

## Supporting Information: Simultaneous quantification of microplastic particles by NoD $^1\text{H}$ -qNMR comprising samples of different polymer types

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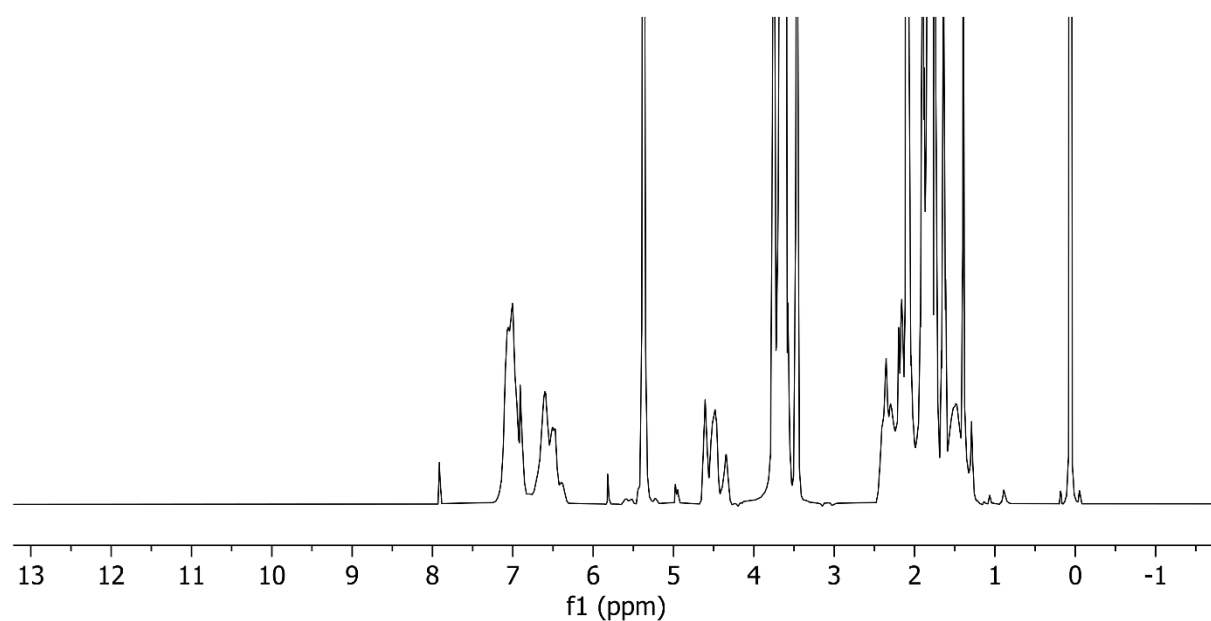


Figure S1:  $^1\text{H}$ -NMR spectra of PS, BR and PVC measured in non-deuterated THF using HMDSO as INST.

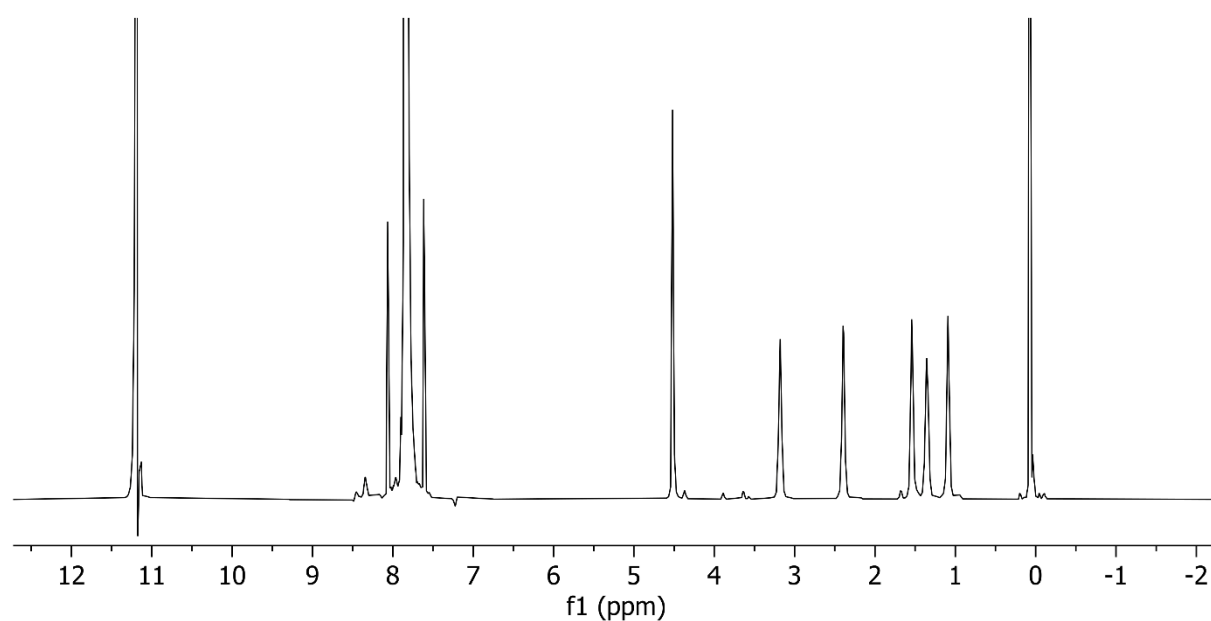


Figure S2:  $^1\text{H}$ -NMR spectra of PET and PA measured in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST.

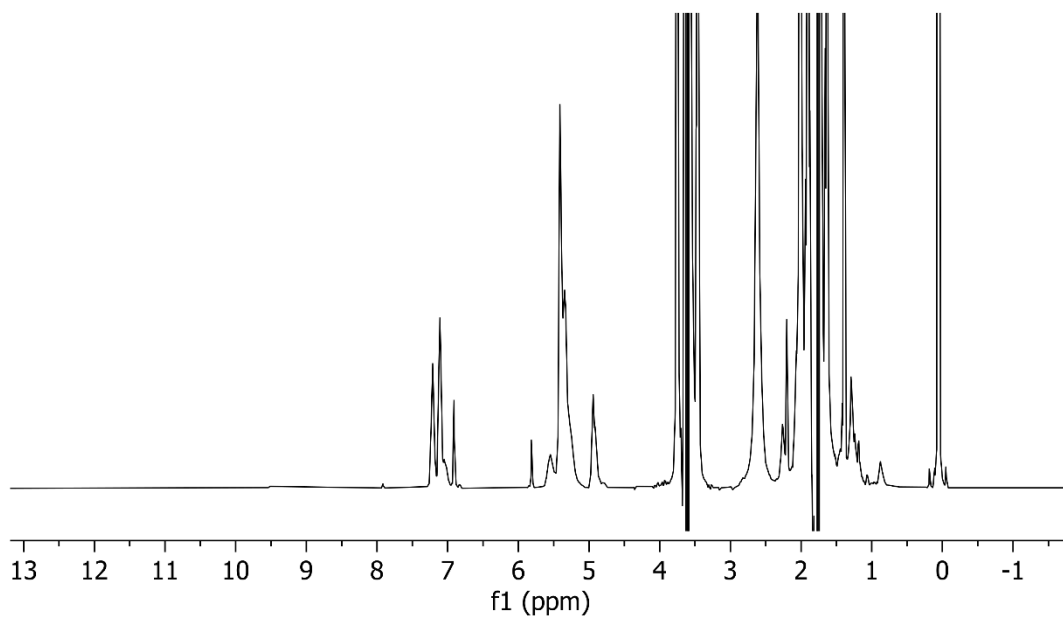


Figure S3: <sup>1</sup>H-NMR spectra of SBR measured in non-deuterated THF using HMDSO as INST.

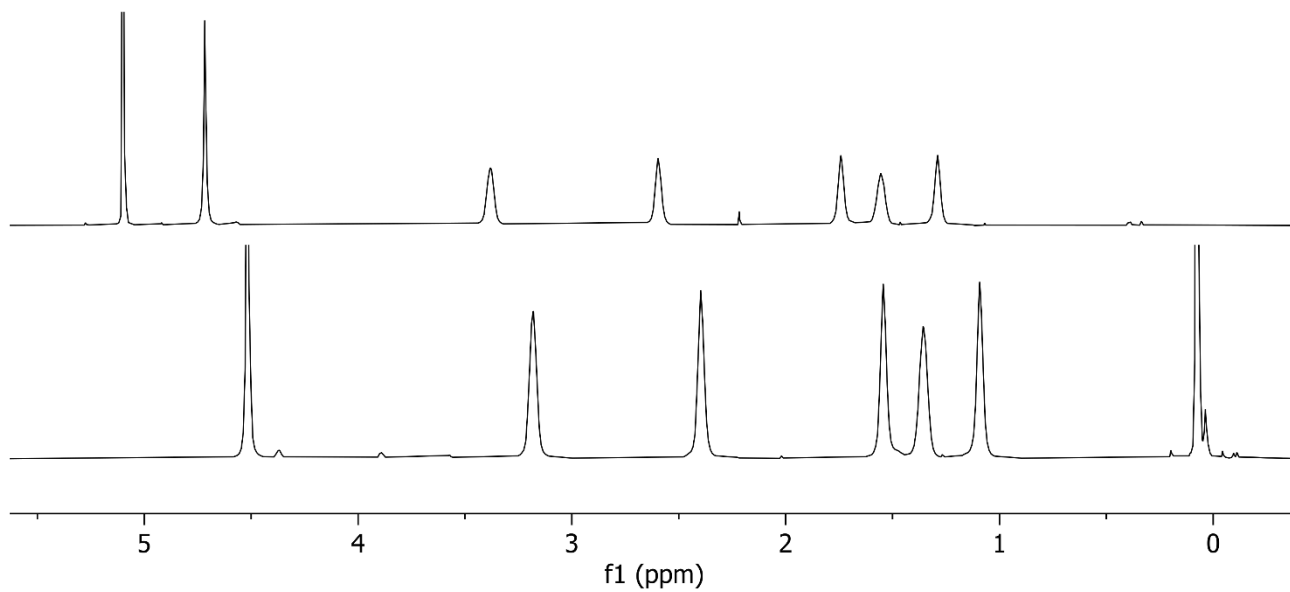


Figure S4: Comparison of PET and PA measured by <sup>1</sup>H-NMR in TFA/FA (85:15 Vol.-%) either using DCM (top) or HMDSO (bottom) as INST.

Table S1: Intensities of PVC, BR and PS calibration samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR simultaneously dissolved in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured three repetitive times within one day.

Sample		Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
K1	1				1.7457	0.8125	1.8558	2.6204			
	2	2.51	2.49	2.51	5.4027	2.4740	5.7077	8.0638	1.37	3.13	4.43
	3				1.7224	0.7996	1.8269	2.5767			
K2	1				5.4720	2.0447	4.6595	6.6445			
	2	2.00	1.99	2.01	5.4606	2.0078	4.6247	6.5628	1.10	2.51	3.57
	3				5.5087	2.0530	4.6697	6.6210			
K3	1				5.4817	1.5422	3.5277	5.0463			
	2	1.50	1.49	1.51	5.5121	1.5580	3.5321	5.0376	0.83	1.90	2.71
	3				5.4968	1.5218	3.5137	5.0155			
K4	1				5.5273	1.0318	2.3836	3.4654			
	2	1.00	1.00	1.00	5.5345	1.0114	2.3724	3.4492	0.54	1.27	1.84
	3				1.7483	0.3140	0.7503	1.0839			
K5	1				5.5284	0.4820	1.1022	1.7069			
	2	0.50	0.50	0.50	5.5236	0.4638	1.0909	1.6869	0.25	0.58	0.91
	3				5.4148	0.4642	1.0623	1.6475			

Table S2: Intensities of PVC, BR and PS calibration samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR simultaneously dissolved in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured three repetitive times within one day.

Sample		Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
K1	1				6.1380	0.4321	1.1042	1.6610			
	2	0.50	0.51	0.49	6.3363	0.4839	1.1455	1.7382	0.47	1.13	1.71
	3				6.3363	0.4828	1.1448	1.7241			
K2	1				6.2789	0.3495	0.8843	1.4024			
	2	0.40	0.40	0.40	6.3066	0.3902	0.9160	1.4245	0.37	0.90	1.41
	3				6.3773	0.3904	0.9228	1.4452			
K3	1				6.2336	0.2580	0.6837	1.0883			
	2	0.30	0.30	0.30	6.2462	0.2925	0.6785	1.0928	0.28	0.69	1.09
	3				6.3244	0.3023	0.6957	1.0825			
K4	1				6.4252	0.1606	0.4666	0.8219			
	2	0.20	0.20	0.20	6.3395	0.2089	0.4664	0.8267	0.18	0.46	0.81
	3				6.4322	0.1942	0.4804	0.8376			
K5	1				6.4583	0.1036	0.2368	0.5216			
	2	0.10	0.10	0.10	6.4775	0.1093	0.2528	0.5281	0.10	0.24	0.51
	3				6.4788	0.1029	0.2435	0.5186			

Table S3: Intensities of PA and PET calibration samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR simultaneously dissolved in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured three repetitive times within one day.

Sample	Concentration [mg/mL]			Absolute Intensity				Normalised Intensity				
	PA	PET	INST	PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET	PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET	
K1	1			1.8569	2.7662	0.9128	0.9025	1.1196				
	2	2.50	2.50	1.8622	2.7686	0.9166	0.9034	1.1111	2.77	0.92	0.90	1.12
	3			1.8603	2.7690	0.9165	0.8997	1.1166				
K2	1			1.8421	2.2088	0.7314	0.7200	0.8930				
	2	2.00	2.00	1.8467	2.2094	0.7300	0.7206	0.8929	2.23	0.74	0.73	0.90
	3			1.8380	2.2012	0.7319	0.7155	0.8854				
K3	1			1.8522	1.6775	0.5495	0.5475	0.6690				
	2	1.50	1.50	1.8425	1.6699	0.5441	0.5406	0.6683	1.68	0.55	0.55	0.67
	3			1.8465	1.6710	0.5508	0.5436	0.6714				
K4	1			1.8953	1.1685	0.3864	0.3787	0.4680				
	2	1.00	1.00	1.8977	1.1633	0.3842	0.3784	0.4684	1.14	0.38	0.37	0.46
	3			1.9001	1.1696	0.3807	0.3785	0.4614				
K5	1			1.8667	0.5839	0.1898	0.1911	0.2327				
	2	0.50	0.50	1.8560	0.5907	0.1936	0.1939	0.2302	0.59	0.19	0.19	0.23
	3			1.8647	0.5837	0.1875	0.1900	0.2236				

Table S4: Intensities of PA and PET calibration samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR simultaneously dissolved in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured three repetitive times within one day.

Sample	Concentration [mg/mL]			Absolute Intensity				Normalised Intensity				
	PA	PET	INST	PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET	PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET	
K1	1			1.8646	0.5525	0.1898	0.1838	0.2293				
	2	0.50	0.50	1.8843	0.5666	0.1824	0.1854	0.2268	0.56	0.19	0.18	0.23
	3			1.8748	0.5502	0.1839	0.1833	0.2235				
K2	1			1.8296	0.4454	0.1467	0.1418	0.1780				
	2	0.40	0.40	1.8517	0.4510	0.1461	0.1483	0.1824	0.46	0.15	0.15	0.18
	3			1.8233	0.4444	0.1462	0.1437	0.1759				
K3	1			1.8188	0.3376	0.1100	0.1090	0.1346				
	2	0.30	0.30	1.8476	0.3360	0.1105	0.1177	0.1516	0.35	0.11	0.12	0.15
	3			1.8334	0.3408	0.1115	0.1113	0.1395				
K4	1			1.8752	0.2343	0.0696	0.0782	0.0957				
	2	0.20	0.20	1.8768	0.2499	0.0850	0.0774	0.0957	0.24	0.08	0.08	0.09
	3			1.8643	0.2335	0.0785	0.0770	0.0850				
K5	1			1.8966	0.1260	0.0425	0.0391	0.0536				
	2	0.10	0.10	1.8917	0.1246	0.0310	0.0378	0.0485	0.12	0.04	0.04	0.05
	3			1.8842	0.1273	0.0411	0.0419	0.0481				

Table S5: Intensities of PVC, BR and PS model samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured five times distributed over five hours.

Sample	t [h]	Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
M1	0				1.9420	0.5172	1.8242	0.8938	0.79	2.78	1.36
	1				6.0715	1.5842	5.7108	2.7963	0.77	2.78	1.36
	2	1.38	2.17	0.75	5.9471	1.5627	5.5810	2.7407	0.78	2.77	1.36
	3				6.0940	1.5996	5.6973	2.7990	0.78	2.76	1.36
	4				6.0652	1.6115	5.6969	2.7801	0.79	2.78	1.36
M2	0				5.4153	0.5355	3.1433	7.3554	0.29	1.72	4.02
	1				5.3968	0.5348	3.1253	7.3253	0.29	1.71	4.01
	2	0.65	1.34	2.20	5.3733	0.5366	3.1202	7.2809	0.30	1.72	4.01
	3				5.3978	0.5347	3.1348	7.3150	0.29	1.72	4.01
	4				5.4076	0.5447	3.1342	7.3058	0.30	1.71	3.99
M3	0				5.3889	2.3490	1.7330	5.5672	1.29	0.95	3.05
	1				5.3526	2.3284	1.7255	5.5001	1.29	0.95	3.04
	2	2.37	0.76	1.73	5.3218	2.3138	1.7122	5.4585	1.29	0.95	3.03
	3				5.3191	2.3443	1.7091	5.4561	1.30	0.95	3.03
	4				5.3715	2.3303	1.7313	5.5172	1.28	0.95	3.04

Table S6: Intensities of PVC, BR and PS model samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured five times distributed over one week.

Sample	t [d]	Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
M1	0				6.1132	1.5786	5.7489	2.8137	0.76	2.78	1.36
	1				6.1255	1.5704	5.7330	2.8086	0.76	2.77	1.36
	2	1.38	2.17	0.75	1.9441	0.5128	1.8225	0.8929	0.78	2.77	1.36
	3				6.0919	1.5358	5.7004	2.7939	0.75	2.77	1.36
	4				1.9388	0.4922	1.8223	0.8890	0.75	2.78	1.36
M2	0				5.3885	0.5521	3.1463	7.3826	0.30	1.73	4.05
	1				1.7227	0.1659	1.0006	2.3401	0.28	1.72	4.02
	2	0.65	1.34	2.20	5.4258	0.5410	3.1372	7.3616	0.29	1.71	4.01
	3				5.4653	0.5831	3.1774	7.3838	0.32	1.72	3.99
	4				1.7253	0.1847	0.9964	2.3115	0.32	1.71	3.96
M3	0				5.3218	2.3625	1.7254	5.5141	1.31	0.96	3.06
	1				1.7057	0.7357	0.5508	1.7625	1.28	0.95	3.06
	2	2.37	0.76	1.73	5.3921	2.3509	1.7282	5.5929	1.29	0.95	3.07
	3				5.4003	2.2871	1.7535	5.5287	1.25	0.96	3.03
	4				5.3630	2.3040	1.7225	5.5246	1.27	0.95	3.05

Table S7: Intensities of PVC, BR and PS model samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured five times distributed over five hours.

Sample	t [h]	Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
M1	0				6.4495	0.1701	0.9927	1.0101	0.17	0.97	0.98
	1				6.3522	0.1357	0.9747	0.9929	0.13	0.96	0.98
	2	0.17	0.43	0.27	6.3797	0.1735	1.0004	1.0173	0.17	0.98	1.00
	3				6.3600	0.1376	0.9811	0.9824	0.14	0.97	0.97
	4				6.4062	0.1534	0.9940	1.0218	0.15	0.97	1.00
M2	0				6.2975	0.2737	0.5374	1.7692	0.27	0.54	1.76
	1				6.2351	0.2540	0.5436	1.7598	0.26	0.55	1.77
	2	0.26	0.24	0.49	6.3078	0.2483	0.5486	1.7719	0.25	0.55	1.76
	3				6.3024	0.2620	0.5475	1.7574	0.26	0.54	1.75
	4				6.2435	0.2421	0.5472	1.7652	0.24	0.55	1.77
M3	0				6.1761	0.4066	0.3224	1.3146	0.41	0.33	1.33
	1				6.1360	0.4159	0.3311	1.3061	0.42	0.34	1.33
	2	0.43	0.17	0.36	6.1673	0.4069	0.3346	1.2942	0.41	0.34	1.32
	3				1.9334	0.1203	0.1017	0.4108	0.39	0.33	1.33
	4				6.0950	0.4054	0.3166	1.3048	0.42	0.33	1.34

Table S8: Intensities of PVC, BR and PS model samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured five times distributed over one week.

Sample	t [d]	Concentration [mg/mL]			INST	Absolute Intensity			Normalised Intensity		
		PVC	BR	PS		PVC	BR	PS	PVC	BR	PS
M1	0				6.2759	0.1560	0.9619	1.0051	0.16	0.96	1.00
	1				6.3663	0.1471	0.9719	1.0035	0.14	0.96	0.99
	2	0.17	0.43	0.27	6.4439	0.1521	0.9921	1.0161	0.15	0.97	0.99
	3				6.4630	0.1441	0.9950	1.0197	0.14	0.97	0.99
	4				2.0543	0.0496	0.3192	0.3231	0.15	0.97	0.99
M2	0				6.2413	0.2510	0.5374	1.7634	0.25	0.54	1.77
	1				6.2975	0.2629	0.5417	1.7713	0.26	0.54	1.76
	2	0.26	0.24	0.49	6.3063	0.2716	0.5243	1.7585	0.27	0.52	1.75
	3				2.0045	0.0885	0.1778	0.5564	0.28	0.56	1.74
	4				2.0028	0.0725	0.1730	0.5635	0.23	0.54	1.76
M3	0				6.1892	0.4104	0.3216	1.3019	0.42	0.33	1.32
	1				6.1816	0.3979	0.3144	1.3143	0.40	0.32	1.33
	2	0.43	0.17	0.36	6.1785	0.4063	0.3223	1.3163	0.41	0.33	1.34
	3				6.2086	0.4180	0.3261	1.3324	0.42	0.33	1.35
	4				6.1552	0.4184	0.3346	1.3072	0.43	0.34	1.33

Table S9: Intensities of PA and PET model samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured five times distributed over five hours.

Sample	t [h]	Concentration [mg/mL]		INST	Absolute Intensity			PET	Normalised Intensity			
		PA	PET		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET
M1	0			1.9080	0.7610	0.2465	0.2437	1.0470	0.74	0.24	0.24	1.02
	1			1.9015	0.7616	0.2478	0.2443	1.0555	0.74	0.24	0.24	1.03
	2	0.65	2.30	1.9001	0.7604	0.2483	0.2422	1.0428	0.74	0.24	0.24	1.02
	3			1.9002	0.7543	0.2485	0.2412	1.0488	0.74	0.24	0.24	1.03
	4			1.8904	0.7558	0.2468	0.2443	1.0383	0.74	0.24	0.24	1.02
M2	0			1.8069	2.4578	0.8210	0.8029	0.6599	2.53	0.85	0.83	0.68
	1			1.7992	2.4467	0.8112	0.8020	0.6520	2.53	0.84	0.83	0.67
	2	2.27	1.50	1.8003	2.4587	0.8205	0.8062	0.6597	2.54	0.85	0.83	0.68
	3			1.8123	2.4703	0.8206	0.8082	0.6614	2.54	0.84	0.83	0.68
	4			1.7963	2.4399	0.8085	0.7979	0.6558	2.53	0.84	0.83	0.68
M3	0			1.8528	1.6435	0.5443	0.5343	0.3321	1.65	0.55	0.54	0.33
	1			1.8388	1.6269	0.5396	0.5318	0.3256	1.65	0.55	0.54	0.33
	2	1.47	0.69	1.8593	1.6456	0.5443	0.5356	0.3362	1.65	0.54	0.54	0.34
	3			1.8459	1.6343	0.5438	0.5318	0.3241	1.65	0.55	0.54	0.33
	4			1.8350	1.6202	0.5409	0.5284	0.3254	1.64	0.55	0.54	0.33

Table S10: Intensities of PA and PET model samples within the range of 2.5-0.5 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured five times distributed over one week.

Sample	t [d]	Concentration [mg/mL]		INST	Absolute Intensity			PET	Normalised Intensity			
		PA	PET		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET
M1	0			1.9028	0.7597	0.2477	0.2425	1.0479	0.74	0.24	0.24	1.02
	1			1.9147	0.7656	0.2440	0.2464	1.0547	0.74	0.24	0.24	1.02
	2	0.65	2.30	1.9041	0.7606	0.2473	0.2438	1.0483	0.74	0.24	0.24	1.02
	3			1.9270	0.7701	0.2482	0.2481	1.0591	0.74	0.24	0.24	1.02
	4			1.8992	0.7629	0.2478	0.2447	1.0503	0.75	0.24	0.24	1.03
M2	0			1.8036	2.4541	0.8147	0.8029	0.6622	2.53	0.84	0.83	0.68
	1			1.8092	2.4673	0.8262	0.8052	0.6631	2.54	0.85	0.83	0.68
	2	2.27	1.50	1.8097	2.4570	0.8199	0.8028	0.6512	2.53	0.84	0.83	0.67
	3			1.8239	2.4790	0.8228	0.8081	0.6643	2.53	0.84	0.82	0.68
	4			1.7972	2.4349	0.8110	0.7984	0.6583	2.52	0.84	0.83	0.68
M3	0			1.8529	1.6381	0.5436	0.5326	0.3344	1.64	0.55	0.53	0.34
	1			1.8526	1.6383	0.5497	0.5358	0.3374	1.64	0.55	0.54	0.34
	2	1.47	0.69	1.8591	1.6366	0.5399	0.5329	0.3405	1.64	0.54	0.53	0.34
	3			1.8655	1.6530	0.5482	0.5414	0.3359	1.65	0.55	0.54	0.33
	4			1.8440	1.6269	0.5342	0.5328	0.3285	1.64	0.54	0.54	0.33

Table S11: Intensities of PA and PET model samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured five times distributed over five hours.

Sample	t [h]	Concentration [mg/mL]		INST	Absolute Intensity			PET	Normalised Intensity			
		PA	PET		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET
M1	0			1.8468	0.3828	0.1242	0.1219	0.1845	0.39	0.13	0.12	0.19
	1			1.8483	0.3872	0.1235	0.1231	0.1907	0.39	0.13	0.12	0.19
	2	0.34	0.43	1.8745	0.3929	0.1261	0.1228	0.2024	0.39	0.13	0.12	0.20
	3			1.8573	0.3872	0.1253	0.1251	0.1971	0.39	0.13	0.13	0.20
	4			1.8517	0.3827	0.1248	0.1244	0.1921	0.39	0.13	0.13	0.19
M2	0			1.8502	0.4660	0.1538	0.1530	0.1389	0.47	0.16	0.16	0.14
	1			1.8405	0.4669	0.1461	0.1521	0.1452	0.48	0.15	0.15	0.15
	2	0.43	0.32	1.8444	0.4595	0.1525	0.1497	0.1337	0.47	0.15	0.15	0.14
	3			1.8563	0.4651	0.1538	0.1488	0.1500	0.47	0.16	0.15	0.15
	4			1.8419	0.4626	0.1481	0.1501	0.1487	0.47	0.15	0.15	0.15
M3	0			1.8744	0.2178	0.0705	0.0714	0.0864	0.22	0.07	0.07	0.09
	1			1.8738	0.2206	0.0700	0.0712	0.0891	0.22	0.07	0.07	0.09
	2	0.20	0.19	1.8762	0.2148	0.0728	0.0748	0.0811	0.21	0.07	0.07	0.08
	3			1.8722	0.2184	0.0728	0.0699	0.0801	0.22	0.07	0.07	0.08
	4			1.8684	0.2167	0.0725	0.0739	0.0901	0.22	0.07	0.07	0.09

Table S12: Intensities of PA and PET model samples within the range of 0.5-0.1 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated TFA/FA (85:15 Vol.-%) using HMDSO as INST (0.1%). Each sample is measured five times distributed over one week.

Sample	t [d]	Concentration [mg/mL]		INST	Absolute Intensity			PET	Normalised Intensity			
		PA	PET		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>		PA <sub>1</sub>	PA <sub>2</sub>	PA <sub>3</sub>	PET
M1	0			1.8767	0.3905	0.1236	0.1269	0.1963	0.39	0.12	0.13	0.20
	1			1.8660	0.3899	0.1301	0.1282	0.1934	0.39	0.13	0.13	0.19
	2	0.34	0.43	1.8522	0.3857	0.1249	0.1216	0.1906	0.39	0.13	0.12	0.19
	3			1.8652	0.3866	0.1254	0.1250	0.1910	0.39	0.13	0.13	0.19
	4			1.8698	0.3888	0.1298	0.1272	0.1997	0.39	0.13	0.13	0.20
M2	0			1.8568	0.4663	0.1590	0.1546	0.1464	0.47	0.16	0.16	0.15
	1			1.8398	0.4608	0.1499	0.1502	0.1453	0.47	0.15	0.15	0.15
	2	0.43	0.32	1.8492	0.4652	0.1479	0.1503	0.1509	0.47	0.15	0.15	0.15
	3			1.8643	0.4675	0.1520	0.1505	0.1397	0.47	0.15	0.15	0.14
	4			1.8444	0.4647	0.1487	0.1503	0.1462	0.47	0.15	0.15	0.15
M3	0			1.8742	0.2176	0.0742	0.0722	0.0899	0.22	0.07	0.07	0.09
	1			1.8689	0.2214	0.0755	0.0750	0.0912	0.22	0.08	0.08	0.09
	2	0.20	0.19	1.8778	0.2229	0.0716	0.0742	0.0850	0.22	0.07	0.07	0.08
	3			1.8783	0.2230	0.0705	0.0710	0.0856	0.22	0.07	0.07	0.09
	4			1.8595	0.2213	0.0712	0.0698	0.0910	0.22	0.07	0.07	0.09



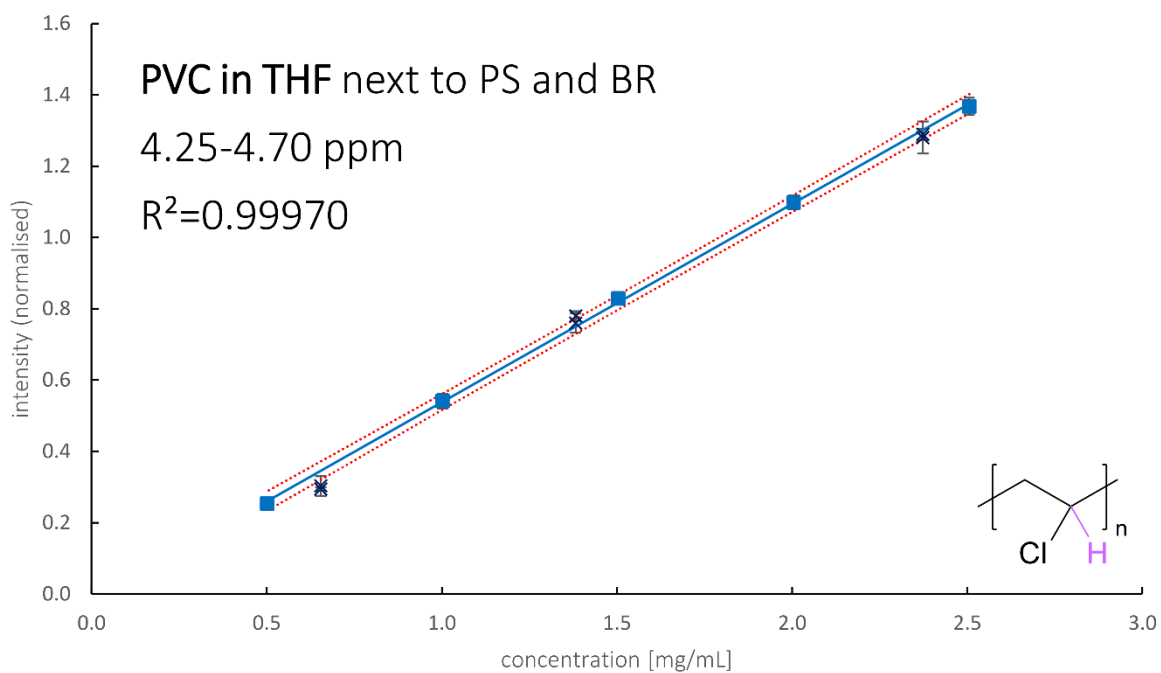


Figure S5: Calibration graph (—) of PVC in THF at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

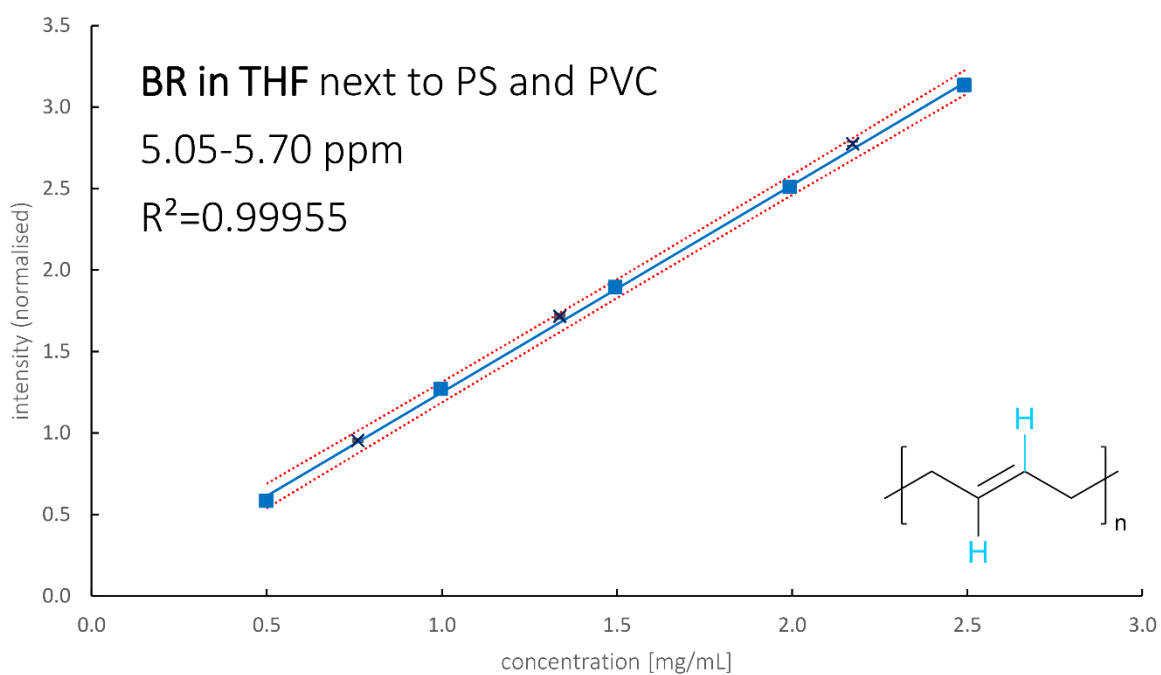


Figure S6: Calibration graph (—) of BR in THF at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

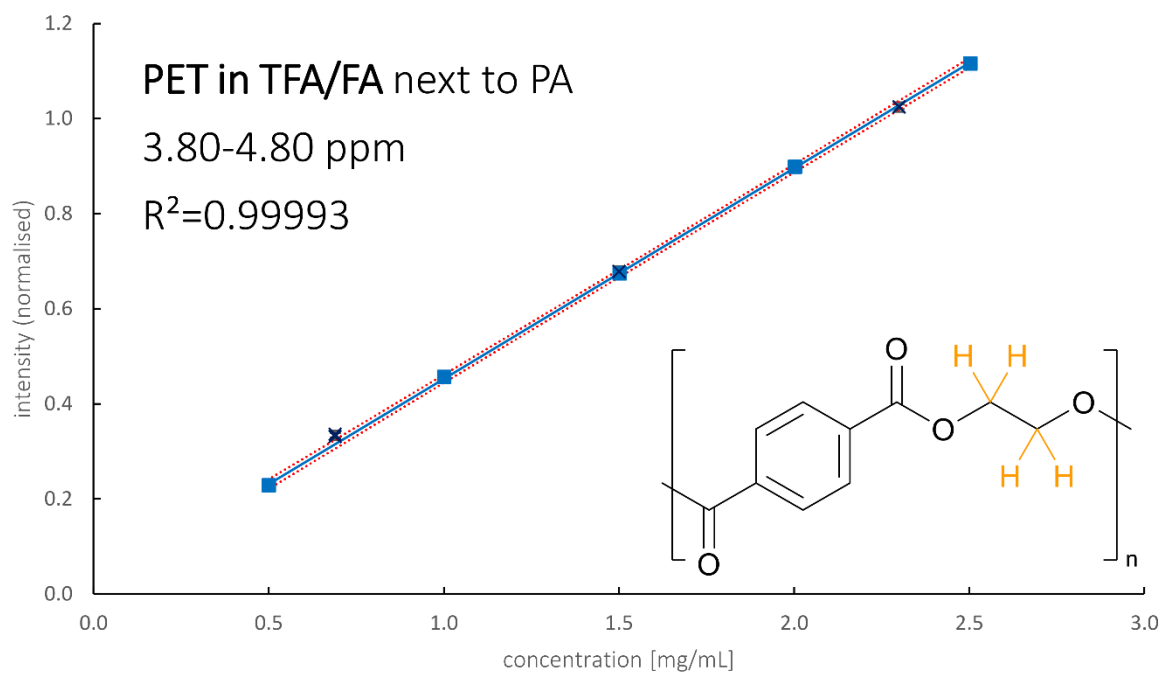


Figure S7: Calibration graph (—) of PET in TFA/FA at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

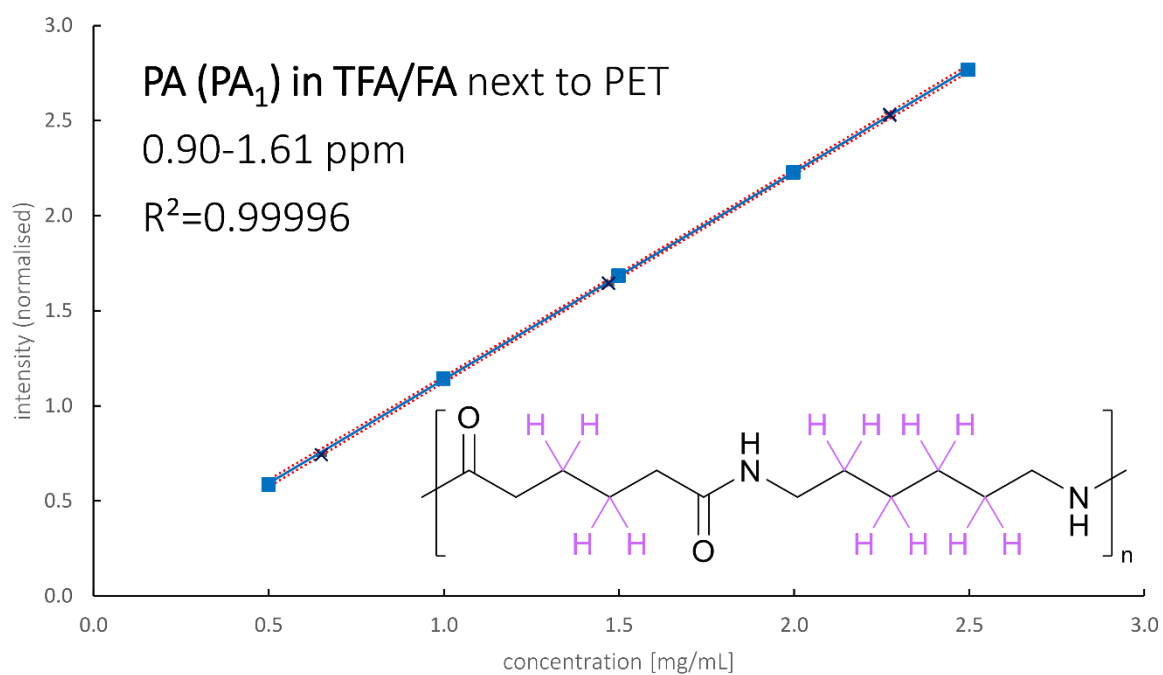


Figure S8: Calibration graph (—) of PA<sub>1</sub> in TFA/FA at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

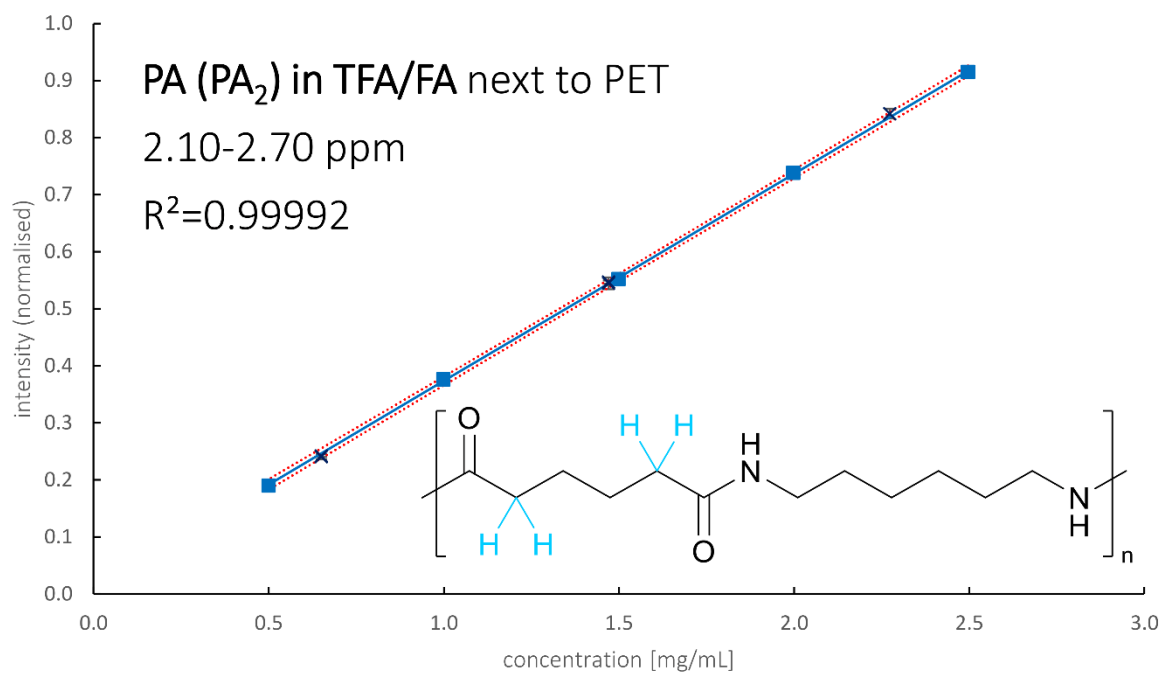


Figure S9: Calibration graph (—) of PA<sub>2</sub> in TFA/FA at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

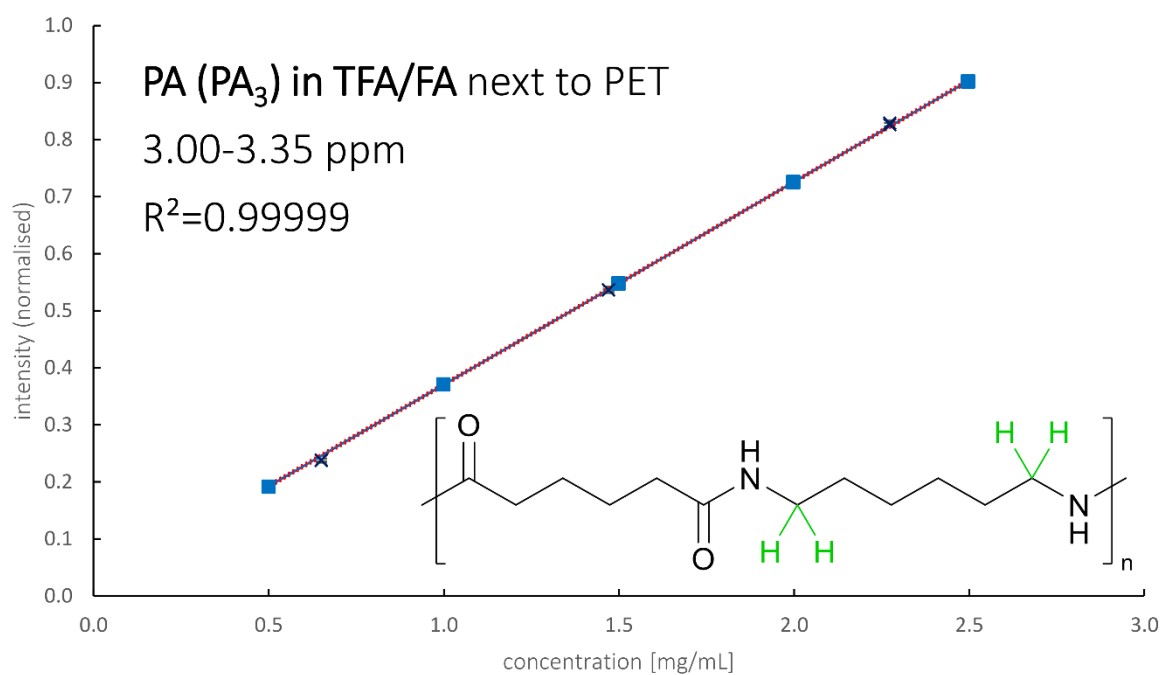


Figure S10: Calibration graph (—) of PA<sub>3</sub> in TFA/FA at 2.5-0.5 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

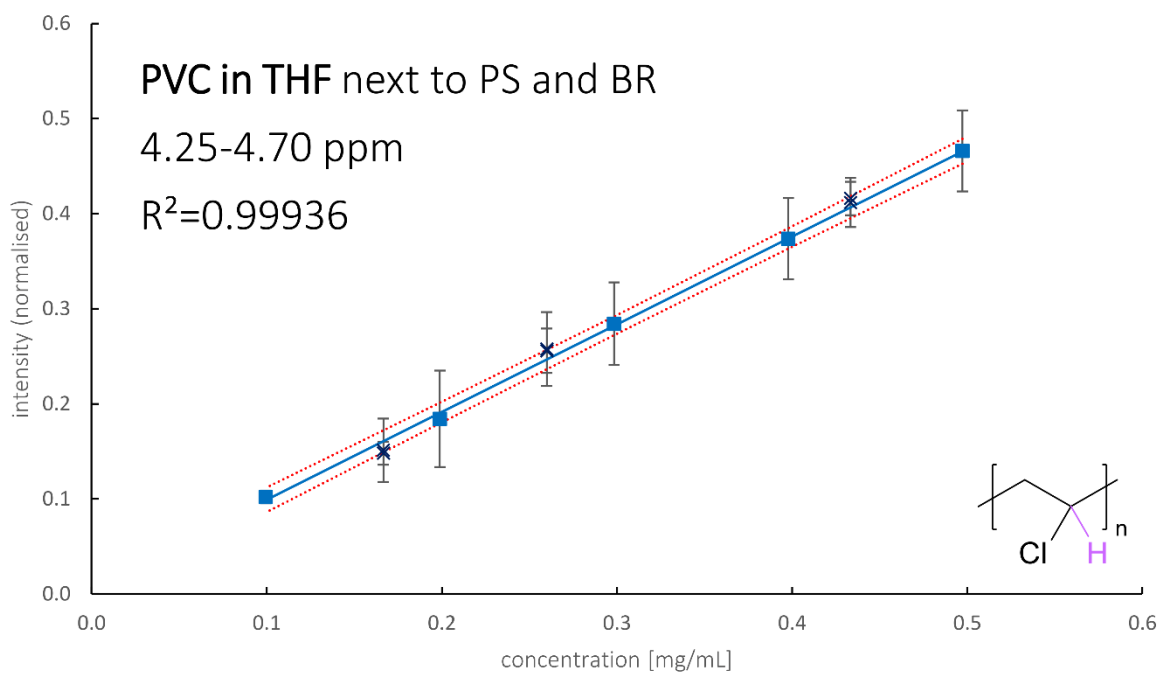


Figure S11: Calibration graph (—) of PVC in THF at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

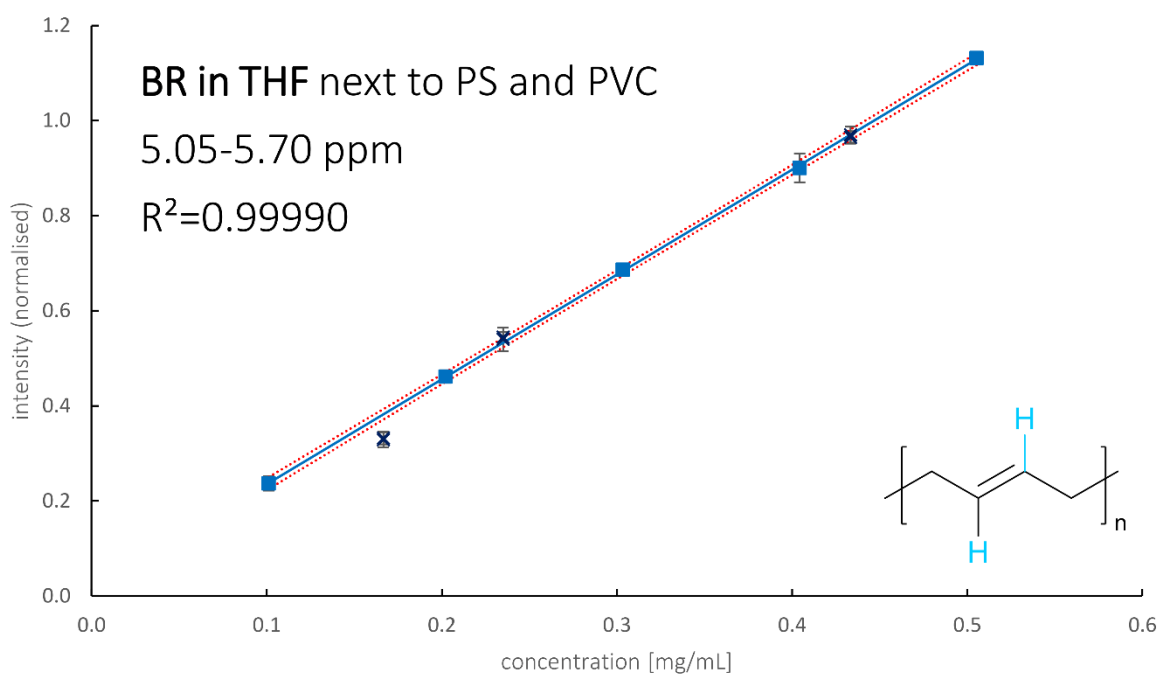


Figure S12: Calibration graph (—) of BR in THF at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

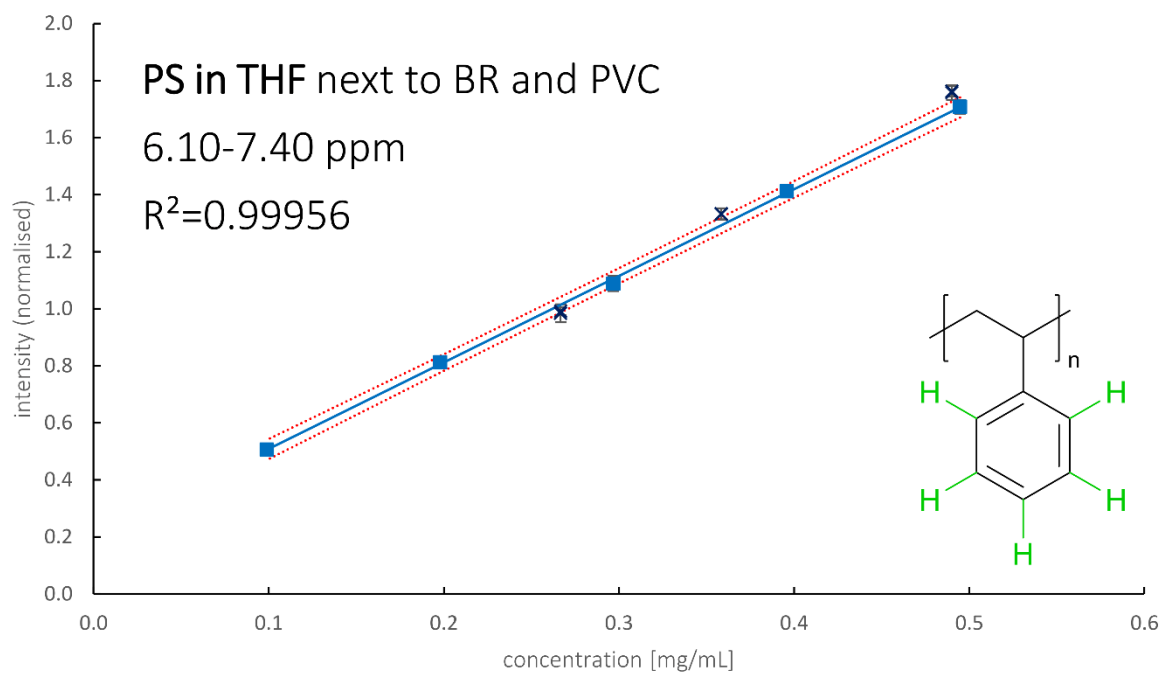


Figure S13: Calibration graph (—) of PS in THF at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

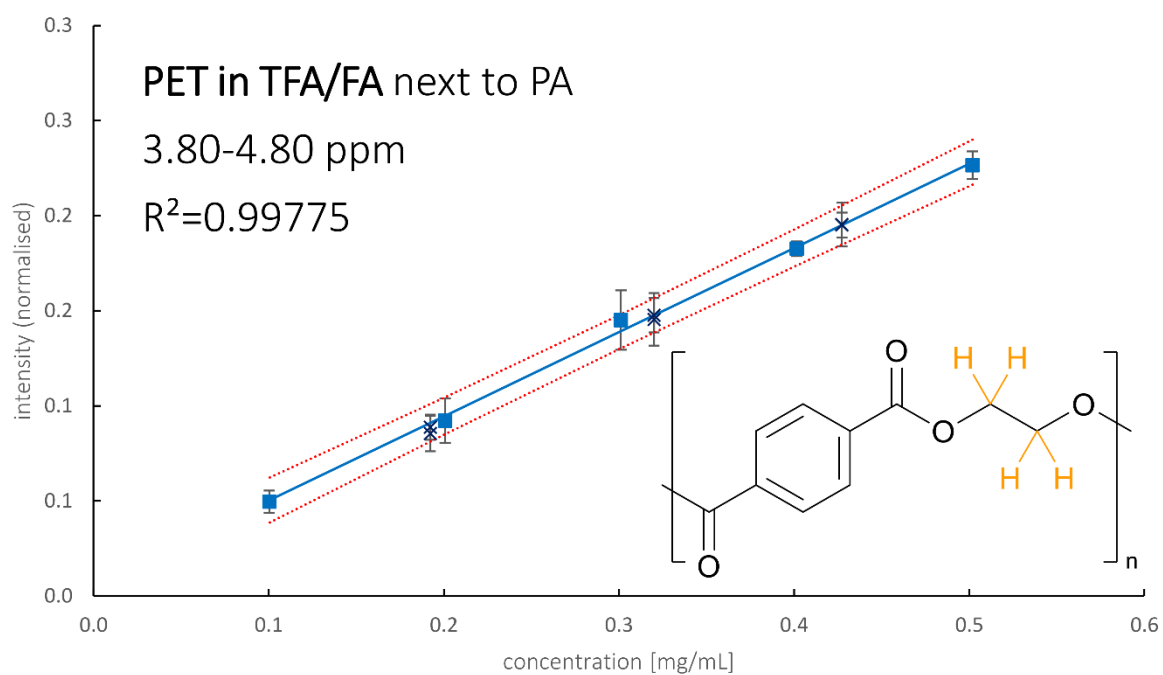


Figure S14: Calibration graph (—) of PET in TFA/FA at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

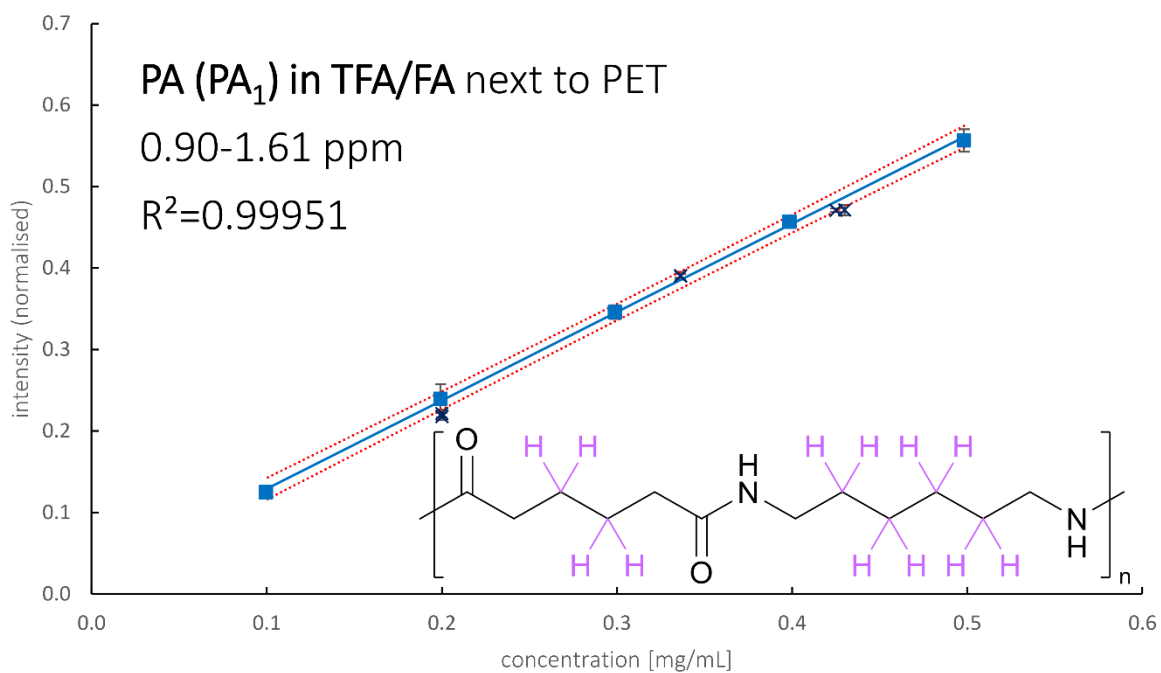


Figure S15: Calibration graph (—) of PA<sub>1</sub> in TFA/FA at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

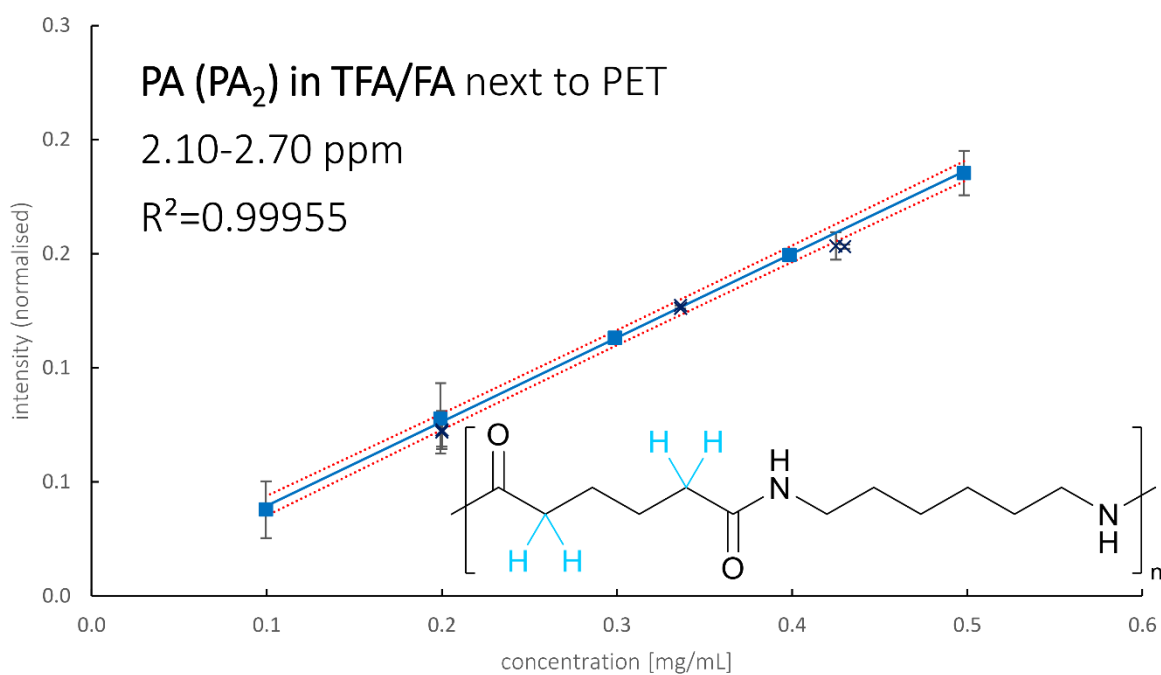


Figure S16: Calibration graph (—) of PA<sub>2</sub> in TFA/FA at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

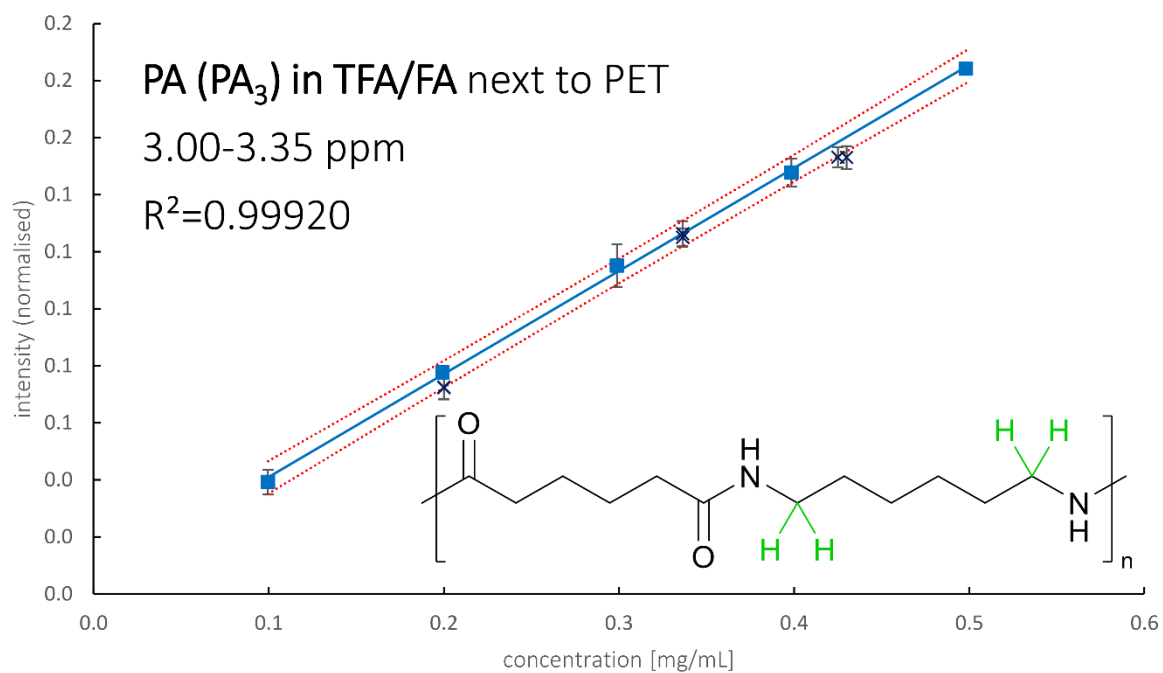


Figure S17: Calibration graph (—) of PA<sub>3</sub> in TFA/FA at 0.5-0.1 mg/mL. Additionally, the confidence interval (.....) and data points for the calibration samples (■), that were used for the linear regression as well as model samples (x), which allow subsequent method validation are depicted.

Table S13: Intensities of styrene- and butadiene-units of SBR model samples within the range of 3.2-2.3 mg/mL measured by <sup>1</sup>H-NMR in non-deuterated THF using HMDSO as INST (0.1%). Each sample is measured five times distributed over five hours.

Sample	count	INST	Absolute Intensity		Normalised Intensity	
			Styrene-Unit	Butadiene-Unit	Styrene-Unit	Butadiene-Unit
SBR1	1	14.1160	5.2480	13.9186	1.10	2.92
	2	4.7824	1.7775	4.6991	1.10	2.91
	3	14.2683	5.3223	14.1598	1.10	2.93
	4	14.3163	5.2713	14.0959	1.09	2.91
	5	4.8009	1.8080	4.7309	1.11	2.91
SBR2	1	14.0359	4.7359	12.5453	1.00	2.64
	2	14.2379	4.8215	12.6085	1.00	2.62
	3	4.7953	1.6198	4.2783	1.00	2.64
	4	14.2459	4.8358	12.6263	1.00	2.62
	5	4.8973	1.6723	4.3535	1.01	2.63
SBR3	1	4.8714	1.5418	3.9701	0.94	2.41
	2	4.8585	1.5237	3.9721	0.93	2.42
	3	4.8596	1.5139	3.9585	0.92	2.41
	4	4.8693	1.5307	3.9403	0.93	2.39
	5	14.6531	4.6182	11.9492	0.93	2.41