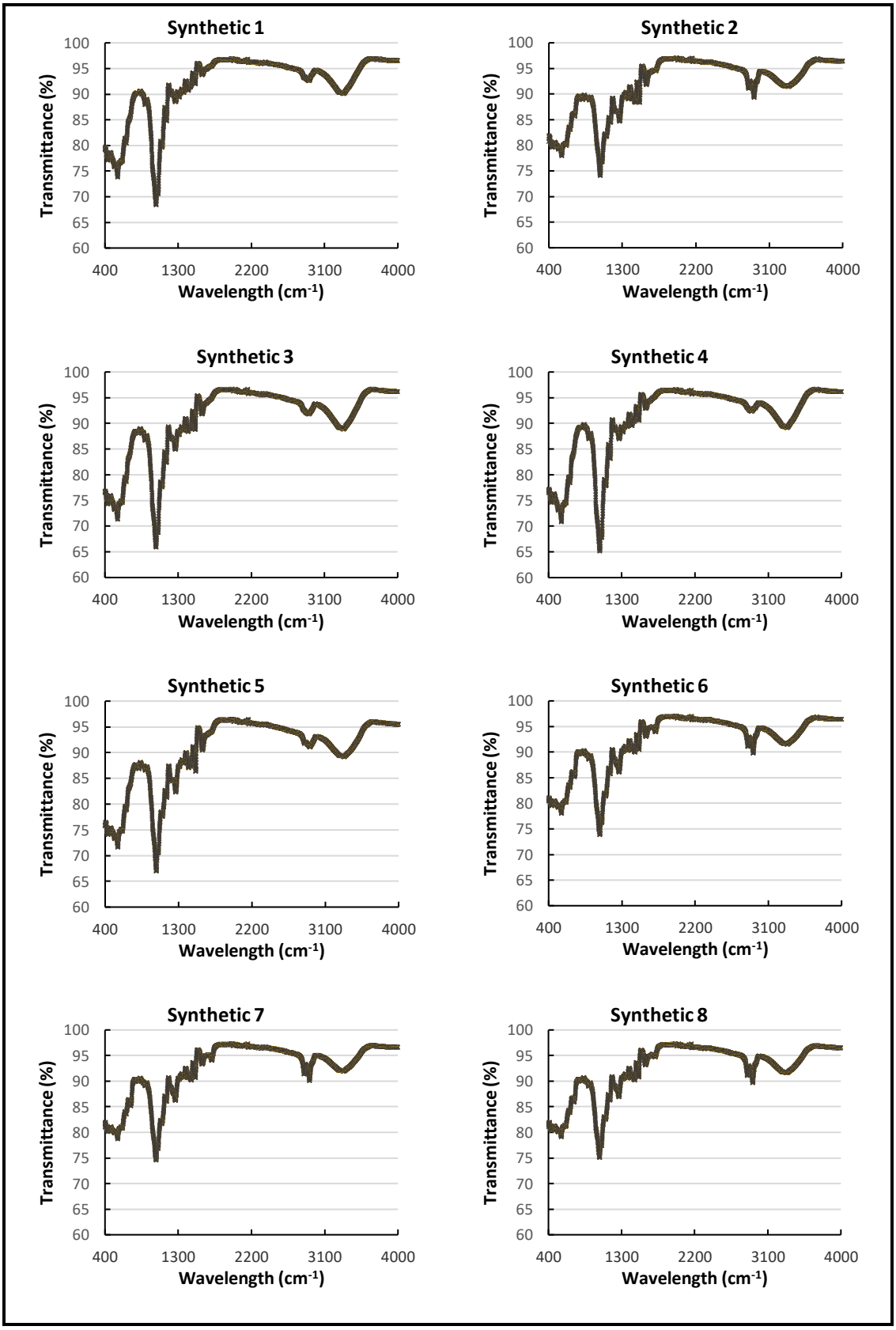
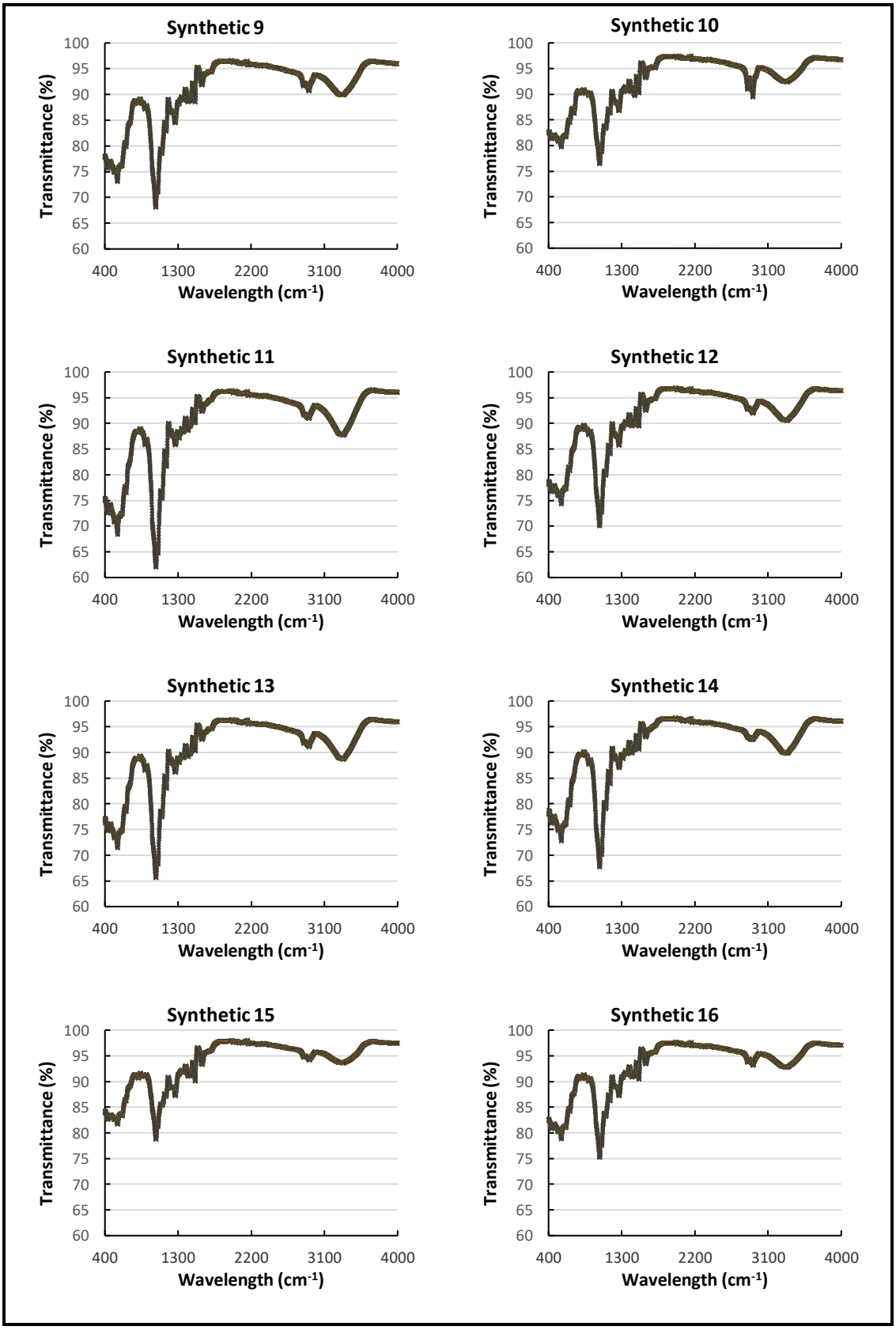
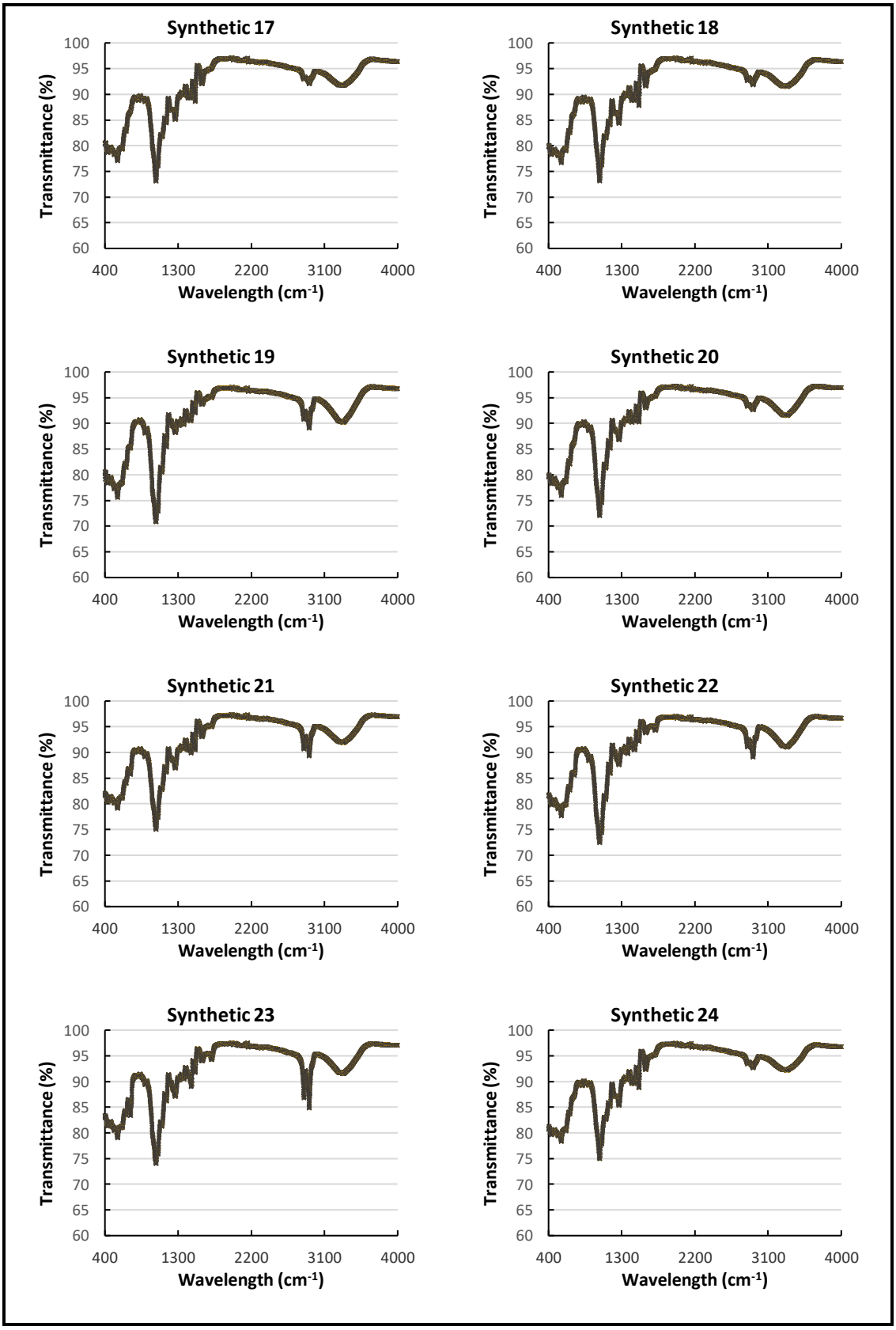
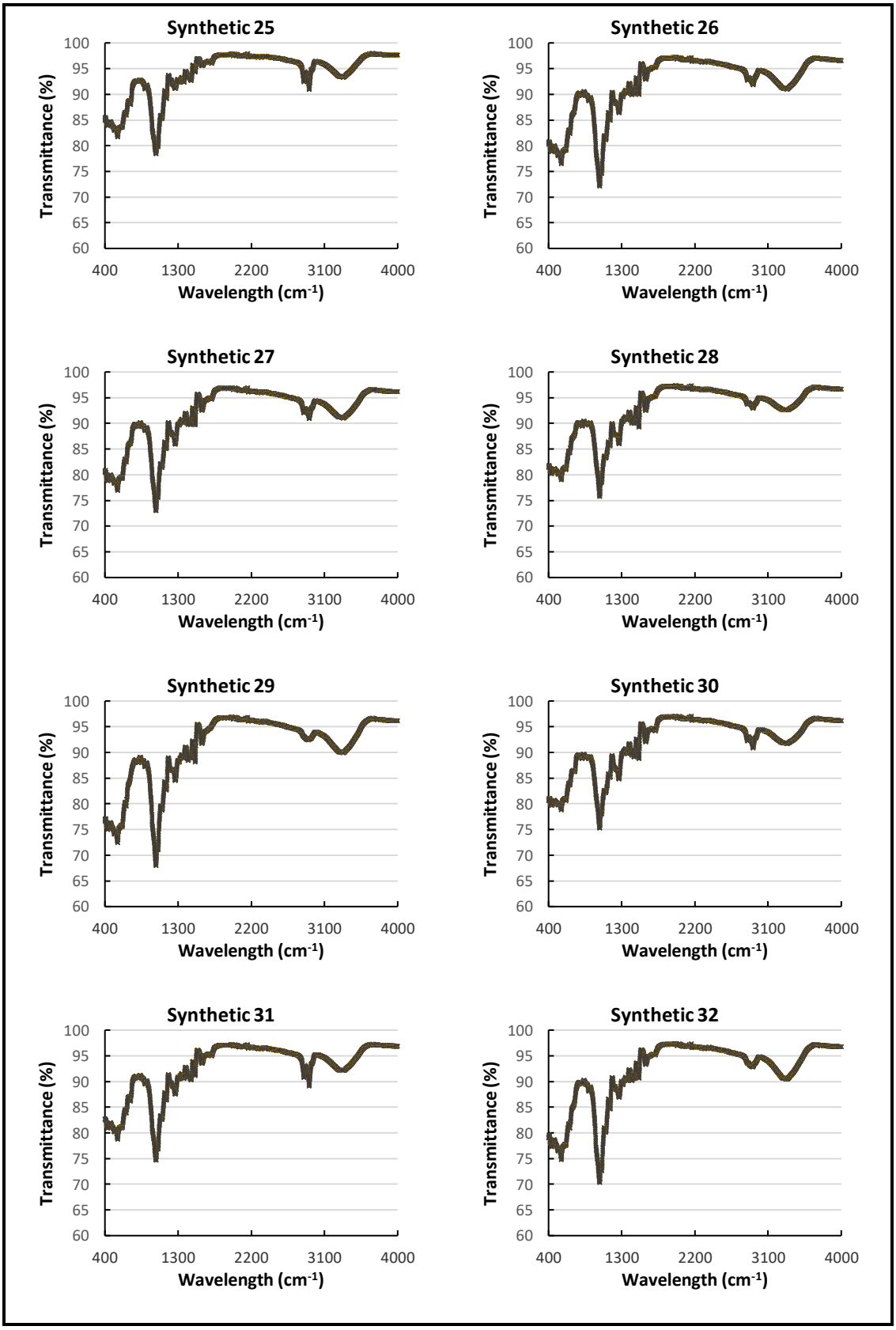


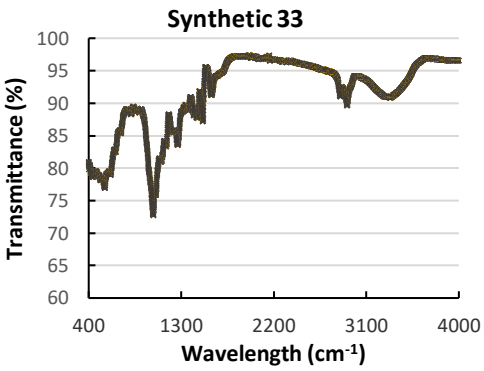
Figure SI.2-1. TG-DTG thermograms of synthetic mixtures (training set): Raw data of DTG (rate of mass loss every second) used for the ML model training and cross-validation.

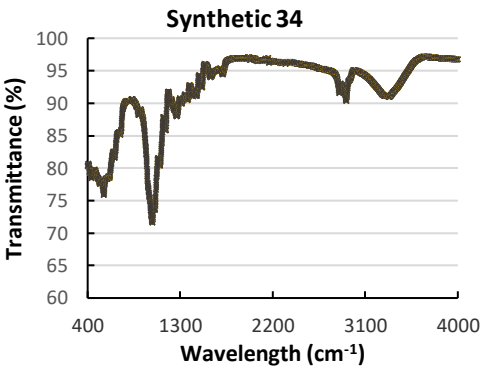

Synthetic 1
Synthetic 2
Synthetic 3
Synthetic 4
Synthetic 5
Synthetic 6
Synthetic 7
Synthetic 8
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

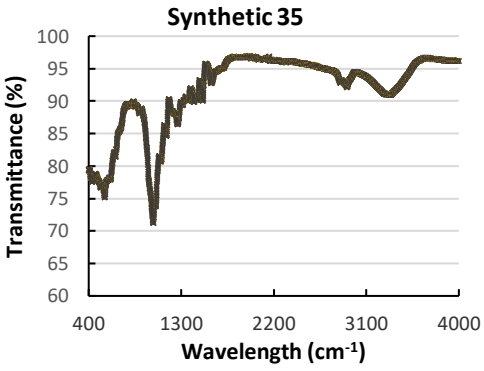

Synthetic 9
Synthetic 10
Synthetic 11
Synthetic 12
Synthetic 13
Synthetic 14
Synthetic 15
Synthetic 16
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

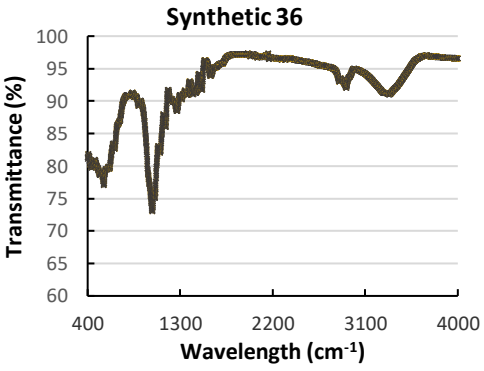

Synthetic 17
Synthetic 18
Synthetic 19
Synthetic 20
Synthetic 21
Synthetic 22
Synthetic 23
Synthetic 24
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

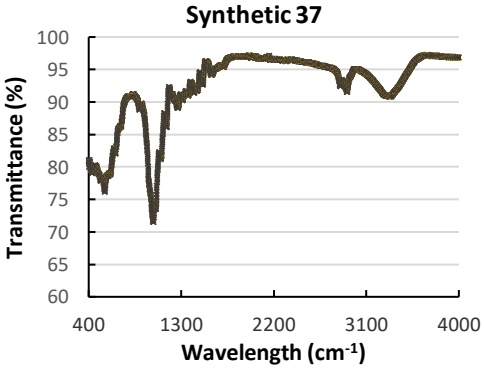

Synthetic 25
Synthetic 26
Synthetic 27
Synthetic 28
Synthetic 29
Synthetic 30
Synthetic 31
Synthetic 32
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

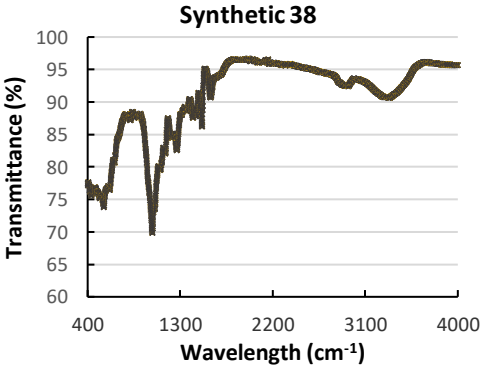

Synthetic 33
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

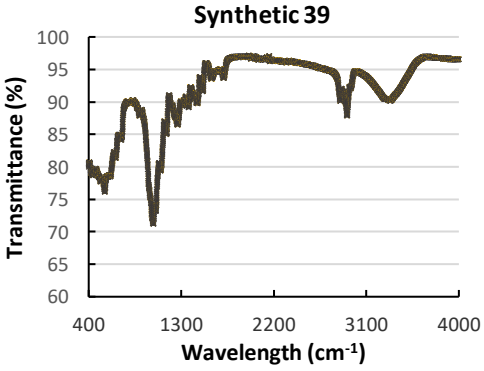

Synthetic 34
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

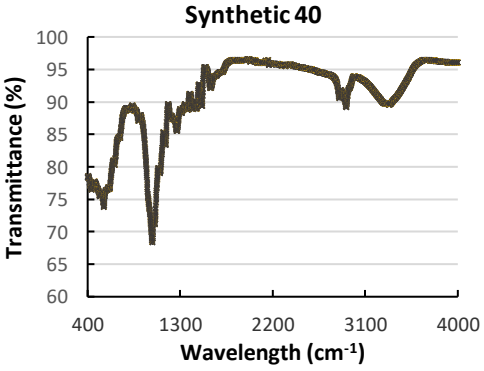

Synthetic 35
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

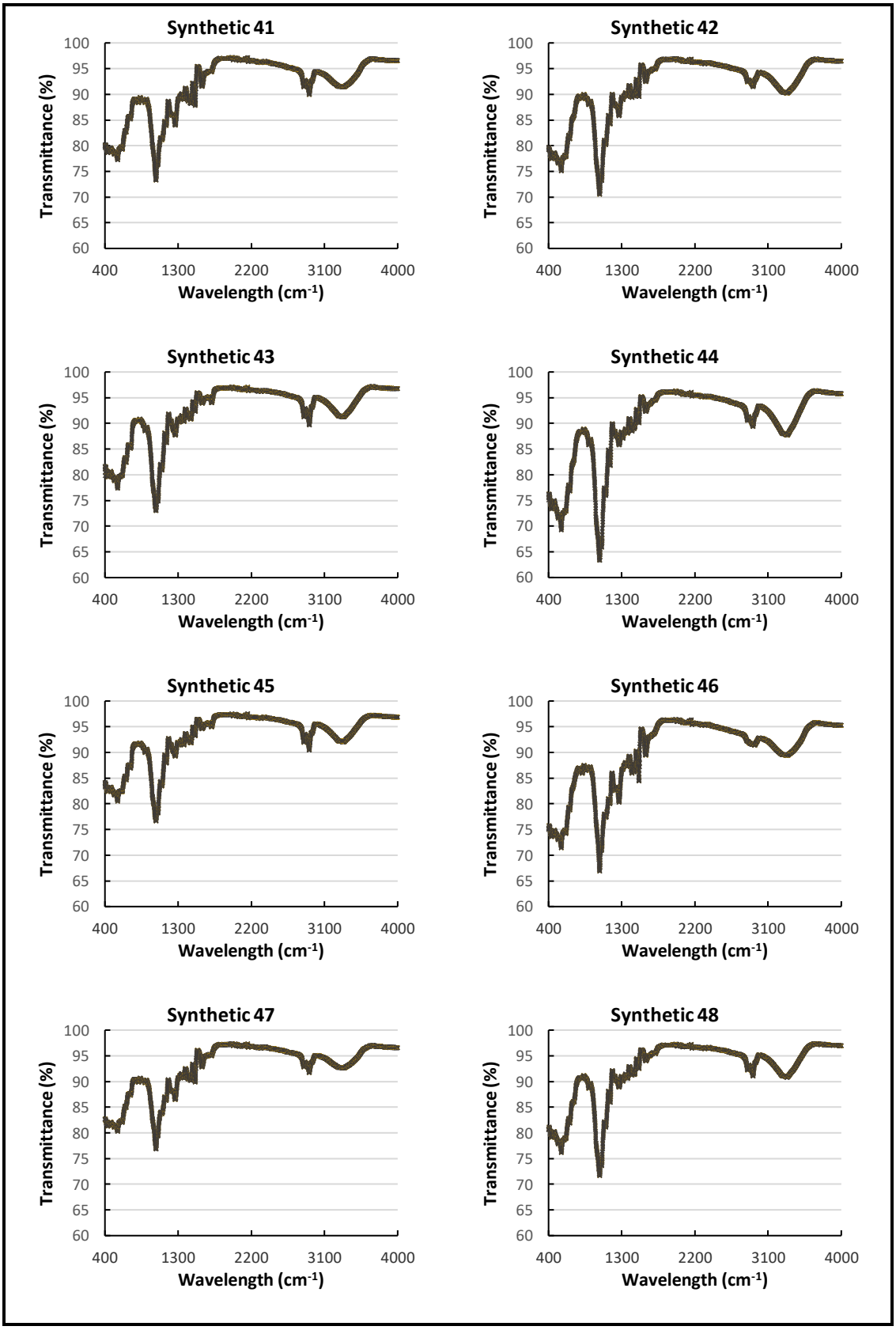

Synthetic 36
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)


Synthetic 37
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)


Synthetic 38
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)


Synthetic 39
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)


Synthetic 40
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)


Synthetic 41
Synthetic 42
Synthetic 43
Synthetic 44
Synthetic 45
Synthetic 46
Synthetic 47
Synthetic 48
Transmittance (%)
100
95
90
85
80
75
70
65
60
400
1300
2200
3100
4000
Wavelength (cm-1)

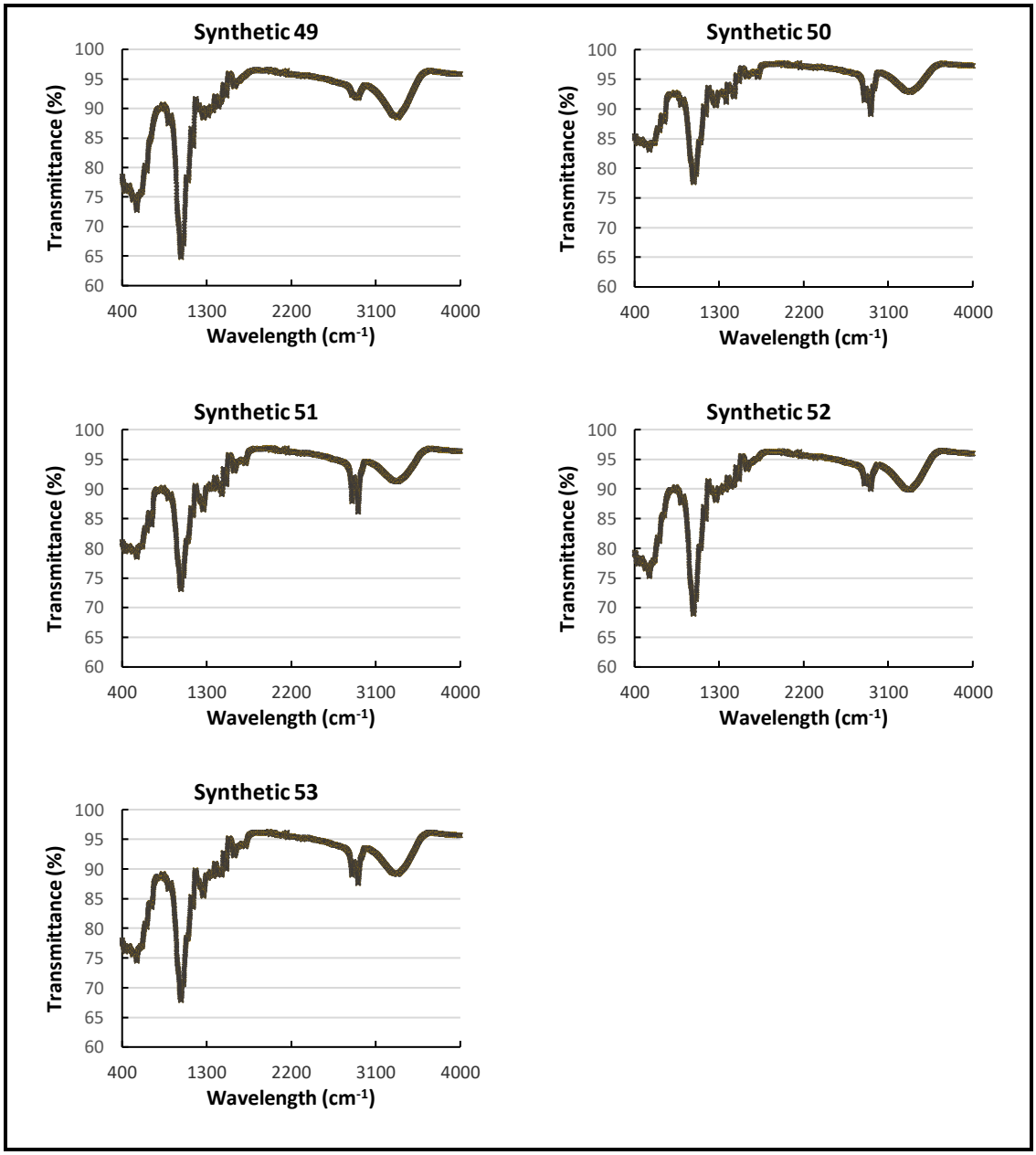


Figure SI.2-2. FTIR spectrum of synthetic mixtures (training set): Raw data of FTIR (absorbance per wavelength) used for the ML model training and cross-validation.

II. TG-DTG and FTIR profiles of validation set (waste mixtures)

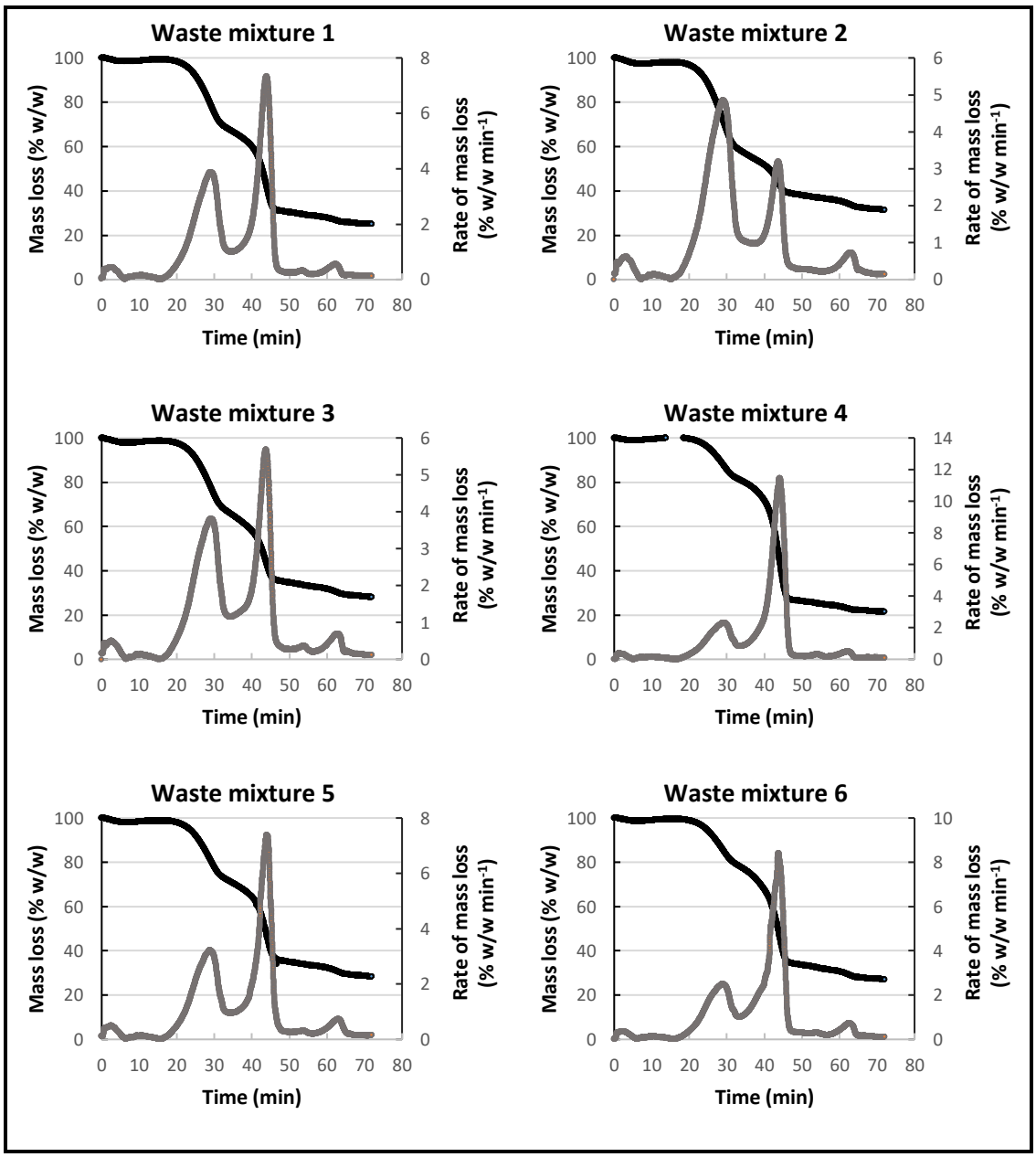


Figure SI.2-3. TG-DTG thermograms of waste mixtures (hold-out validation set): Raw data of DTG (rate of mass loss every second) used for the ML model validation.

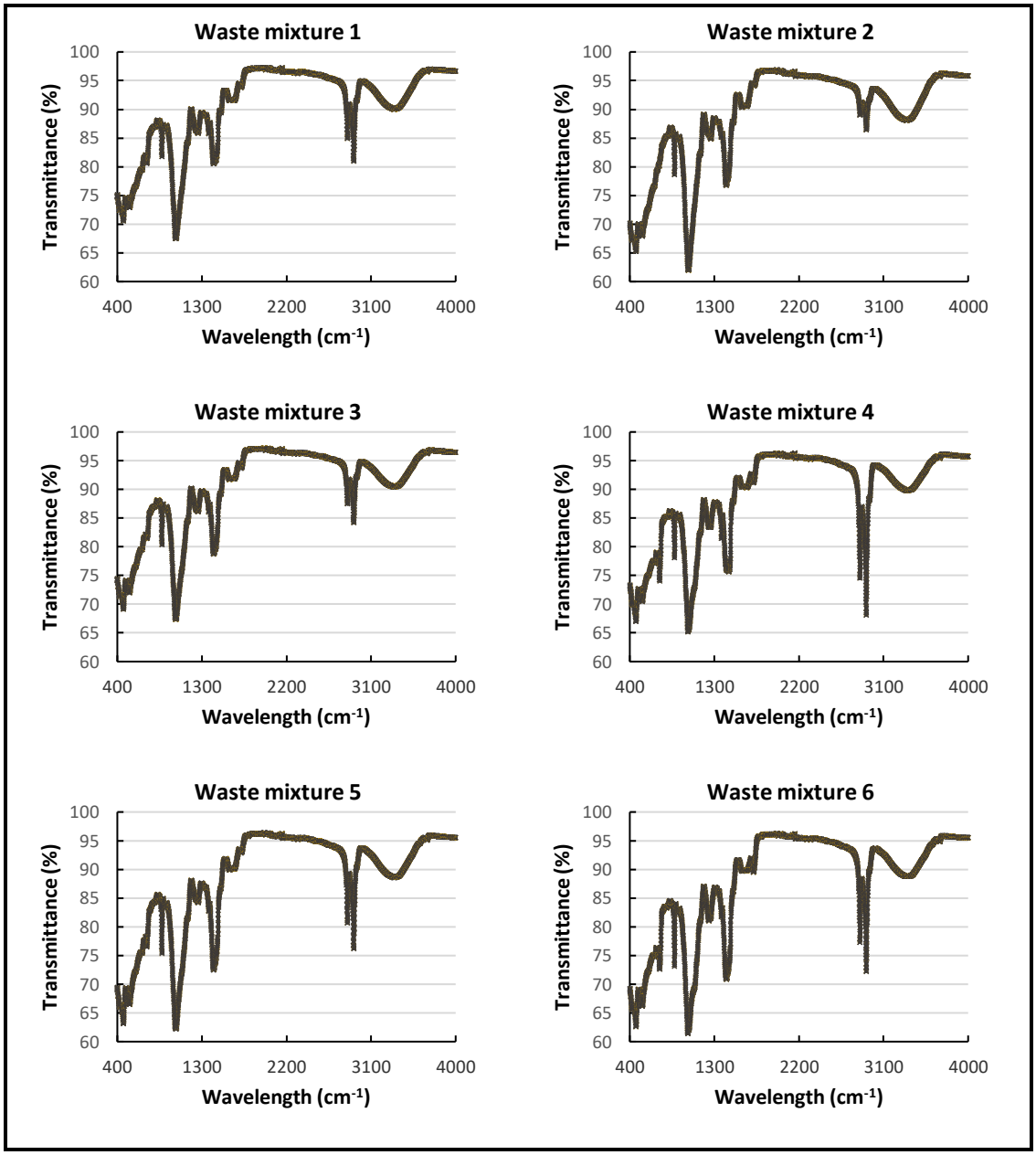


Figure SI.2-4. FTIR spectrum of waste mixtures (hold-out validation set): Raw data of FTIR (absorbance per wavelength) used for the ML model validation.

III. FTIR profiles of testing set (commercially produced SRF samples)

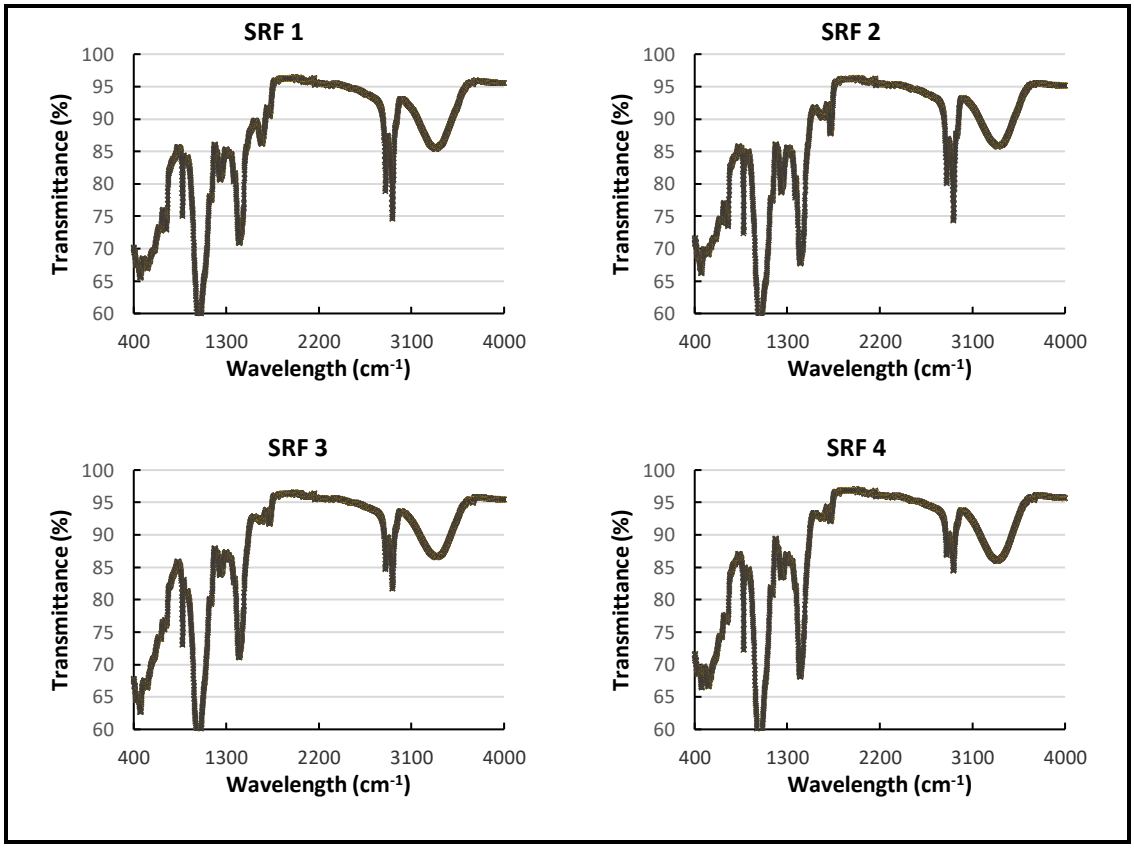


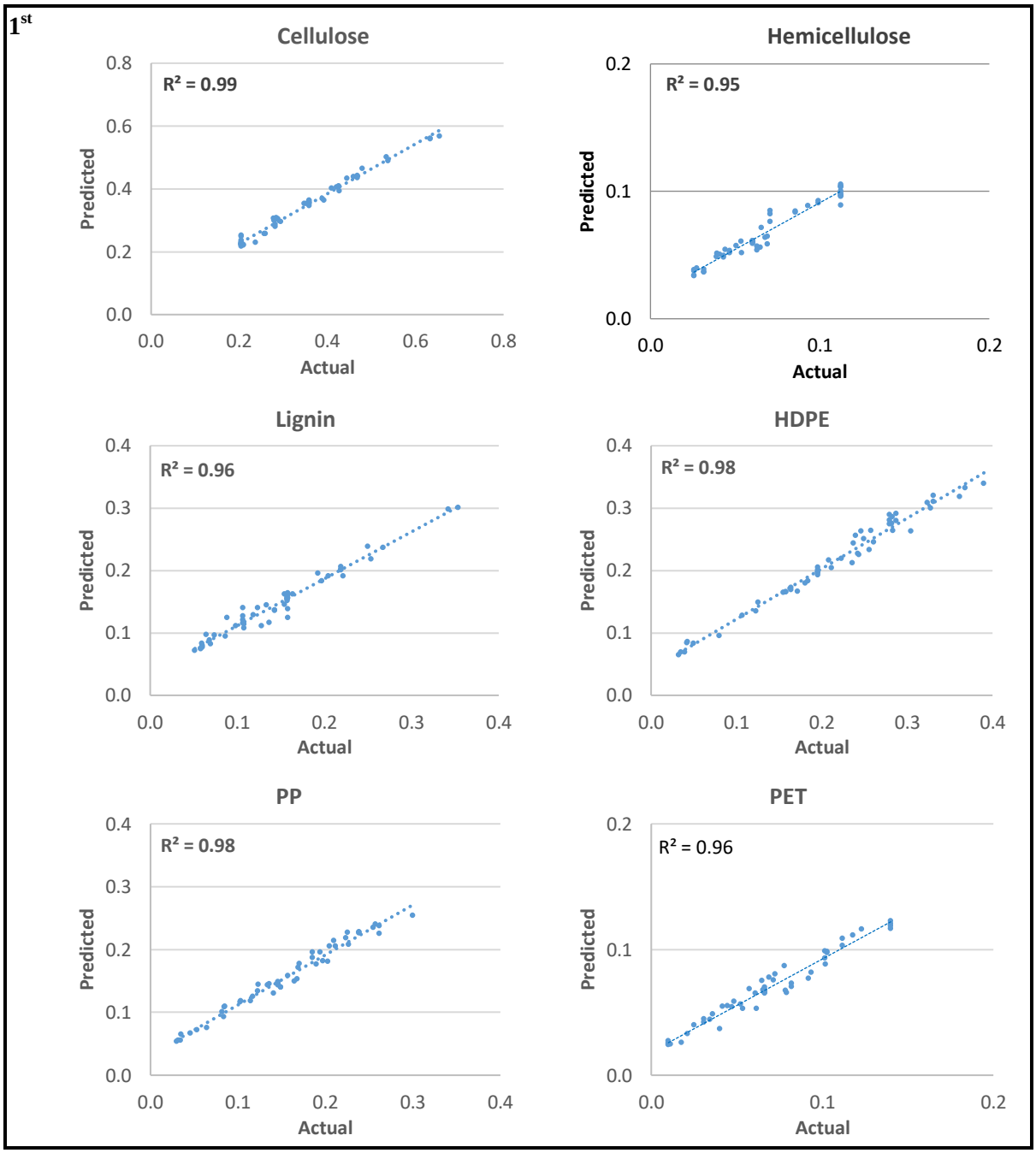
Figure SI.2-5. FTIR spectrum of SRF samples obtained from two MT plants in the UK (testing set): Raw data of FTIR (absorbance per wavelength) used for the ML model testing.

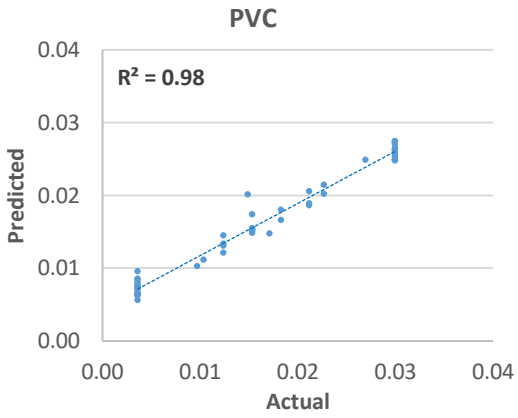
Noted that TG-DTG thermograms are provided in the Results chapter (Section 5.7.8)

SI.3 Scatter plots of observed vs predicted values for each dataset combination

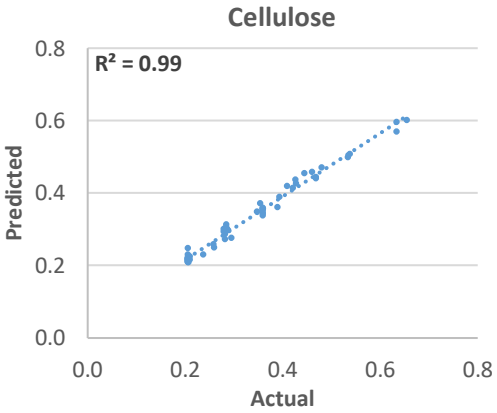
Dataset combinations are provided in **Table 4.10**.

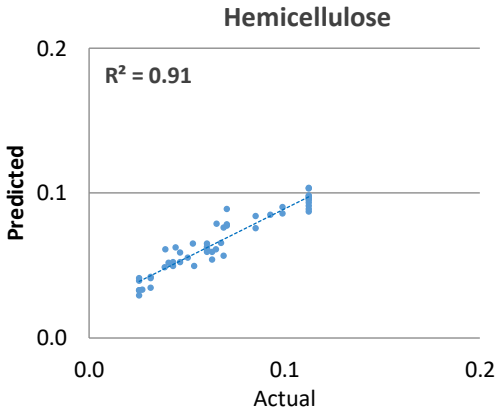
I. Scatter plots (Obs. vs Pred.) of dataset combination under constant *mtry*

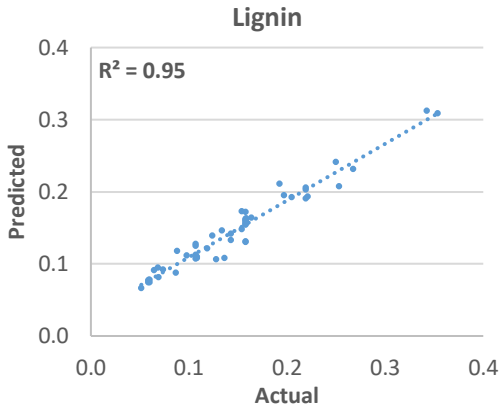


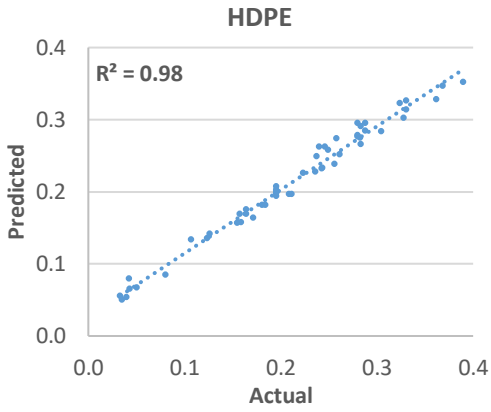

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

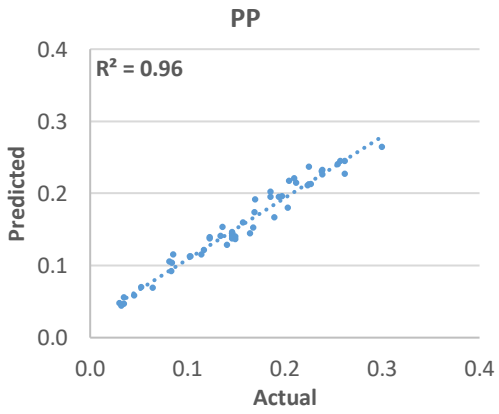
2nd:

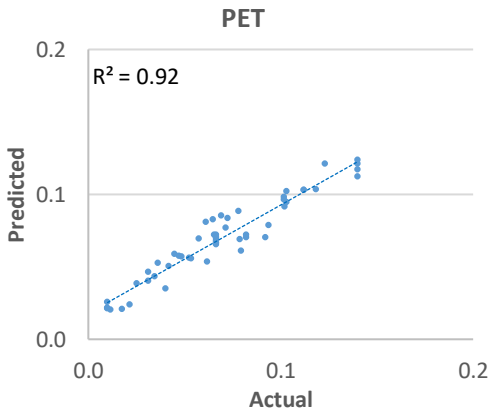

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

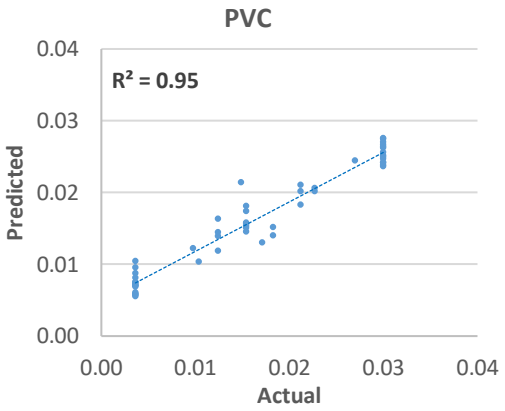

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

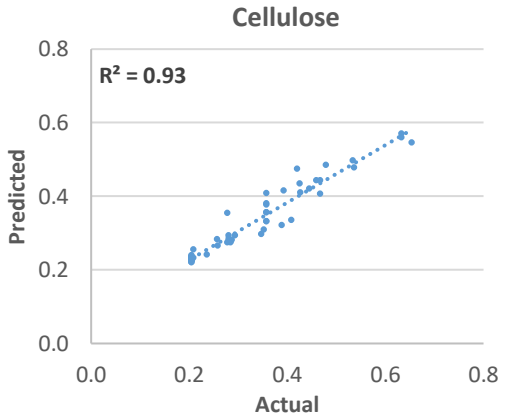

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

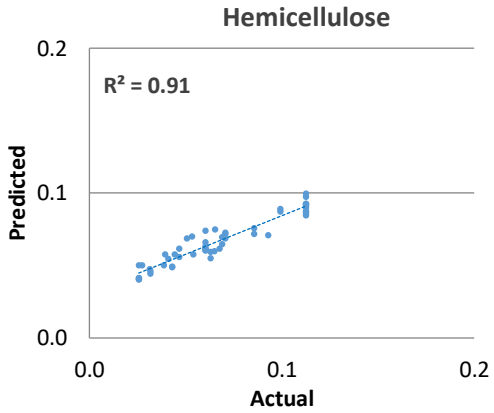

PP
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

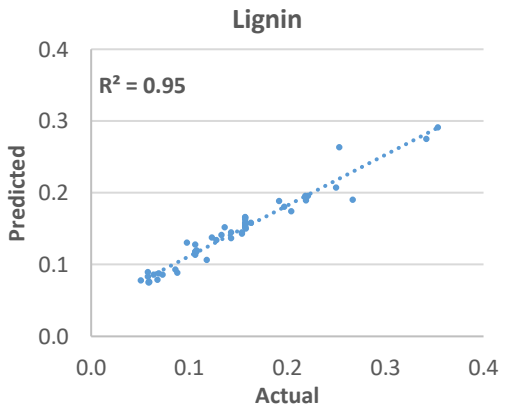

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

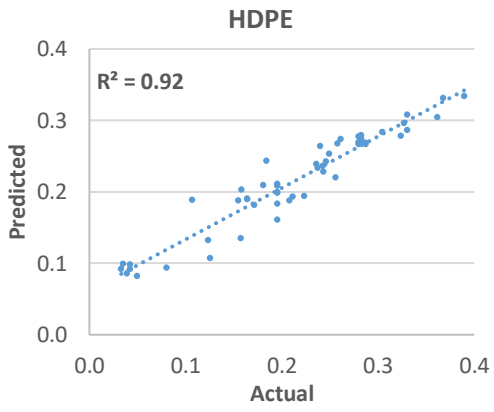

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

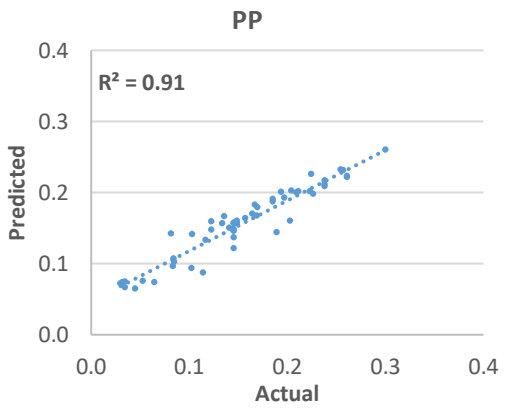
3rd:

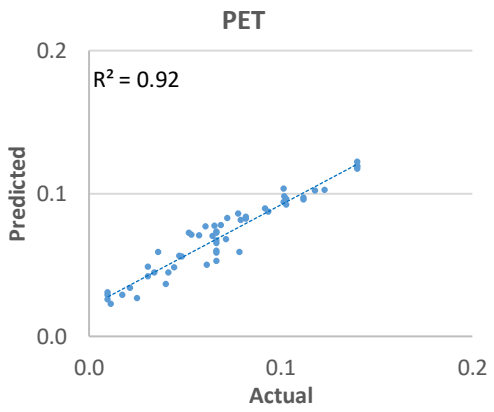

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

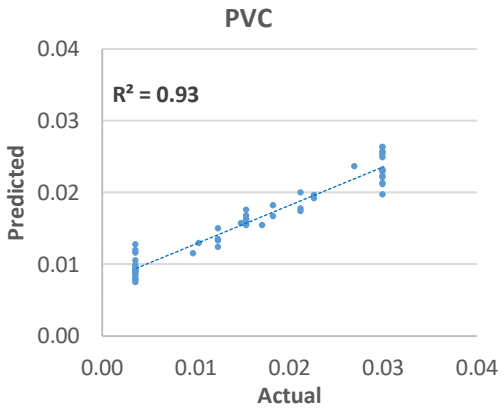

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

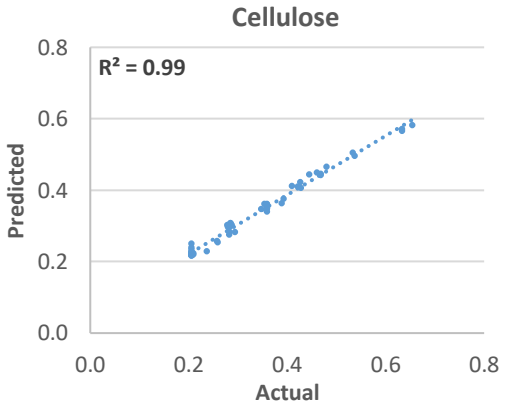

HDPE
R² = 0.92
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

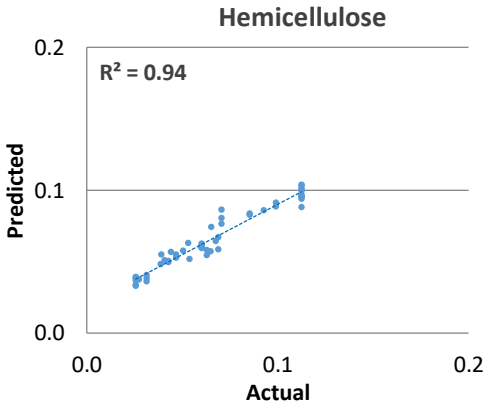

PP
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

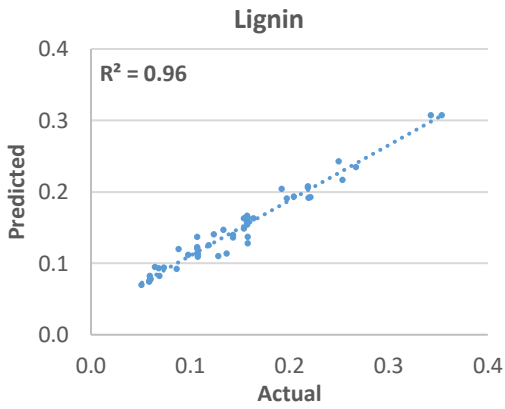

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

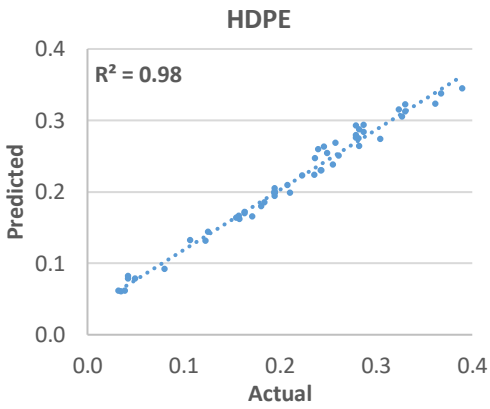

PVC
R² = 0.93
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

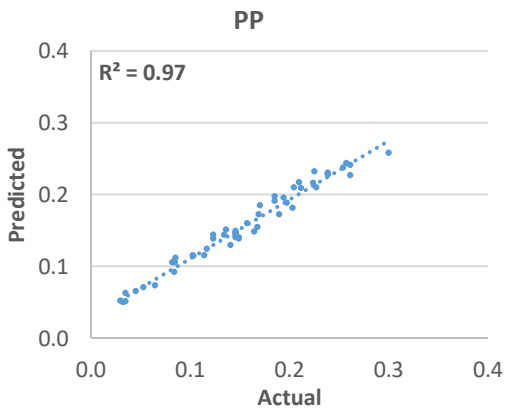
4th:

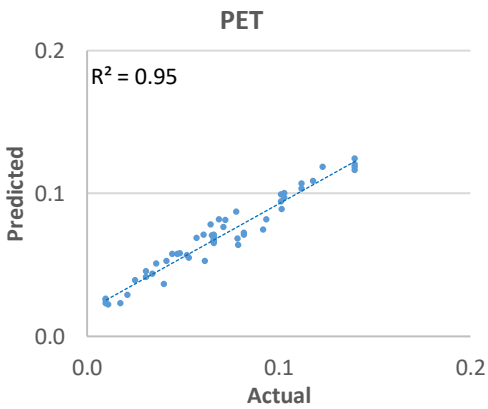

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

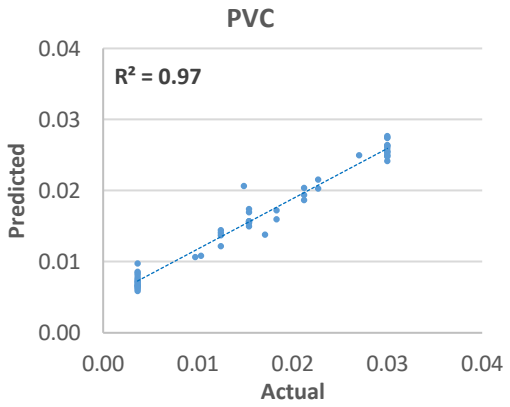

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

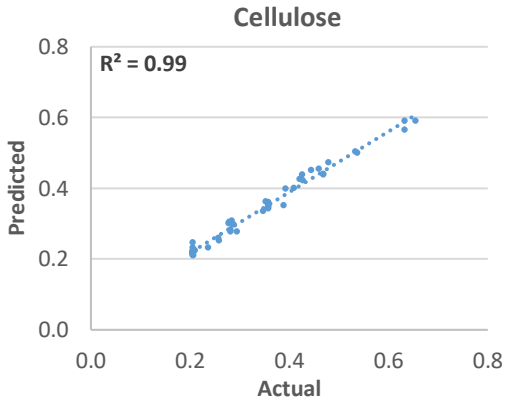

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

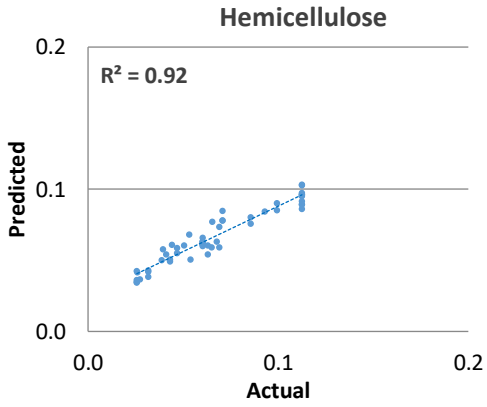

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

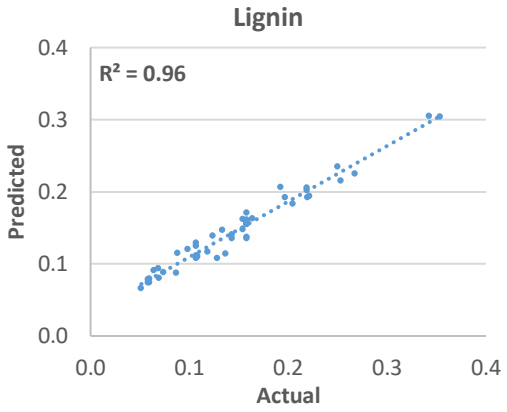

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

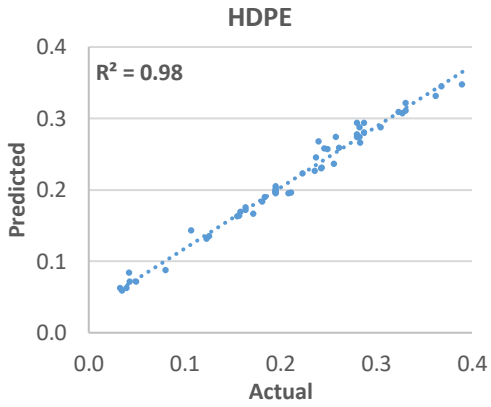

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

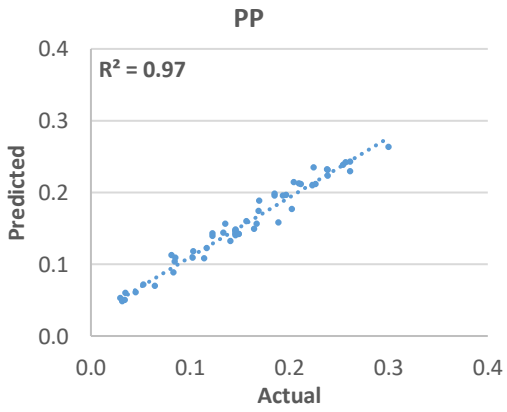
5th:

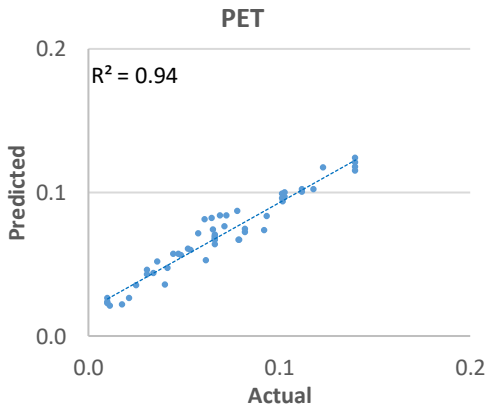

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

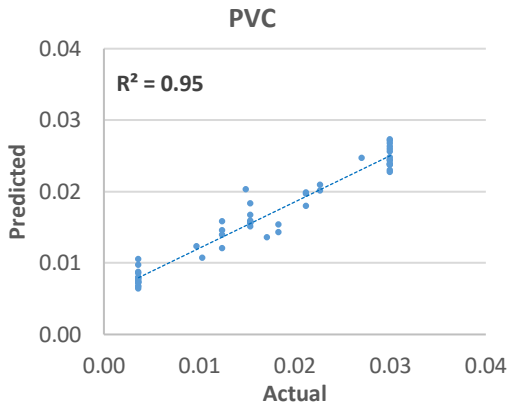

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

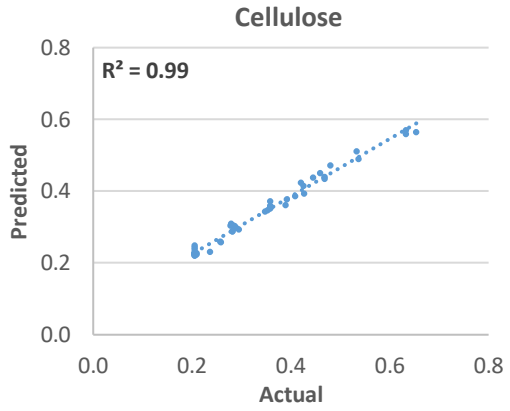

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

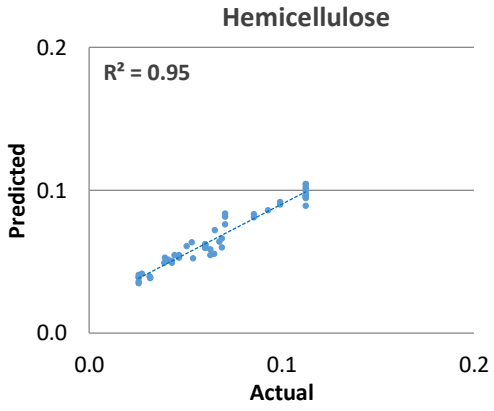

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

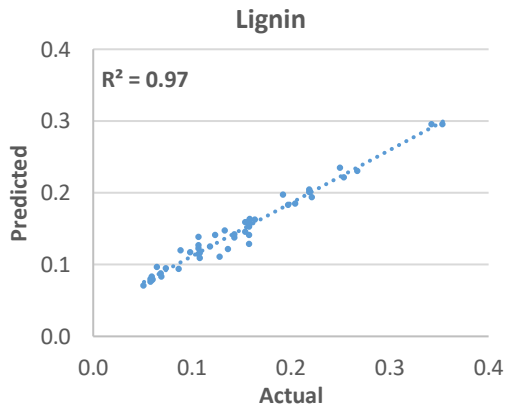

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

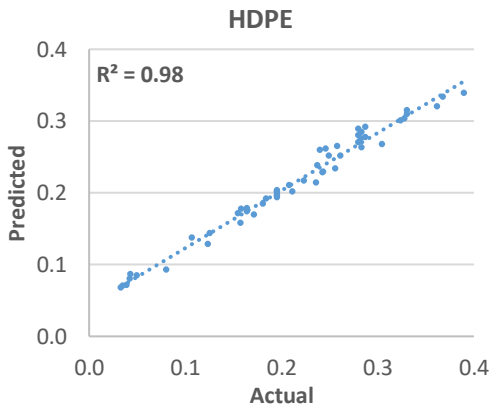

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

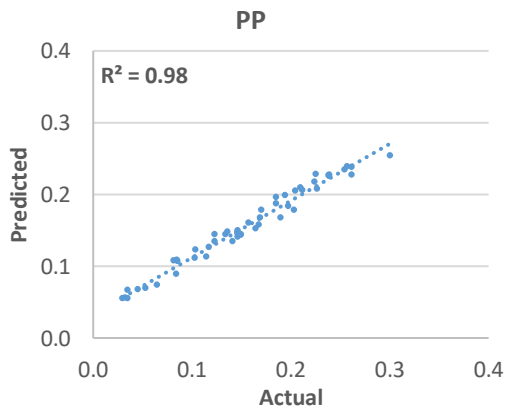
6th:

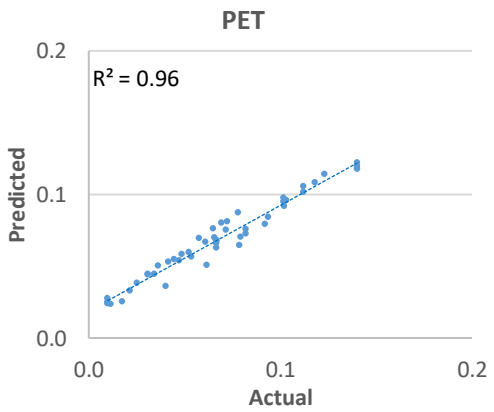

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

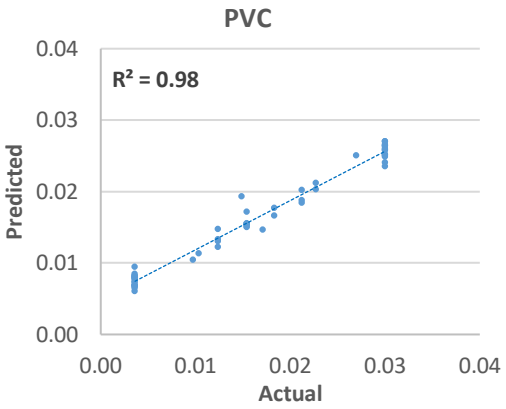

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

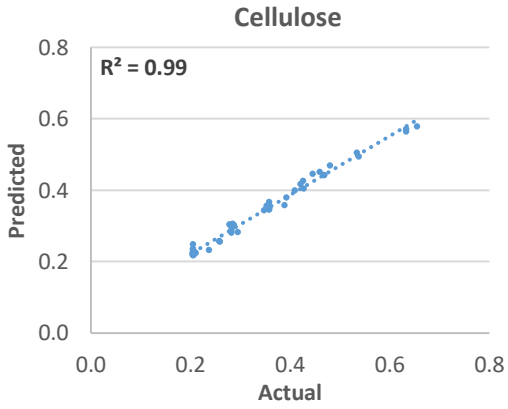

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

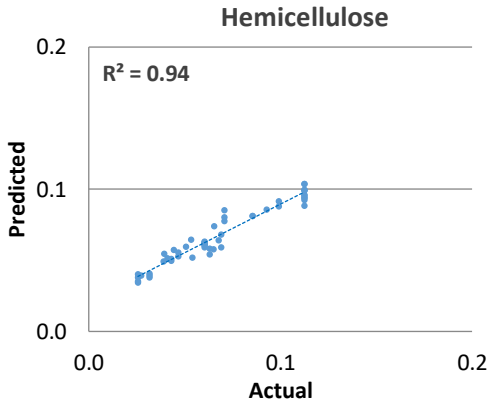

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

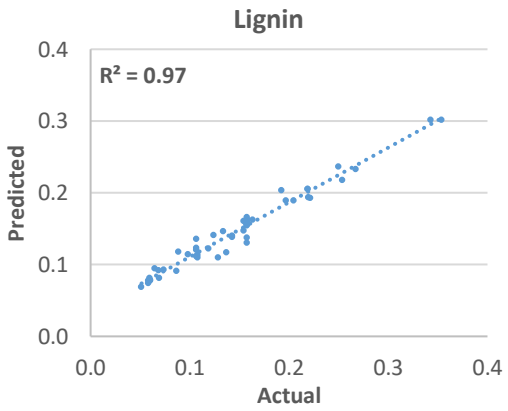

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

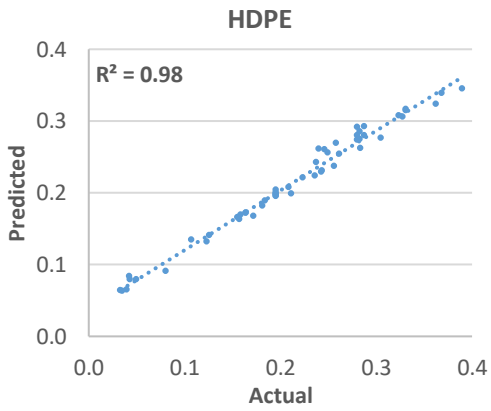

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

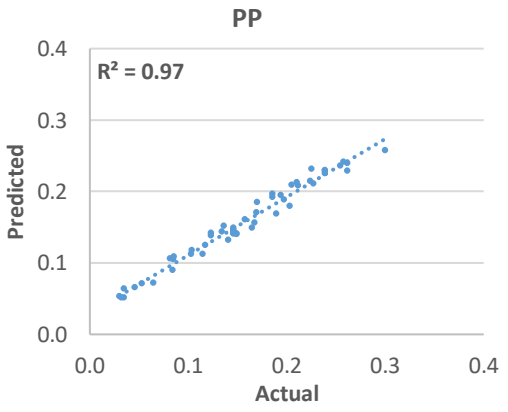
7th:

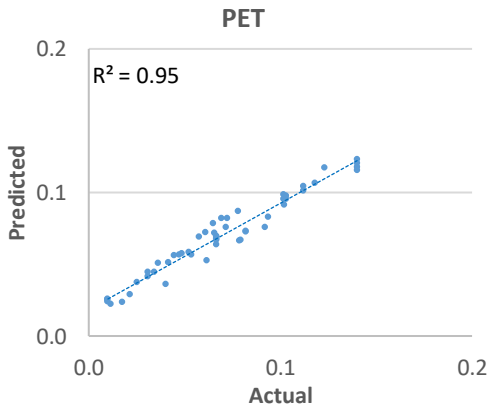

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

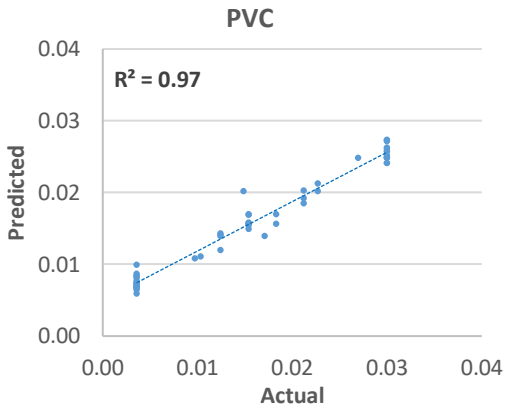

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

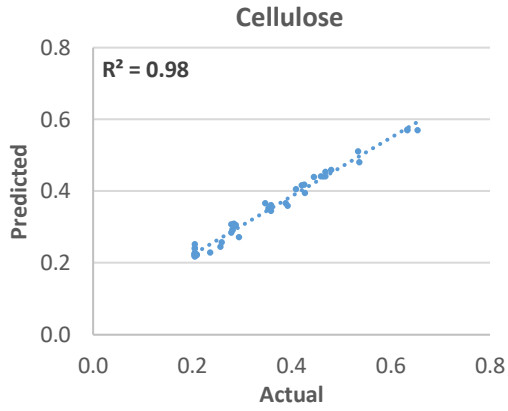

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

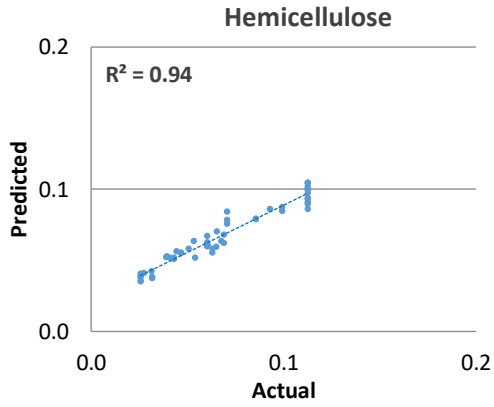

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

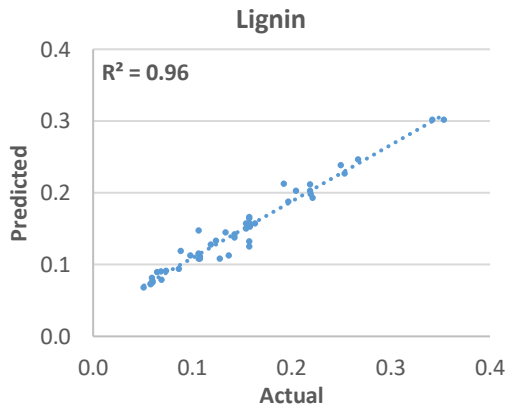

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

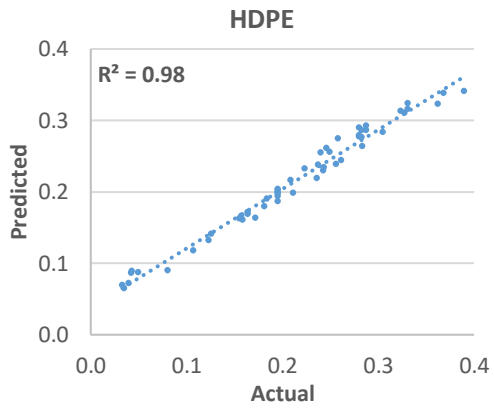

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

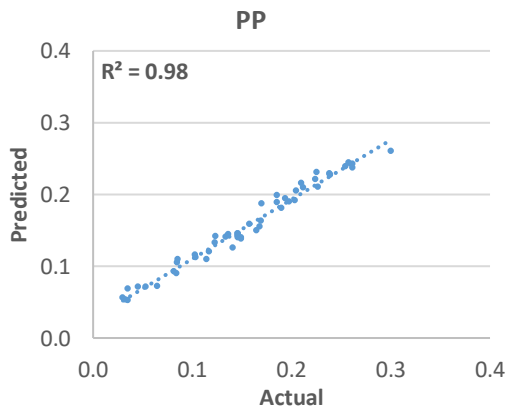
8th:


Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PP
R² = 0.98
Predicted
Actual
0.0
0.1
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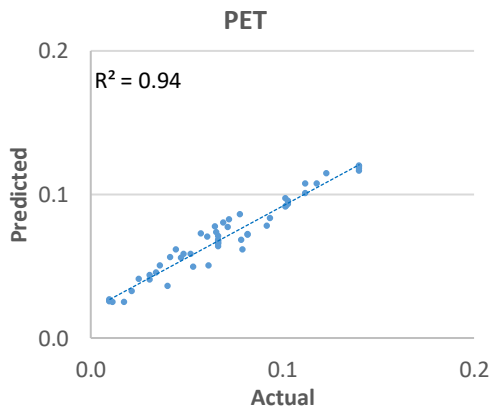
0.3
0.4


PET
R² = 0.94
Predicted
Actual
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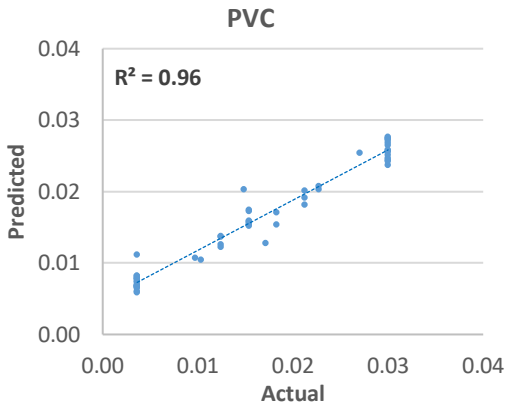
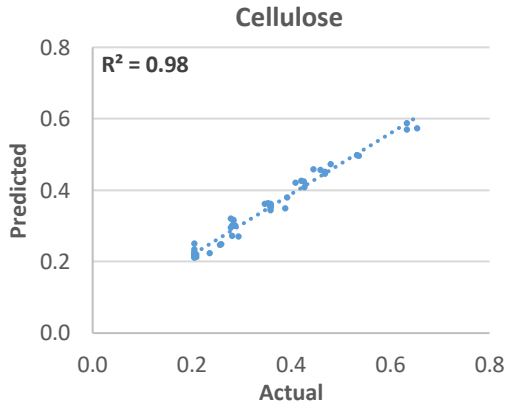
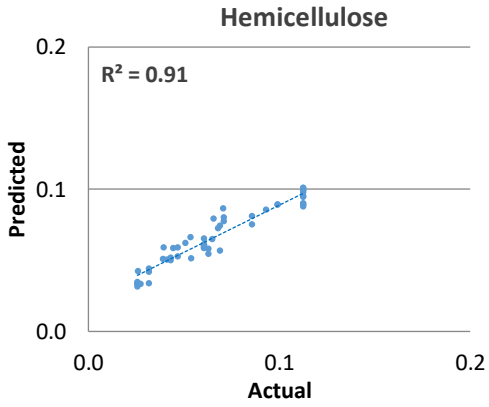
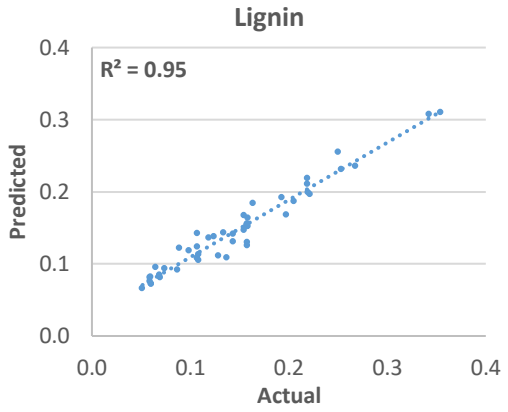
0.1
0.2

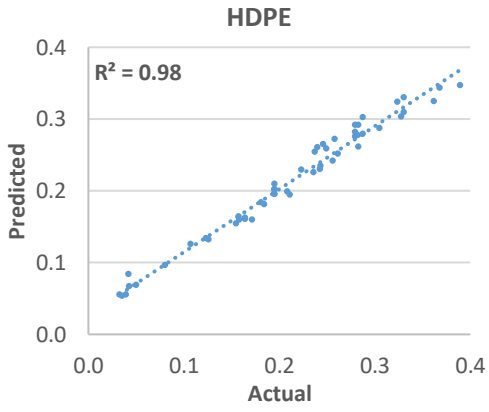

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

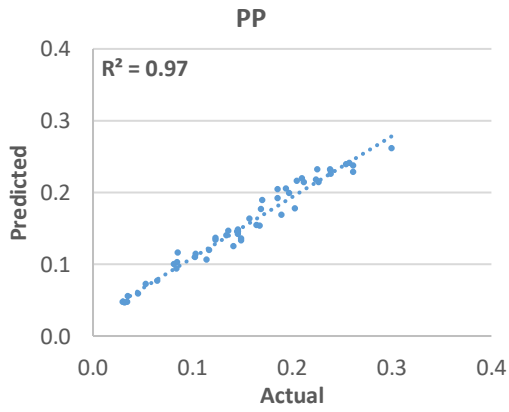
9th:

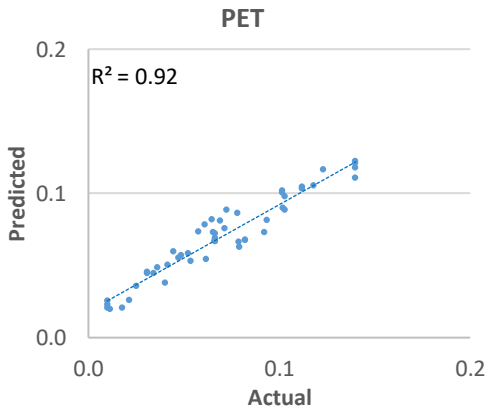

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

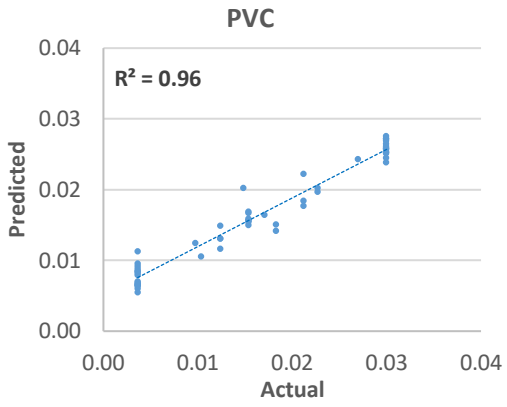

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

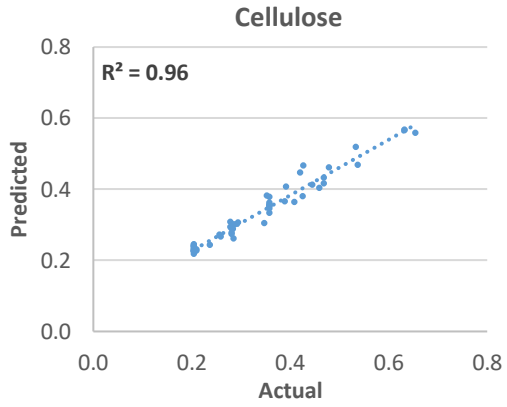

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

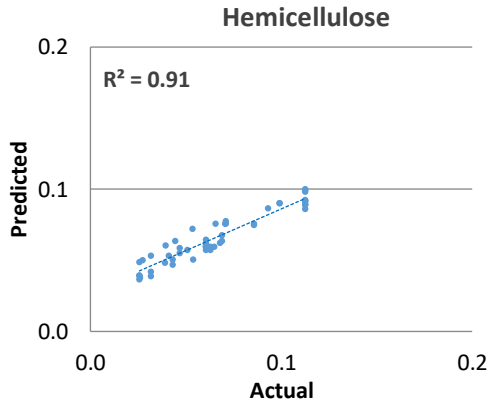

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

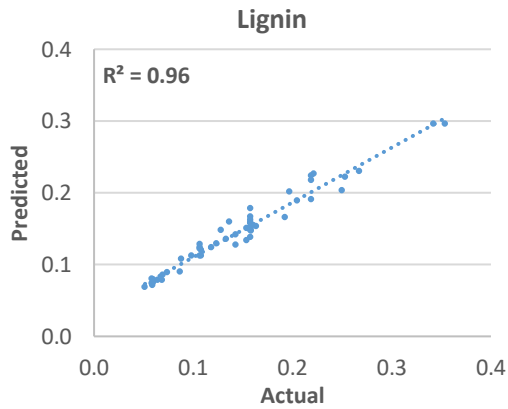

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

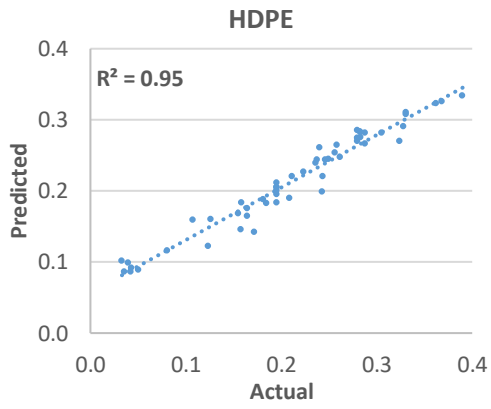

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

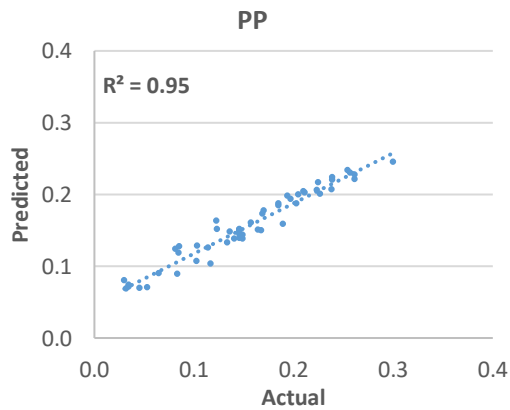
10th:

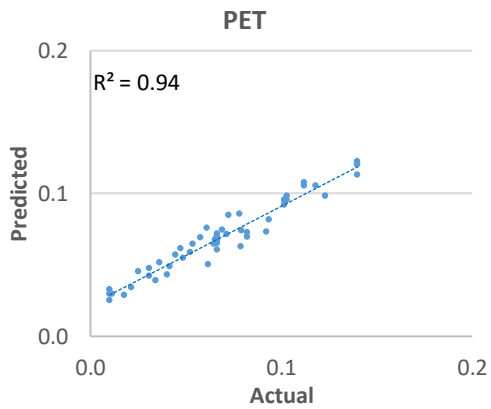

Cellulose
R² = 0.96
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

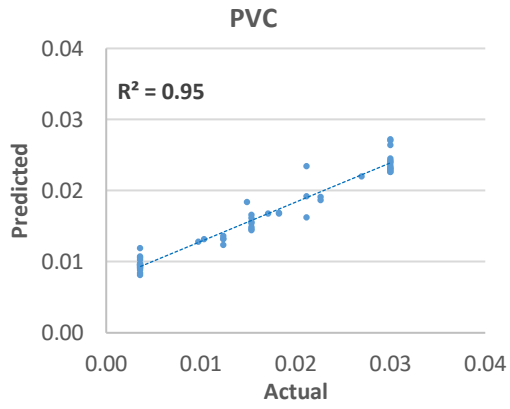

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

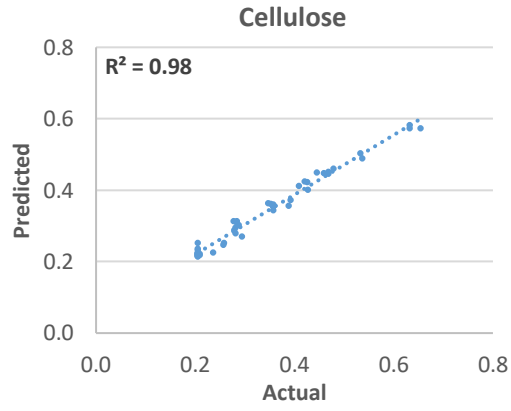

HDPE
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

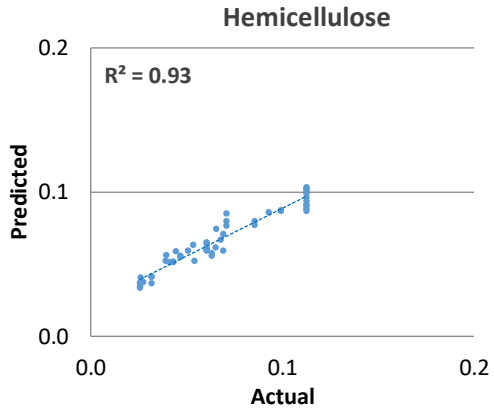

PP
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

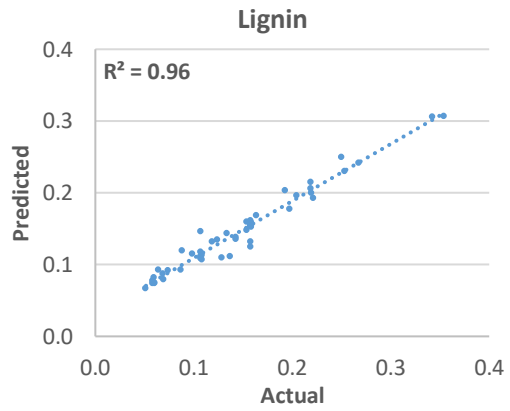

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

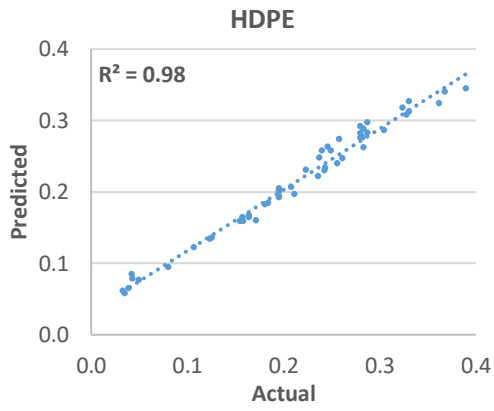

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

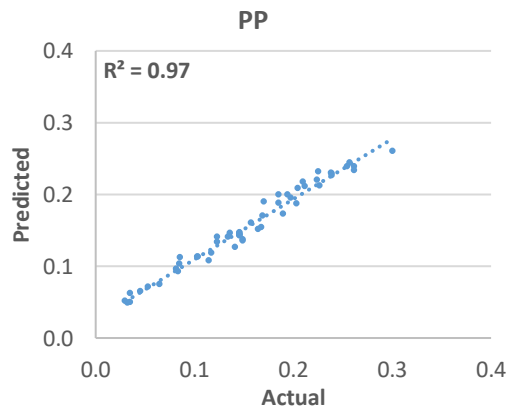
11th:

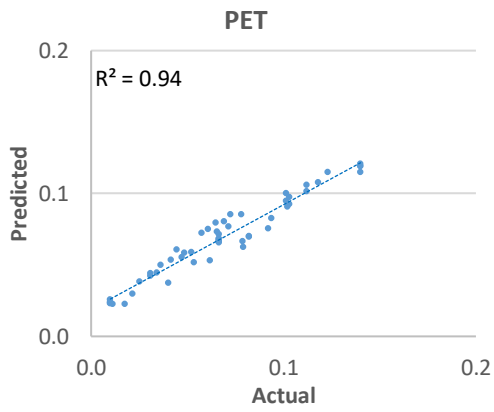

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

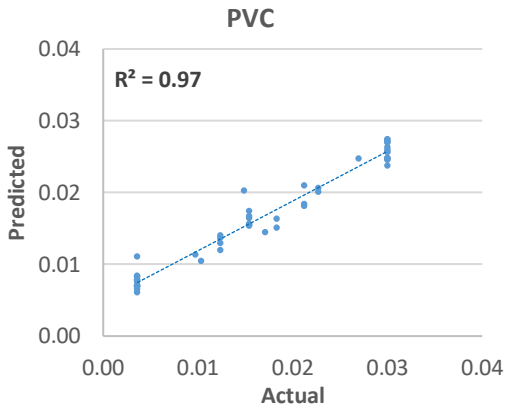

Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

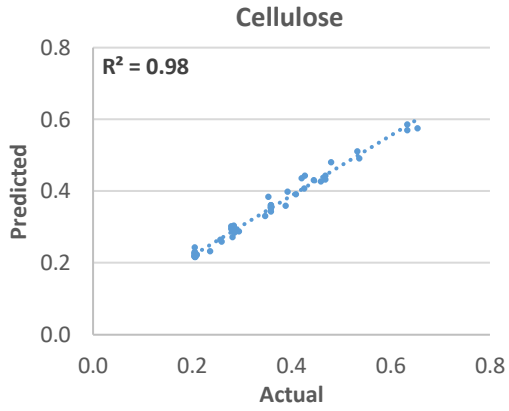

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

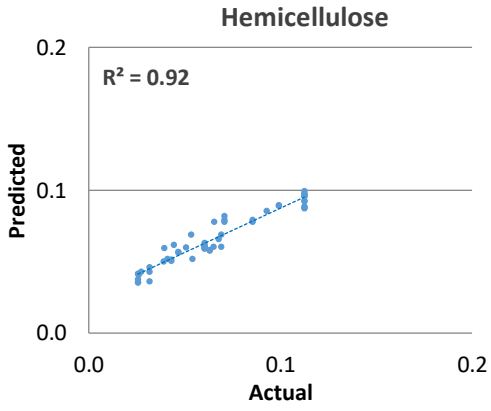

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

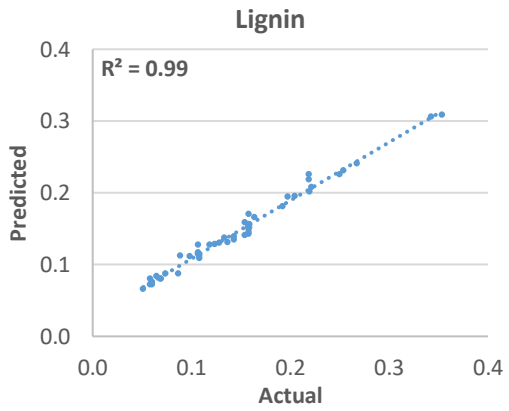

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

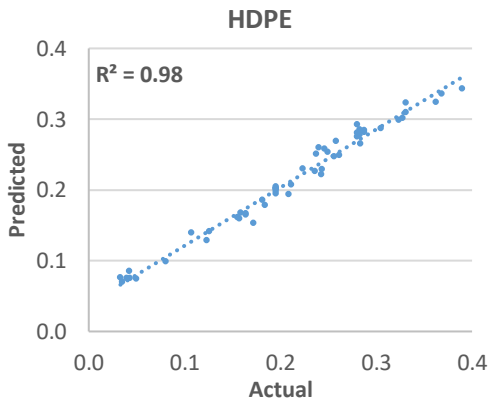

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

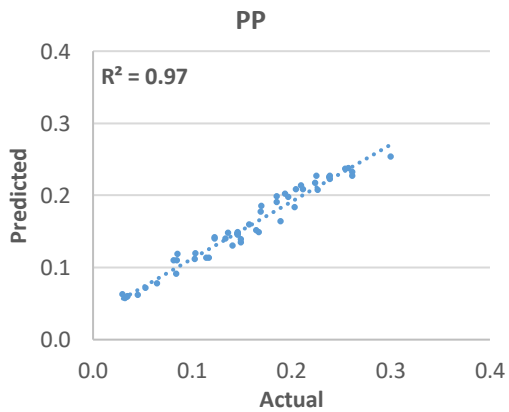
12th:

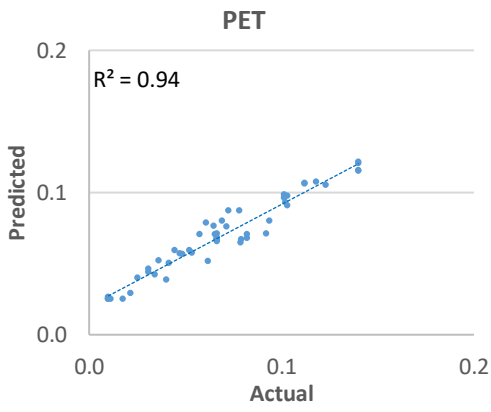

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

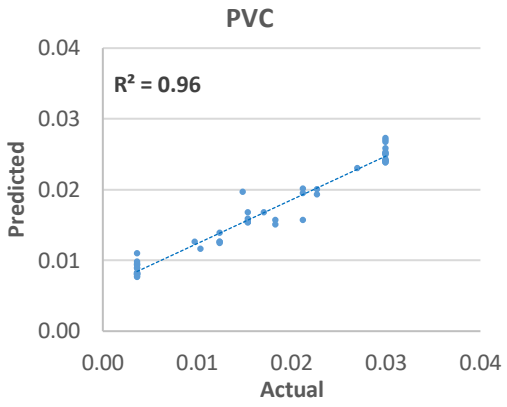

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

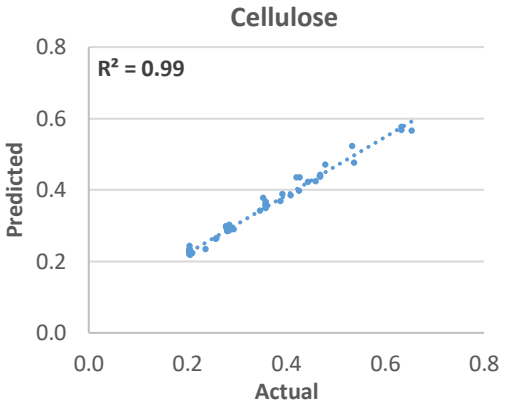

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

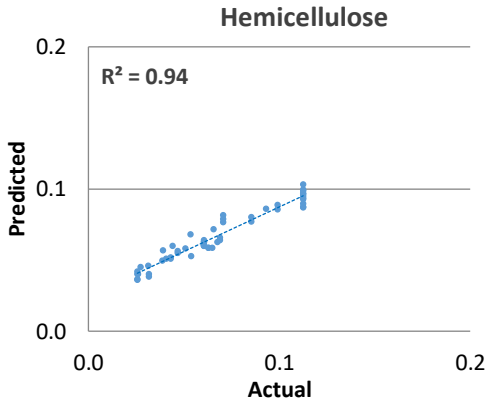

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

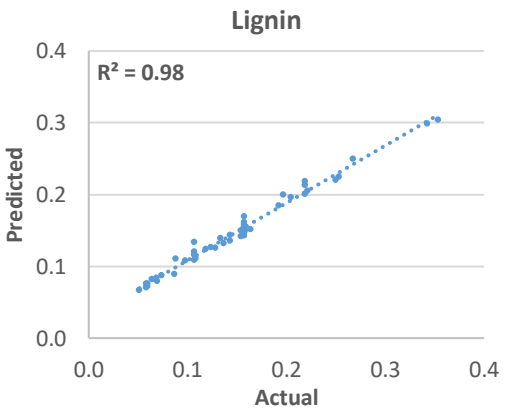

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

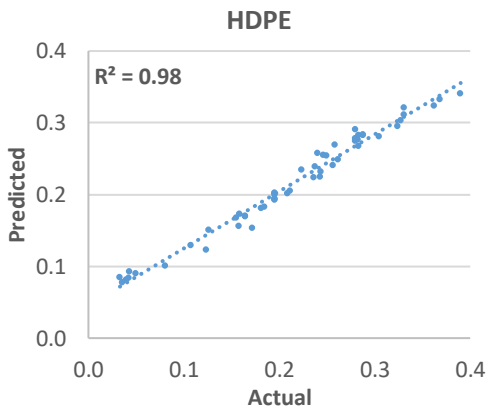

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

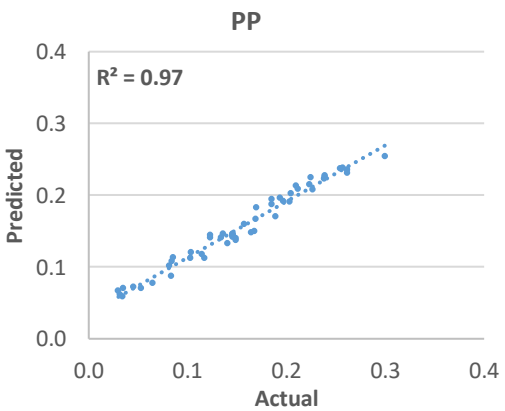
13th:

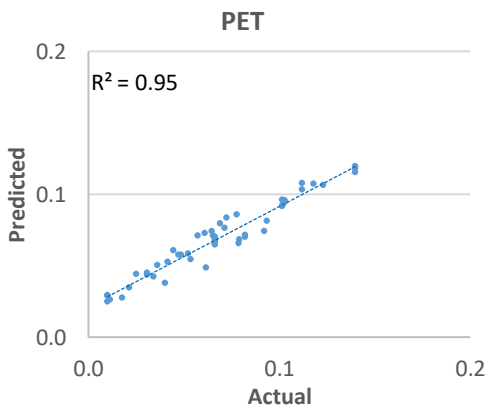

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

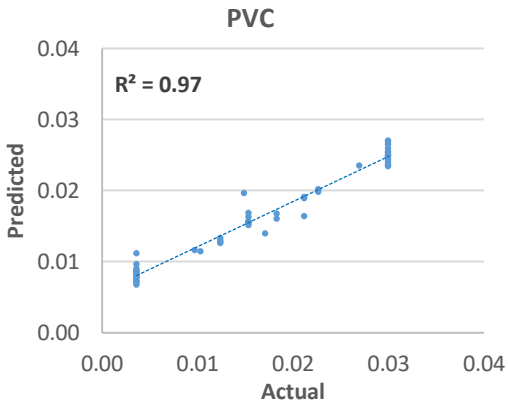

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

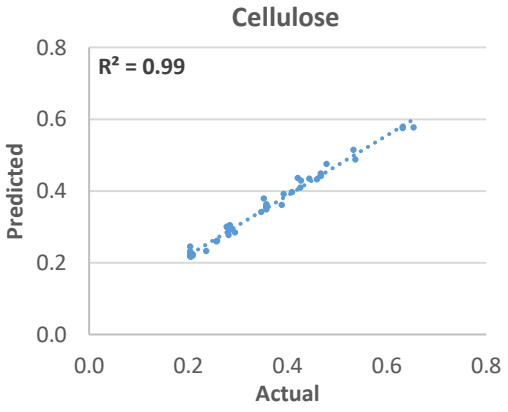

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

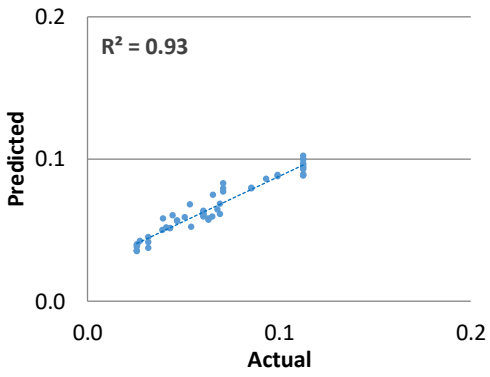

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

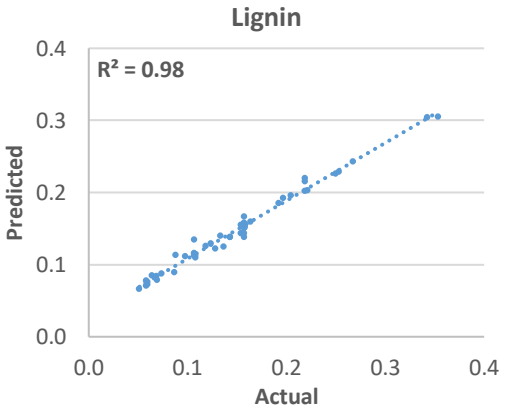

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

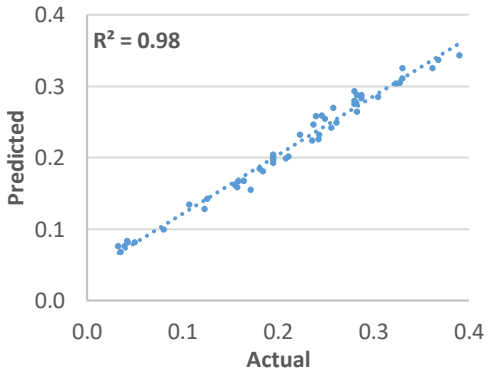

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

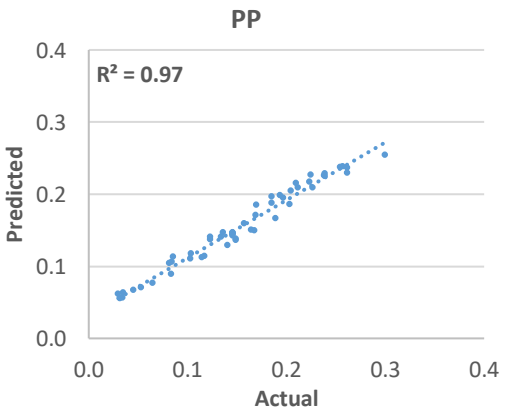
14th:

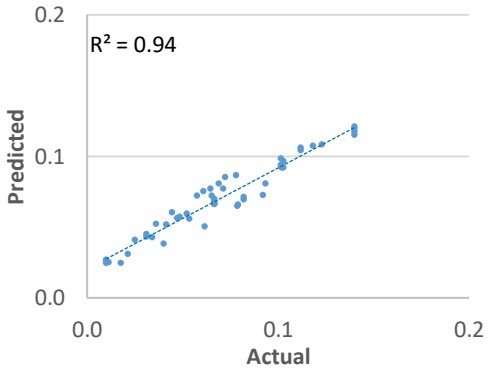

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

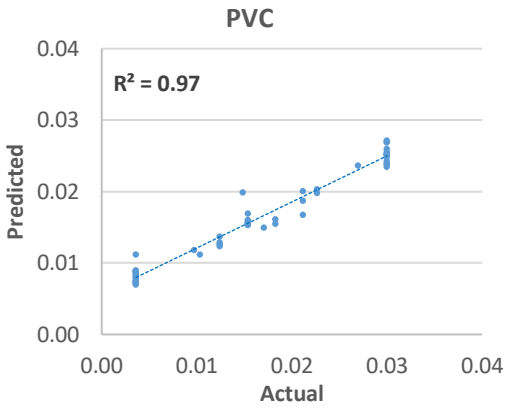

Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

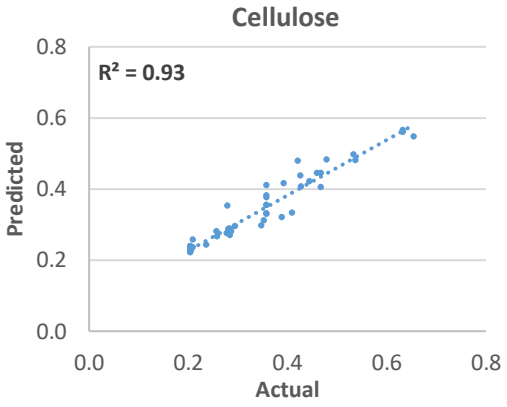

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

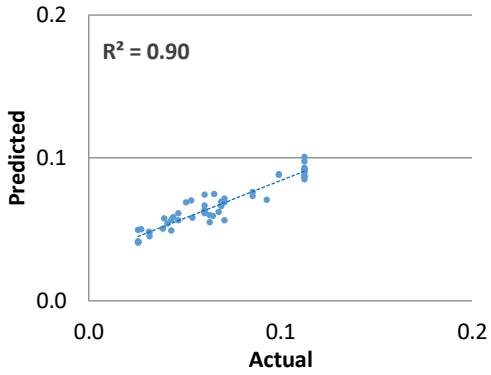

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

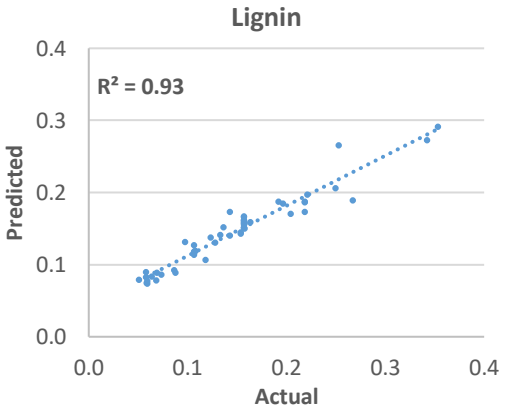

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

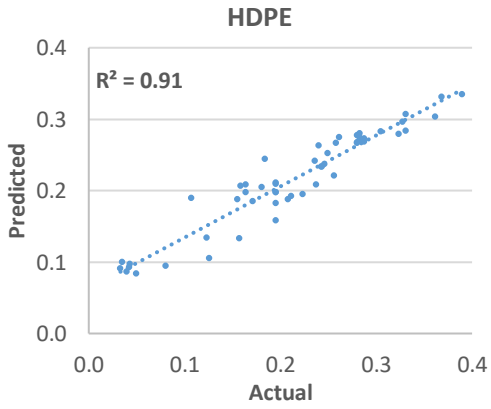

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

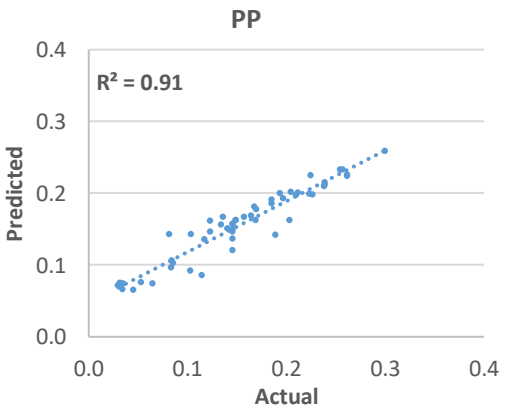
15th:

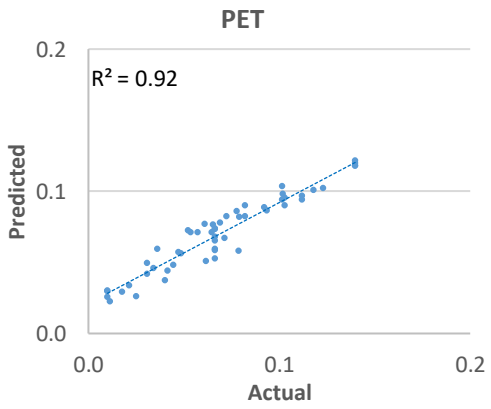

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

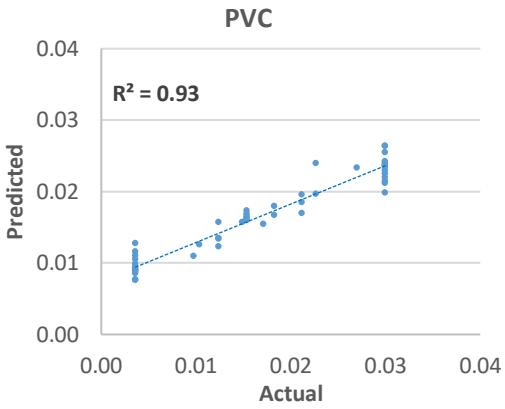

Hemicellulose
R² = 0.90
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.93
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

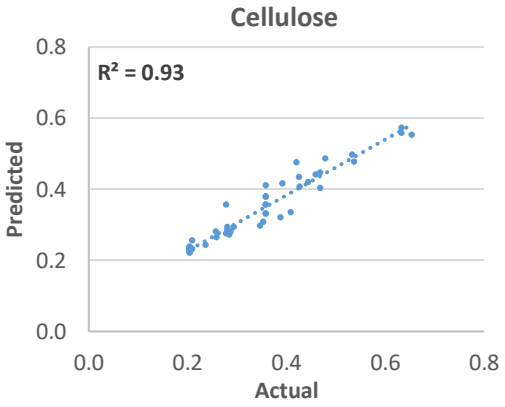

HDPE
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

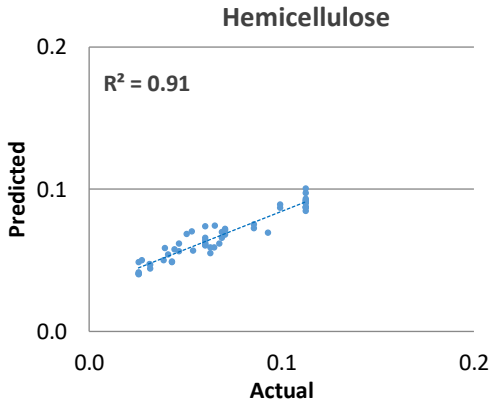

PP
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

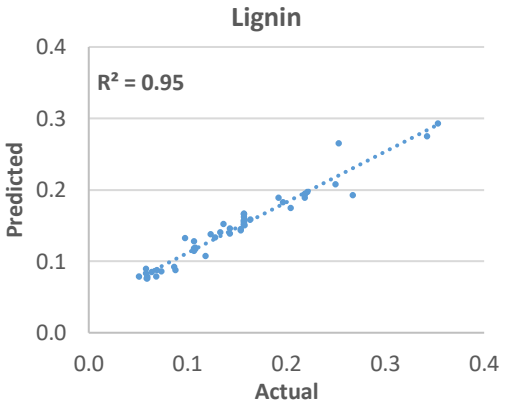

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

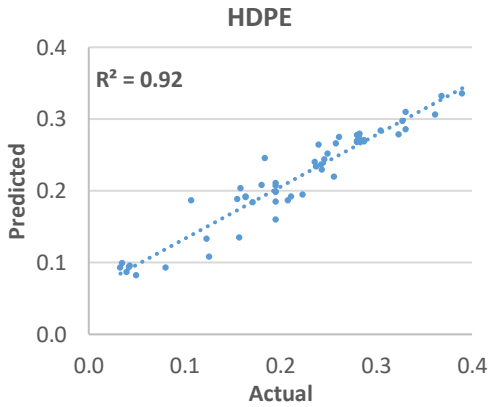

PVC
R² = 0.93
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

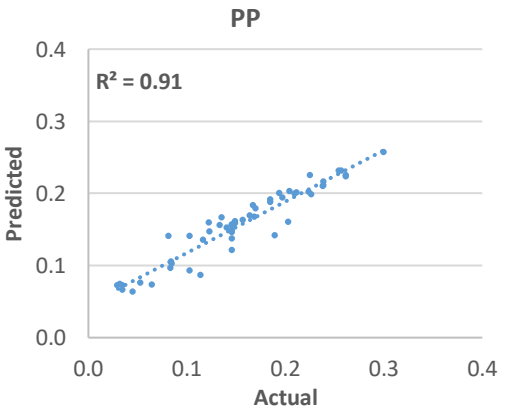
16th:

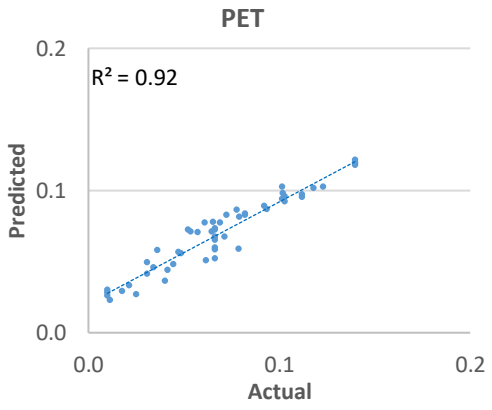

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

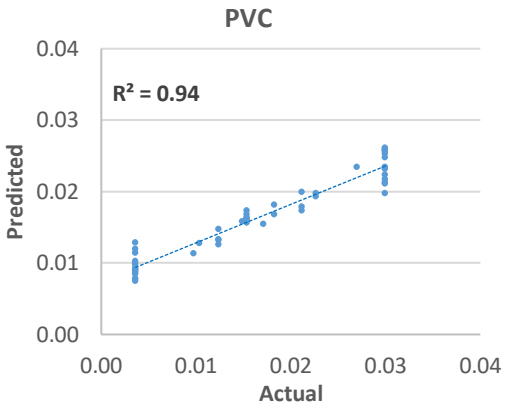

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

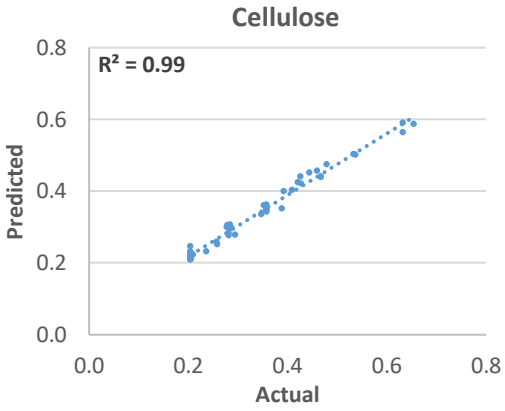

HDPE
R² = 0.92
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

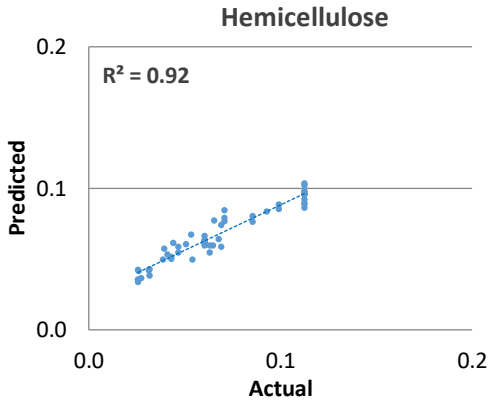

PP
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

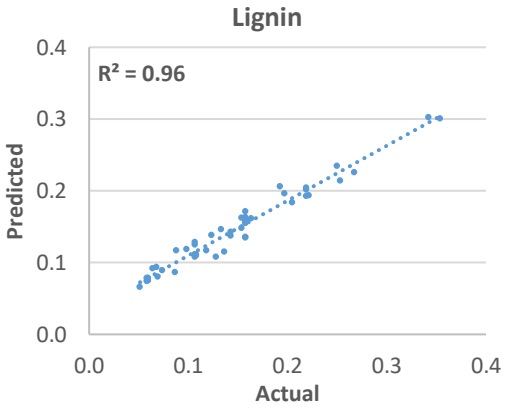

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

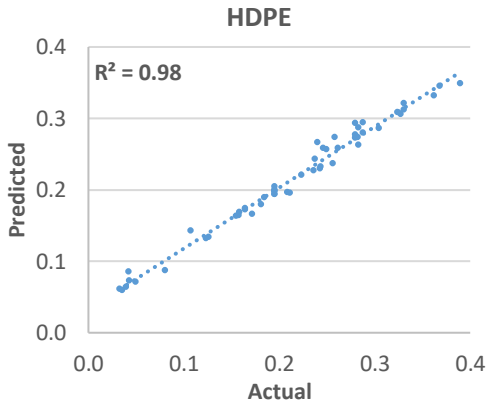

PVC
R² = 0.94
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

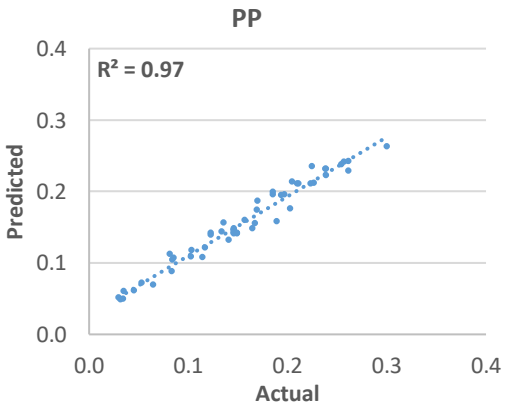
17th:

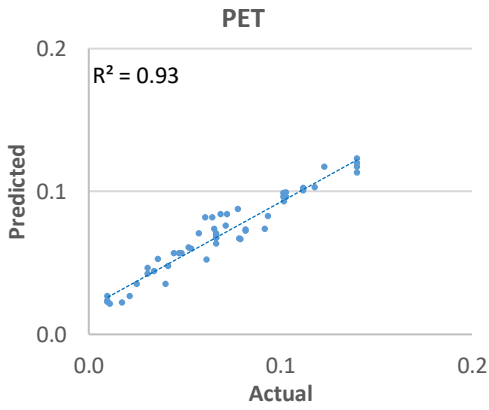

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

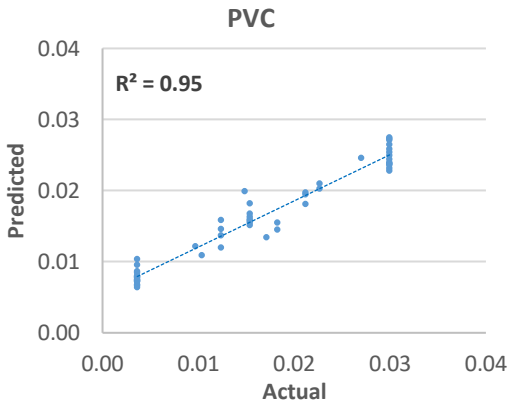

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

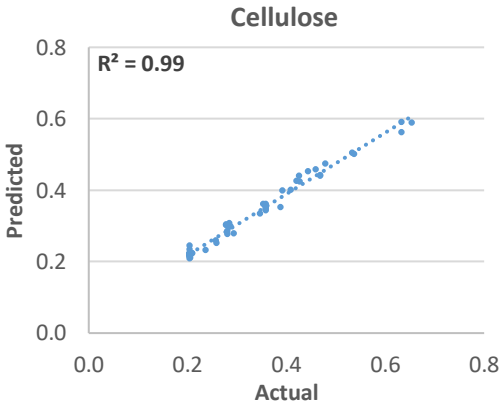

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

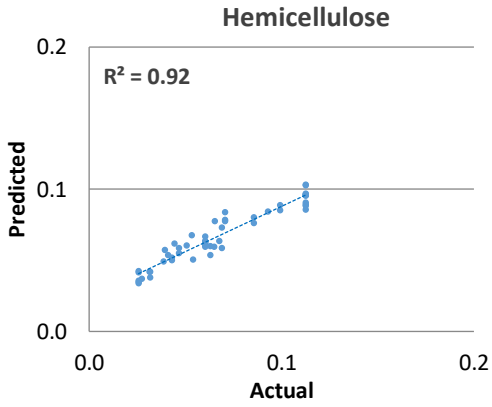

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

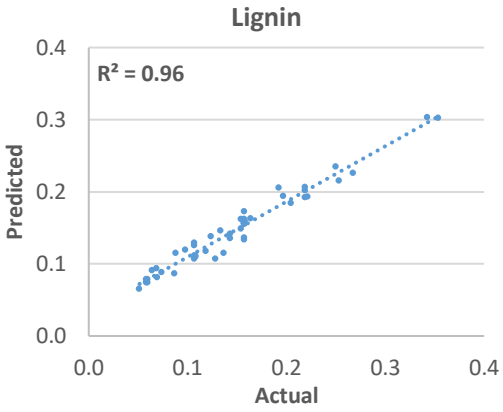

PET
R² = 0.93
Predicted
Actual
0.0
0.1
0.2

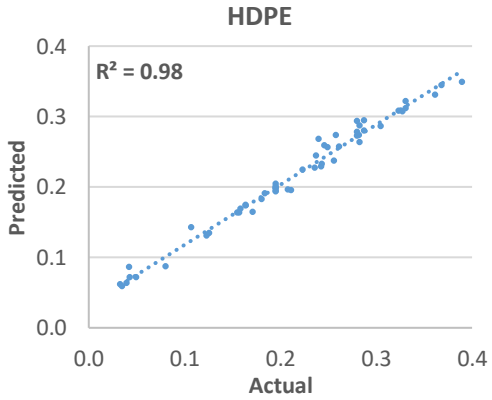

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

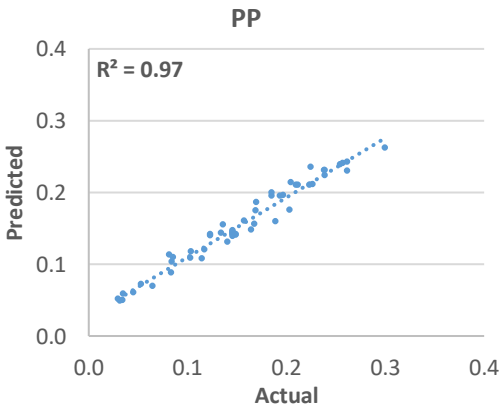
18th:

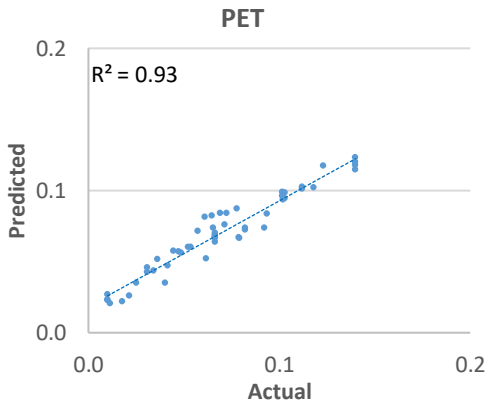

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

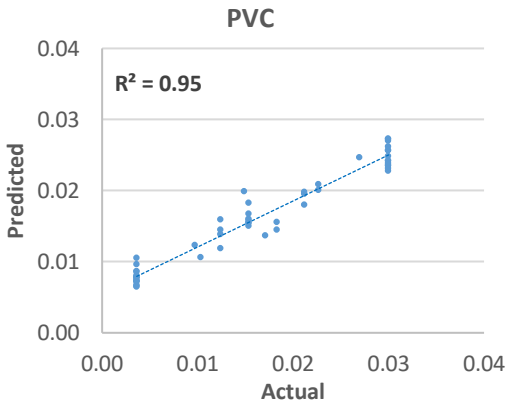

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

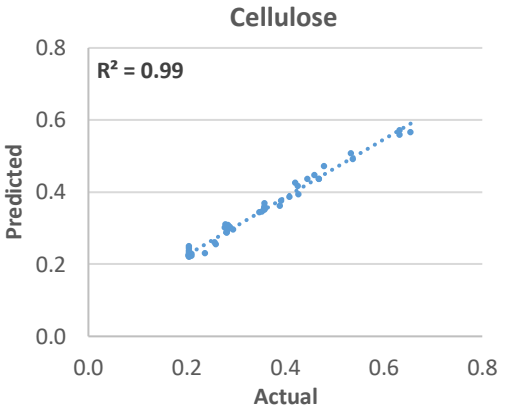

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

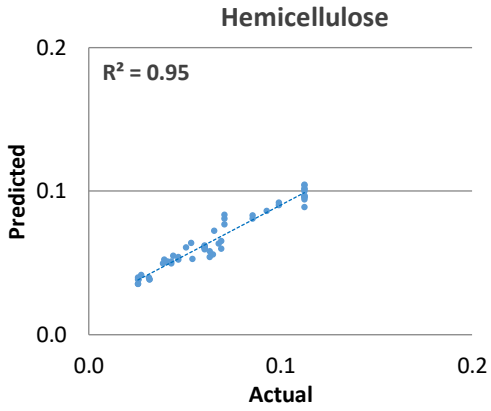

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

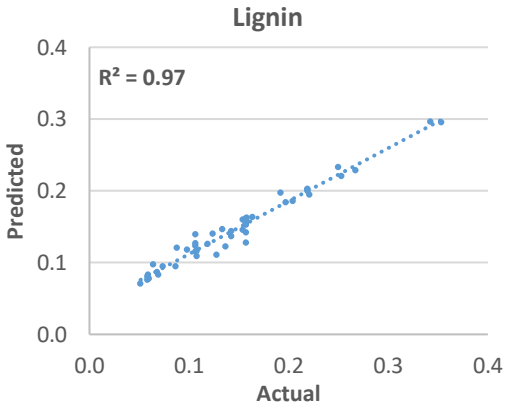

PET
R² = 0.93
Predicted
Actual
0.0
0.1
0.2

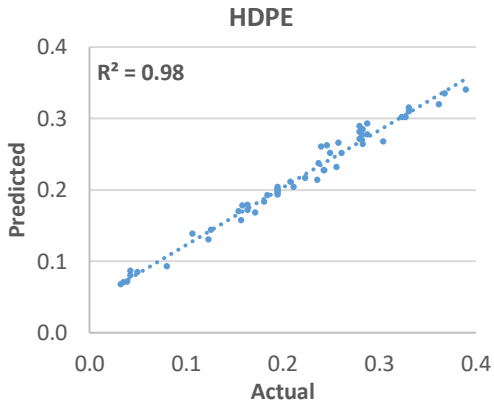

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

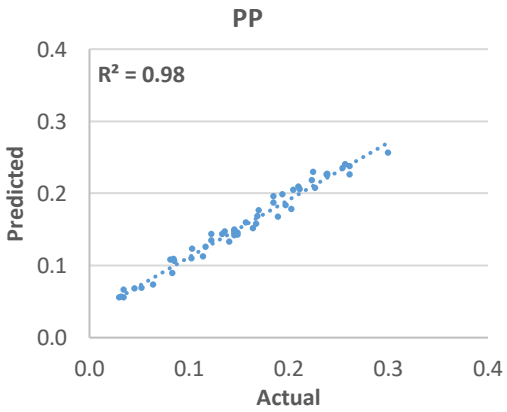
19th:

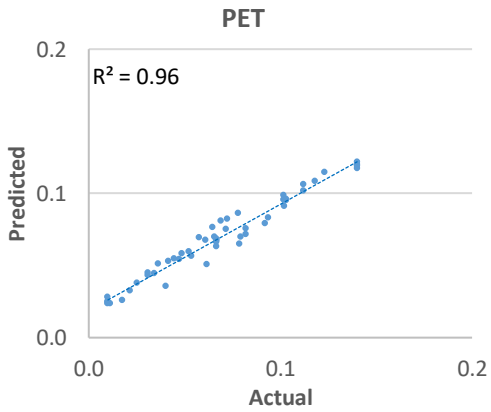

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

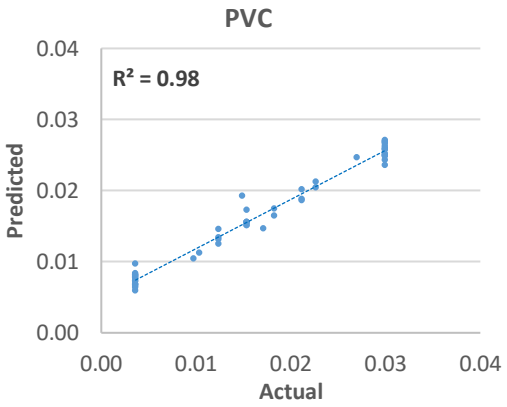

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

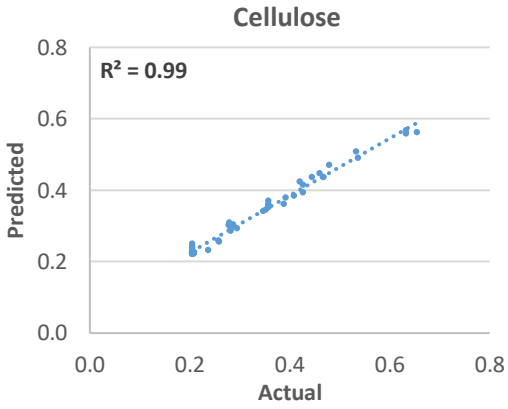

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

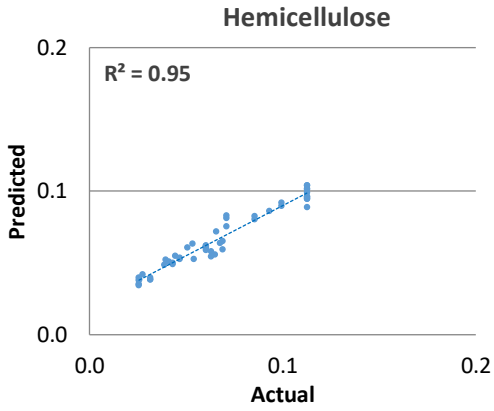

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

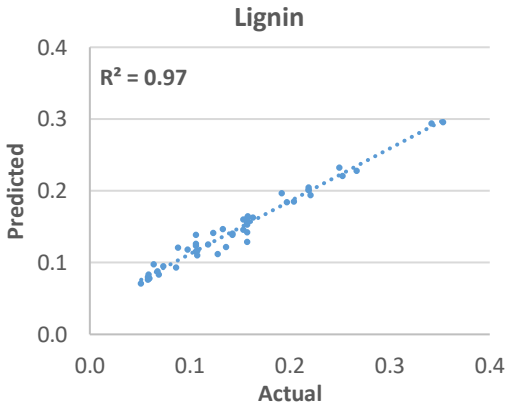

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

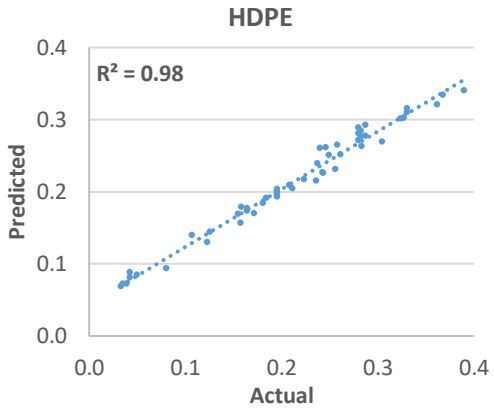

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

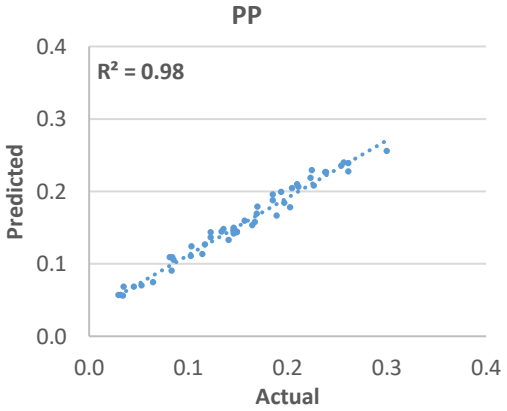
20th:

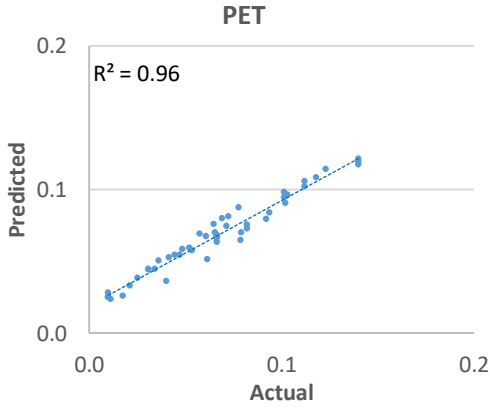

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

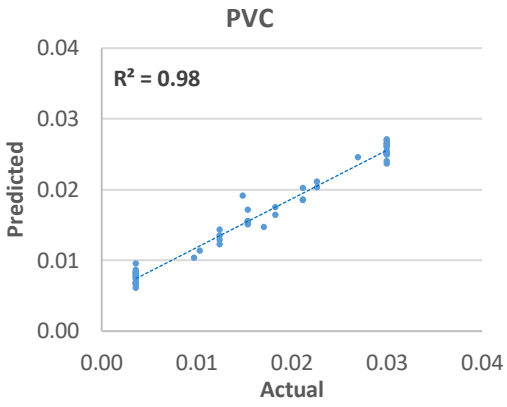

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

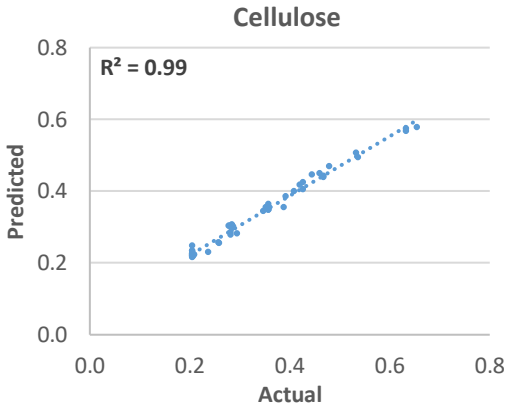

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

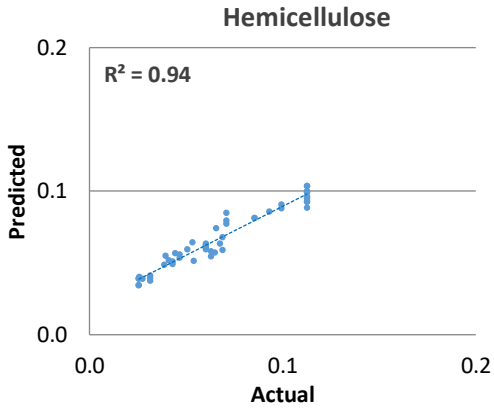

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

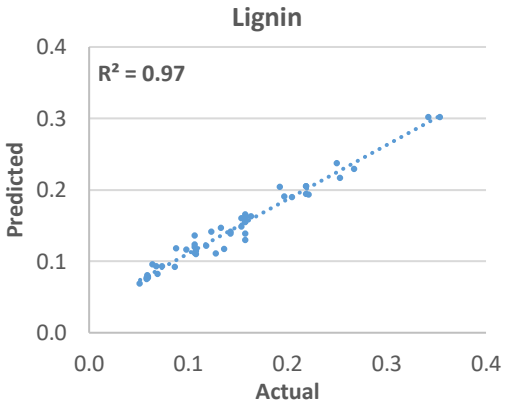

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

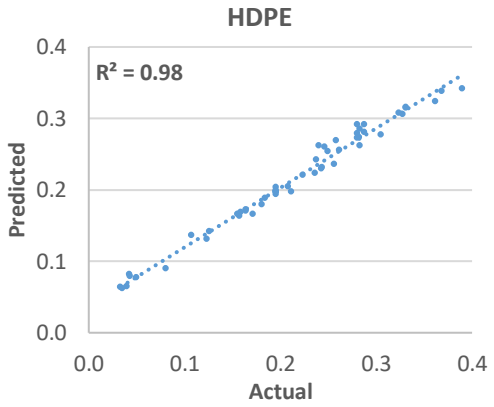

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

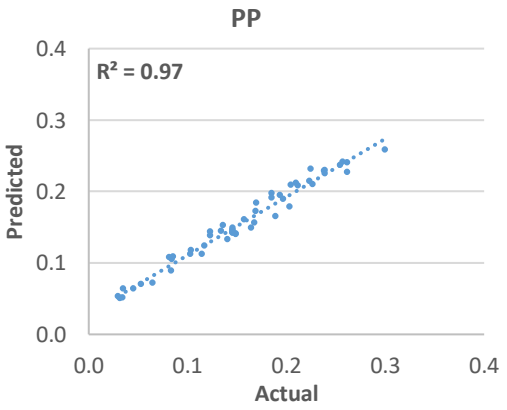
21th:


Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PP
R² = 0.97
Predicted
Actual
0.0
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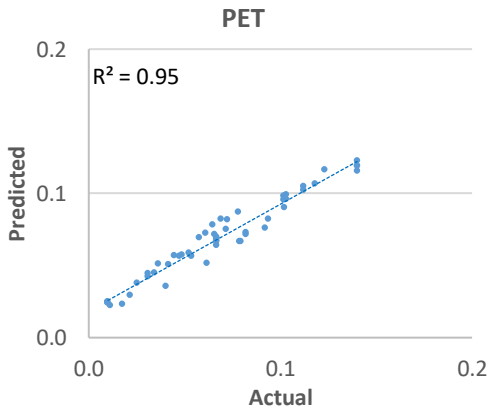
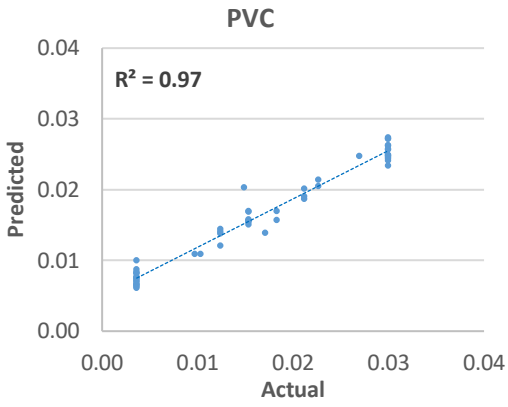
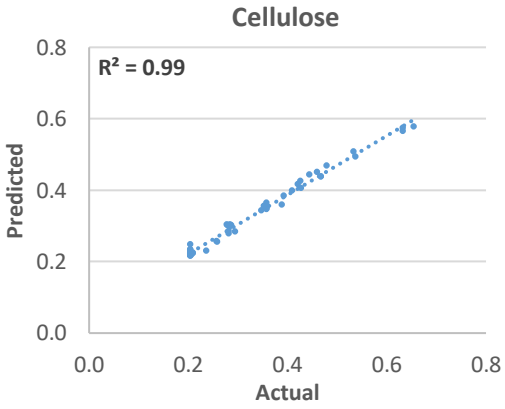
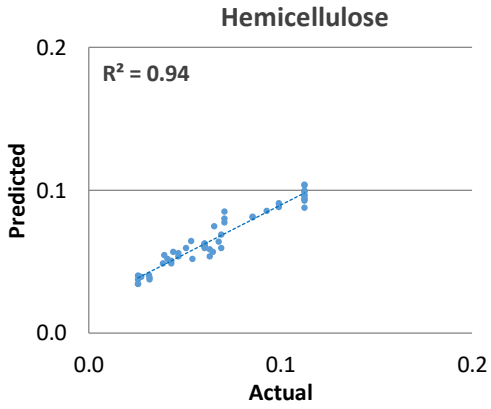
0.2
0.3
0.4

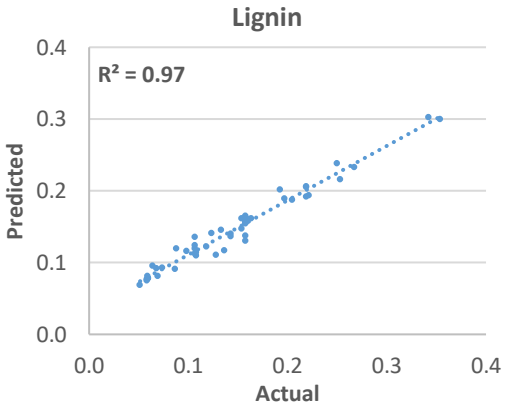

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

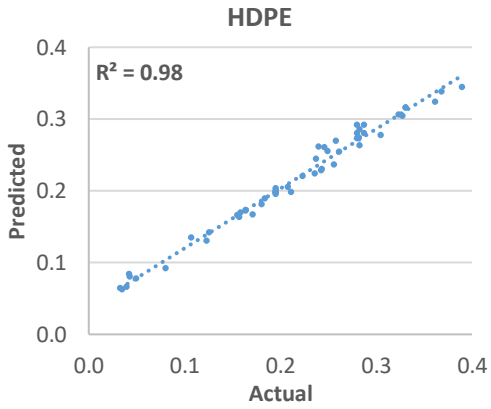

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

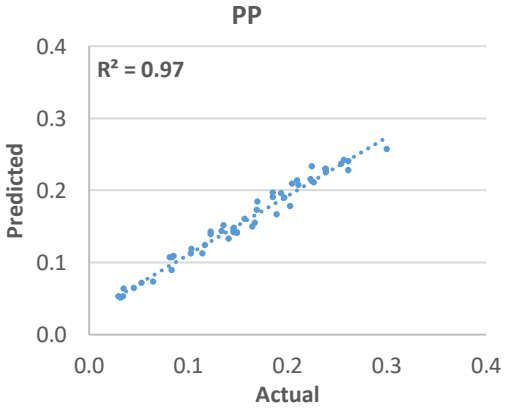
22nd:

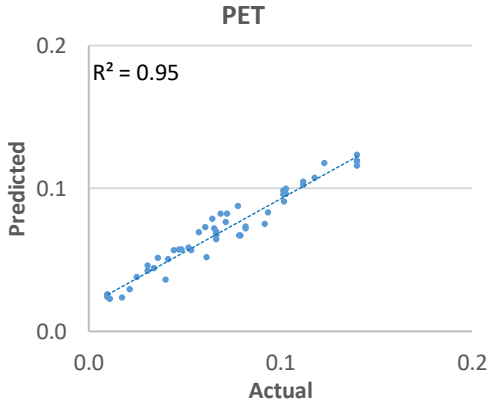

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

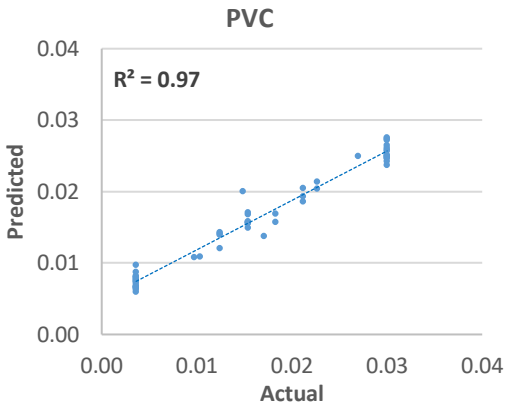

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

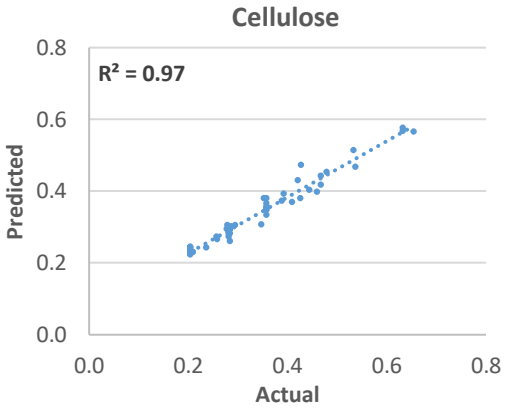

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

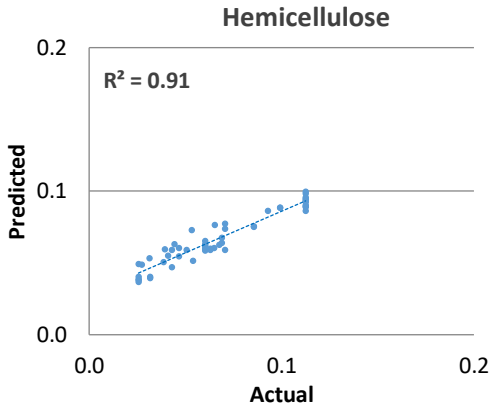

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

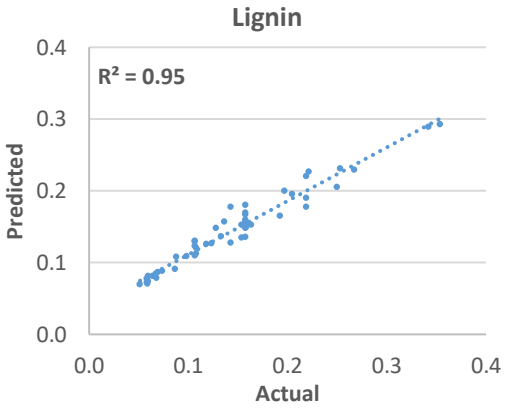

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

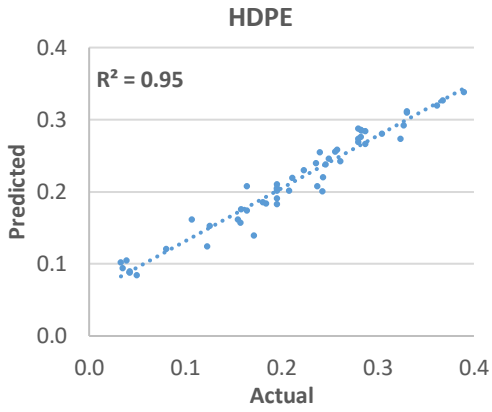

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

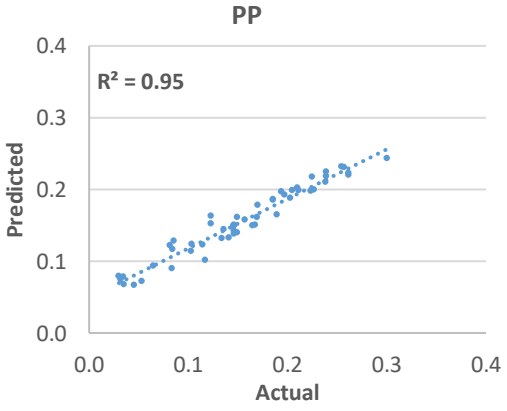
23rd:

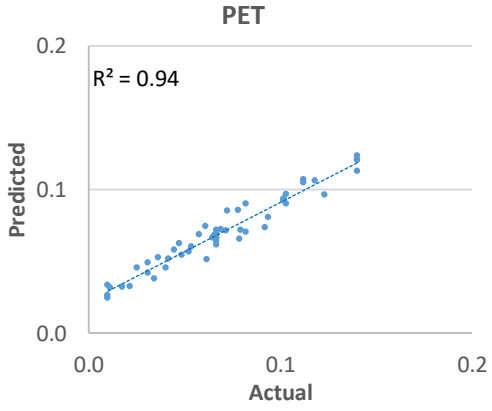

Cellulose
R² = 0.97
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

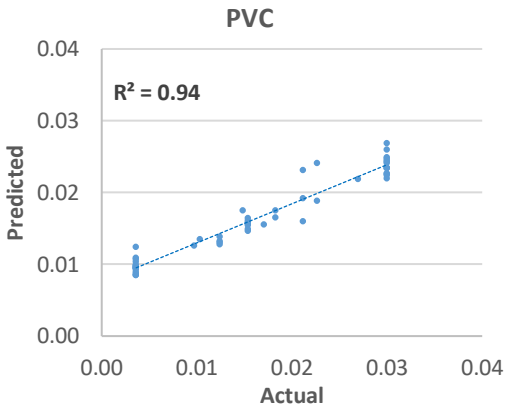

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

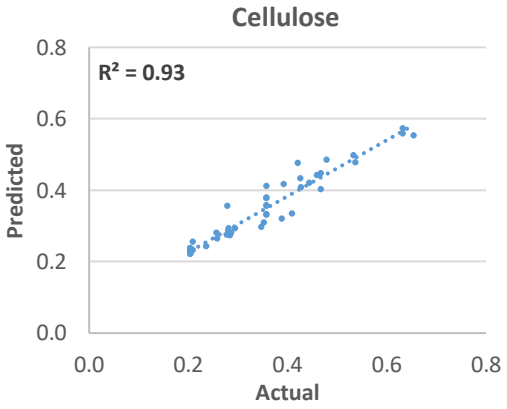

HDPE
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

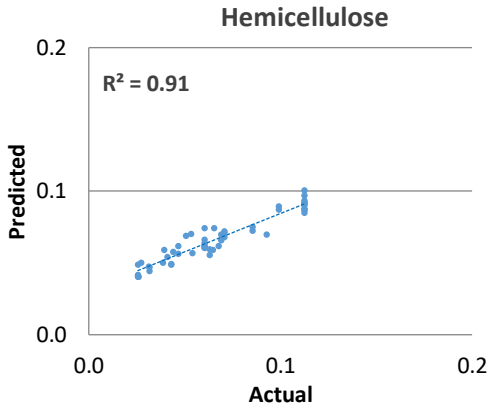

PP
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

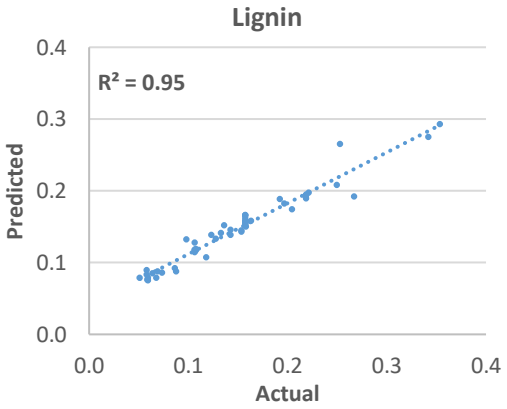

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

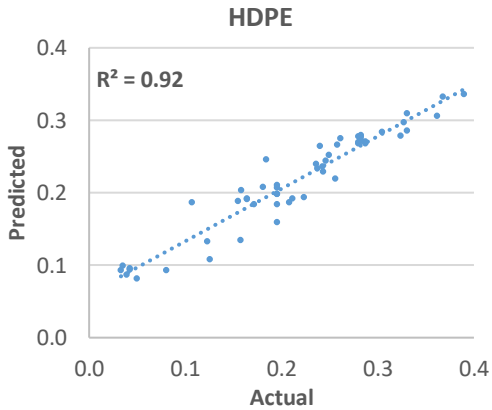

PVC
R² = 0.94
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

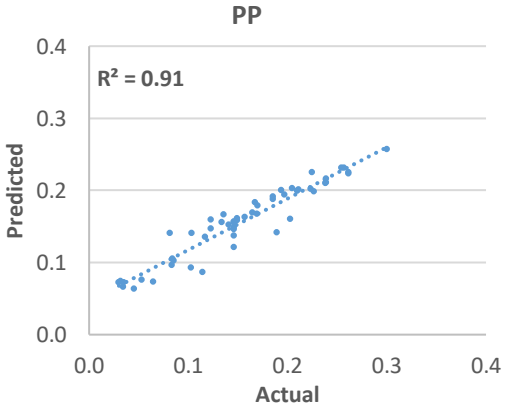
24th:

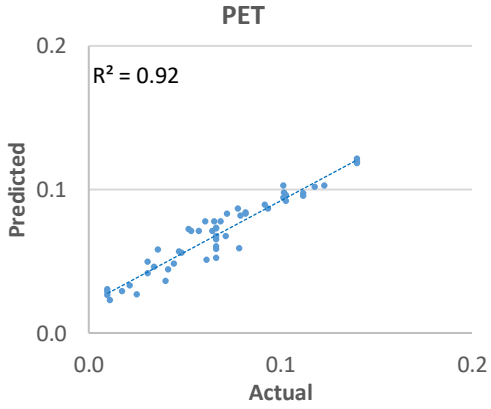

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

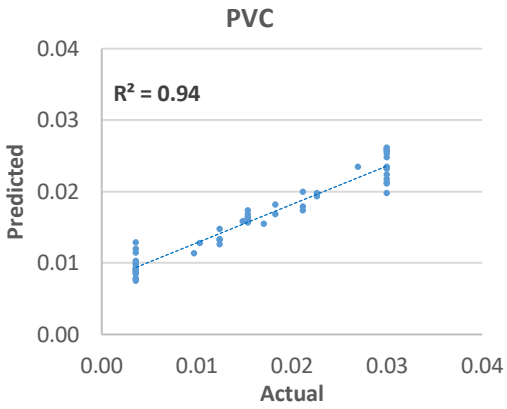

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

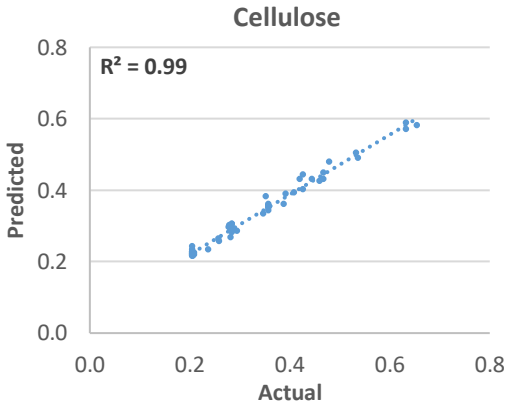

HDPE
R² = 0.92
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

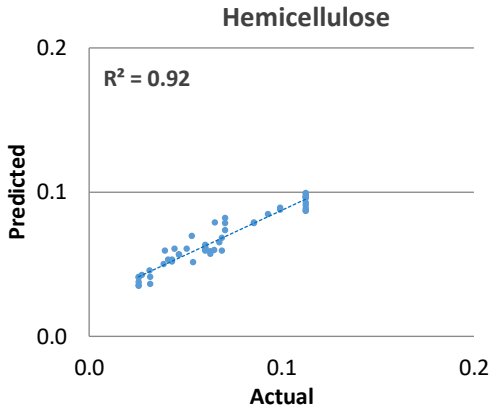

PP
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

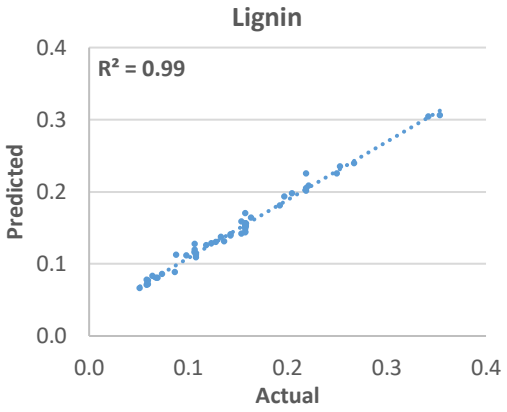

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

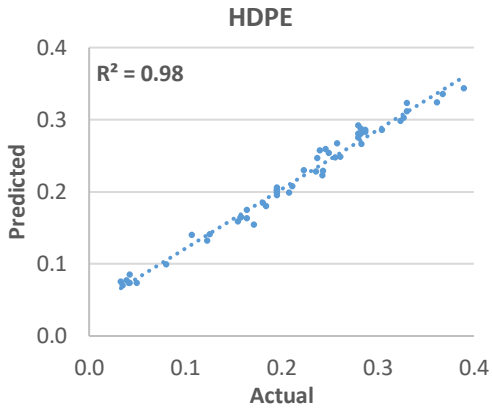

PVC
R² = 0.94
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

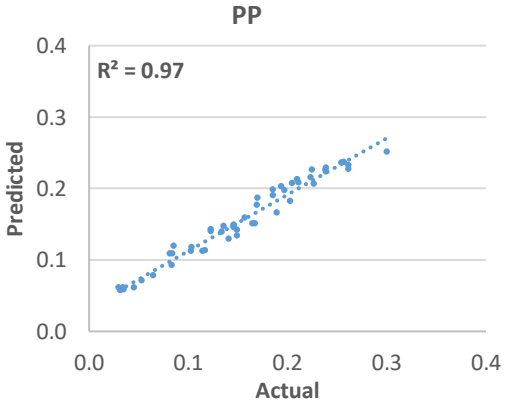
25th:

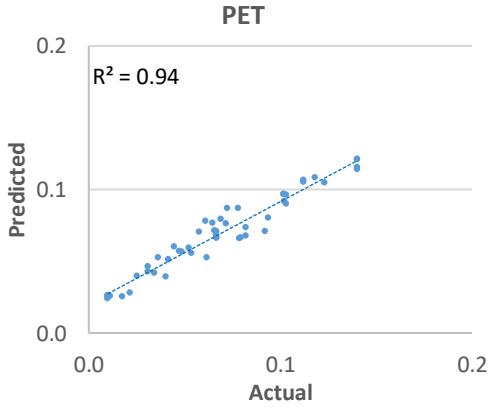

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

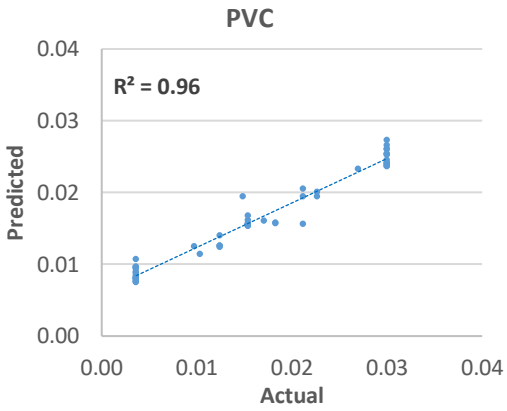

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

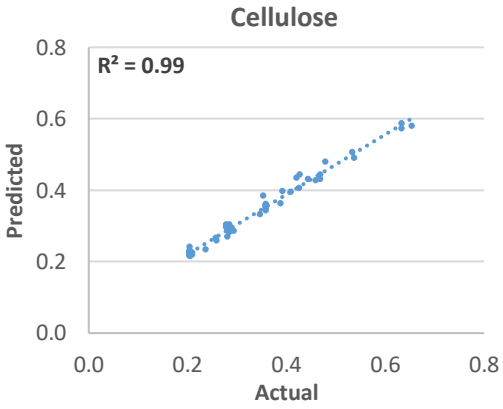

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

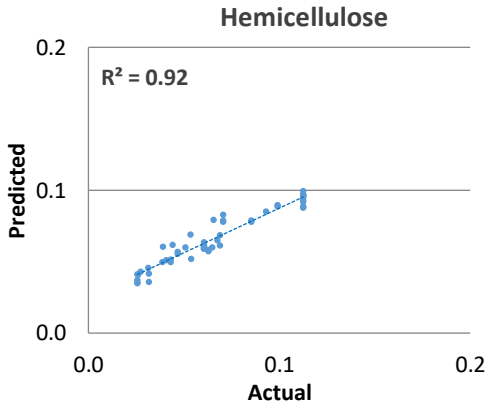

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

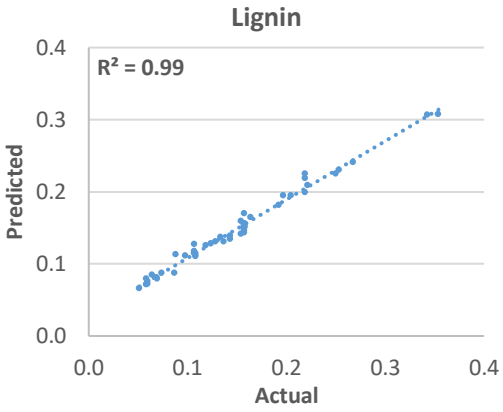

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

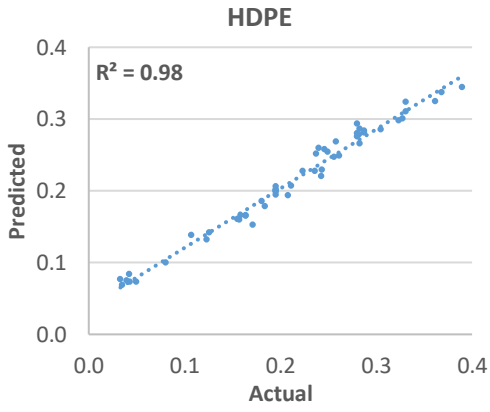

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

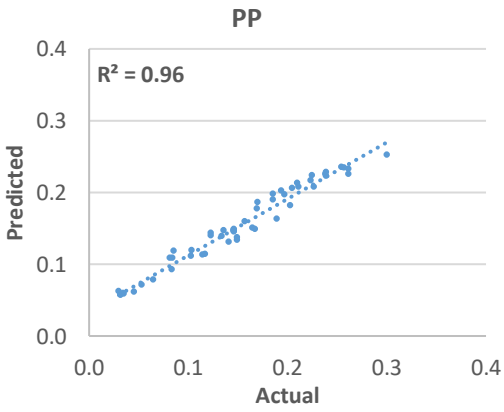
26th:

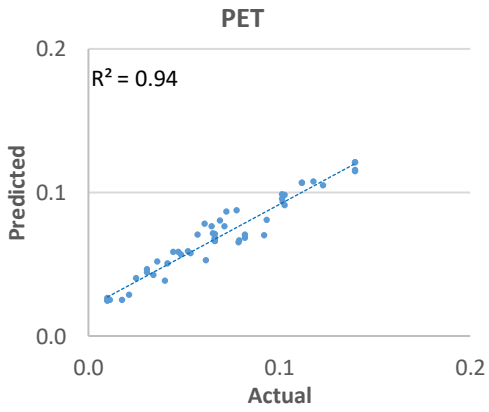

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

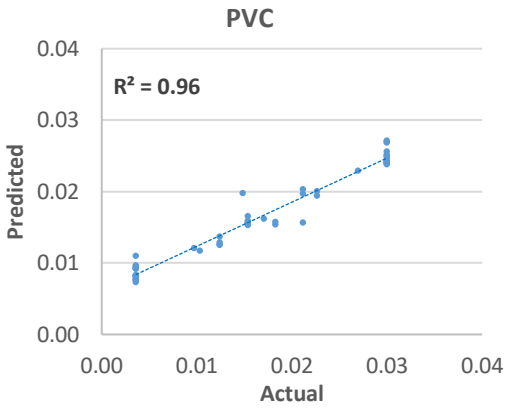

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

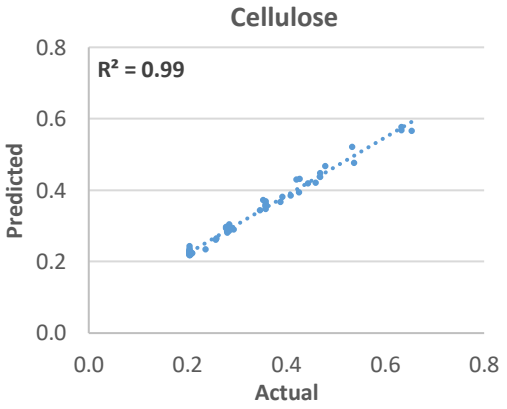

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

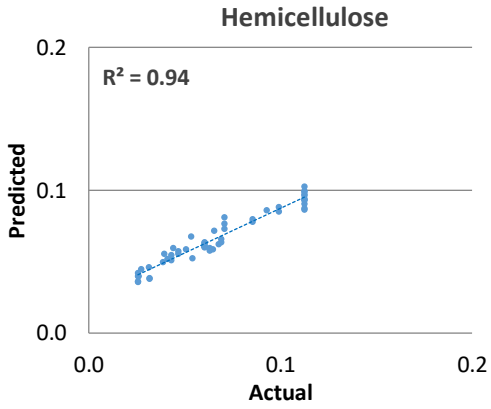

PP
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

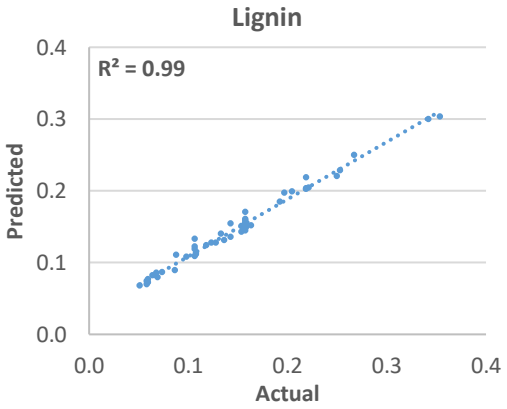

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

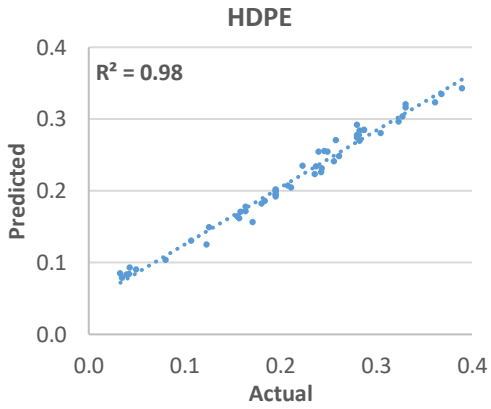

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

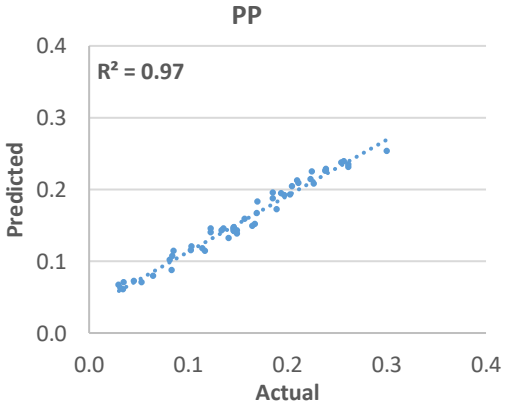
27th:

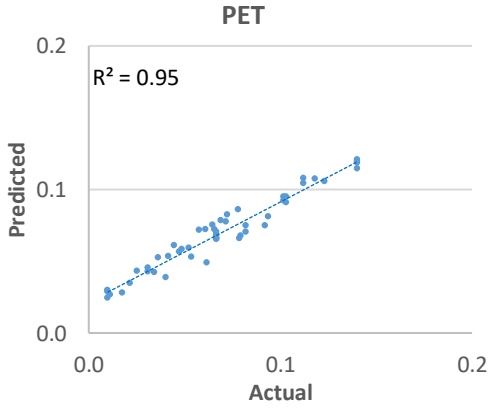

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

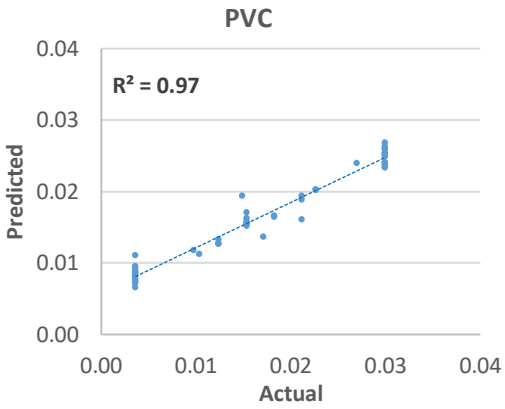

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

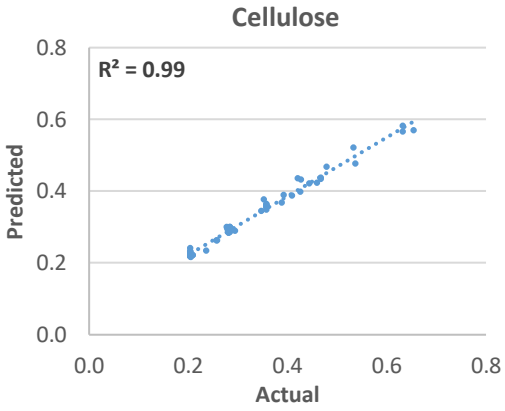

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

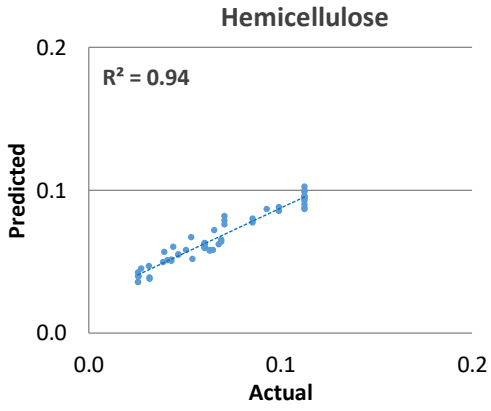

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

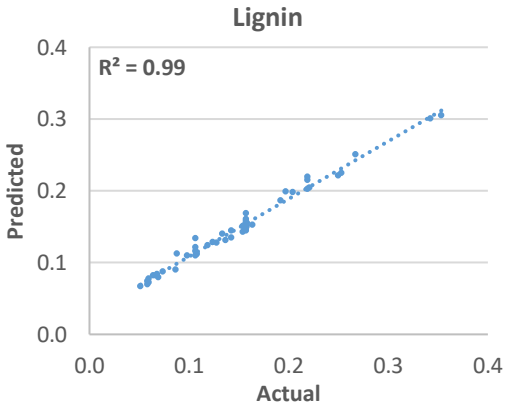

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

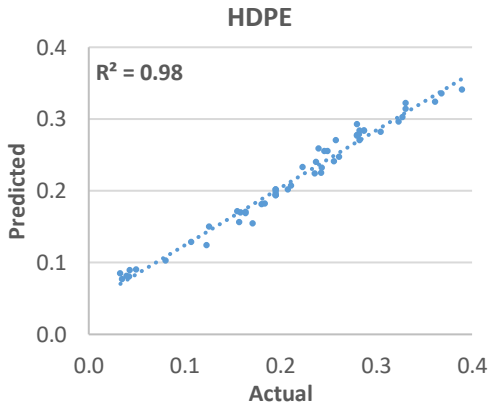

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

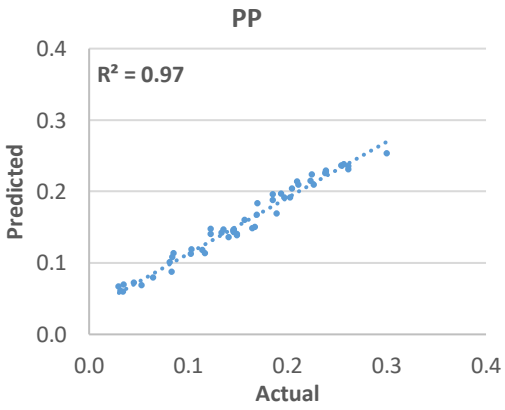
28th:

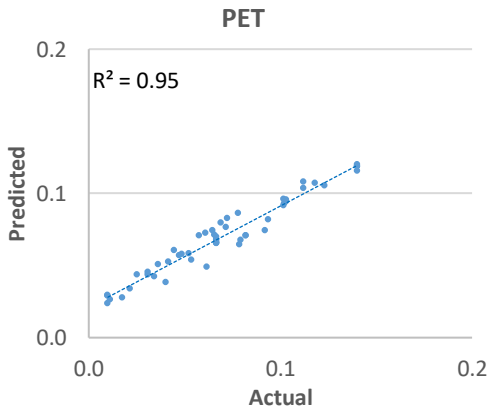

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

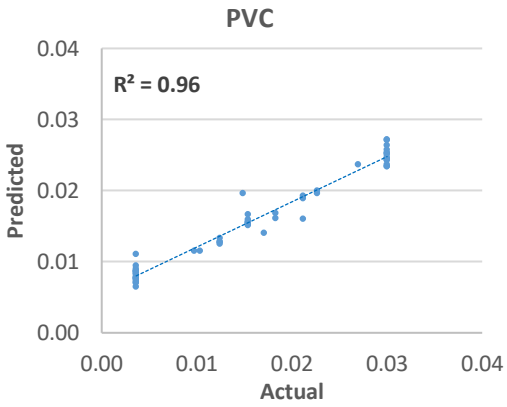

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

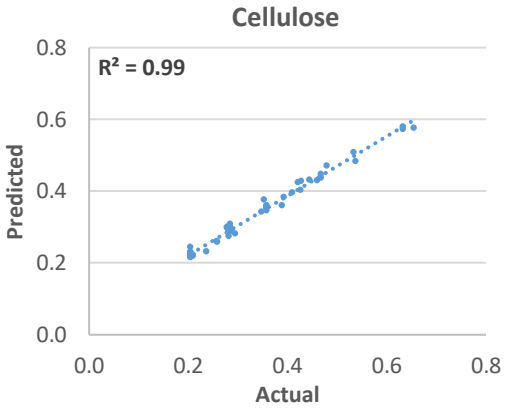

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

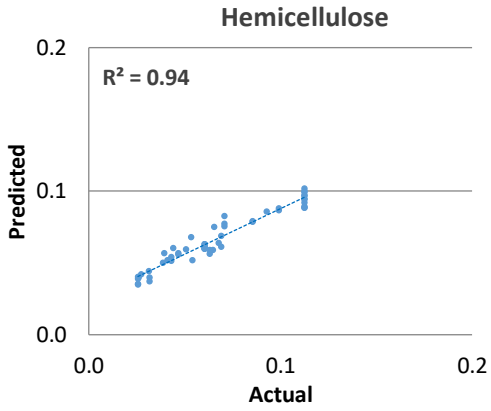

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

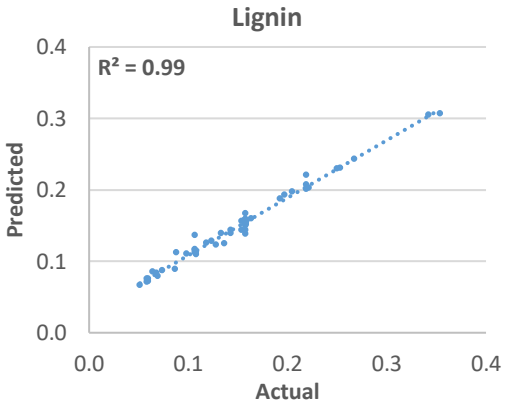

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

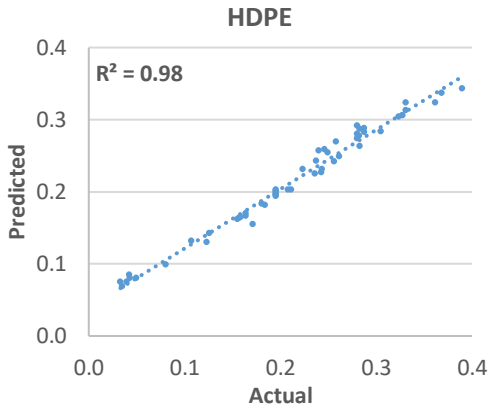

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

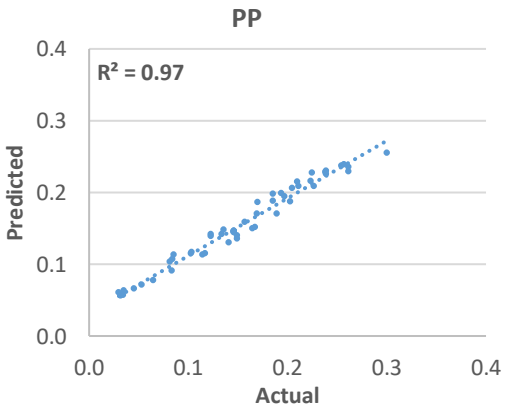
29th:

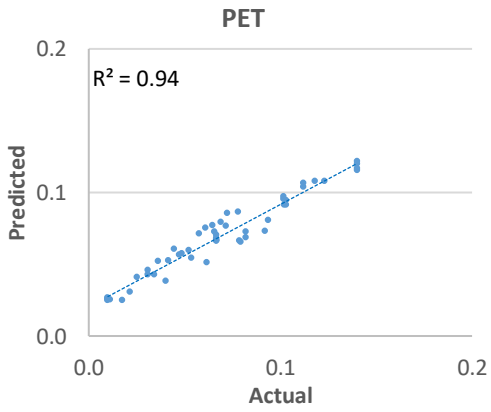

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

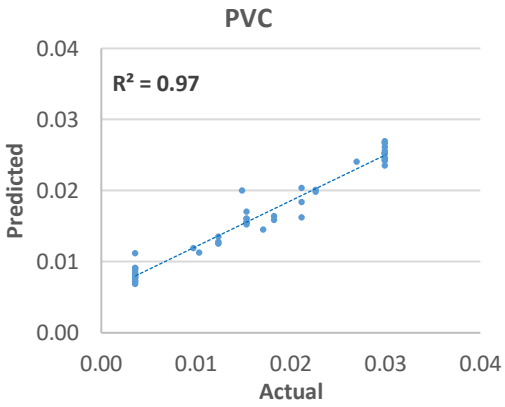

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

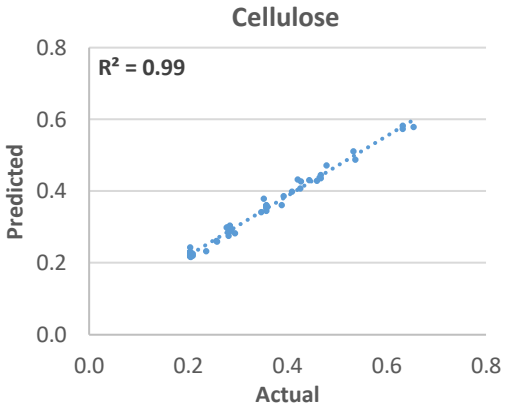

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

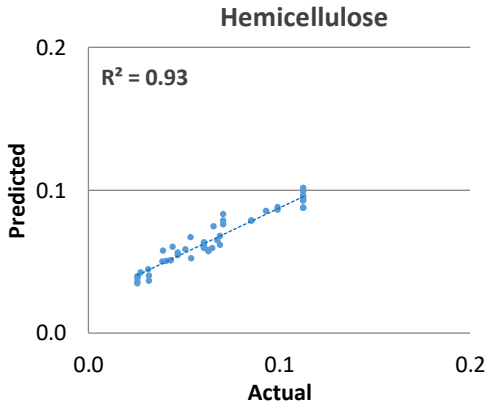

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

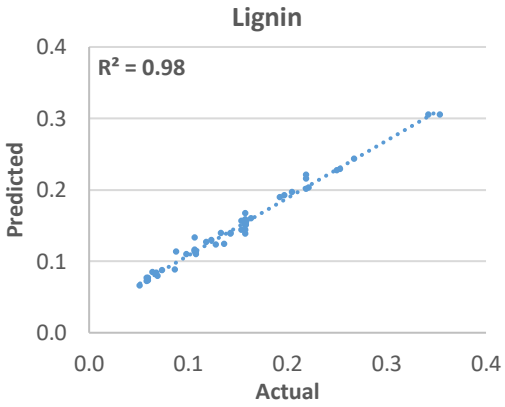

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

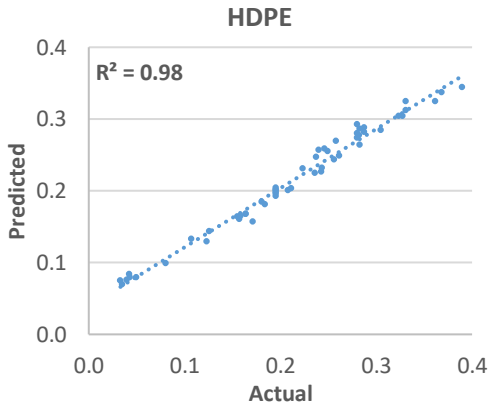

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

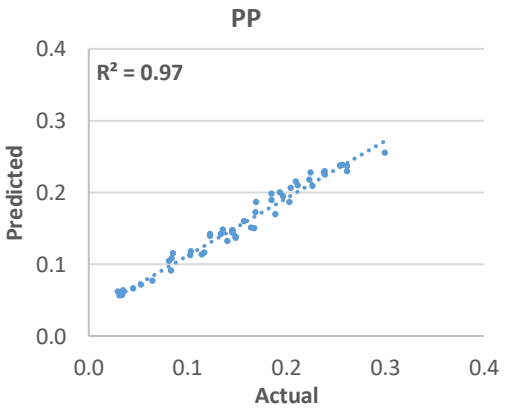
30th:

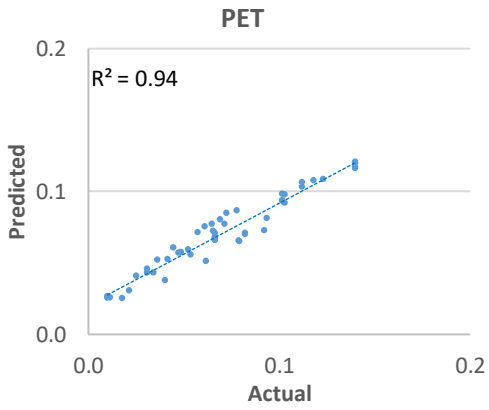

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

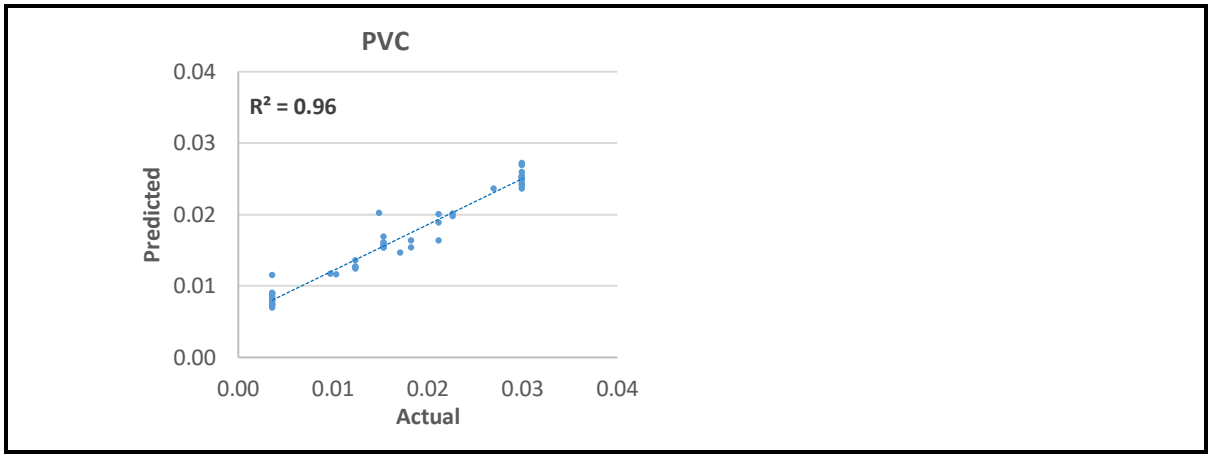
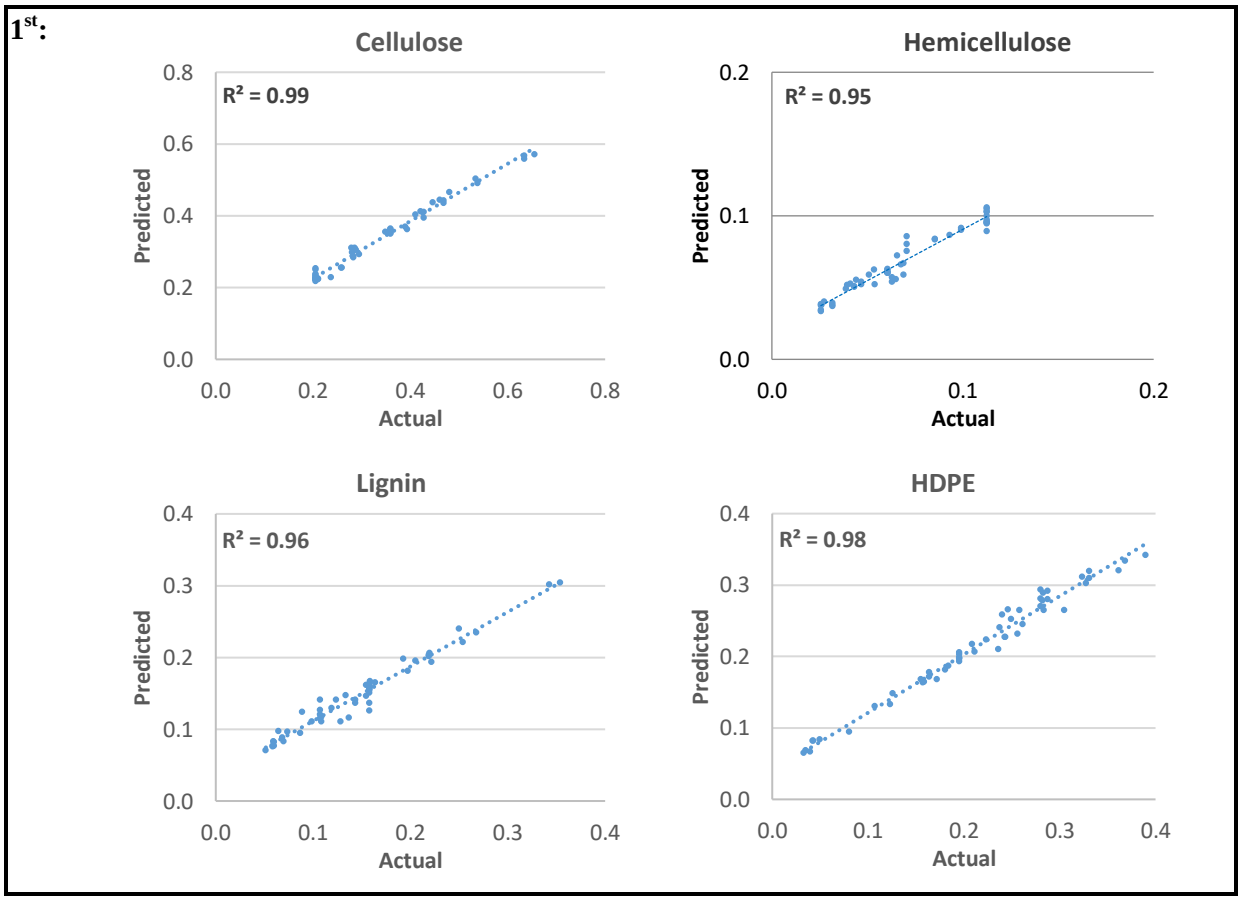
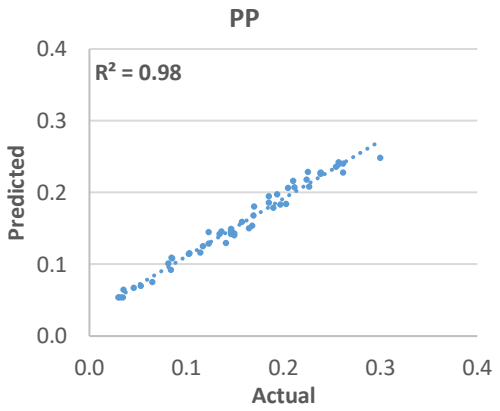
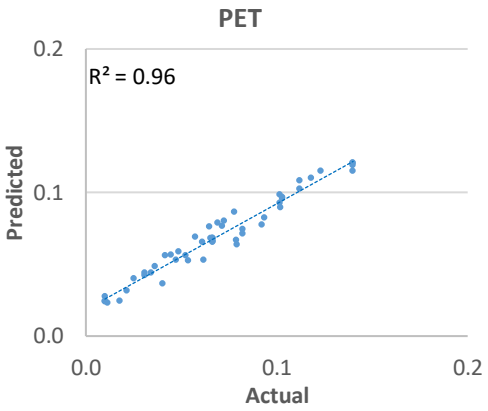


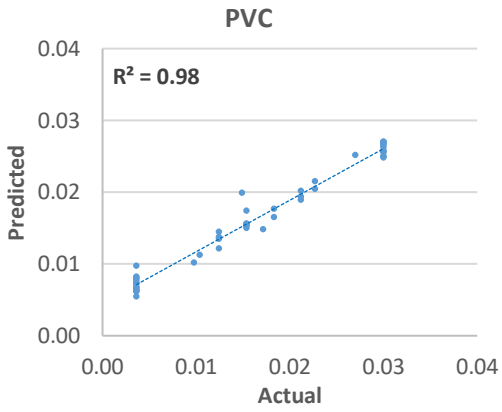
Figure SI.3-1. Observed vs predicted values of prevalent polymers (cellulose, xylan, lignin, HDPE, PP, PET, and PVC) of model training using dataset combinations (n=30) derived from TGA, DTG, and FTIR analytical techniques as input matrix following the first approach of ML model training (under constant *mtry*).

I. Scatter plots (Obs. vs Pred.) of dataset combination under variable *mtry*

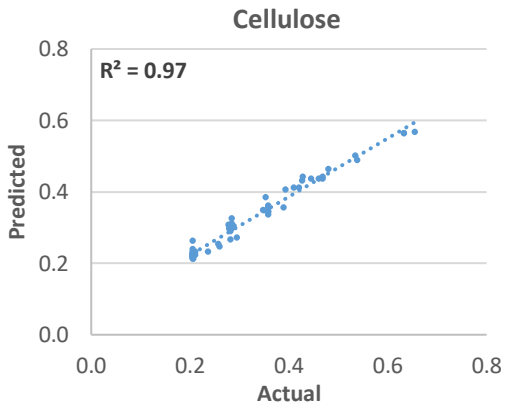


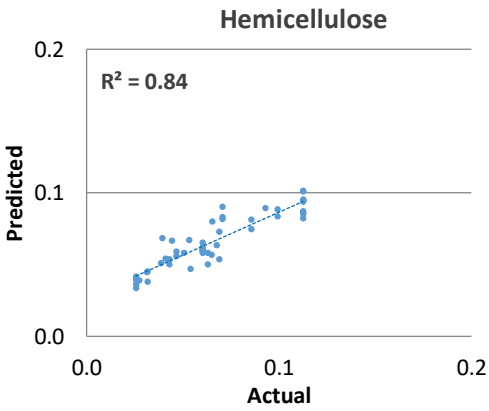

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

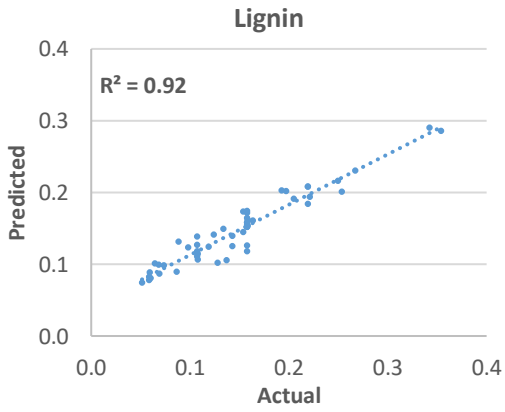

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

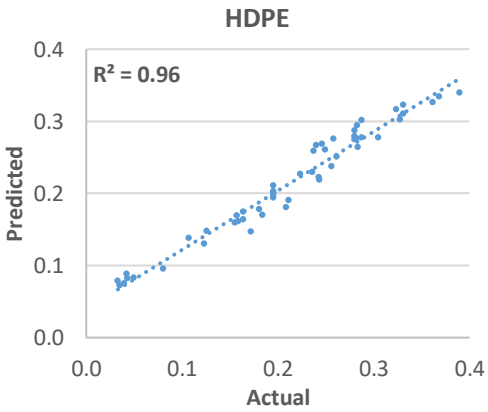

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

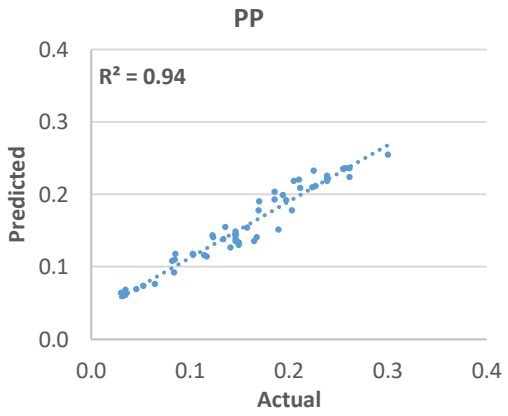
2nd:

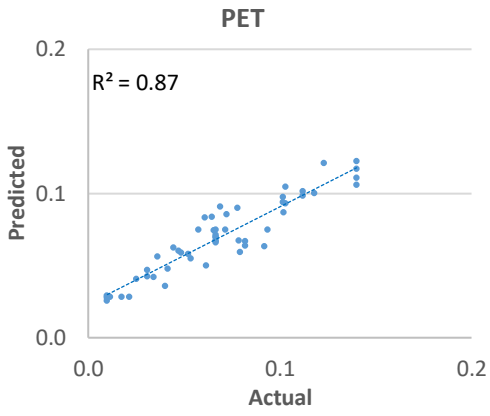

Cellulose
R² = 0.97
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

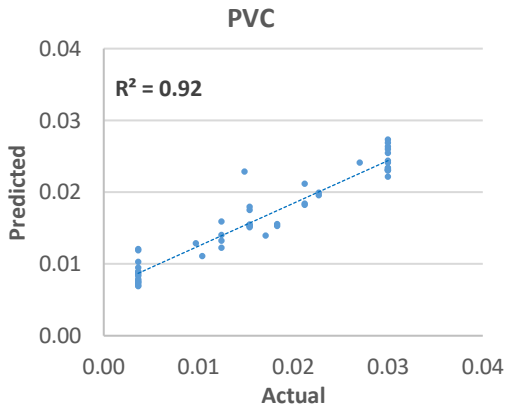

Hemicellulose
R² = 0.84
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.92
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

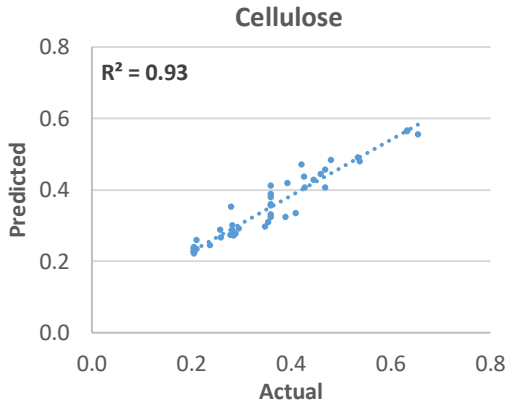

HDPE
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

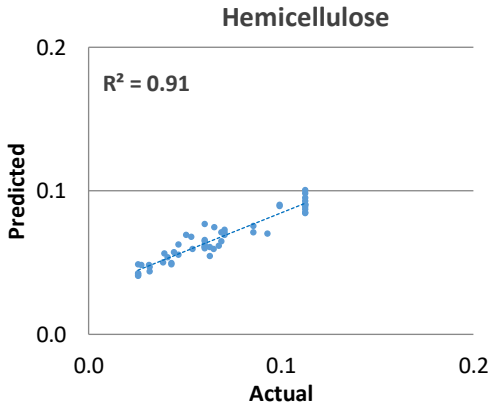

PP
R² = 0.94
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

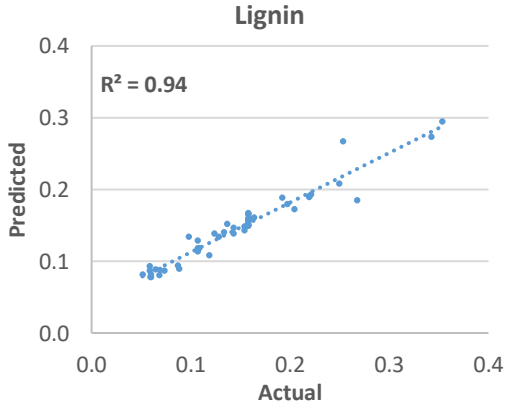

PET
R² = 0.87
Predicted
Actual
0.0
0.1
0.2

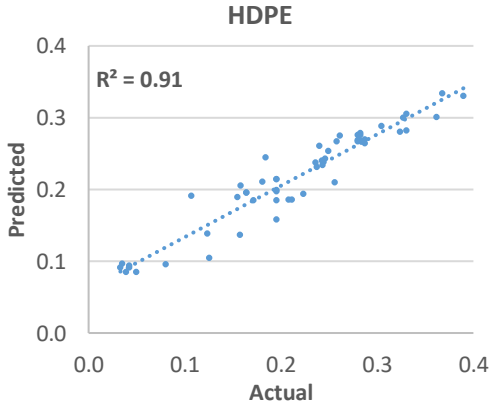

PVC
R² = 0.92
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

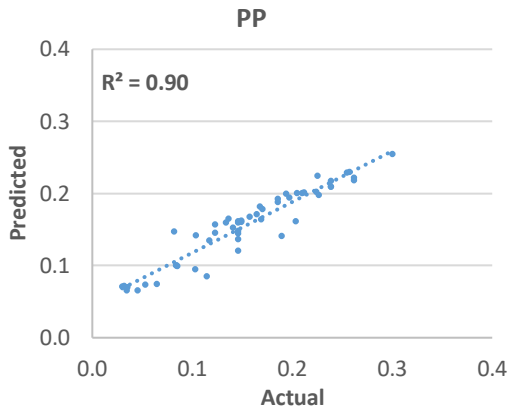
3rd:

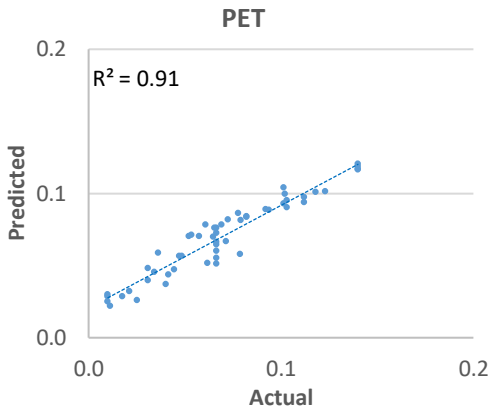

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

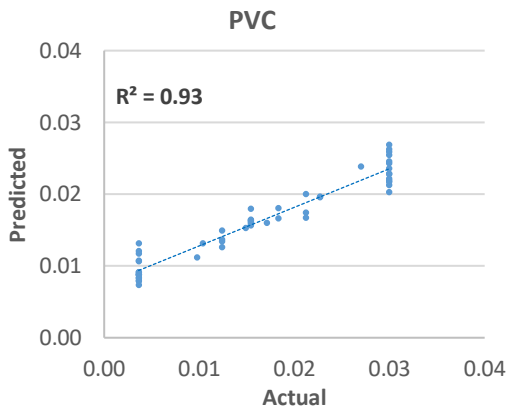

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.94
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

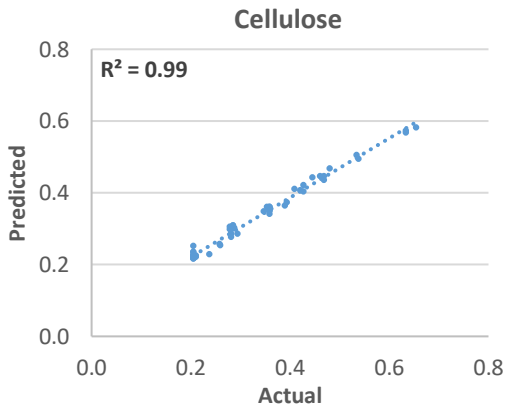

HDPE
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

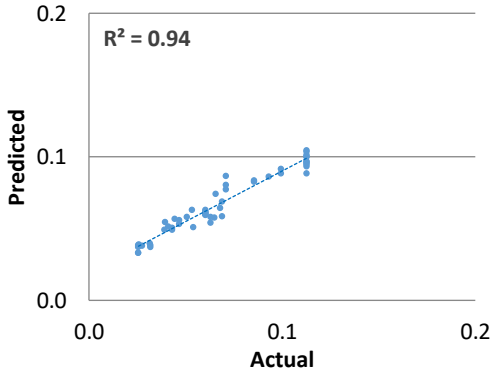

PP
R² = 0.90
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

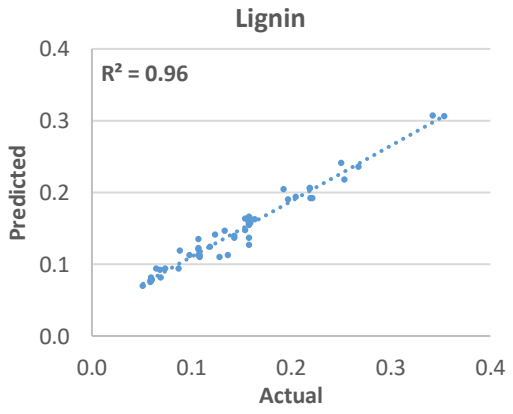

PET
R² = 0.91
Predicted
Actual
0.0
0.1
0.2

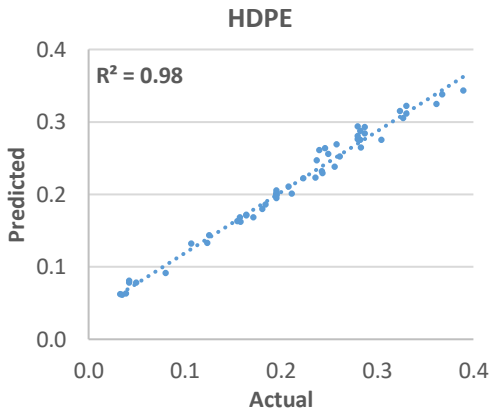

PVC
R² = 0.93
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

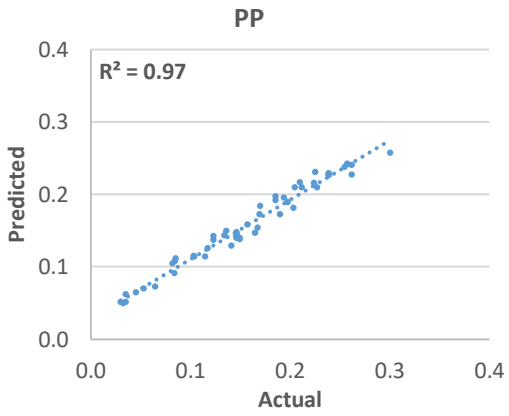
4th:

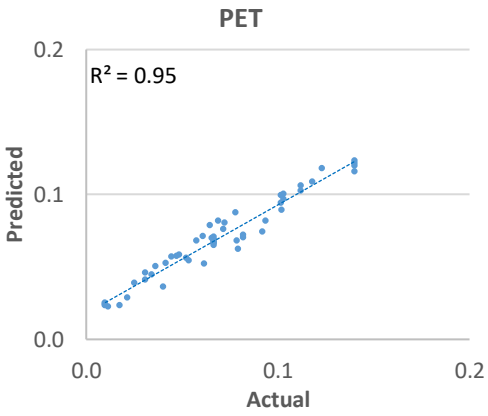

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

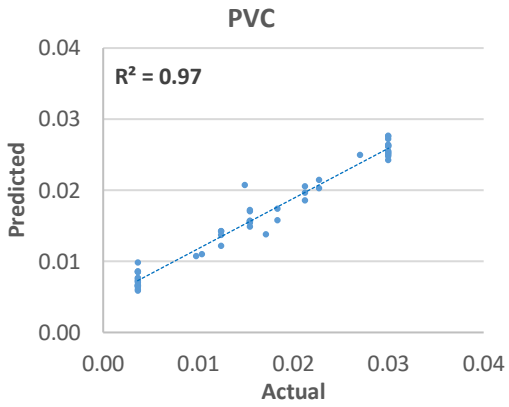

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

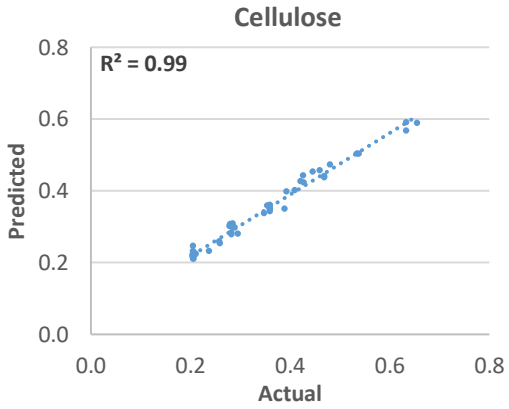

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

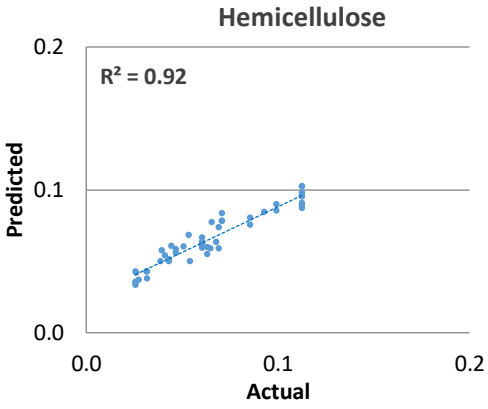

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

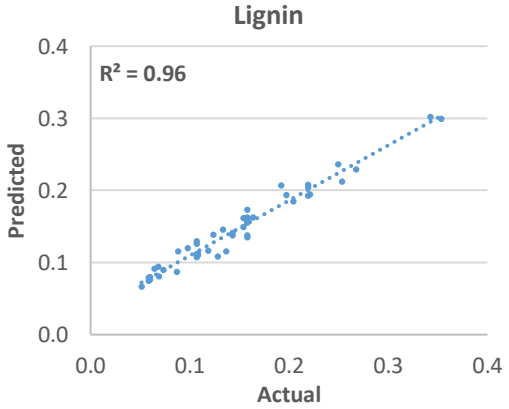

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

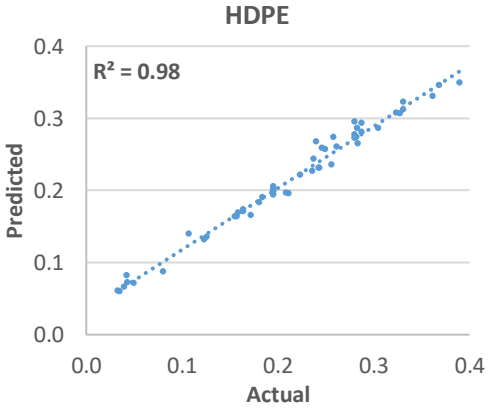

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

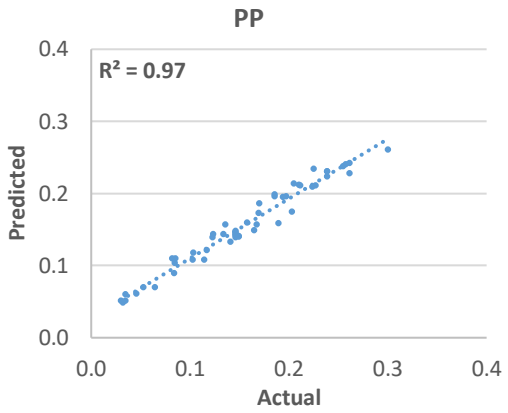
5th:

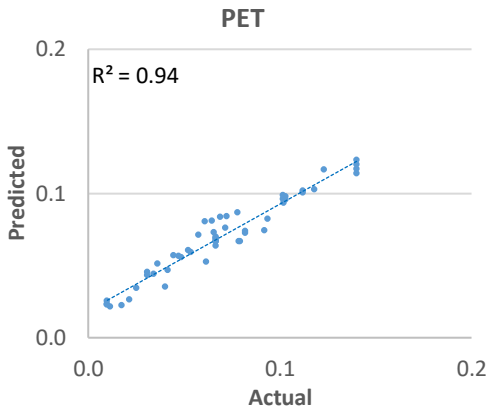

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

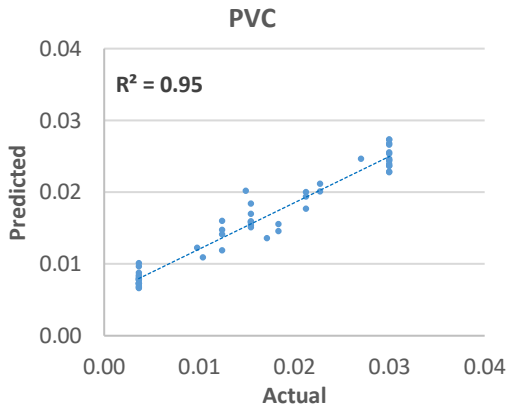

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

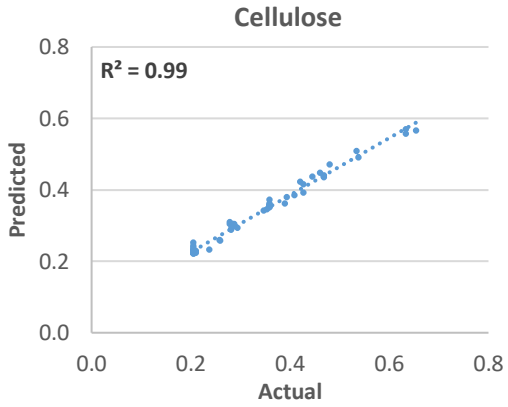

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

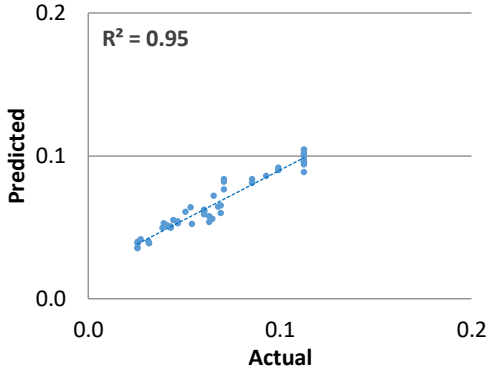

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

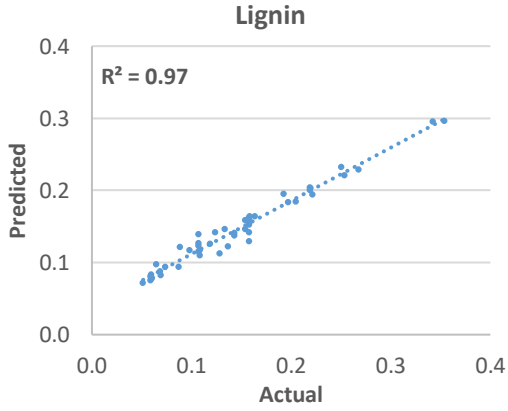

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

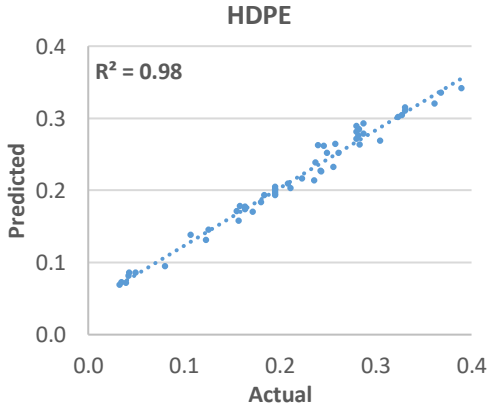

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

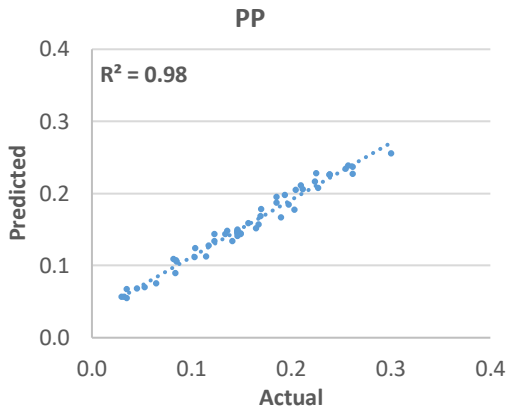
6th:

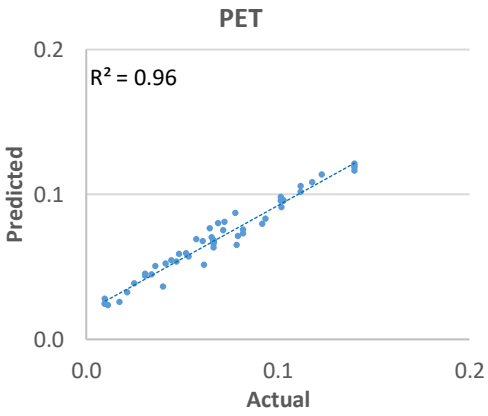

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

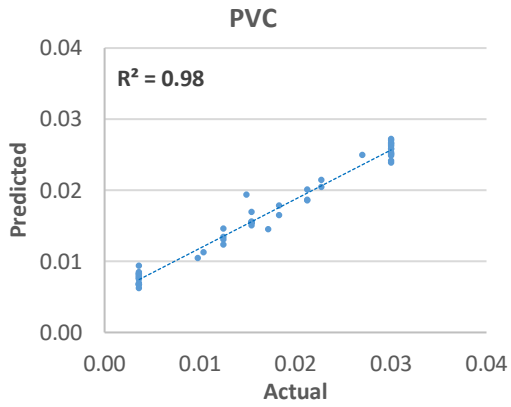

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

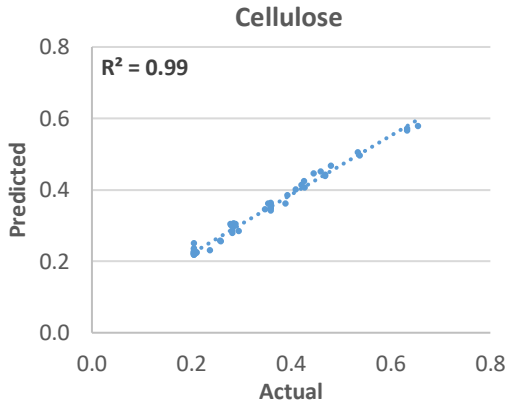

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

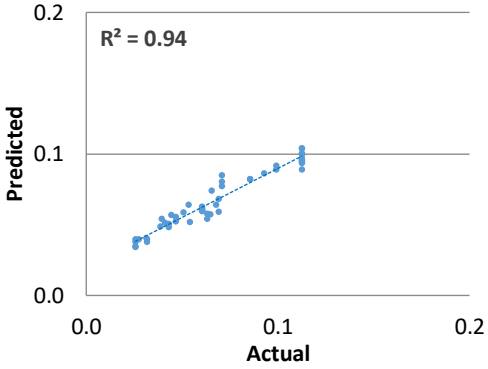

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

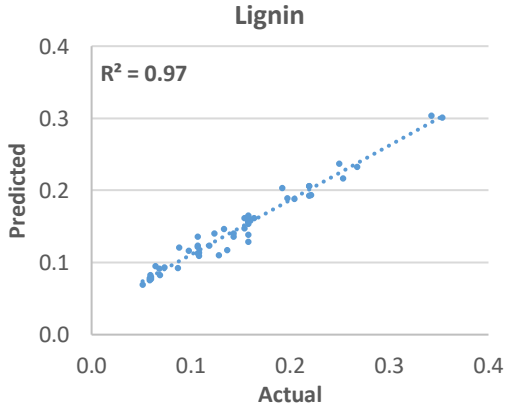

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

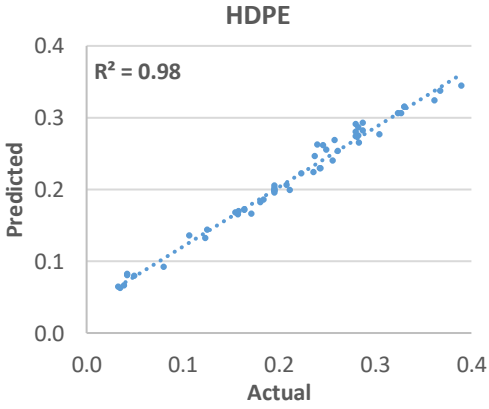

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

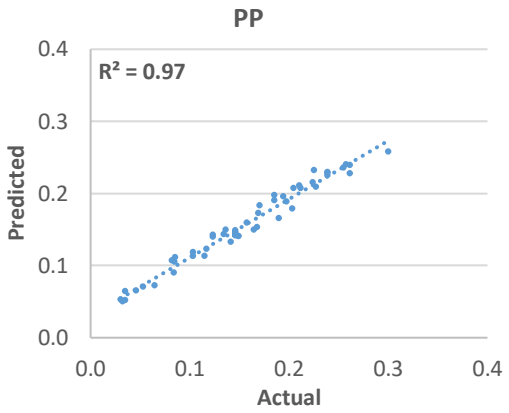
7th:

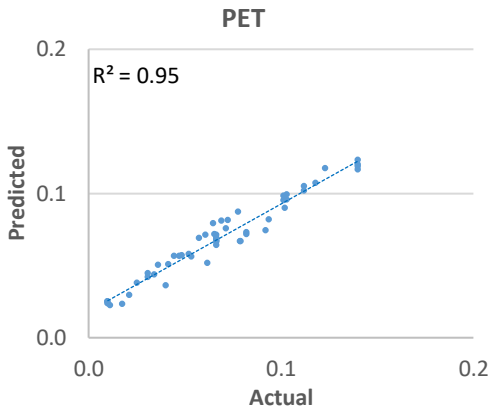

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

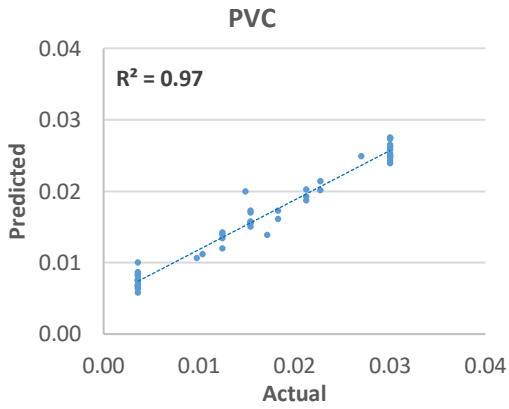

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

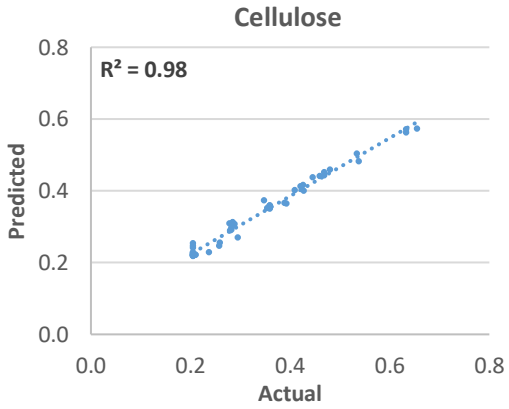

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

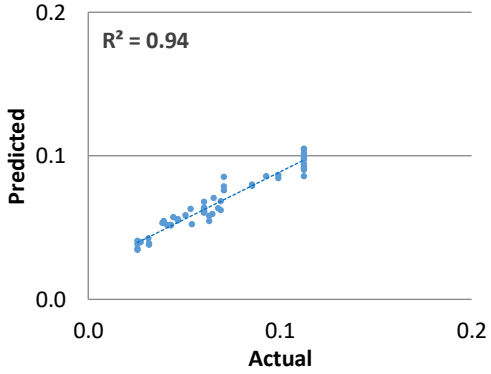

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

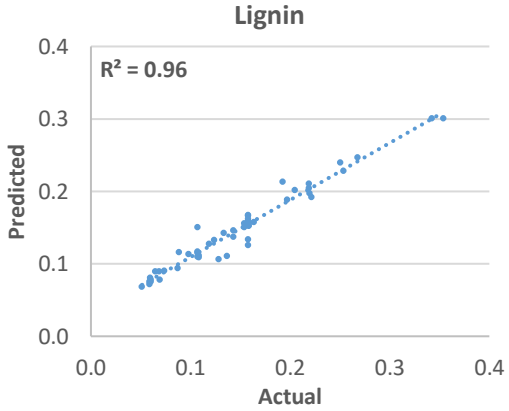

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

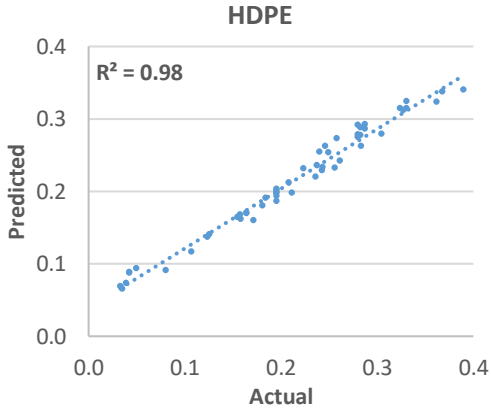

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

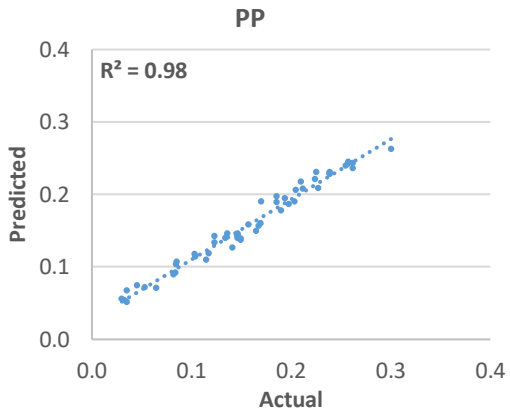
8th:

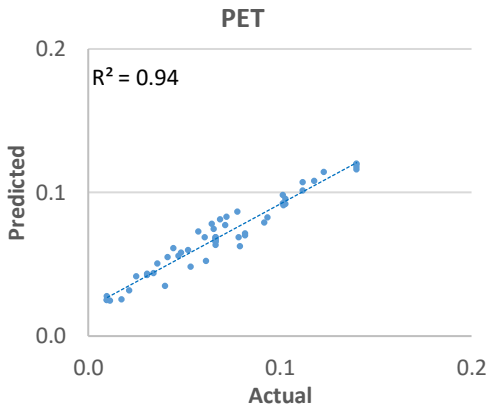

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

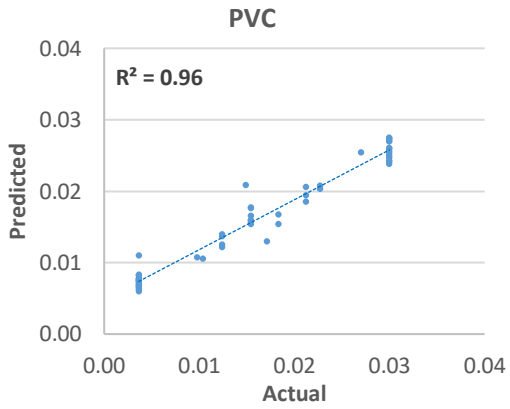

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

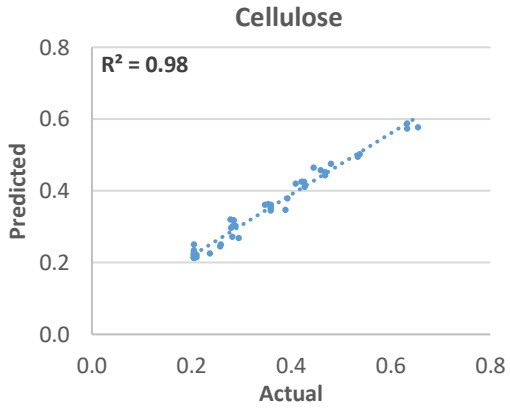

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

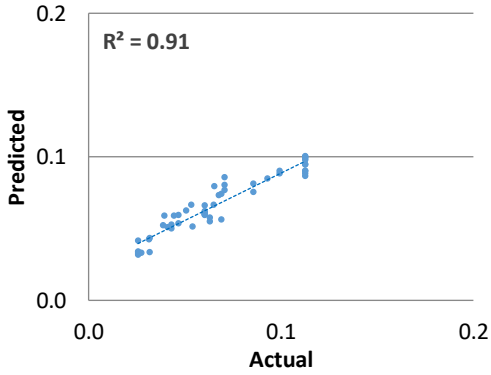

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

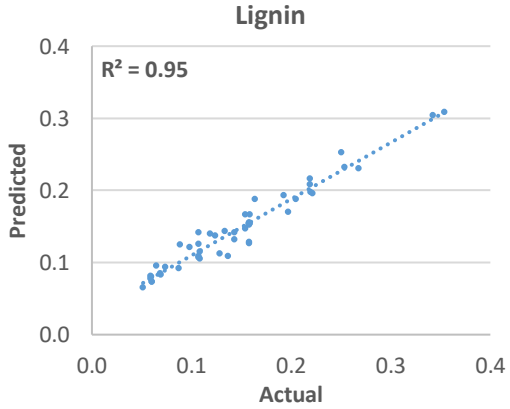

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

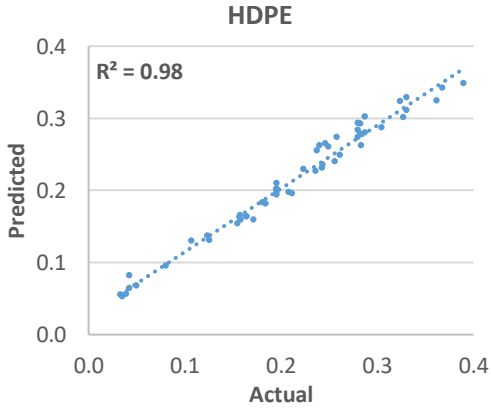

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

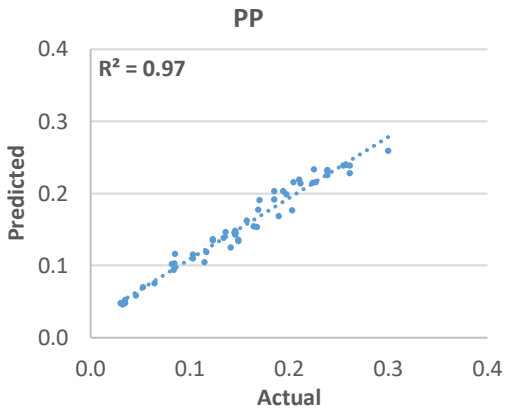
9th:

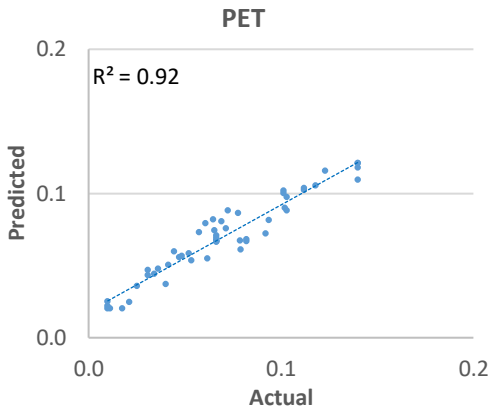

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PET
R² = 0.92
Predicted
Actual
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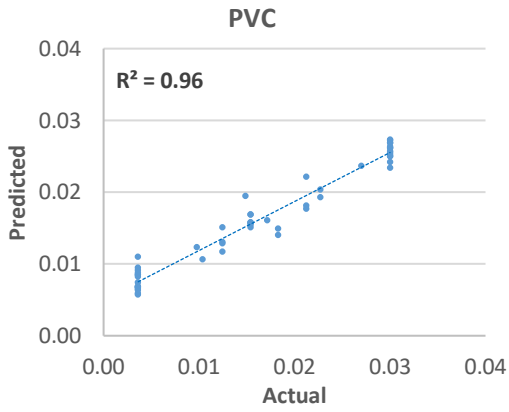
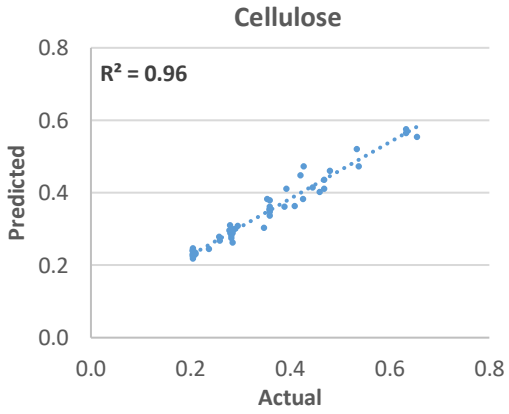
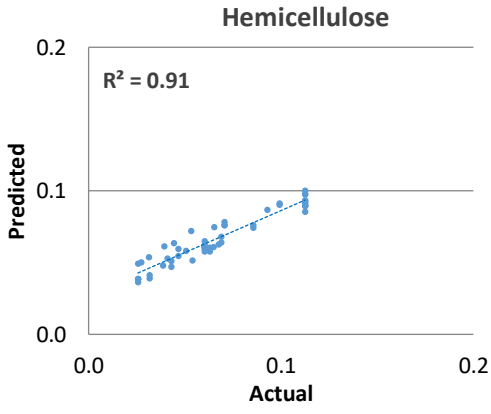
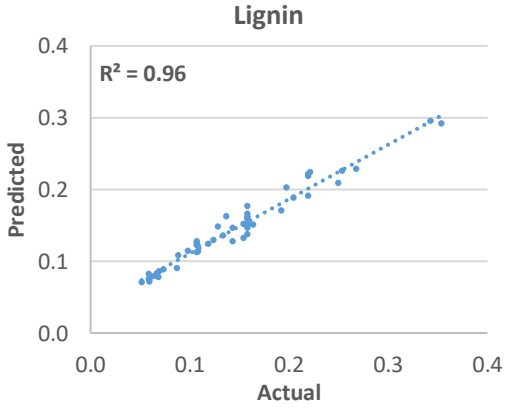
0.1
0.2

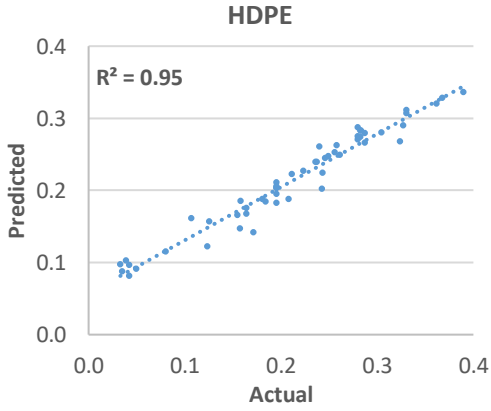

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

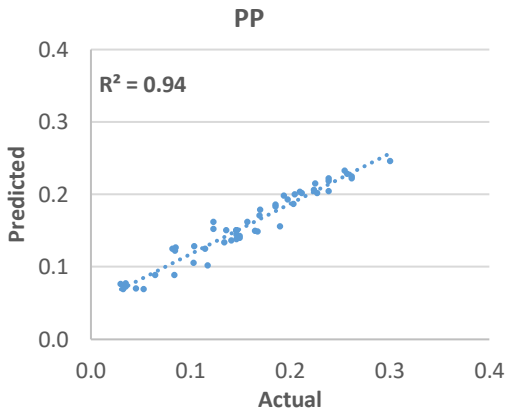
10th:

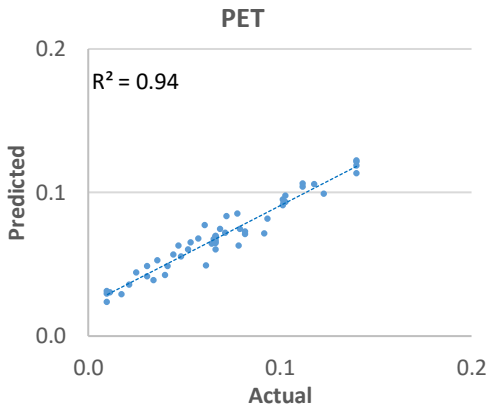

Cellulose
R² = 0.96
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

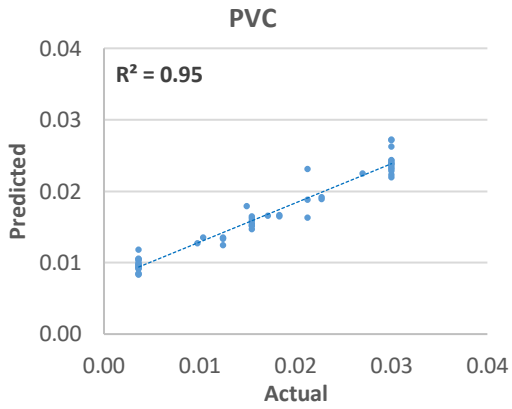

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

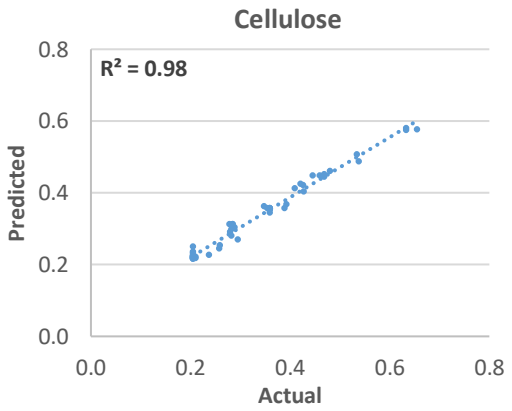

HDPE
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

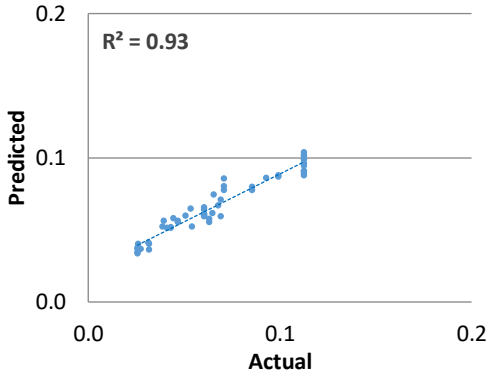

PP
R² = 0.94
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

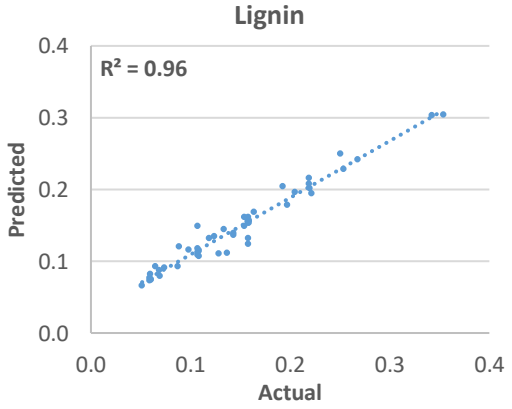

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

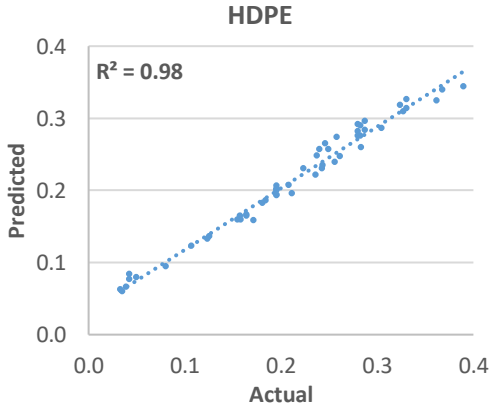

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

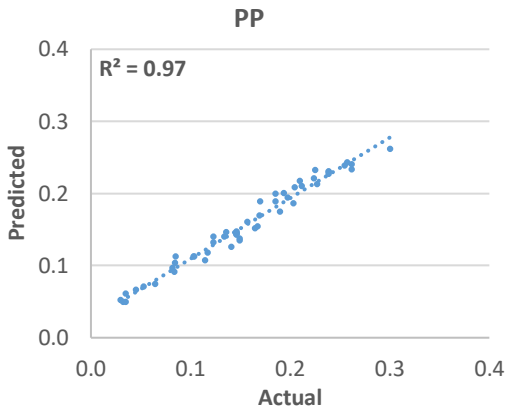
11th:

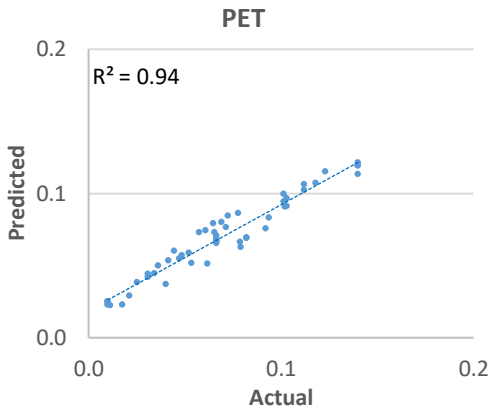

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

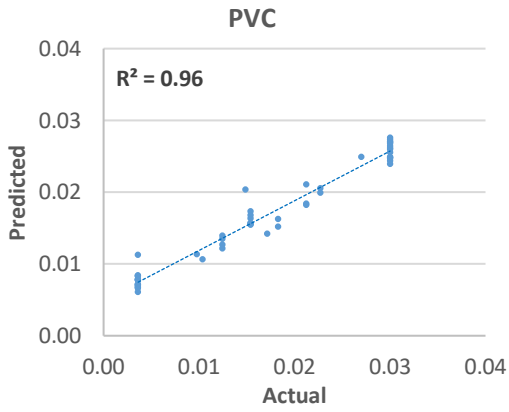

Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

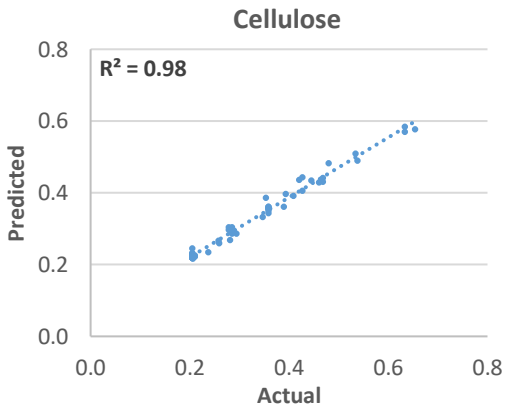

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

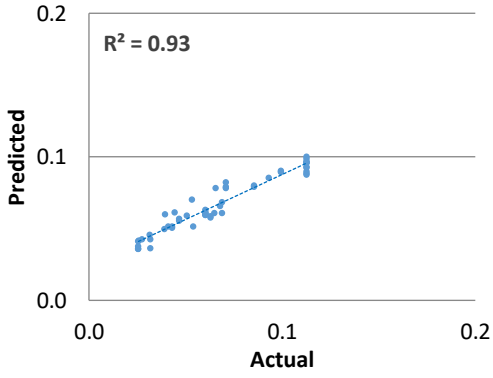

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

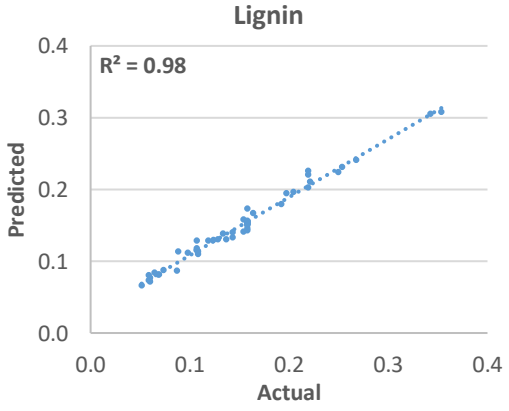

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

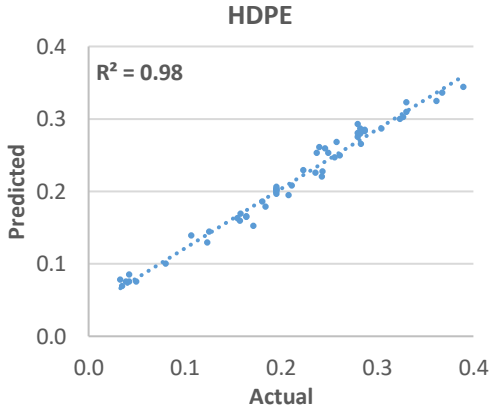

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

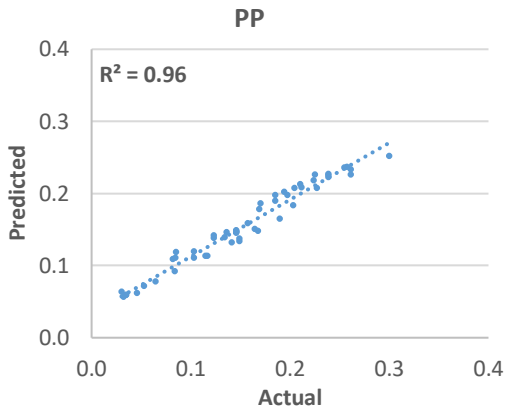
12th:

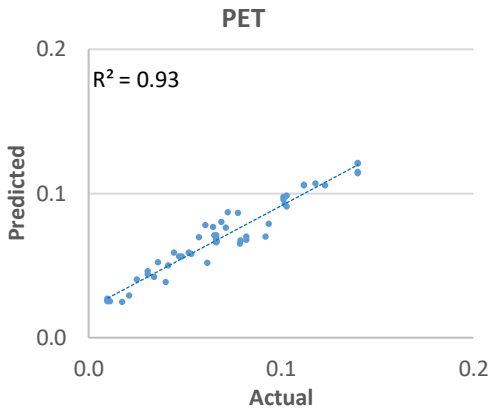

Cellulose
R² = 0.98
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

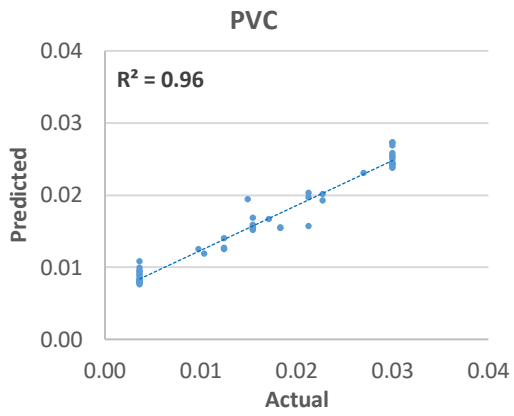

Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

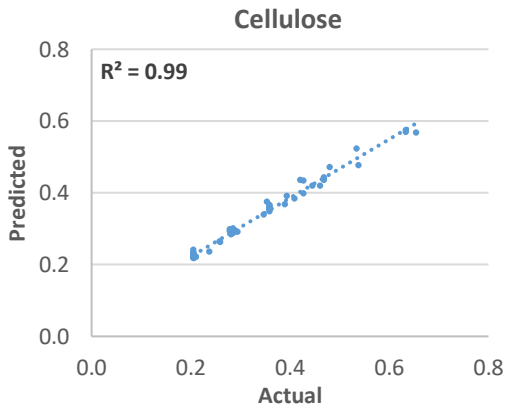

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

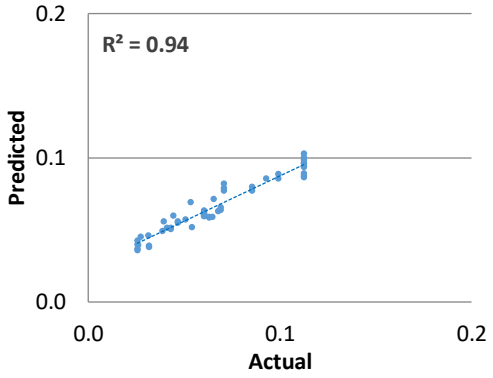

PP
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

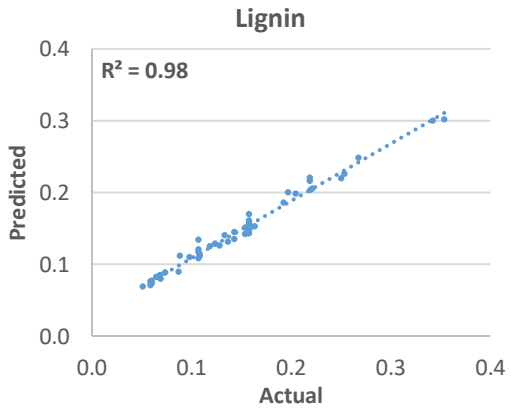

PET
R² = 0.93
Predicted
Actual
0.0
0.1
0.2

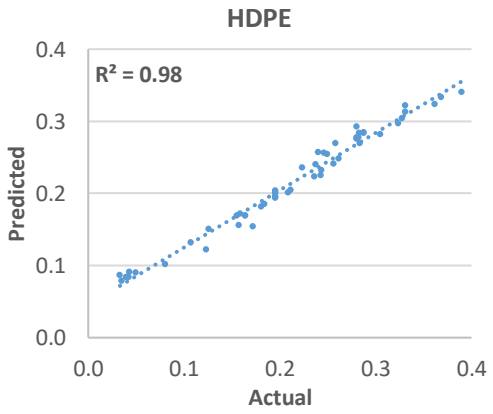

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

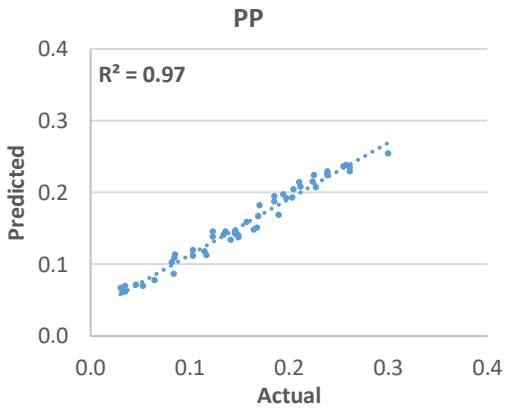
13th:

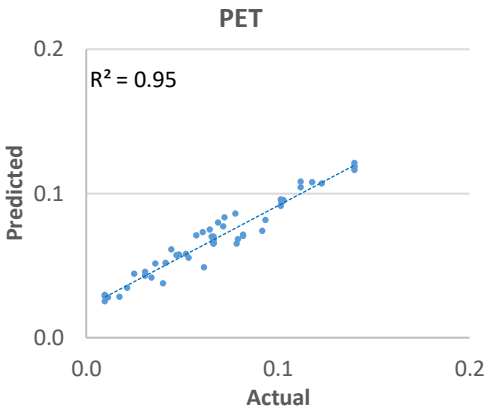

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

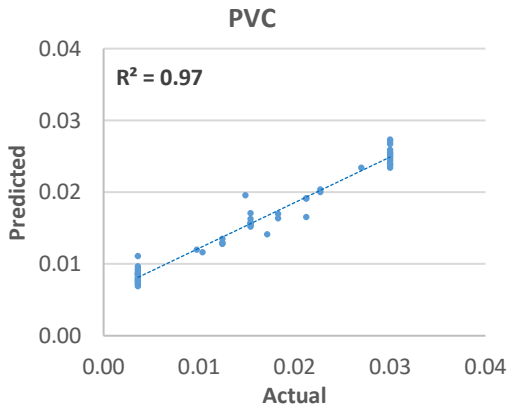

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

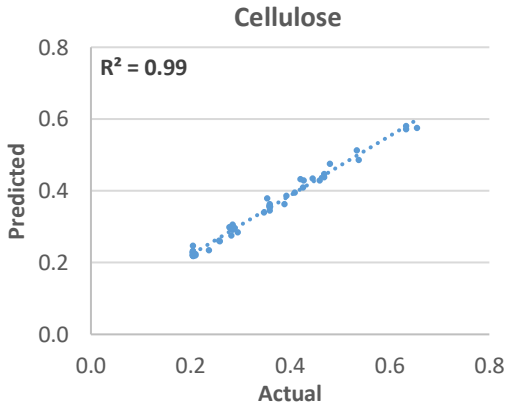

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

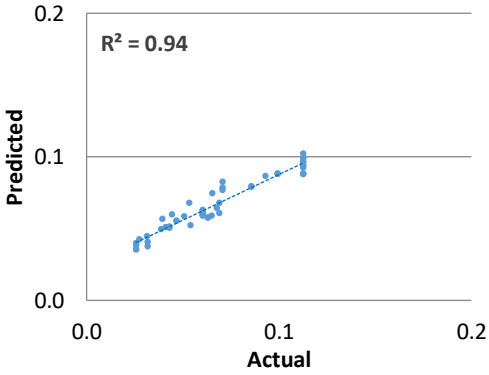

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

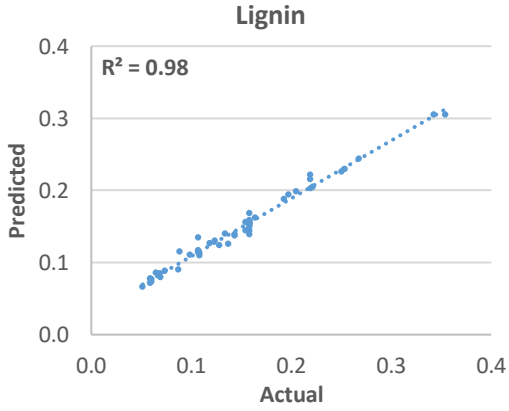

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

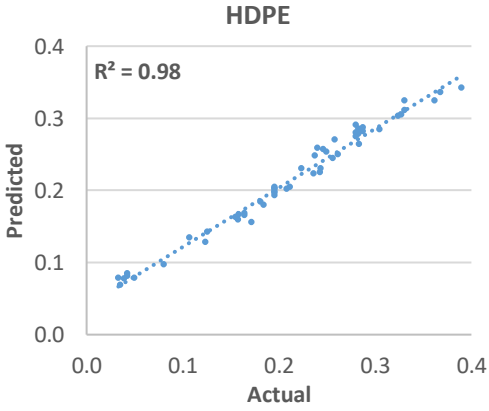

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

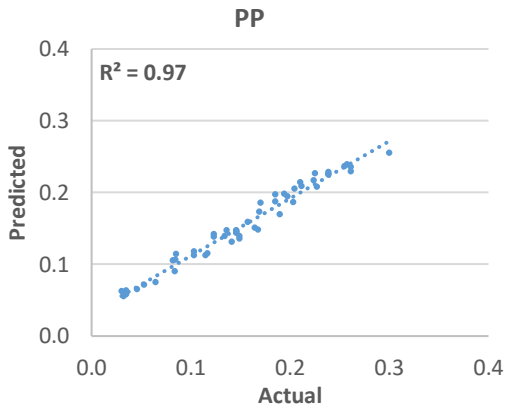
14th:

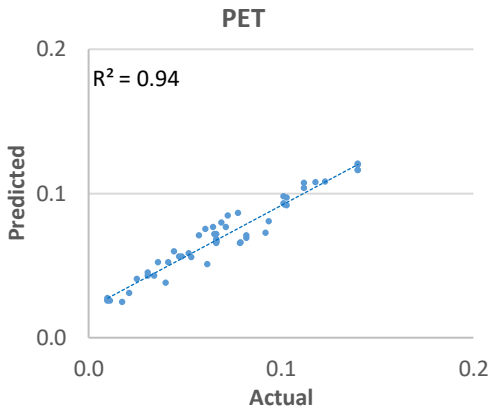

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

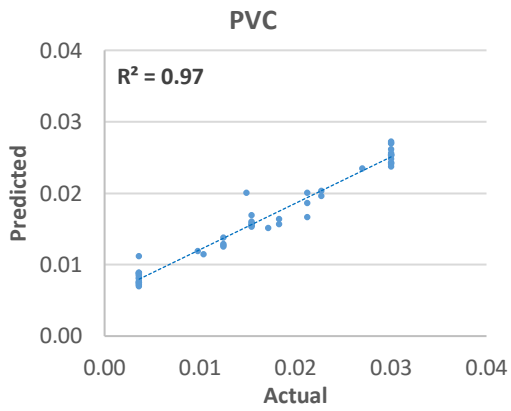

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

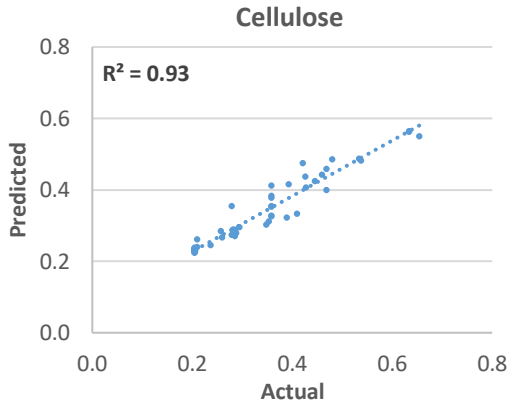

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

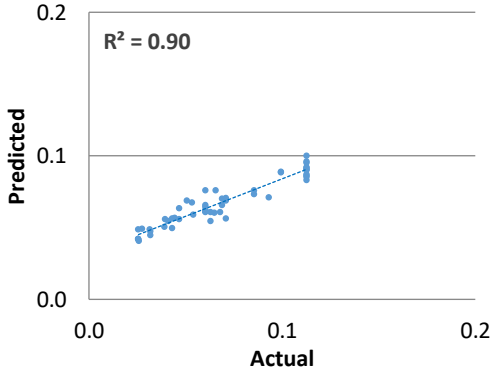

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

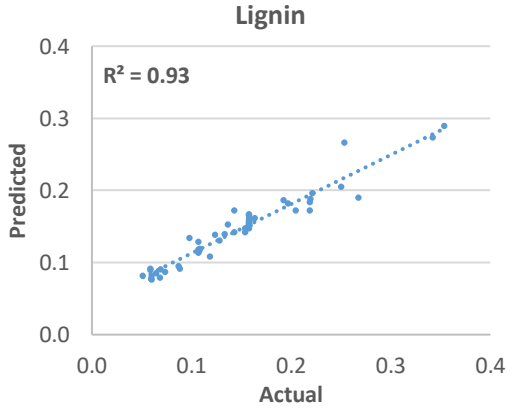

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

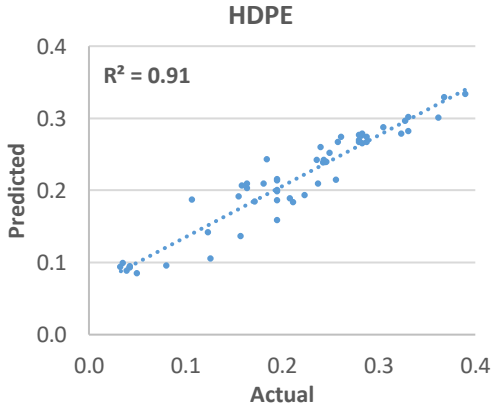

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

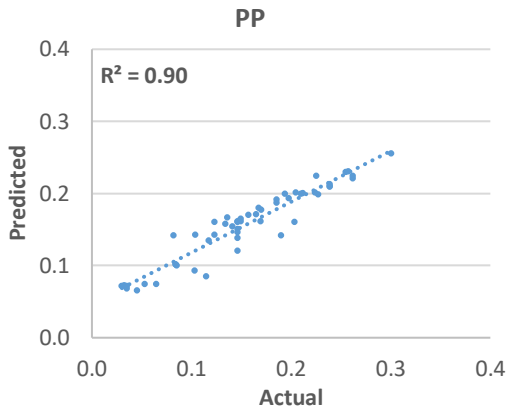
15th:

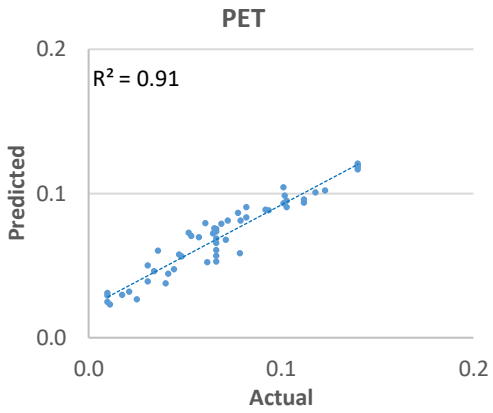

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

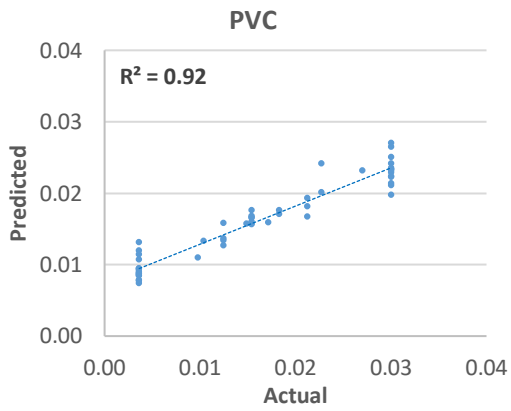

Hemicellulose
R² = 0.90
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.93
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

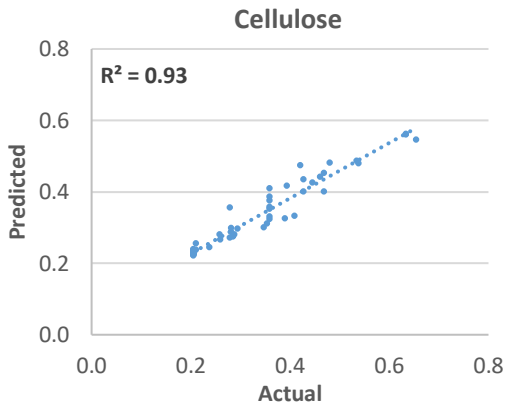

HDPE
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

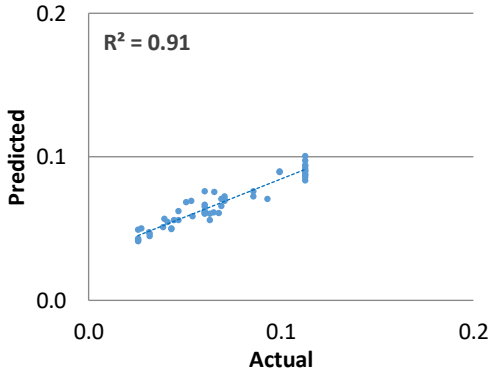

PP
R² = 0.90
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

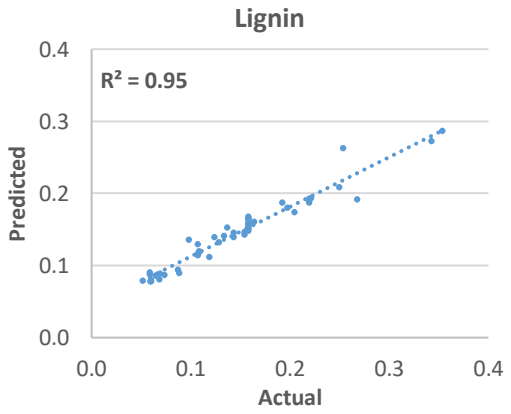

PET
R² = 0.91
Predicted
Actual
0.0
0.1
0.2

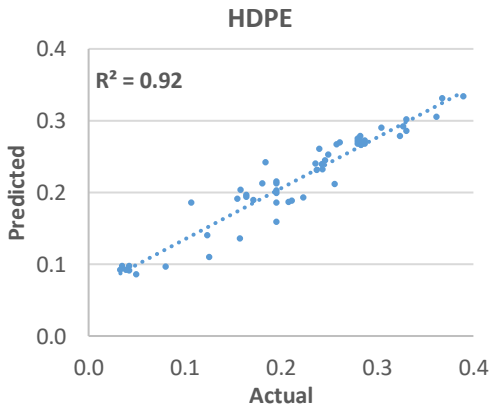

PVC
R² = 0.92
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

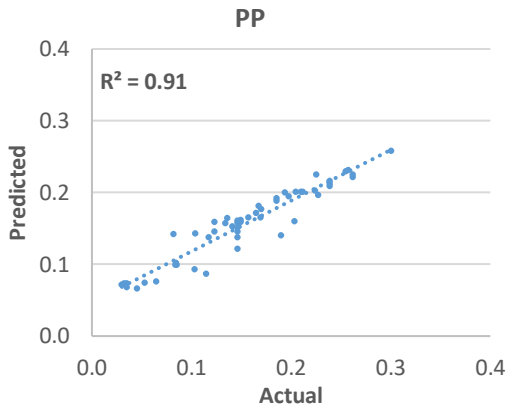
16th:

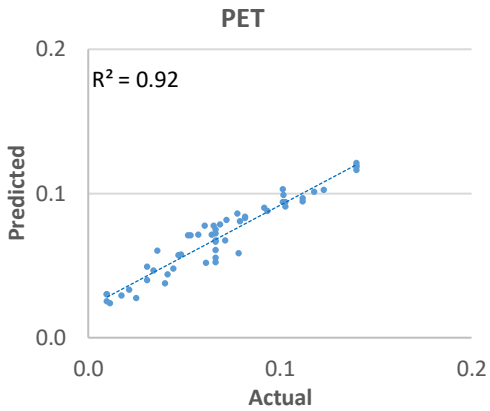

Cellulose
R² = 0.93
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

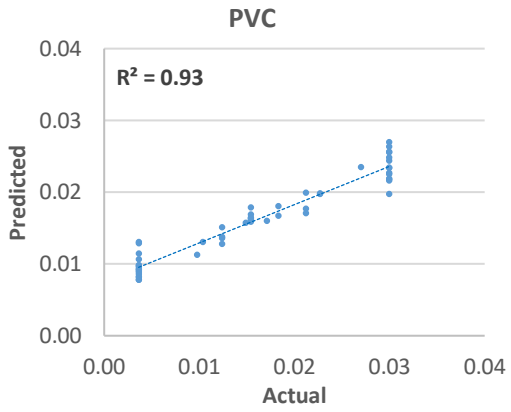

Hemicellulose
R² = 0.91
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

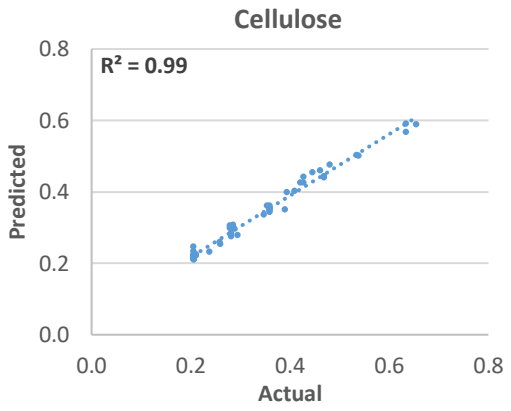

HDPE
R² = 0.92
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

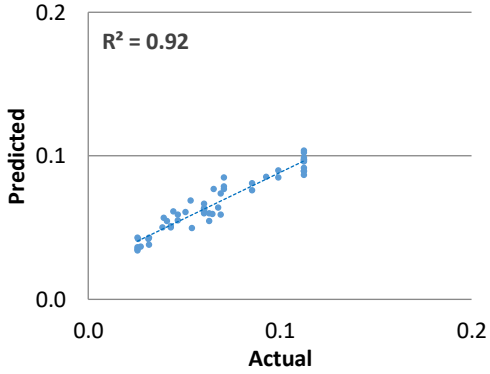

PP
R² = 0.91
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

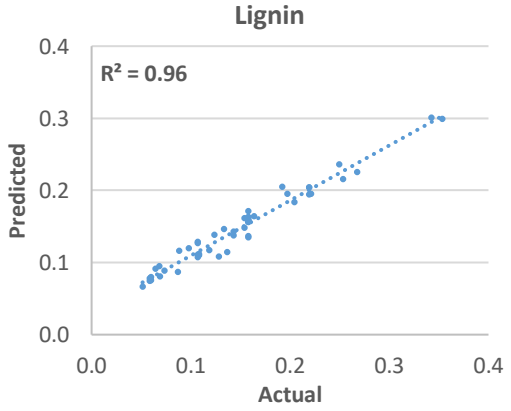

PET
R² = 0.92
Predicted
Actual
0.0
0.1
0.2

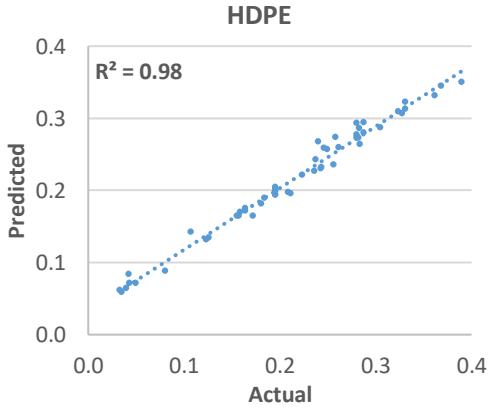

PVC
R² = 0.93
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

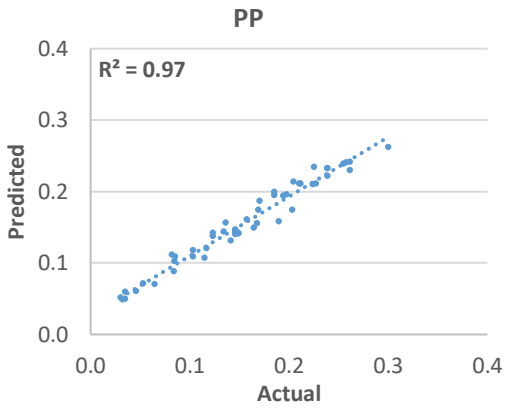
17th:

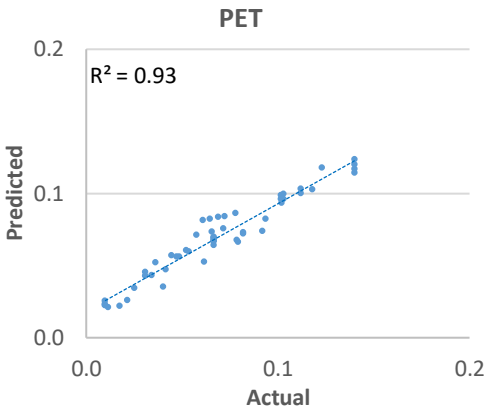

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

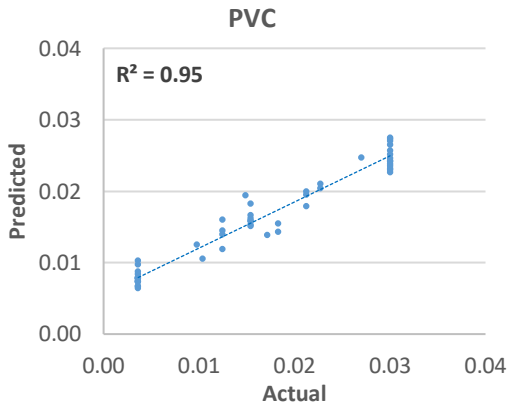

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

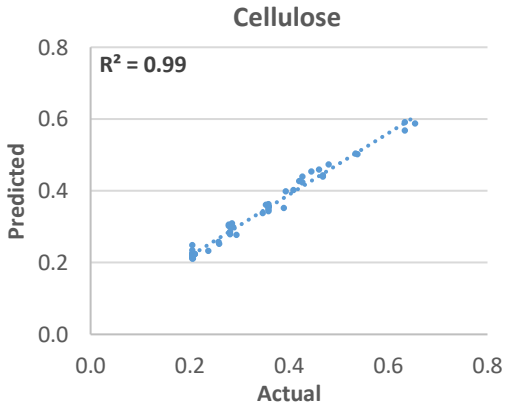

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

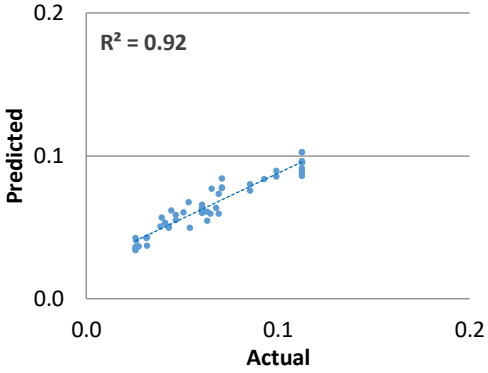

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

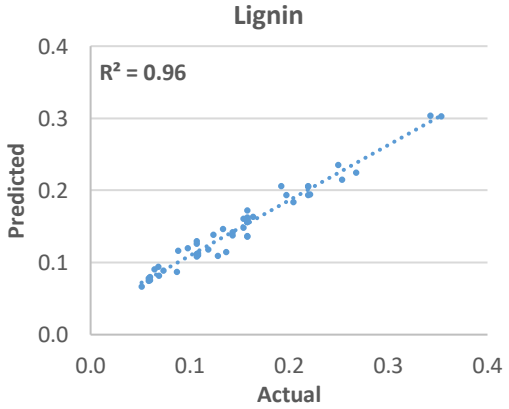

PET
R² = 0.93
Predicted
Actual
0.0
0.1
0.2

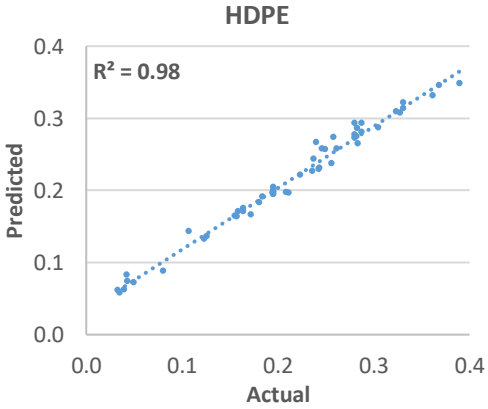

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

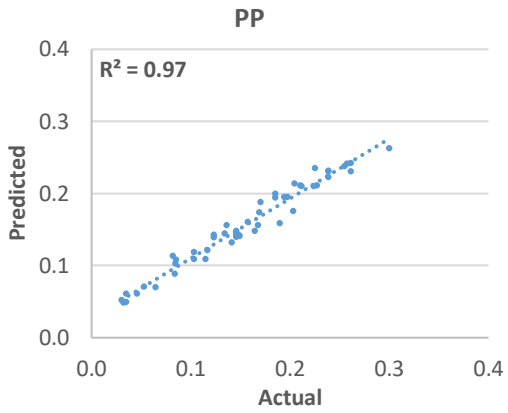
18th:

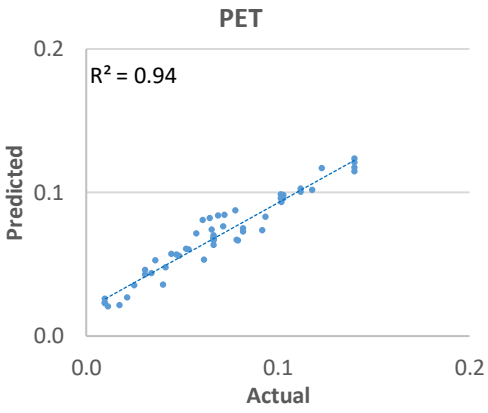

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

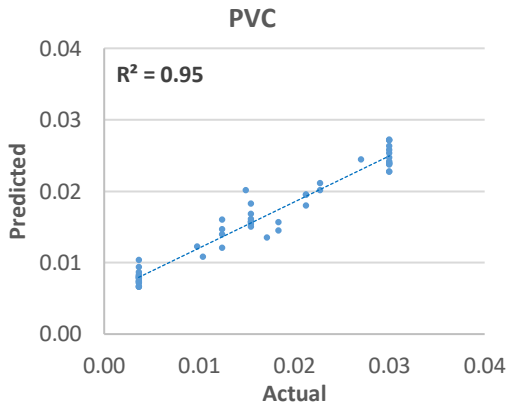

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

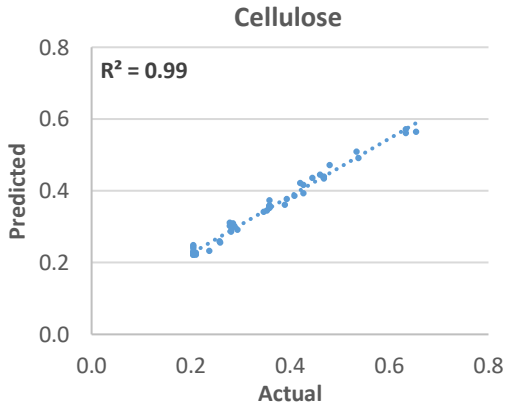

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

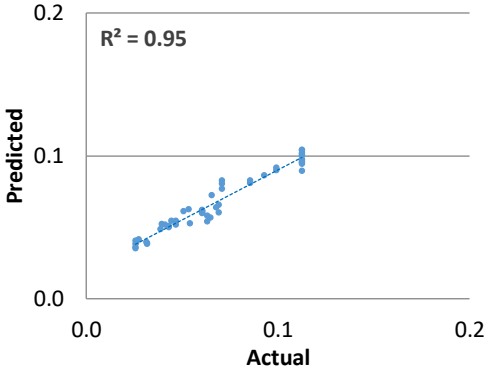

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

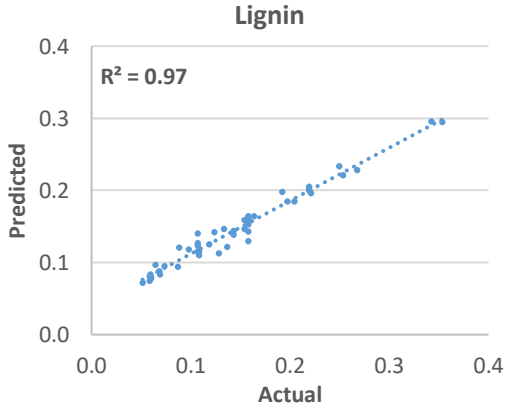

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

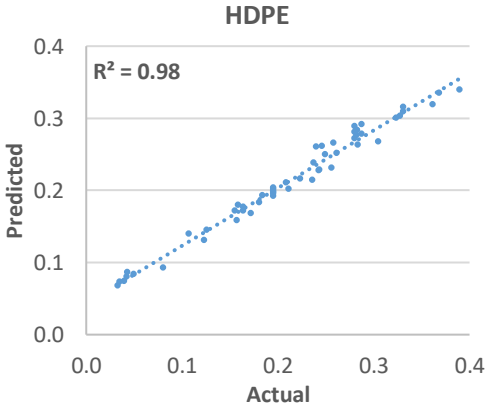

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

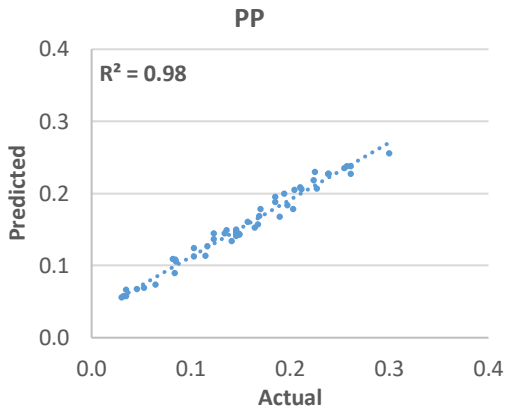
9th:

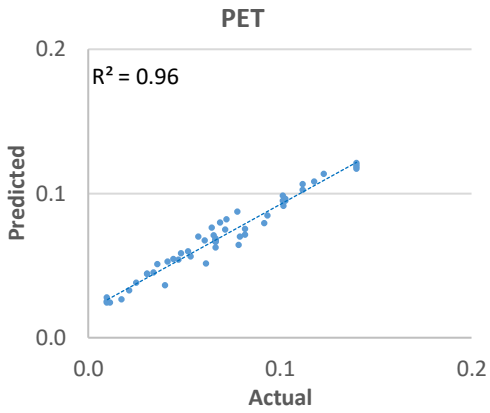

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

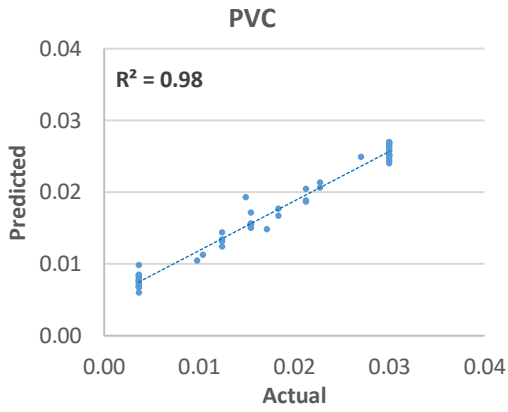

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

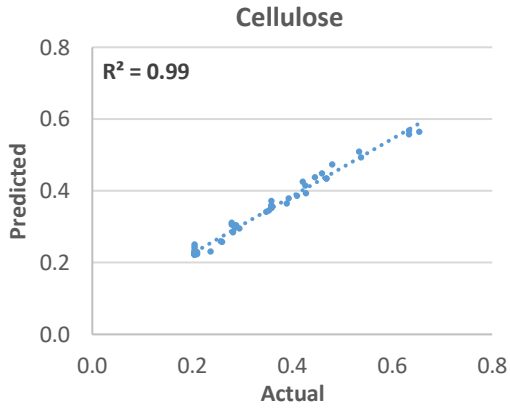

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

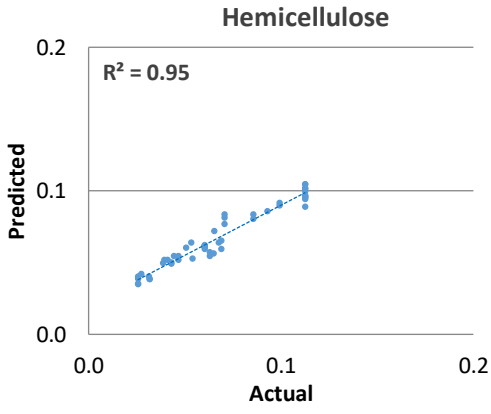

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

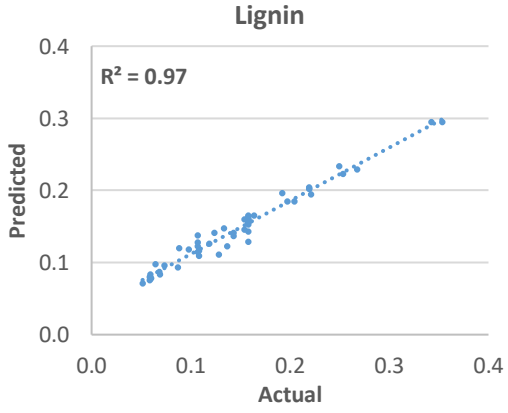

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

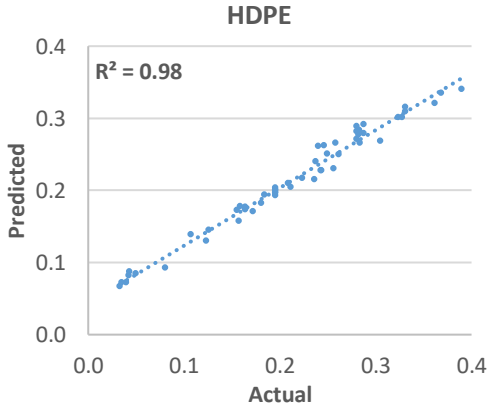

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

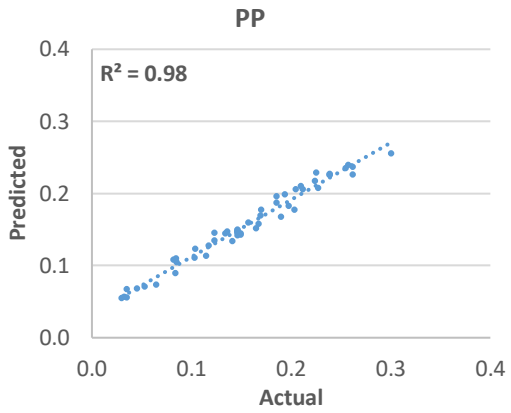
20th:

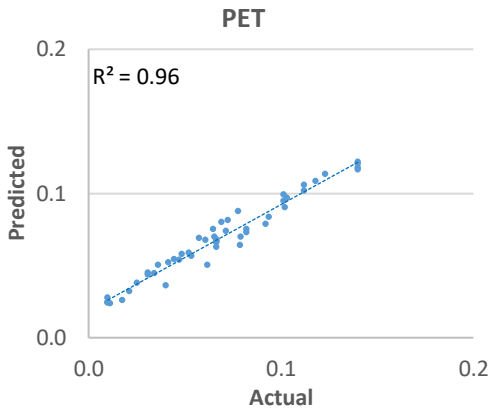

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

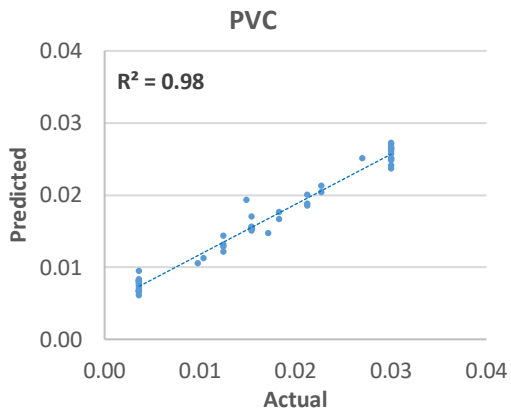

Hemicellulose
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

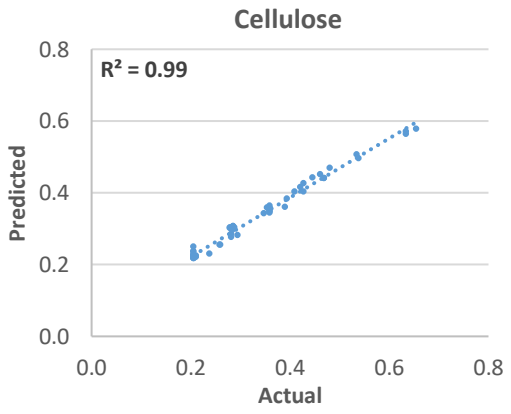

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

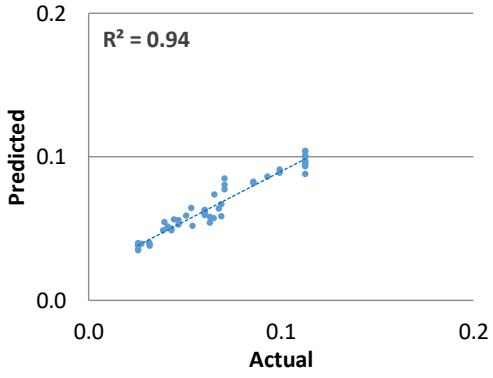

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

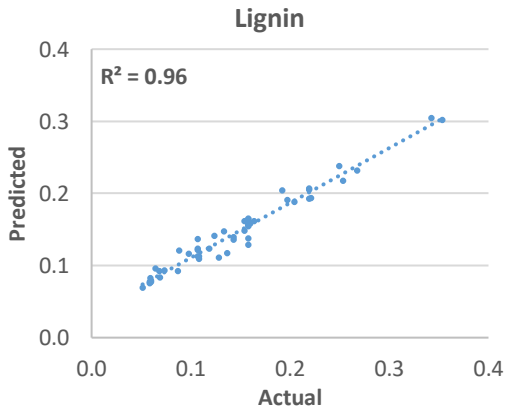

PET
R² = 0.96
Predicted
Actual
0.0
0.1
0.2

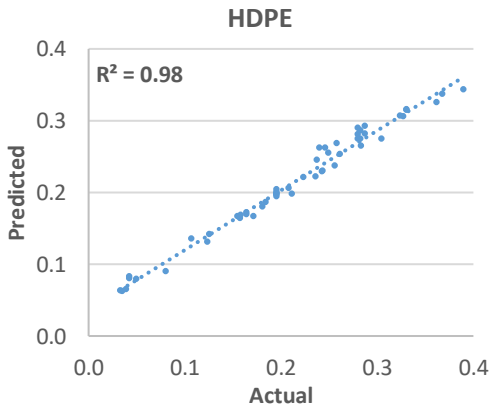

PVC
R² = 0.98
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

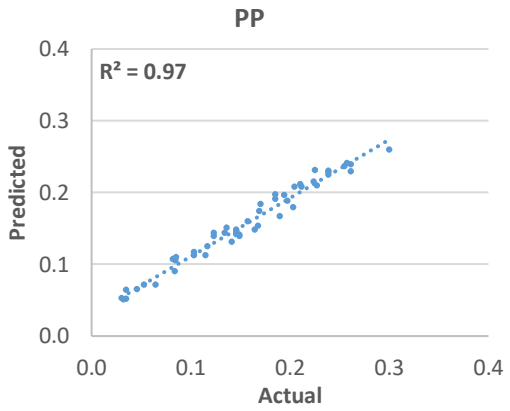
21th:

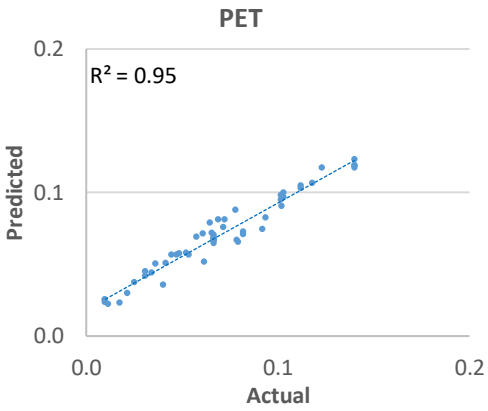

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PET
R² = 0.95
Predicted
Actual
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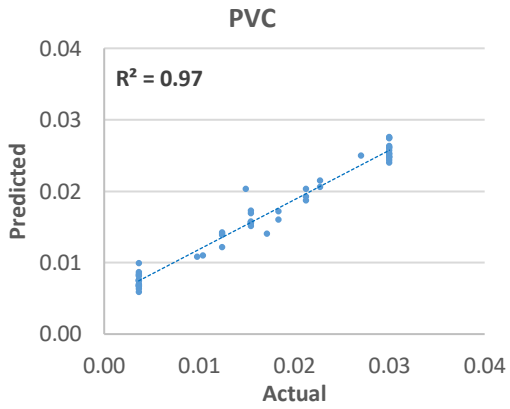
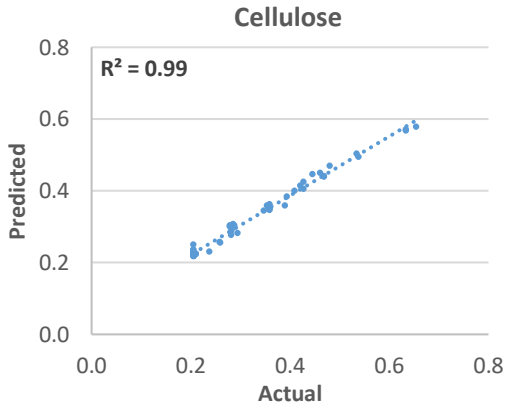
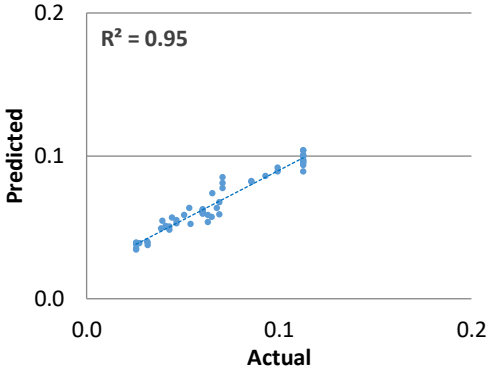
0.1
0.2


PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

22nd:


Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.95
Predicted
Actual
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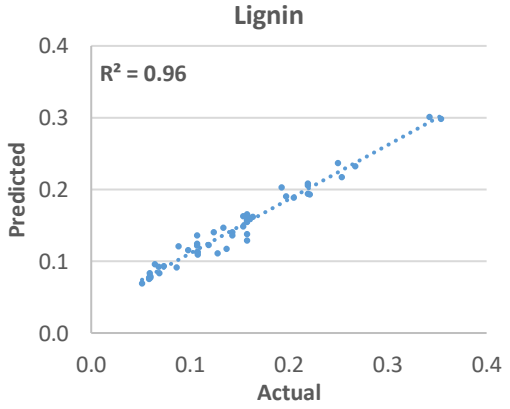
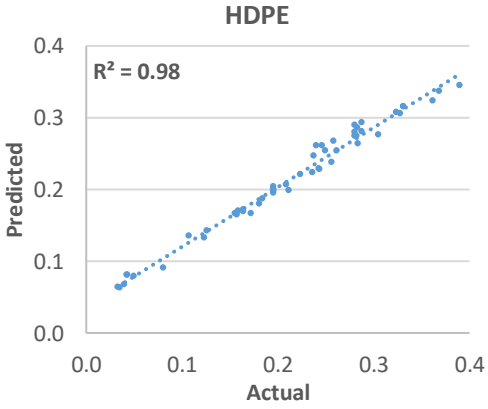
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
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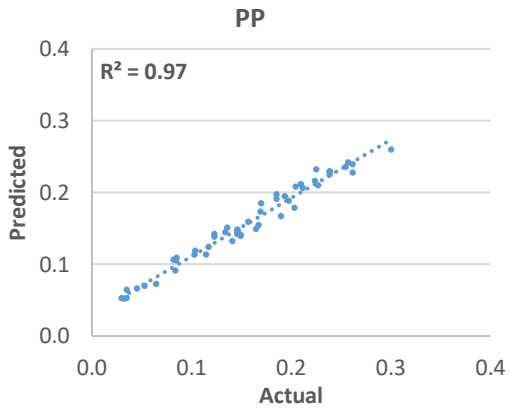
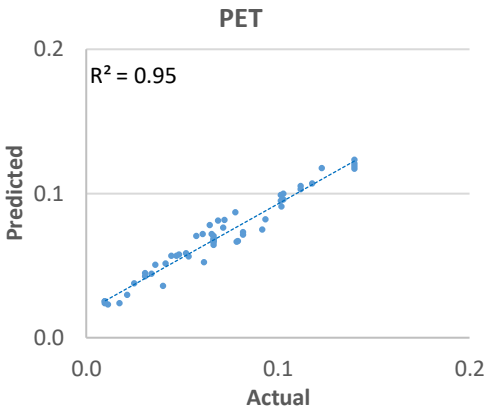
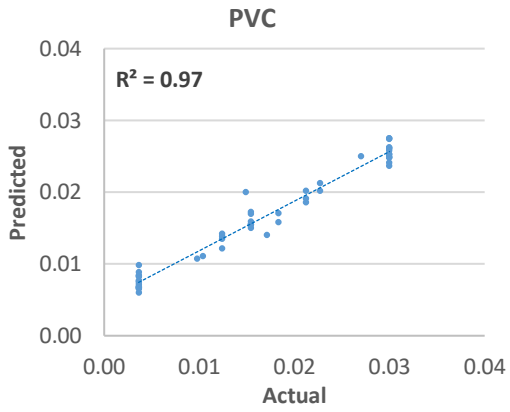
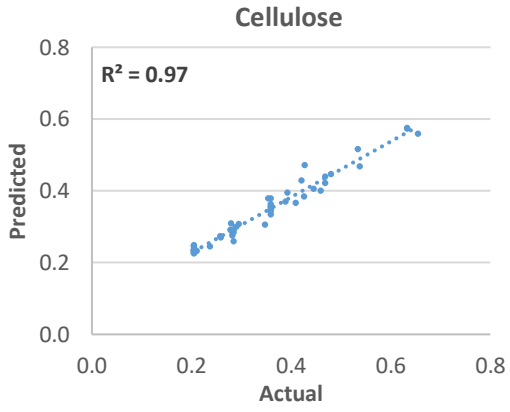
0.3
0.4

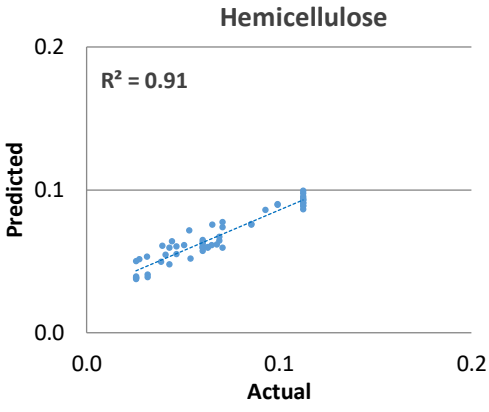

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2


PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

23rd:


Cellulose
R² = 0.97
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.91
Predicted
Actual
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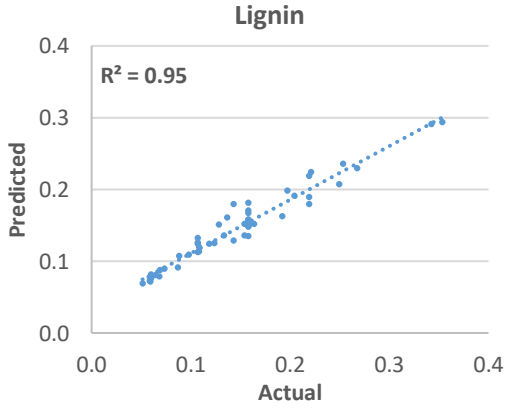
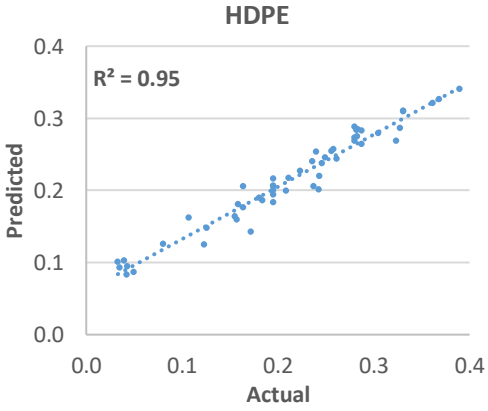
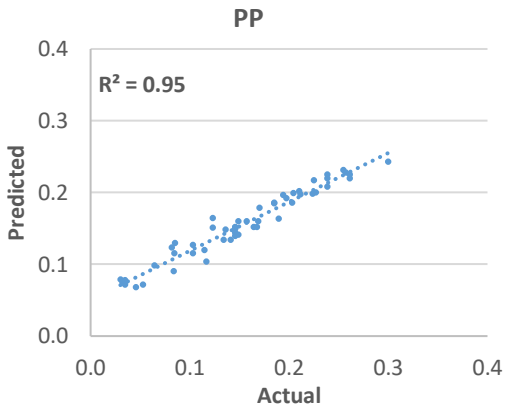
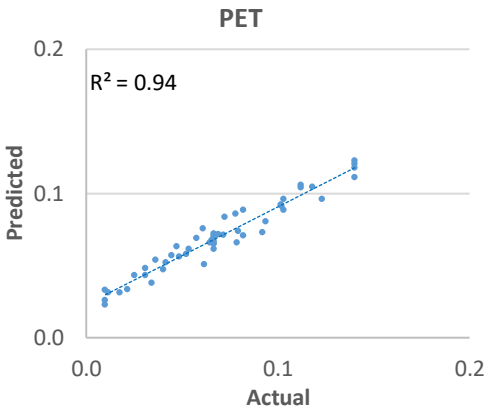
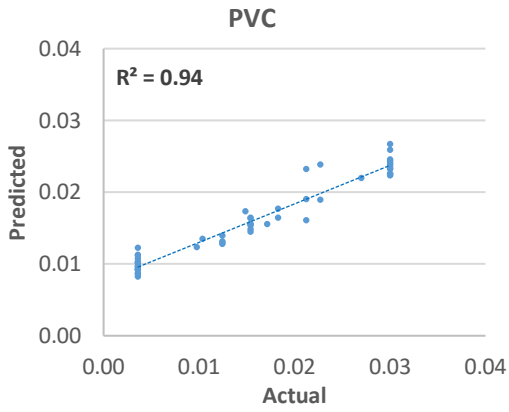
0.1
0.2


Lignin
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

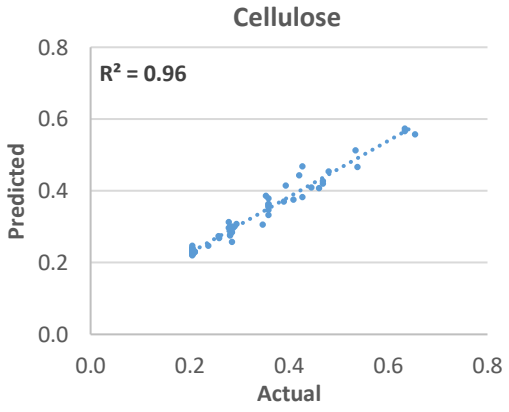

HDPE
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

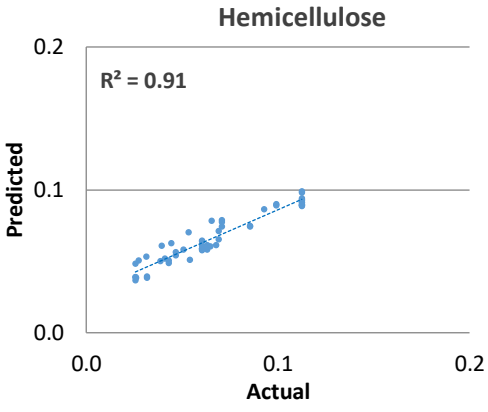

PP
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


PVC
R² = 0.94
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

24th:


Cellulose
R² = 0.96
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.91
Predicted
Actual
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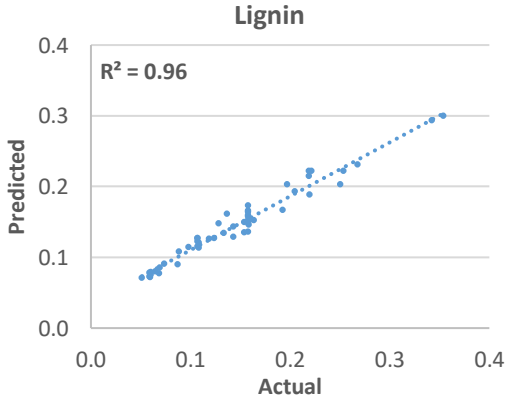
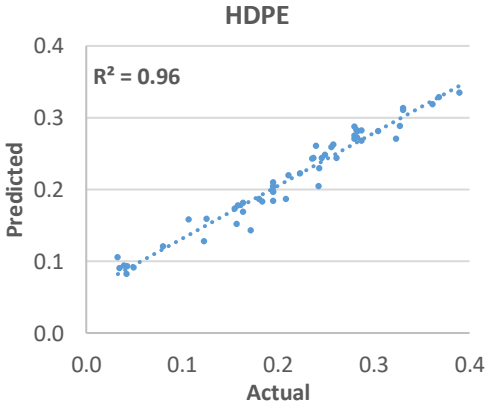
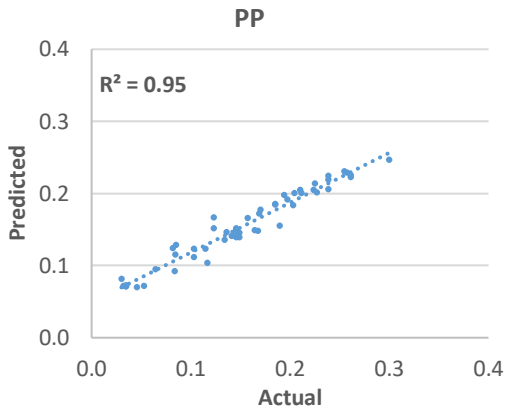
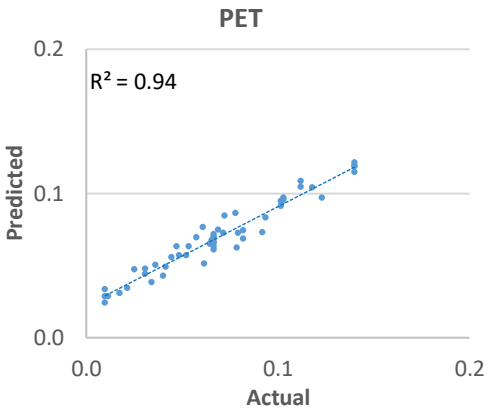
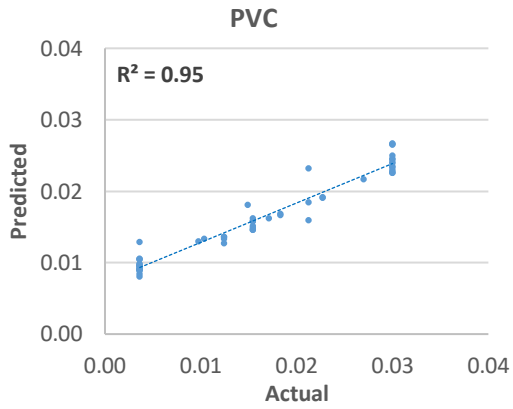
0.1
0.2


Lignin
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

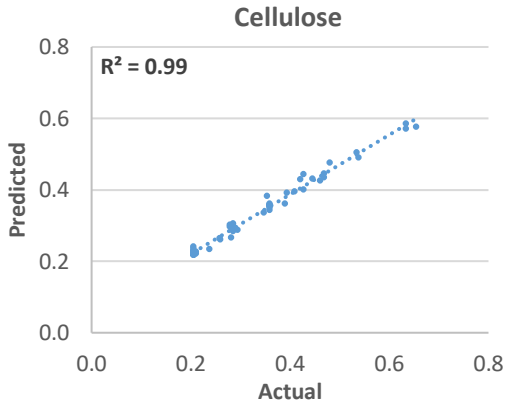

HDPE
R² = 0.96
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

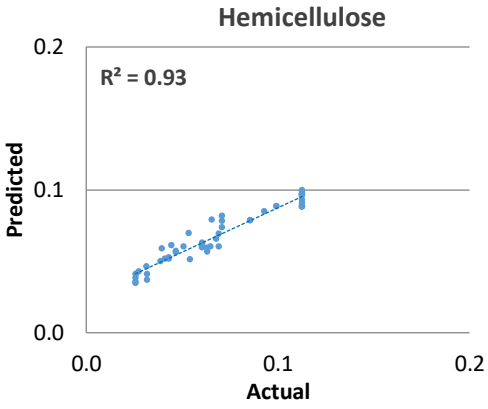

PP
R² = 0.95
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

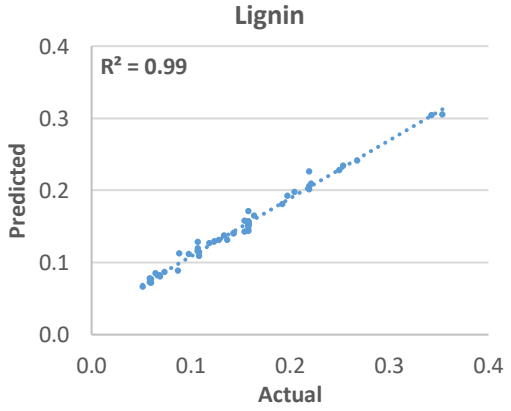

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

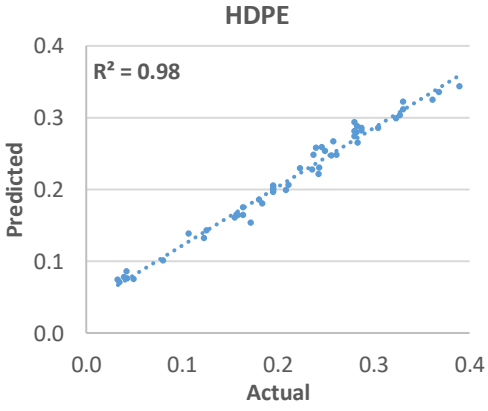

PVC
R² = 0.95
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

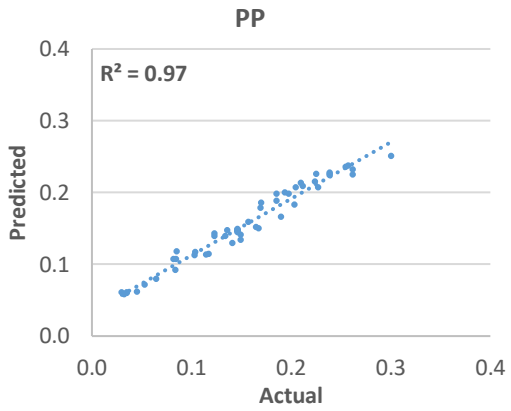
25th:

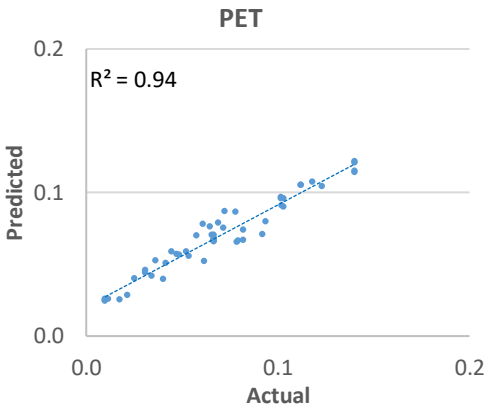

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

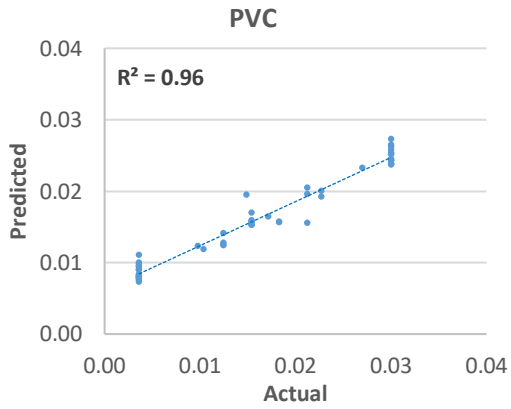

Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

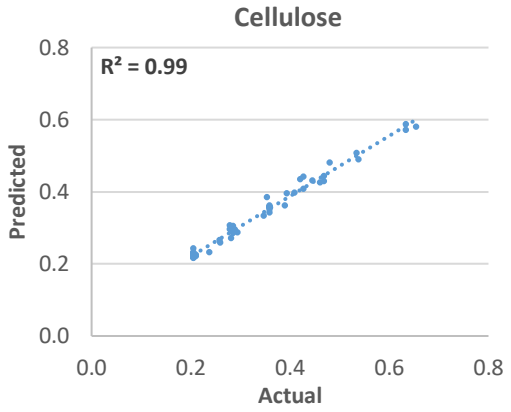

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

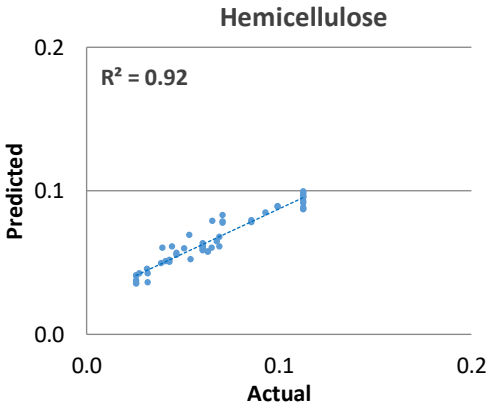

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

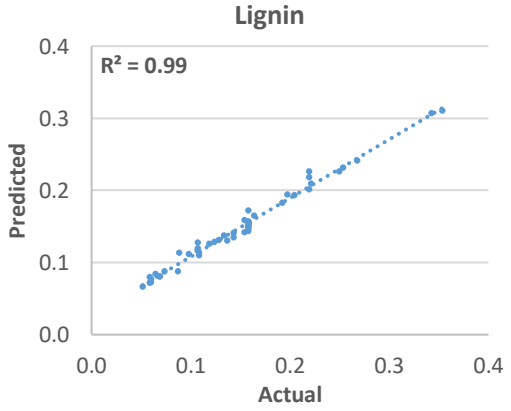

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

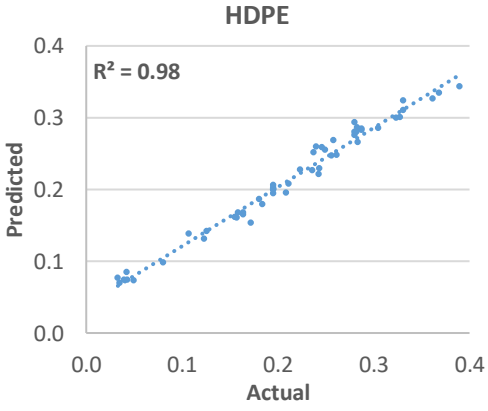

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

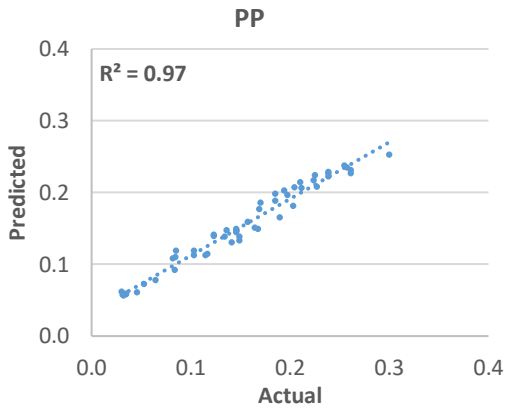
26th:

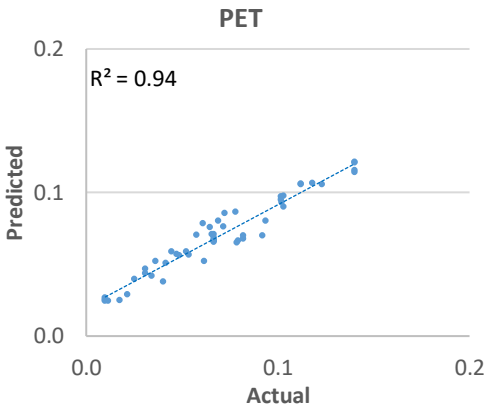

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

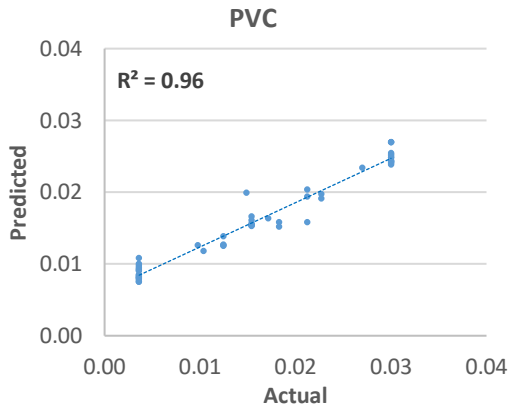

Hemicellulose
R² = 0.92
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

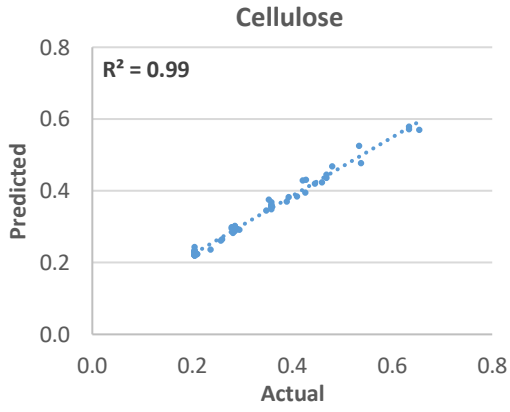

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

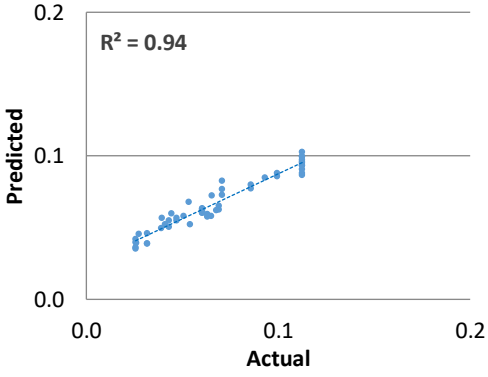

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

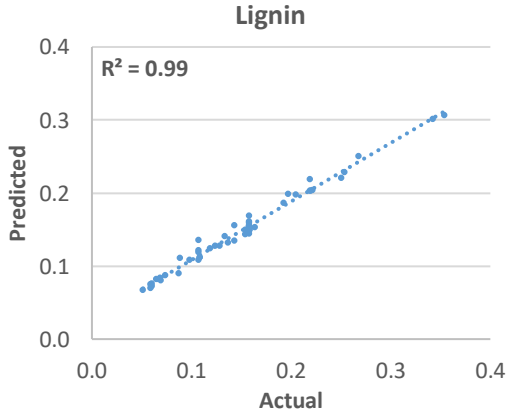

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

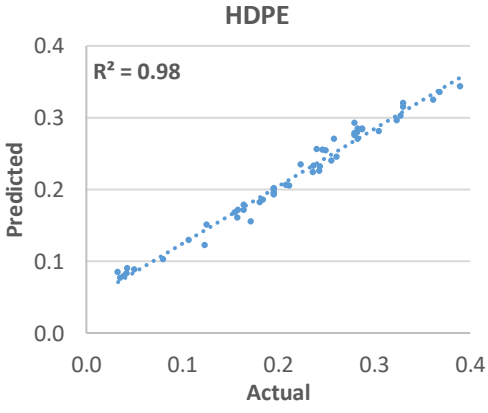

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

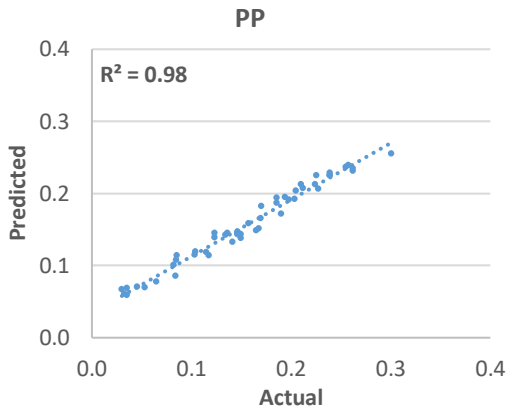
27th:

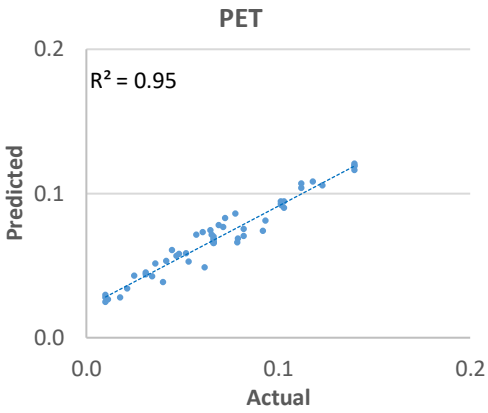

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

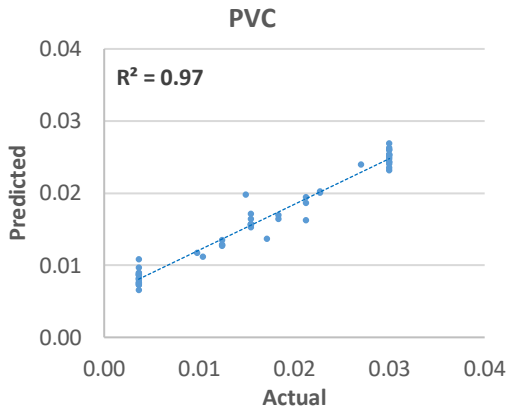

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

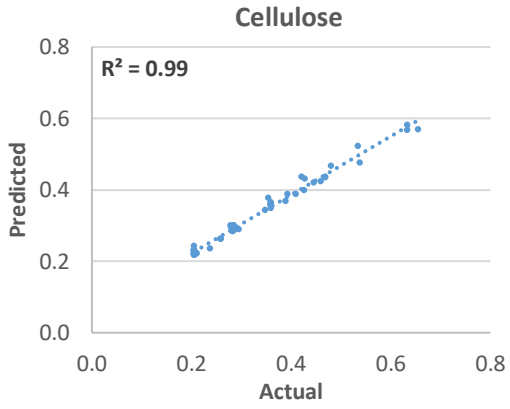

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

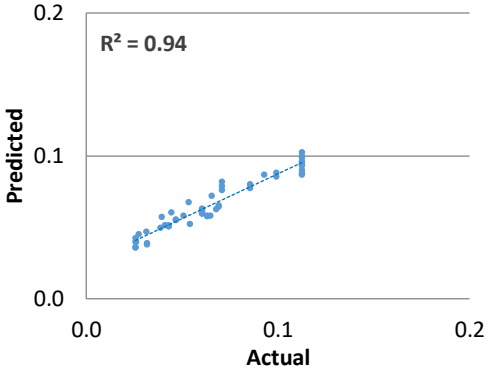

PP
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

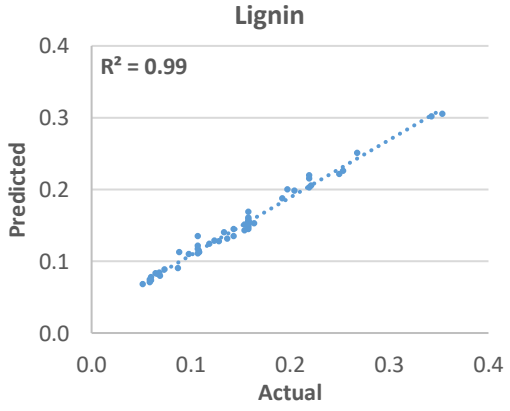

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

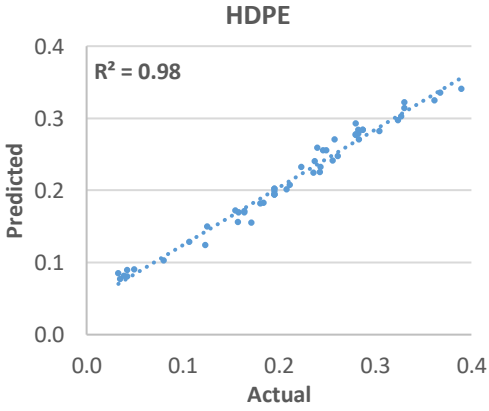

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

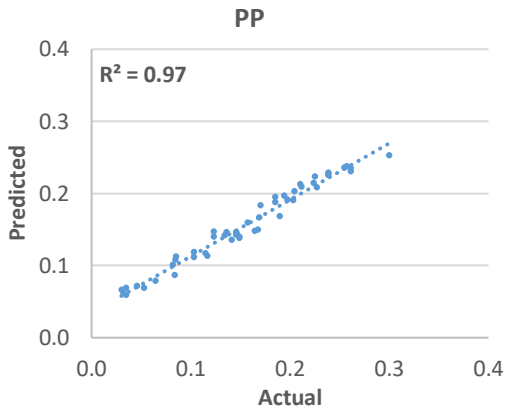
28th:

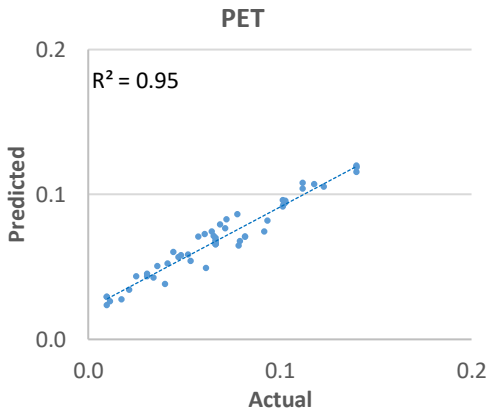

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

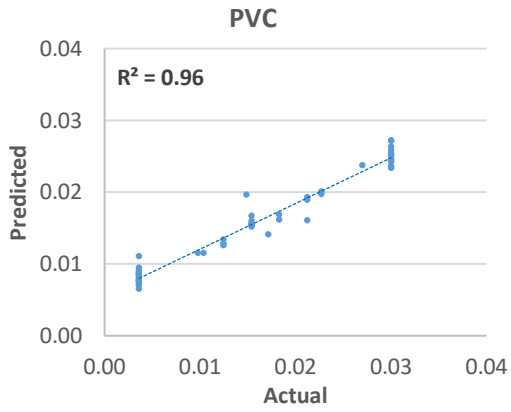

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

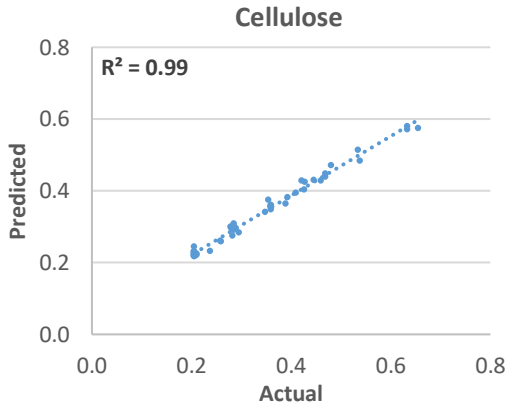

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

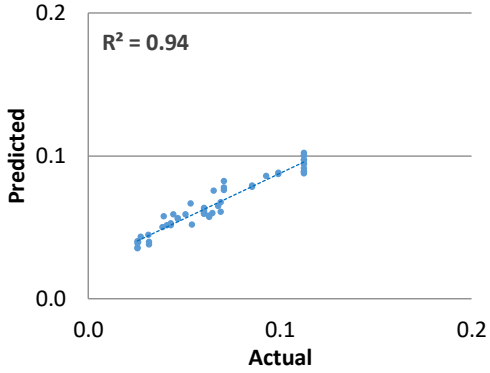

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

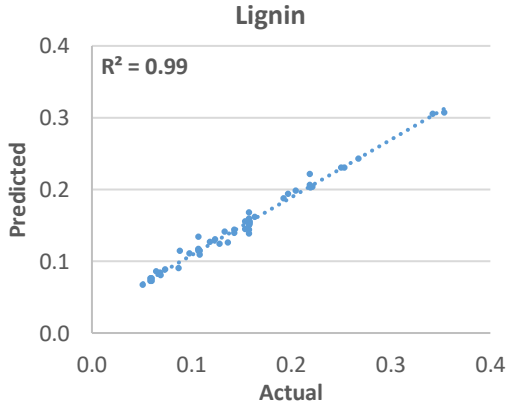

PET
R² = 0.95
Predicted
Actual
0.0
0.1
0.2

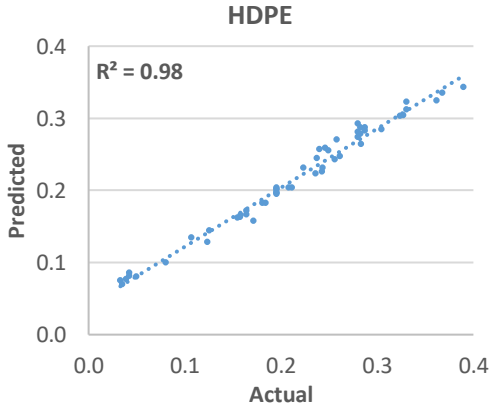

PVC
R² = 0.96
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

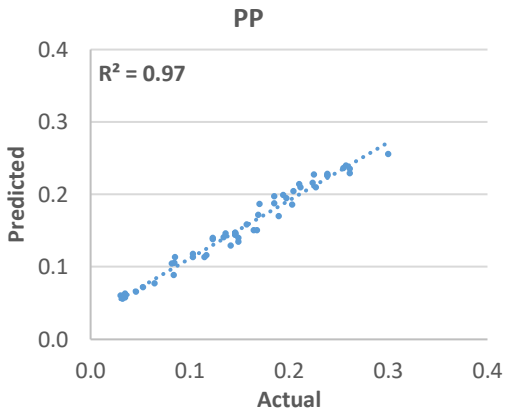
29th:

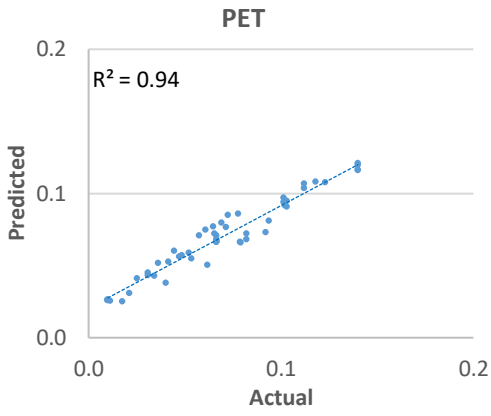

Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8

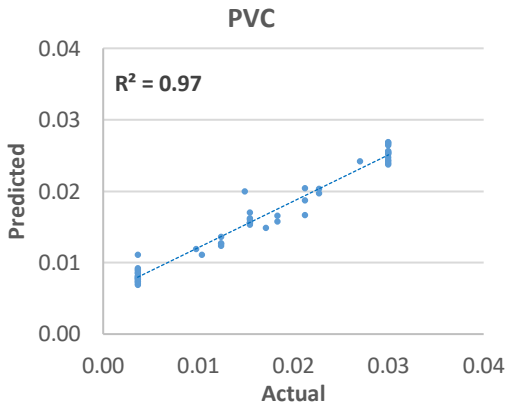

Hemicellulose
R² = 0.94
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

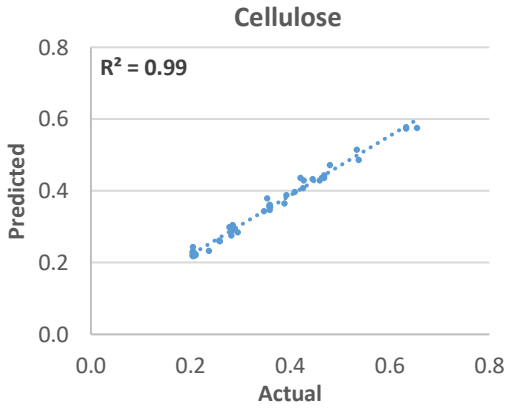

HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

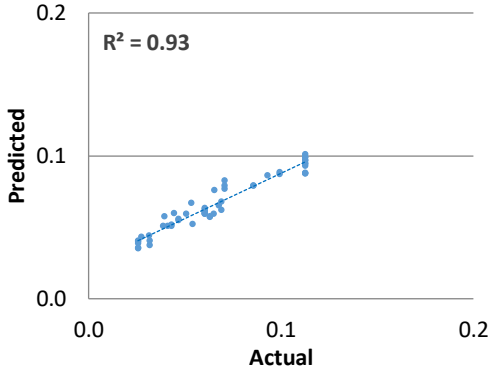

PP
R² = 0.97
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

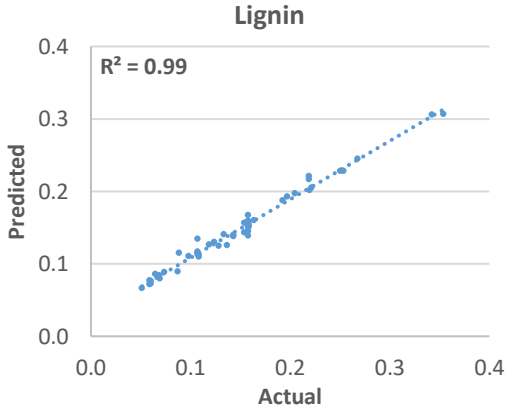

PET
R² = 0.94
Predicted
Actual
0.0
0.1
0.2

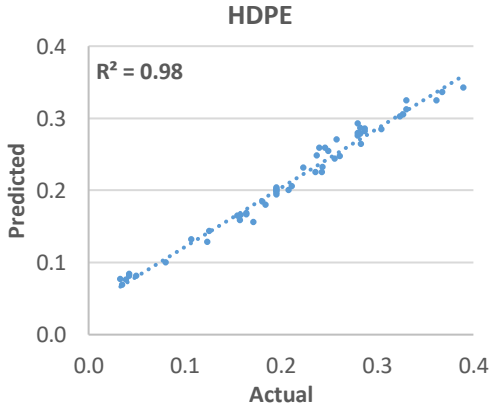

PVC
R² = 0.97
Predicted
Actual
0.00
0.01
0.02
0.03
0.04

30th:


Cellulose
R² = 0.99
Predicted
Actual
0.0
0.2
0.4
0.6
0.8


Hemicellulose
R² = 0.93
Predicted
Actual
0.0
0.1
0.2


Lignin
R² = 0.99
Predicted
Actual
0.0
0.1
0.2
0.3
0.4


HDPE
R² = 0.98
Predicted
Actual
0.0
0.1
0.2
0.3
0.4

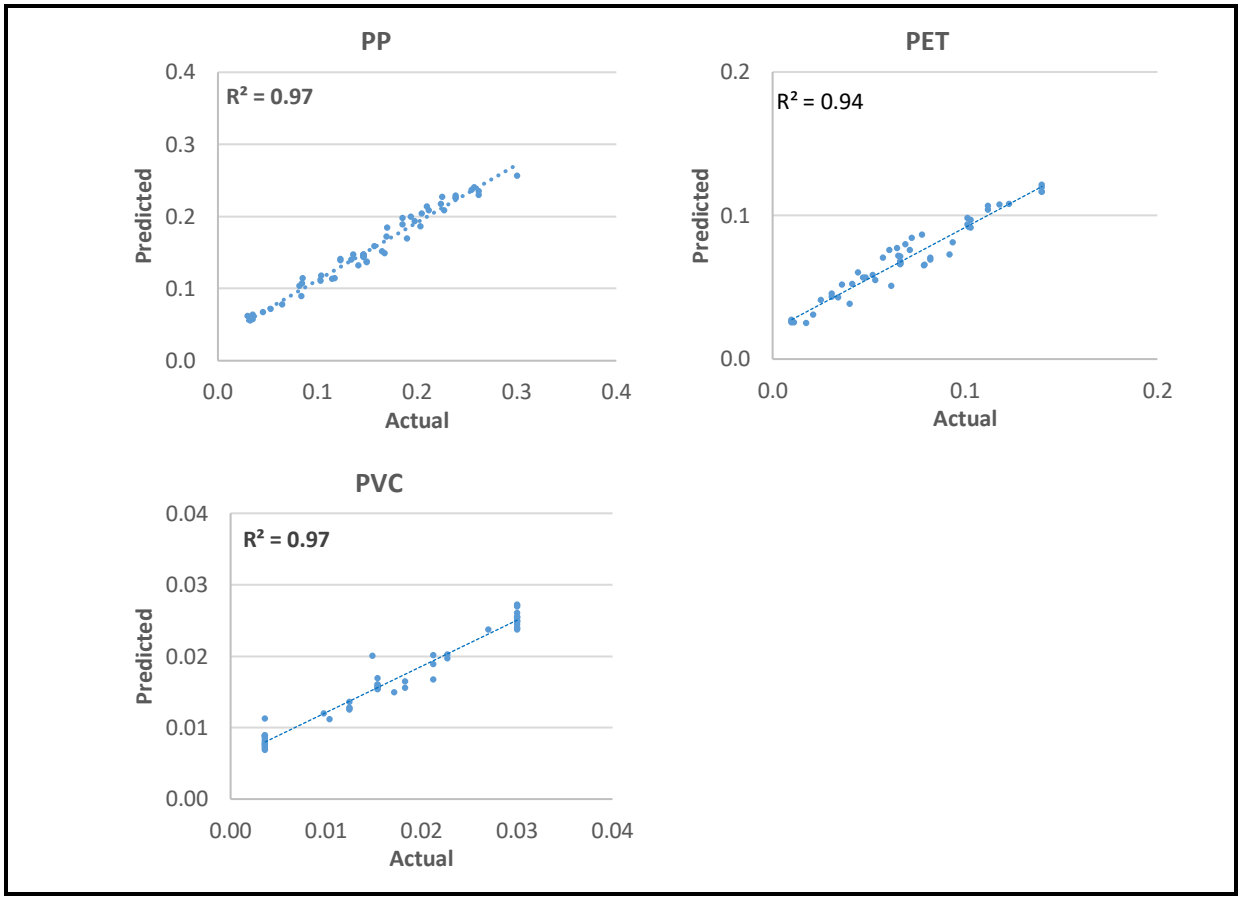


Figure SI.3-3. Observed vs predicted values of prevalent polymers (cellulose, xylan, lignin, HDPE, PP, PET, and PVC) of model training using dataset combinations (n=30) derived from TGA, DTG, and FTIR analytical techniques as input matrix following the second approach of ML model training (under variable *mtry* depending on the number of predictors).

SI.4 Training set of ML model (20th dataset: DTG-FTIR_SG)

An excel file is provided, namely *Training set of ML model*, as it was introduced into the model.