Electronic Supplementary Material (ESI) for Analytical Methods.

Comparison of Three Sorbents for Thin Film Solid Phase Microextraction of Haloacetic Acids from Water

Supplementary Information

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Table S1: Gaussian 16 coordinates of the analyte molecules

Analyte	Element	X	Y	Z
BCAA	C	-1.02162	1.329868	-0.21771
	H	-1.27932	1.632269	-1.22462
	C	-0.7288	-0.16634	-0.20659
	O	-0.23113	-0.59524	0.951876
	O	-0.95086	-0.85735	-1.16909
	Cl	0.381747	2.303074	0.309465
	Br	-2.62463	1.675459	0.879407
	H	-0.08052	-1.55318	0.897802
BDCAA	C	-1.04393	1.409457	-0.12892
	C	-0.44103	-0.01805	-0.26159
	O	-0.09221	-0.49571	0.928982
	O	-0.3359	-0.59268	-1.3087
	Cl	0.027968	2.451437	0.856318
	Br	-2.8036	1.20274	0.764614
	Cl	-1.27343	2.128956	-1.73766
	H	0.254334	-1.39658	0.819324
CDBAA	C	-1.14073	1.326537	-0.02447
	C	-0.67024	-0.15249	-0.00173
	O	0.646685	-0.23148	0.167612
	O	-1.41791	-1.08251	-0.12406
	Br	-0.24043	2.244148	-1.52441
	Cl	-2.89918	1.408573	-0.24467
	Br	-0.64729	2.168374	1.693011
	H	0.908308	-1.16683	0.175573
DBAA	C	-2.33623	0.587849	0.052565
	C	-1.91473	-0.87317	0.0088
	O	-0.60984	-1.04219	-0.20091
	O	-2.71542	-1.76339	0.154399
	Br	-1.48097	1.512747	1.557599
	H	-3.40312	0.644782	0.222376
	Br	-1.99766	1.462597	-1.67128
	H	-0.41194	-1.99263	-0.21821
DCAA	C	-0.76124	-0.20454	0.178684
	H	-1.47924	0.032782	0.953895
	C	-0.15403	-1.57627	0.473159

	O	0.744497	-1.95159	-0.43446
	O	-0.48399	-2.21693	1.438562
	Cl	-1.64614	-0.22592	-1.38537
	Cl	0.506279	1.068541	0.210081
	H	1.093043	-2.82623	-0.19612
MBAA	C	-2.41979	0.623503	0.039063
	C	-1.87012	-0.75794	-0.222
	O	-0.70677	-0.71861	-0.88954
	O	-2.41575	-1.78059	0.119306
	H	-2.26168	1.290495	-0.80288
	H	-3.46516	0.563988	0.318579
	Br	-1.47444	1.436591	1.574343
	H	-0.38865	-1.62694	-1.01794
MCAA	C	-1.2526	1.338115	0.075279
	H	-1.46417	1.81908	1.029716
	C	-0.80296	-0.08194	0.354599
	O	0.505916	-0.30027	0.215004
	O	-1.5978	-0.92106	0.70965
	H	-2.16619	1.299771	-0.51206
	Cl	-0.07561	2.384835	-0.80456
	H	0.689798	-1.22665	0.442051
TBAA	C	-2.31917	0.640624	0.180722
	C	-2.00283	-0.83952	-0.16051
	O	-0.69144	-1.02556	-0.29696
	O	-2.8425	-1.68813	-0.27992
	Br	-4.24588	0.894137	0.372807
	Br	-1.64537	1.777948	-1.28201
	Br	-1.41932	1.095213	1.875623
	H	-0.52562	-1.95926	-0.50727
TCAA	C	-3.55385	-0.2456	-0.05567
	C	-3.13267	0.476405	1.261159
	O	-2.56939	1.533711	1.284154
	O	-3.4866	-0.24635	2.318675
	H	-3.21618	0.219396	3.127265
	Cl	-5.33722	-0.47318	-0.04521
	Cl	-3.08147	0.734861	-1.46447
	Cl	-2.73103	-1.84355	-0.1249

Table S2: Gaussian 16 coordinates of the sorbent monomers.

Sorbent	**Element**	**X**	**Y**	**Z**
HLB	C	-3.34362	0.45914	-0.34806
	H	-3.46742	-0.23351	0.491035
	H	-3.15353	-0.13411	-1.24449
	C	-4.61654	1.296954	-0.53176
	H	-4.78502	1.911041	0.359846
	H	-4.46926	1.987603	-1.36967

	C	-5.84812	0.422811	-0.78873
	H	-5.98647	-0.27281	0.047376
	H	-5.68285	-0.1927	-1.68077
	C	-7.13675	1.246696	-0.97644
	H	-7.29972	1.859392	-0.08342
	H	-6.99691	1.938546	-1.81381
	C	-8.35676	0.388306	-1.22991
	C	-9.1328	-0.08453	-0.16495
	C	-8.71535	0.014875	-2.53071
	C	-10.2431	-0.91324	-0.36476
	H	-8.86488	0.201115	0.849135
	C	-9.81639	-0.81204	-2.75084
	H	-8.13088	0.372265	-3.3728
	C	-10.5749	-1.27464	-1.67619
	H	-10.0838	-1.09686	-3.76295
	N	-2.14869	1.255917	-0.1044
	C	-1.90001	1.931033	1.173203
	C	-1.24405	1.565158	-1.06638
	C	-0.43064	2.380042	1.057436
	H	-2.07061	1.241899	2.003651
	C	-0.20104	2.493333	-0.45739
	H	0.222029	1.611588	1.477672
	H	0.800933	2.210687	-0.78182
	O	-1.27519	1.173972	-2.23524
	H	-0.24479	3.310546	1.593519
	H	-0.39574	3.50473	-0.83044
	H	-2.5777	2.783564	1.295777
	H	-11.4295	-1.91954	-1.85589
	C	-11.0871	-1.37229	0.805186
	H	-10.4526	-1.47995	1.690491
	H	-11.4973	-2.36375	0.588942
	C	-12.2427	-0.40837	1.127304
	H	-12.8277	-0.77408	1.97599
	H	-11.8645	0.586128	1.380252
	H	-12.9161	-0.30403	0.271947
PDMS	C	-0.43971	0.389071	-0.17739
	H	-0.00387	-0.57049	-0.46988
	H	0.19697	0.82893	0.595401
	H	-1.42231	0.197221	0.262799
	Si	-0.57676	1.528574	-1.6459
	O	0.939263	1.772583	-2.26262
	O	-1.51726	0.693652	-2.75915
	H	-1.8082	1.166418	-3.545
	C	-1.35117	3.184504	-1.25054
	H	-2.34604	3.055365	-0.81447
	H	-0.73665	3.738912	-0.53517
	H	-1.4522	3.797024	-2.15154
	Si	2.087022	2.220829	-3.35603
	C	3.772375	1.871677	-2.62804
	H	4.566917	2.21451	-3.29805

	H	3.894867	2.3813	-1.66804
	H	3.91188	0.798744	-2.46521
	C	1.820294	1.345542	-4.98796
	H	1.909321	0.261679	-4.86754
	H	0.827119	1.563289	-5.39107
	H	2.562793	1.661788	-5.72733
	O	1.859816	3.877297	-3.54192
	H	2.410007	4.332592	-4.18652

Table S3: Gaussian 16 coordinates of interfaces between the analytes and sorbent monomers.

Interaction (sorbent x analyte)	**Element**	**X**	**Y**	**Z**
HLB x BCAA	C	-3.75338	2.203156	-0.48984
	H	-4.39107	3.00289	-0.10242
	H	-3.17679	1.812028	0.349318
	C	-4.61106	1.092343	-1.11024
	H	-5.17392	1.495757	-1.95895
	H	-3.95186	0.312647	-1.5074
	C	-5.58347	0.483158	-0.09508
	H	-6.22995	1.268742	0.313237
	H	-5.0219	0.070585	0.750829
	C	-6.46173	-0.62522	-0.70708
	H	-7.0277	-0.2066	-1.54609
	H	-5.81314	-1.40475	-1.12038
	C	-7.41758	-1.24217	0.290531
	C	-8.68476	-0.68693	0.504962
	C	-7.04372	-2.35833	1.048384
	C	-9.57616	-1.21188	1.447966
	H	-8.98624	0.17855	-0.07968
	C	-7.91628	-2.8948	1.994634
	H	-6.06734	-2.8079	0.897129
	C	-9.17326	-2.32567	2.194836
	H	-7.6155	-3.7587	2.577879
	N	-2.81559	2.805841	-1.43385
	C	-3.25425	3.779221	-2.44657
	C	-1.53026	2.443891	-1.57215
	C	-1.93145	4.337255	-3.00252
	H	-3.88005	4.54268	-1.98069
	C	-0.91642	3.218177	-2.72197
	H	-1.65326	5.239871	-2.45477
	H	0.081187	3.570216	-2.45849
	O	-0.92274	1.597486	-0.8899
	H	-2.00859	4.592431	-4.05875
	H	-0.81108	2.530075	-3.56765
	H	-3.84521	3.276328	-3.21881
	H	-9.84603	-2.74825	2.934629
	C	-10.9561	-0.61521	1.625261
	H	-10.915	0.460363	1.426913
	H	-11.2698	-0.73174	2.667359
	C	-12.0109	-1.25727	0.706794
	H	-12.9921	-0.80074	0.864784
	H	-11.7437	-1.12954	-0.34599

	H	-12.1009	-2.32942	0.902783
	C	-0.74413	-1.04248	3.10703
	H	0.077787	-1.01117	3.810617
	C	-0.52147	0.005941	2.01445
	O	-1.35099	-0.09863	1.002817
	O	0.354889	0.833104	2.149937
	Cl	-0.84505	-2.70849	2.458744
	Br	-2.35509	-0.5571	4.143505
	H	-1.19172	0.613159	0.296929
HLB x BDCAA	C	-3.60599	0.240158	-0.57147
	H	-3.68512	-0.39009	0.31918
	H	-3.50518	-0.41467	-1.43821
	C	-4.85306	1.122174	-0.7136
	H	-4.92986	1.793207	0.148738
	H	-4.74185	1.755011	-1.6009
	C	-6.13242	0.286963	-0.8272
	H	-6.23522	-0.35134	0.058086
	H	-6.05696	-0.38604	-1.68917
	C	-7.39793	1.153826	-0.97326
	H	-7.47114	1.823937	-0.11018
	H	-7.29311	1.788863	-1.85929
	C	-8.66526	0.334922	-1.08691
	C	-9.37634	-0.04576	0.057311
	C	-9.13421	-0.09362	-2.33456
	C	-10.5293	-0.83653	-0.01319
	H	-9.02228	0.283323	1.031011
	C	-10.2791	-0.88427	-2.42596
	H	-8.60143	0.192407	-3.2361
	C	-10.9718	-1.25496	-1.27397
	H	-10.6324	-1.21263	-3.39772
	N	-2.36583	1.005039	-0.46468
	C	-1.9773	1.715365	0.763384
	C	-1.53888	1.234329	-1.49065
	C	-0.51193	2.108593	0.497743
	H	-2.09507	1.057139	1.625999
	C	-0.40581	2.131306	-1.03642
	H	0.153884	1.345771	0.905833
	H	0.548142	1.775026	-1.42578
	O	-1.70879	0.782343	-2.64422
	H	-0.25632	3.06242	0.957356
	H	-0.58142	3.129451	-1.45192
	H	-2.61937	2.589767	0.908855
	H	-11.8613	-1.8721	-1.35351
	C	-11.3004	-1.19462	1.239367
	H	-10.6053	-1.28779	2.079669
	H	-11.7693	-2.17485	1.108132
	C	-12.3842	-0.16108	1.593784
	H	-12.9179	-0.45481	2.502111
	H	-11.9441	0.825587	1.763783
	H	-13.1159	-0.0679	0.786414

	C	1.774898	0.953579	-5.89511
	C	1.010585	0.766427	-4.54162
	O	-0.22929	1.157337	-4.64013
	O	1.558003	0.294705	-3.57379
	Cl	1.499093	2.59717	-6.55599
	Br	1.055902	-0.4069	-7.15297
	Cl	3.52201	0.686947	-5.67643
	H	-0.76826	1.005562	-3.76365
HLB x CDBAA	C	-3.80043	2.361588	-0.26039
	H	-4.54275	3.109585	0.032833
	H	-3.29318	2.033967	0.648225
	C	-4.48684	1.174782	-0.94921
	H	-4.96044	1.515054	-1.87641
	H	-3.72725	0.437935	-1.23166
	C	-5.54022	0.519706	-0.04984
	H	-6.29226	1.263737	0.237582
	H	-5.07089	0.176021	0.879058
	C	-6.24337	-0.67014	-0.73129
	H	-6.7076	-0.32268	-1.6604
	H	-5.49066	-1.41406	-1.01253
	C	-7.29199	-1.32031	0.144712
	C	-8.61319	-0.85718	0.142161
	C	-6.95859	-2.37427	1.003703
	C	-9.59712	-1.41297	0.968202
	H	-8.88365	-0.04078	-0.52275
	C	-7.92364	-2.94004	1.836244
	H	-5.94123	-2.75209	1.020971
	C	-9.23357	-2.46279	1.820496
	H	-7.65372	-3.75506	2.499464
	N	-2.81393	3.030704	-1.10498
	C	-3.21478	3.942563	-2.18879
	C	-1.49299	2.801058	-1.07212
	C	-1.89443	4.626722	-2.58741
	H	-3.96831	4.642842	-1.82384
	C	-0.81646	3.622024	-2.15153
	H	-1.78125	5.560426	-2.03292
	H	0.097233	4.078316	-1.77
	O	-0.89358	2.029354	-0.29819
	H	-1.86037	4.858333	-3.65128
	H	-0.53168	2.939347	-2.95934
	H	-3.64882	3.37239	-3.01621
	H	-9.97855	-2.9076	2.47293
	C	-11.0267	-0.91835	0.910458
	H	-11.0324	0.147745	0.662935
	H	-11.4834	-1.0144	1.900489
	C	-11.8847	-1.67885	-0.11609
	H	-12.9082	-1.2935	-0.12745
	H	-11.473	-1.57579	-1.124
	H	-11.9273	-2.74541	0.121908
	C	-1.37684	-1.96099	2.302931

	C	-1.30793	-0.97031	1.097418
	O	-1.30088	0.273503	1.504292
	O	-1.25925	-1.36609	-0.041
	Br	-2.95975	-1.54072	3.407557
	Cl	-1.48504	-3.64139	1.734759
	Br	0.274384	-1.73541	3.371989
	H	-1.2136	0.935853	0.731761
HLB x DBAA	C	-3.32975	1.097067	-0.56801
	H	-3.8789	1.168717	-1.51142
	H	-3.40305	2.067138	-0.0743
	C	-3.9372	0.000218	0.316537
	H	-3.82805	-0.97082	-0.17844
	H	-3.37366	-0.05604	1.254278
	C	-5.41814	0.258421	0.612289
	H	-5.97481	0.322679	-0.32989
	H	-5.53169	1.229267	1.10808
	C	-6.04795	-0.83622	1.495196
	H	-5.92614	-1.80528	0.999649
	H	-5.49707	-0.89213	2.439943
	C	-7.51451	-0.59492	1.779171
	C	-8.49933	-1.07382	0.906855
	C	-7.91897	0.144599	2.896942
	C	-9.86167	-0.83307	1.119795
	H	-8.19646	-1.65102	0.036872
	C	-9.27116	0.397554	3.125578
	H	-7.17361	0.523408	3.589179
	C	-10.2364	-0.08606	2.243307
	H	-9.57333	0.973736	3.993722
	N	-1.92435	0.86913	-0.89383
	C	-1.51349	-0.11357	-1.90905
	C	-0.88809	1.416738	-0.23922
	C	-0.021	0.19734	-2.12502
	H	-2.11308	0.013716	-2.81234
	C	0.405804	0.872397	-0.81227
	H	0.093347	0.894001	-2.9579
	H	1.137396	1.671533	-0.9338
	O	-0.95425	2.230491	0.701018
	H	0.553285	-0.69982	-2.3531
	H	0.814931	0.157853	-0.08996
	H	-1.67188	-1.12956	-1.53346
	H	-11.2868	0.116938	2.427557
	C	-10.9045	-1.40145	0.181112
	H	-10.4915	-1.45484	-0.83107
	H	-11.7608	-0.72128	0.136533
	C	-11.3927	-2.79929	0.600745
	H	-12.1438	-3.17432	-0.10032
	H	-10.5645	-3.51318	0.62359
	H	-11.8425	-2.77457	1.597307
	C	-3.3376	4.85345	3.925595
	C	-2.33876	4.314469	2.903224

	O	-2.70324	3.182184	2.346997
	O	-1.32009	4.933845	2.678973
	Br	-5.05592	5.279452	3.071721
	H	-2.96684	5.780764	4.34153
	Br	-3.53637	3.612098	5.436677
	H	-2.02178	2.841382	1.678399
HLB x DCAA	C	-4.40618	2.080187	-0.05595
	H	-5.07736	2.913967	-0.28251
	H	-4.25902	2.052061	1.024702
	C	-5.01422	0.758866	-0.54385
	H	-5.13657	0.788788	-1.63201
	H	-4.31622	-0.05641	-0.32402
	C	-6.3682	0.475959	0.114797
	H	-7.06119	1.297861	-0.09971
	H	-6.24822	0.446087	1.203977
	C	-6.99484	-0.84912	-0.36049
	H	-7.11558	-0.81484	-1.44843
	H	-6.30007	-1.66767	-0.14467
	C	-8.3311	-1.13809	0.287861
	C	-9.52079	-0.67688	-0.28808
	C	-8.40602	-1.83961	1.497161
	C	-10.7684	-0.89474	0.308298
	H	-9.4744	-0.133	-1.22817
	C	-9.63882	-2.06485	2.108604
	H	-7.49698	-2.21001	1.960686
	C	-10.8123	-1.59492	1.520032
	H	-9.68505	-2.60789	3.046647
	N	-3.10866	2.377241	-0.65709
	C	-2.96679	2.832346	-2.04815
	C	-1.93558	2.149637	-0.05244
	C	-1.49659	3.28501	-2.12571
	H	-3.67459	3.638537	-2.24983
	C	-0.80574	2.492894	-1.00325
	H	-1.42942	4.355418	-1.92194
	H	-0.01702	3.042596	-0.48878
	O	-1.81507	1.704377	1.107833
	H	-1.06415	3.099475	-3.10805
	H	-0.37242	1.553194	-1.36217
	H	-3.18083	2.008334	-2.73614
	H	-11.7679	-1.77296	2.003358
	C	-12.0403	-0.42065	-0.36185
	H	-11.8345	0.494977	-0.92499
	H	-12.7779	-0.16058	0.403874
	C	-12.6471	-1.47007	-1.31
	H	-13.5624	-1.09099	-1.77322
	H	-11.9458	-1.72895	-2.10828
	H	-12.8959	-2.38836	-0.77069
	C	2.138154	0.001384	3.190925
	H	2.385521	-1.0479	3.293241
	C	0.810271	0.139554	2.432967

	O	0.416217	1.378988	2.288023
	O	0.243685	-0.85758	2.036434
	Cl	2.007235	0.681722	4.852182
	Cl	3.477831	0.774469	2.267533
	H	-0.47208	1.458304	1.775668
HLB x MBAA	C	-3.95391	2.451739	0.168609
	H	-4.49667	3.132936	-0.49333
	H	-4.15525	2.764404	1.19448
	C	-4.42745	1.008824	-0.05127
	H	-4.1973	0.700289	-1.07684
	H	-3.86594	0.343906	0.614013
	C	-5.93006	0.853056	0.204163
	H	-6.48822	1.517521	-0.46573
	H	-6.16524	1.172441	1.226033
	C	-6.41978	-0.59403	0.002439
	H	-6.18363	-0.91025	-1.01905
	H	-5.86167	-1.25409	0.674959
	C	-7.90324	-0.75786	0.251575
	C	-8.82431	-0.62085	-0.79351
	C	-8.39129	-1.01382	1.538778
	C	-10.2047	-0.73023	-0.58692
	H	-8.45611	-0.42416	-1.79721
	C	-9.76255	-1.12315	1.76602
	H	-7.69581	-1.12792	2.364368
	C	-10.664	-0.98139	0.711555
	H	-10.1299	-1.31973	2.767705
	N	-2.52741	2.640294	-0.0791
	C	-1.97915	2.728589	-1.44101
	C	-1.57931	2.62523	0.87345
	C	-0.53821	3.222162	-1.21424
	H	-2.57904	3.417049	-2.03927
	C	-0.21839	2.769985	0.219077
	H	-0.5082	4.311802	-1.2778
	H	0.405766	3.464617	0.781751
	O	-1.76699	2.498674	2.096444
	H	0.151727	2.82081	-1.95569
	H	0.270434	1.790178	0.24728
	H	-2.00559	1.745293	-1.92192
	H	-11.7302	-1.06676	0.897247
	C	-11.1718	-0.62164	-1.74644
	H	-10.766	0.066559	-2.49453
	H	-12.1121	-0.18589	-1.39443
	C	-11.4634	-1.97726	-2.41405
	H	-12.1639	-1.85743	-3.24538
	H	-10.5465	-2.42629	-2.80595
	H	-11.9026	-2.67945	-1.69987
	C	-4.6514	0.502516	5.415379
	C	-3.60624	0.709513	4.33878
	O	-3.64749	1.928216	3.821244
	O	-2.83568	-0.16624	3.999375

	H	-5.58682	1.000233	5.178783
	H	-4.79182	-0.55406	5.6122
	Br	-4.02538	1.300713	7.117143
	H	-2.93827	2.065917	3.121092
HLB x MCAA	C	-5.28933	0.654033	2.005806
	H	-6.32752	0.737911	2.341233
	H	-4.96251	-0.37219	2.180091
	C	-5.18236	0.999047	0.514727
	H	-5.49808	2.035337	0.352311
	H	-4.1322	0.934528	0.209268
	C	-6.03343	0.06398	-0.35053
	H	-7.08095	0.118252	-0.03178
	H	-5.714	-0.97297	-0.1946
	C	-5.94548	0.398883	-1.85202
	H	-6.27456	1.432147	-2.00523
	H	-4.89737	0.350618	-2.16569
	C	-6.77279	-0.5289	-2.71475
	C	-8.11489	-0.24236	-2.99138
	C	-6.22713	-1.71333	-3.2242
	C	-8.91632	-1.10078	-3.75325
	H	-8.54817	0.675792	-2.60281
	C	-7.00944	-2.58305	-3.98311
	H	-5.18755	-1.95492	-3.02586
	C	-8.34513	-2.28071	-4.24525
	H	-6.57686	-3.49916	-4.37116
	N	-4.47359	1.512836	2.859543
	C	-4.83382	2.907362	3.153167
	C	-3.27457	1.160373	3.346202
	C	-3.86812	3.292323	4.289791
	H	-5.88413	2.967358	3.444864
	C	-2.68279	2.329515	4.110053
	H	-4.34715	3.11749	5.255172
	H	-2.23315	1.995437	5.04558
	O	-2.73985	0.048097	3.169733
	H	-3.57834	4.341235	4.240732
	H	-1.88488	2.761032	3.496297
	H	-4.68972	3.528319	2.263159
	H	-8.94787	-2.96402	-4.83545
	C	-10.352	-0.74085	-4.07106
	H	-10.7734	-0.16291	-3.24265
	H	-10.9459	-1.65678	-4.15056
	C	-10.4948	0.066808	-5.37326
	H	-11.544	0.306316	-5.56792
	H	-9.93831	1.00646	-5.3146
	H	-10.1121	-0.49735	-6.2284
	C	1.856366	-1.10347	4.084595
	H	2.563106	-0.28083	4.170358
	C	0.561631	-0.56744	3.492366
	O	-0.52219	-0.7497	4.210834
	O	0.608532	-0.01645	2.407743

	H	2.263409	-1.84824	3.403575
	Cl	1.735959	-1.87888	5.714482
	H	-1.35242	-0.37367	3.755596
HLB x TBAA	C	-4.71508	2.741092	0.42727
	H	-5.64425	3.313951	0.355512
	H	-4.51617	2.554786	1.483608
	C	-4.84524	1.414289	-0.33177
	H	-5.01517	1.613698	-1.39533
	H	-3.89846	0.868204	-0.25736
	C	-5.98736	0.551652	0.214789
	H	-6.93214	1.103136	0.143937
	H	-5.82167	0.353187	1.28003
	C	-6.12818	-0.78851	-0.53256
	H	-6.29268	-0.58639	-1.59623
	H	-5.18367	-1.33764	-0.4571
	C	-7.25472	-1.64773	-0.00142
	C	-8.54864	-1.53394	-0.52331
	C	-7.03787	-2.54861	1.048211
	C	-9.619	-2.28769	-0.02739
	H	-8.72766	-0.83905	-1.33989
	C	-8.09129	-3.30644	1.558284
	H	-6.04202	-2.65674	1.466575
	C	-9.37354	-3.17679	1.025947
	H	-7.91244	-4.00004	2.373086
	N	-3.63311	3.586937	-0.07115
	C	-3.73572	4.342109	-1.3292
	C	-2.41947	3.654294	0.48765
	C	-2.51115	5.275054	-1.2841
	H	-4.68438	4.880813	-1.36252
	C	-1.52875	4.551173	-0.34819
	H	-2.796	6.236756	-0.85311
	H	-0.94123	5.217224	0.284229
	O	-2.08893	3.044553	1.527754
	H	-2.10016	5.45663	-2.27628
	H	-0.82753	3.911369	-0.8946
	H	-3.70033	3.65642	-2.18155
	H	-10.1886	-3.76942	1.429654
	C	-10.9971	-2.17362	-0.64338
	H	-11.1499	-1.15201	-1.00516
	H	-11.754	-2.35168	0.126923
	C	-11.2191	-3.1583	-1.80509
	H	-12.2238	-3.04554	-2.22244
	H	-10.4975	-2.9856	-2.60847
	H	-11.1063	-4.19285	-1.46894
	C	2.304982	2.422897	3.24897
	C	0.935136	2.198576	2.530495
	O	0.182156	3.263219	2.603108
	O	0.668745	1.151251	1.991191
	Br	3.406872	0.807804	3.1745
	Br	1.96904	2.894833	5.135959

	Br	3.250919	3.899216	2.339032
	H	-0.72905	3.141344	2.121595
HLB x TCAA	C	-3.466	0.500482	-0.31016
	H	-3.57376	-0.06197	0.621923
	H	-3.24584	-0.21036	-1.10786
	C	-4.75724	1.267626	-0.6223
	H	-4.955	1.995118	0.17234
	H	-4.61833	1.836588	-1.54811
	C	-5.95846	0.327256	-0.76447
	H	-6.0855	-0.24974	0.158952
	H	-5.76431	-0.39969	-1.56161
	C	-7.26806	1.077884	-1.07395
	H	-7.46002	1.801353	-0.27448
	H	-7.13857	1.65278	-1.99694
	C	-8.45852	0.154956	-1.21751
	C	-9.22075	-0.20803	-0.10075
	C	-8.80179	-0.38734	-2.46177
	C	-10.303	-1.09096	-0.19484
	H	-8.96441	0.209051	0.869873
	C	-9.87475	-1.27062	-2.57618
	H	-8.22735	-0.1176	-3.34249
	C	-10.6199	-1.62171	-1.45113
	H	-10.1307	-1.68667	-3.54487
	N	-2.29734	1.366447	-0.17269
	C	-2.07073	2.206817	1.01312
	C	-1.39849	1.568137	-1.14181
	C	-0.61816	2.687203	0.836113
	H	-2.2201	1.617405	1.919527
	C	-0.37671	2.586932	-0.67942
	H	0.059499	2.015437	1.366372
	H	0.633127	2.277895	-0.95081
	O	-1.42978	1.005478	-2.25849
	H	-0.47138	3.693622	1.225768
	H	-0.58396	3.528971	-1.19825
	H	-2.78183	3.038667	1.023499
	H	-11.4527	-2.31128	-1.54832
	C	-11.134	-1.42957	1.024299
	H	-10.4956	-1.41988	1.913246
	H	-11.5223	-2.44815	0.926266
	C	-12.3101	-0.46022	1.237825
	H	-12.8848	-0.73752	2.12608
	H	-11.9536	0.564976	1.371692
	H	-12.9876	-0.47081	0.379385
	C	1.263879	2.220293	-5.98789
	C	0.092224	2.162771	-4.94473
	O	-0.88655	2.859366	-5.05905
	O	0.351332	1.296672	-4.00575
	H	-0.40248	1.237571	-3.28911
	Cl	1.496973	0.583862	-6.70245
	Cl	0.893819	3.385216	-7.28738

	Cl	2.769047	2.732068	-5.13907
PDMS x BCAA	C	-0.97599	1.160183	-0.23481
	H	-0.62507	0.126275	-0.28606
	H	-0.48699	1.651338	0.61056
	H	-2.05106	1.14395	-0.03177
	Si	-0.65687	2.064305	-1.82975
	O	0.992276	1.919512	-2.21864
	O	-1.5199	1.282229	-3.02787
	H	-1.16039	1.43824	-3.91495
	C	-1.0953	3.878002	-1.74788
	H	-2.14726	4.000716	-1.47306
	H	-0.48769	4.394421	-0.99917
	H	-0.93992	4.370245	-2.71207
	Si	1.824841	2.086884	-3.67579
	C	2.671915	3.745085	-3.75769
	H	3.18403	3.869275	-4.71675
	H	1.95618	4.563123	-3.64303
	H	3.421634	3.832321	-2.96593
	C	2.995944	0.648989	-3.8481
	H	3.756541	0.660713	-3.06241
	H	2.457544	-0.3008	-3.79093
	H	3.510681	0.693092	-4.81263
	O	0.576549	1.98958	-4.8038
	H	0.715125	2.343381	-5.68767
	C	4.029952	1.423798	1.657888
	H	4.498848	2.243219	2.187303
	C	3.094974	1.983563	0.58641
	O	2.613391	1.062679	-0.22646
	O	2.852212	3.16835	0.548435
	Cl	5.328429	0.403586	0.966924
	Br	2.963013	0.450961	3.004094
	H	2.008732	1.459143	-0.91265
PDMS x BDCAA	C	-0.96743	0.770277	-0.36134
	H	-0.69636	-0.2583	-0.61267
	H	-0.42523	1.062135	0.541825
	H	-2.03602	0.791946	-0.12698
	Si	-0.61764	1.929358	-1.7742
	O	1.006592	1.734371	-2.24762
	O	-1.56981	1.450201	-3.06021
	H	-1.23048	1.75547	-3.91574
	C	-0.90101	3.724029	-1.34337
	H	-1.93113	3.874265	-1.0066
	H	-0.23219	4.043097	-0.53881
	H	-0.73101	4.373739	-2.20641
	Si	1.807205	2.11718	-3.6848
	C	2.807122	3.675912	-3.47894
	H	3.298264	3.946136	-4.41871
	H	2.178725	4.514017	-3.16694
	H	3.586756	3.533074	-2.72501

	C	2.825268	0.642702	-4.19166
	H	3.606857	0.428302	-3.4574
	H	2.197766	-0.24657	-4.29534
	H	3.312206	0.831853	-5.15304
	O	0.523503	2.357019	-4.74924
	H	0.6525	2.920583	-5.51826
	C	4.055402	0.247961	1.320839
	C	3.147326	1.13501	0.412311
	O	2.586498	0.416683	-0.53657
	O	3.000225	2.312688	0.61077
	Cl	5.160784	-0.74905	0.32303
	Br	2.846747	-0.92703	2.370183
	Cl	5.004917	1.262881	2.431393
	H	1.994275	0.974821	-1.12032
PDMS x CDBAA	C	-1.16892	1.007994	-0.28328
	H	-0.83266	-0.02881	-0.3639
	H	-0.71357	1.452801	0.605449
	H	-2.25263	1.002437	-0.13265
	Si	-0.75929	1.977738	-1.81737
	O	0.91065	1.837777	-2.11954
	O	-1.55563	1.252808	-3.09461
	H	-1.16168	1.467213	-3.95415
	C	-1.1935	3.78909	-1.6823
	H	-2.25826	3.905658	-1.45897
	H	-0.62525	4.269741	-0.88077
	H	-0.98569	4.32127	-2.61479
	Si	1.816252	2.118678	-3.51735
	C	2.661117	3.777206	-3.42786
	H	3.220112	3.97525	-4.34751
	H	1.939475	4.585448	-3.28462
	H	3.370395	3.799877	-2.5954
	C	2.996854	0.696039	-3.73911
	H	3.718398	0.647402	-2.91885
	H	2.458437	-0.25456	-3.78026
	H	3.557376	0.812486	-4.67154
	O	0.62662	2.108115	-4.71028
	H	0.787581	2.576512	-5.53508
	C	3.733635	0.79624	1.778958
	C	2.861152	1.559784	0.737431
	O	2.368338	0.736862	-0.16366
	O	2.693695	2.750576	0.793993
	Br	5.236365	-0.06421	0.823988
	Cl	4.373624	1.915801	2.99976
	Br	2.616	-0.57261	2.663421
	H	1.820089	1.222699	-0.84612
PDMS x DBAA	C	-1.17779	1.096522	-0.25404
	H	-0.85614	0.054761	-0.33086
	H	-0.72081	1.536567	0.63625
	H	-2.26221	1.106951	-0.10878

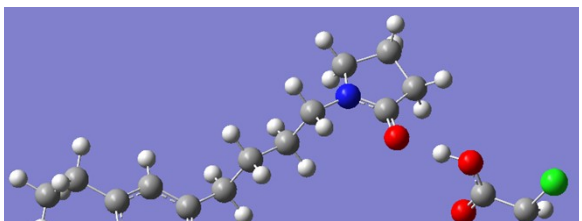
	Si	-0.7446	2.056583	-1.78818
	O	0.919923	1.881682	-2.08873
	O	-1.5567	1.349069	-3.06591
	H	-1.15127	1.545588	-3.9245
	C	-1.1417	3.876754	-1.65352
	H	-2.20438	4.016341	-1.43348
	H	-0.5657	4.34488	-0.85008
	H	-0.91903	4.404496	-2.58516
	Si	1.836634	2.107456	-3.48643
	C	2.741061	3.735614	-3.42076
	H	3.305335	3.900597	-4.34378
	H	2.048252	4.570579	-3.28861
	H	3.451931	3.745299	-2.58939
	C	2.966327	0.640478	-3.68665
	H	3.682173	0.575745	-2.86251
	H	2.393735	-0.29035	-3.71837
	H	3.534491	0.724579	-4.61794
	O	0.650595	2.122623	-4.68369
	H	0.838895	2.552442	-5.52355
	C	3.667622	0.93954	1.917125
	C	2.794024	1.613657	0.86406
	O	2.397946	0.801535	-0.098
	O	2.525457	2.790399	0.95818
	Br	2.694303	-0.50253	2.827338
	H	3.932514	1.659294	2.680153
	Br	5.358009	0.325105	1.125145
	H	1.842045	1.277833	-0.77456
PDMS x DCAA	C	-1.17442	0.958518	-0.30775
	H	-0.77908	-0.05667	-0.39647
	H	-0.75867	1.41511	0.59425
	H	-2.25832	0.890256	-0.17459
	Si	-0.79381	1.966889	-1.82494
	O	0.882546	1.913778	-2.10676
	O	-1.53932	1.219843	-3.12013
	H	-1.12809	1.438646	-3.97073
	C	-1.31617	3.75358	-1.67467
	H	-2.38943	3.819588	-1.47259
	H	-0.78647	4.248536	-0.8556
	H	-1.11215	4.306472	-2.59599
	Si	1.803991	2.175502	-3.49511
	C	2.600624	3.8595	-3.4402
	H	3.170477	4.04745	-4.35531
	H	1.85281	4.649495	-3.33349
	H	3.293467	3.927513	-2.59642
	C	3.028842	0.781413	-3.65152
	H	3.730359	0.775022	-2.81249
	H	2.517537	-0.18455	-3.67905
	H	3.609553	0.887688	-4.57271
	O	0.639318	2.096295	-4.71049
	H	0.814487	2.521591	-5.5555

	C	3.63402	1.430734	1.972532
	H	3.870307	2.226487	2.668009
	C	2.74146	1.986701	0.858333
	O	2.396066	1.078304	-0.03294
	O	2.422183	3.153133	0.85522
	Cl	5.19013	0.830182	1.298063
	Cl	2.776149	0.148409	2.897037
	H	1.824784	1.466241	-0.75279
PDMS x MBAA	C	-0.95386	0.831417	-0.29261
	H	-0.73033	-0.20315	-0.5655
	H	-0.38719	1.082814	0.607761
	H	-2.01739	0.894878	-0.0433
	Si	-0.56698	1.998281	-1.68995
	O	1.038196	1.748586	-2.18226
	O	-1.55267	1.582958	-2.9746
	H	-1.19508	1.865276	-3.83077
	C	-0.77808	3.795319	-1.22556
	H	-1.80115	3.982234	-0.88557
	H	-0.09669	4.073291	-0.4163
	H	-0.58101	4.451874	-2.07772
	Si	1.847617	2.079685	-3.62066
	C	2.911562	3.599483	-3.43911
	H	3.409276	3.838083	-4.38402
	H	2.318067	4.465928	-3.13609
	H	3.687831	3.436002	-2.68587
	C	2.806654	0.56244	-4.11949
	H	3.584625	0.326605	-3.38791
	H	2.145504	-0.30374	-4.20895
	H	3.293726	0.722047	-5.08619
	O	0.572438	2.361592	-4.68738
	H	0.733069	2.875598	-5.48456
	C	4.071901	0.220618	1.452514
	C	3.186899	1.07475	0.5717
	O	2.641398	0.379085	-0.42308
	O	3.015752	2.26048	0.758288
	H	4.66254	-0.48376	0.874477
	H	4.691478	0.845596	2.085124
	Br	2.957692	-0.87115	2.671278
	H	2.063183	0.953482	-0.98846
PDMS x MCAA	C	-1.22542	0.865092	-0.35671
	H	-0.93794	-0.17032	-0.55678
	H	-0.75257	1.182188	0.576539
	H	-2.30879	0.893943	-0.20591
	Si	-0.76014	1.982032	-1.77095
	O	0.895183	1.790331	-2.09716
	O	-1.59658	1.456207	-3.11907
	H	-1.17145	1.714961	-3.95144
	C	-1.09672	3.786072	-1.42316
	H	-2.1556	3.9372	-1.1927

	H	-0.51115	4.13603	-0.56808
	H	-0.84719	4.410546	-2.28564
	Si	1.824319	2.101977	-3.46696
	C	2.780177	3.688956	-3.2619
	H	3.357395	3.912508	-4.16426
	H	2.112468	4.531565	-3.06448
	H	3.483702	3.607247	-2.42824
	C	2.908338	0.622112	-3.78993
	H	3.619799	0.466683	-2.97404
	H	2.307392	-0.28472	-3.89894
	H	3.481288	0.765636	-4.71101
	O	0.647557	2.258805	-4.66428
	H	0.858837	2.744977	-5.46715
	C	3.669831	0.605486	1.868357
	H	3.212679	0.777714	2.840604
	C	2.835346	1.314822	0.816177
	O	2.343726	0.547998	-0.14209
	O	2.667703	2.513541	0.905231
	H	4.666412	1.042516	1.865476
	Cl	3.863907	-1.17992	1.672496
	H	1.817397	1.084596	-0.79235
PDMS x TBAA	C	-1.04635	0.999694	-0.23968
	H	-0.74518	-0.04297	-0.36908
	H	-0.54592	1.398299	0.64665
	H	-2.1236	1.020637	-0.04922
	Si	-0.66261	2.010102	-1.75413
	O	0.988111	1.824817	-2.12804
	O	-1.53412	1.359075	-3.02183
	H	-1.16355	1.584078	-3.88915
	C	-1.02438	3.829507	-1.53891
	H	-2.07602	3.977352	-1.27559
	H	-0.41217	4.258883	-0.74064
	H	-0.82617	4.387501	-2.45831
	Si	1.846913	2.093877	-3.55693
	C	2.77514	3.707244	-3.4689
	H	3.306288	3.897308	-4.40662
	H	2.099573	4.54572	-3.28142
	H	3.517054	3.678705	-2.66562
	C	2.944694	0.621071	-3.862
	H	3.698977	0.51795	-3.07702
	H	2.358257	-0.30089	-3.89873
	H	3.468089	0.731902	-4.81646
	O	0.610293	2.169172	-4.69891
	H	0.760597	2.648076	-5.51963
	C	3.91688	0.710607	1.674224
	C	3.017199	1.495401	0.673695
	O	2.501052	0.688739	-0.23096
	O	2.847365	2.684674	0.753276
	Br	4.647025	1.911336	3.032481
	Br	5.39831	-0.11241	0.66188

	Br	2.830517	-0.68427	2.548662
	H	1.935405	1.187515	-0.88889
PDMS x TCAA	C	-0.83087	0.882664	-0.04547
	H	-0.57353	-0.15499	-0.2732
	H	-0.22224	1.212968	0.800254
	H	-1.87853	0.911613	0.268842
	Si	-0.59362	1.977411	-1.53147
	O	1.000121	1.781647	-2.09887
	O	-1.61899	1.423707	-2.72766
	H	-1.33105	1.673215	-3.61958
	C	-0.87555	3.787514	-1.17068
	H	-1.88722	3.944333	-0.78464
	H	-0.16717	4.152202	-0.42126
	H	-0.76075	4.395335	-2.07252
	Si	1.699421	2.048659	-3.6128
	C	2.698058	3.621477	-3.59929
	H	3.125843	3.815107	-4.58766
	H	2.083359	4.480022	-3.31686
	H	3.524818	3.543119	-2.88736
	C	2.693242	0.539618	-4.06299
	H	3.517459	0.384375	-3.36097
	H	2.065043	-0.35519	-4.05822
	H	3.1223	0.651403	-5.06322
	O	0.348152	2.198717	-4.6078
	H	0.421416	2.706641	-5.42156
	C	4.325843	0.851004	1.408309
	C	3.354554	1.596895	0.433935
	O	3.245855	2.794365	0.425656
	O	2.711437	0.736252	-0.32479
	H	2.082954	1.197098	-0.95375
	Cl	5.480743	-0.13878	0.447055
	Cl	5.229409	2.024525	2.399656
	Cl	3.351466	-0.21838	2.480272

Figures S1 – S9 depict the ball and stick models of the sorbent monomers interacting with the analyte molecules after DFT calculations.



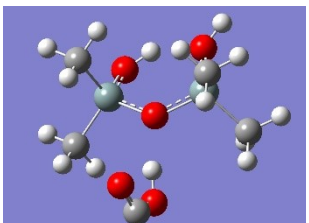


Figure S1 – Ball and stick model of the HLB (left) and PDMS (right) monomers and MCAA interaction after DFT calculations.

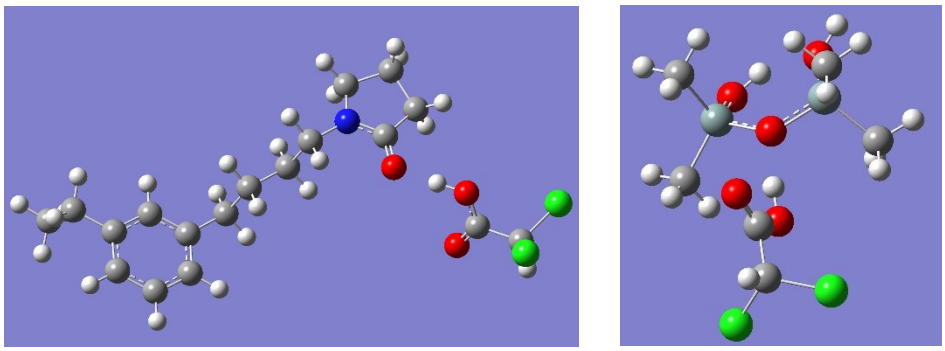


Figure S2 – Ball and stick model of the HLB (left) and PDMS (right) monomers and DCAA interaction after DFT calculations.

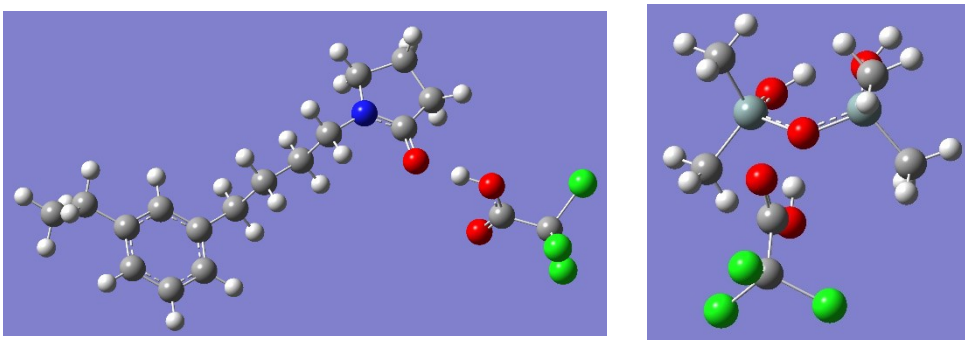


Figure S3 – Ball and stick model of the HLB (left) and PDMS (right) monomers and TCAA interaction after DFT calculations.

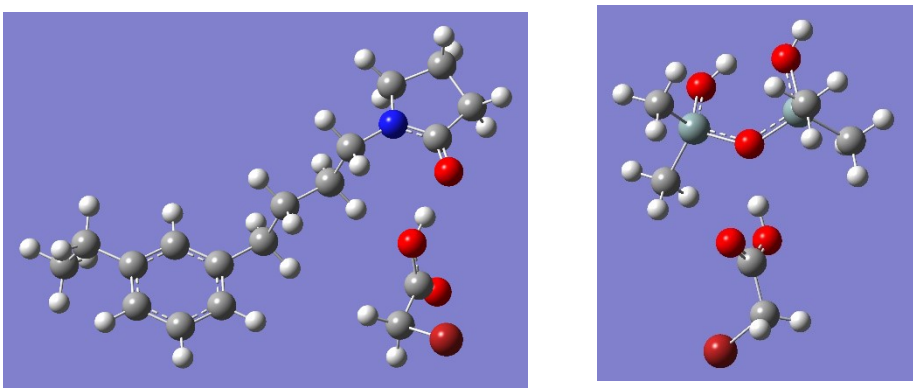


Figure S4 – Ball and stick model of the HLB (left) and PDMS (right) monomers and MBAA interaction after DFT calculations.

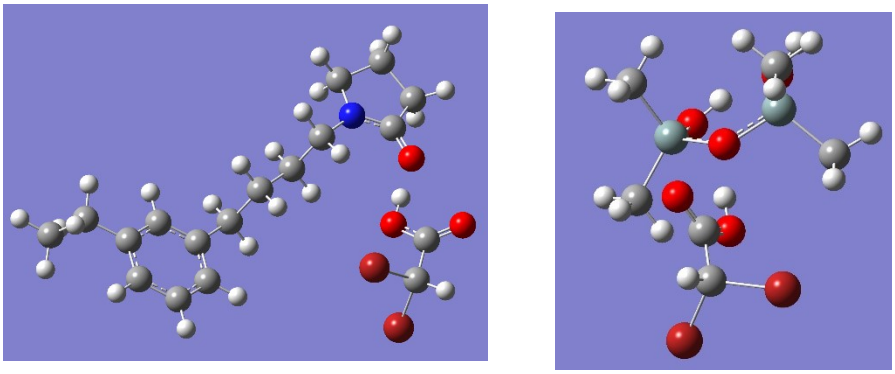


Figure S5 – Ball and stick model of the HLB (left) and PDMS (right) monomers and DBAA interaction after DFT calculations.

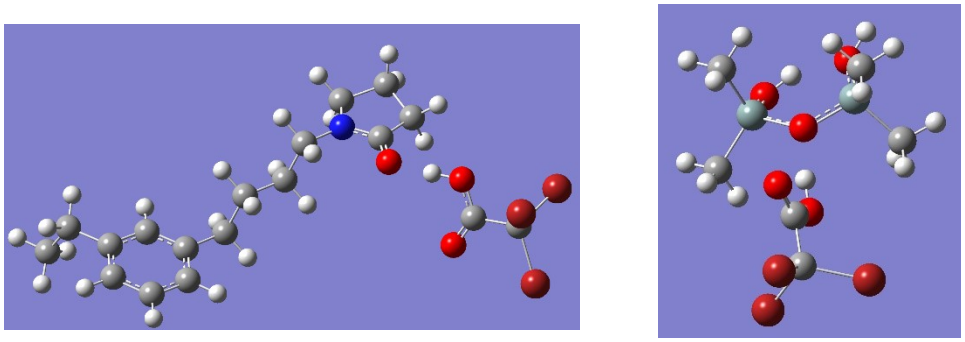


Figure S6 – Ball and stick model of the HLB (left) and PDMS (right) monomers and TBAA interaction after DFT calculations.

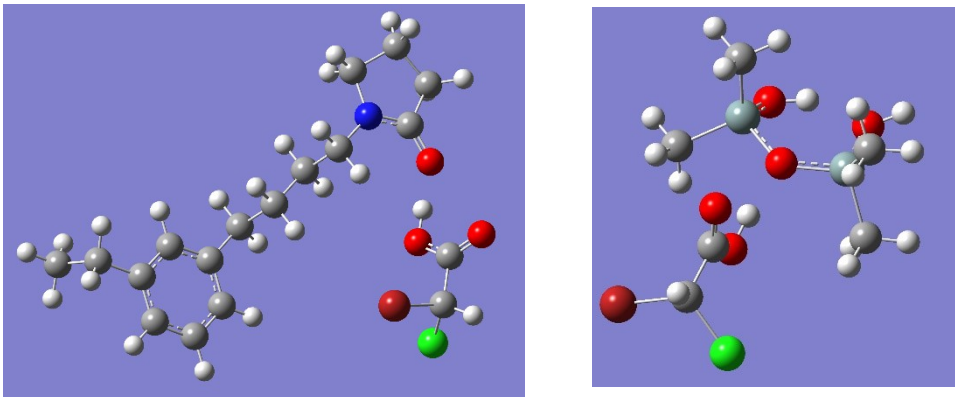


Figure S7 – Ball and stick model of the HLB (left) and PDMS (right) monomers and BCAA interaction after DFT calculations.

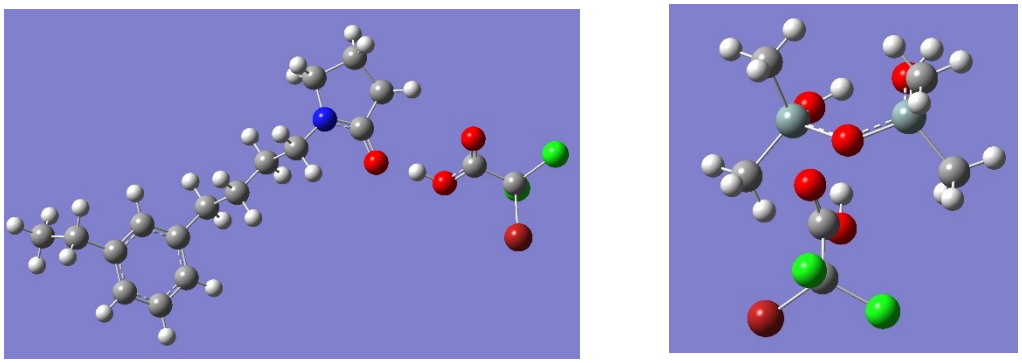


Figure S8 – Ball and stick model of the HLB (left) and PDMS (right) monomers and BDCAA interaction after DFT calculations.

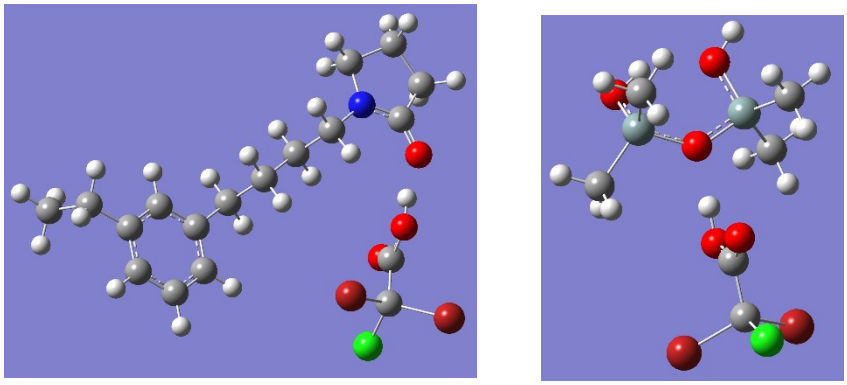


Figure S9 – Ball and stick model of the HLB (left) and PDMS (right) monomers and CDBAA interaction after DFT calculations.

Table S4: Geometries of the analytes and interfaces showing the hydrogen bonding character of the interfaces.

		HLB			PDMS		
	X-H analyte	**X-H interface**	**Bond angle interface**	**H-Y interface**	**X-H interface**	**Bond angle**	**H-Y interface**
MCAA	0.971	1.019	172	1.564	0.994	171	1.746
DCAA	0.971	1.029	174	1.520	0.998	171	1.709
TCAA	0.971	1.042	174	1.474	1.001	173	1.681
MBAA	0.971	1.006	172	1.615	0.991	171	1.763
DBAA	0.971	1.014	176	1.571	0.997	171	1.715
TBAA	0.971	1.038	175	1.487	1.001	172	1.685
CDBAA	0.971	1.021	171	1.536	1.001	172	1.681
BDCAA	0.971	1.040	172	1.479	1.001	172	1.680
BCAA	0.971	1.015	174	1.565	0.997	172	1.718

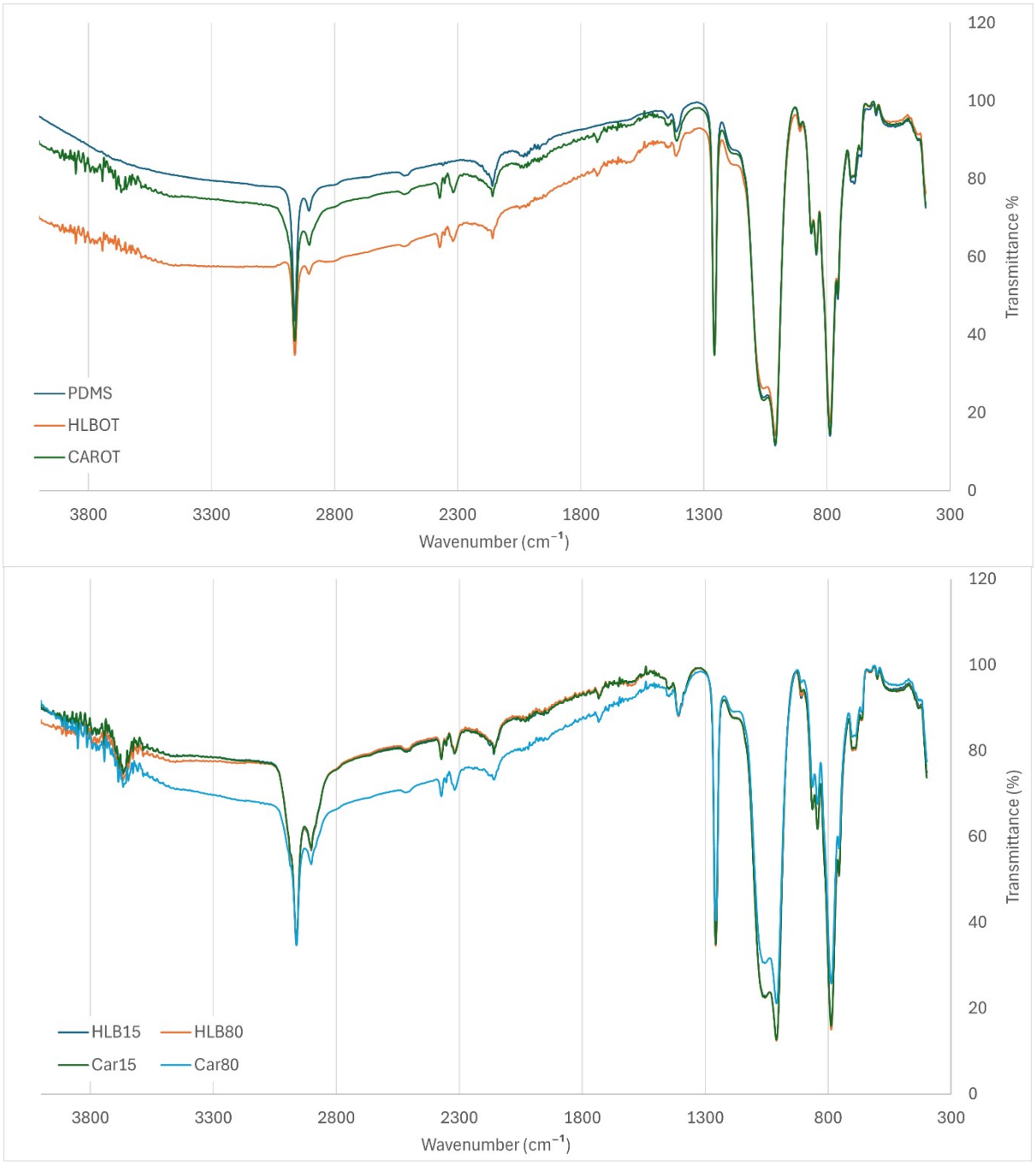


Figure S10 – FTIR spectra of the PDMS thin film, and the HLB and Carboxen® impregnated thin films. At the top the PDMS thin film and the film with the sorbent added to the surface directly are shown. At the bottom the PDMS thin films with the sorbent added to the PDMS prior to synthesis are shown.

Table S5: Amounts of sorbents added to achieve different film coverages, as well as the percent coverage and average particle sizes, as determined with ImageJ from micrographs.

	Mass added	**% coverage**	**Average particle**		**Mass added**	**% coverage**	**Average particle**

	(g)	size (µm)			(g)		size (µm)
		HLB15				**Car15**	
film4_2	0.203	17.5	565	**film4_1**	0.509	14.4	740.1
film2_1		15.3	676.6	**film4_1**		18.4	766.9
film5_2		13.1	613.7	**film1_1**		20.2	2704.3
				film1_1		22.3	2770.3
average		15.3	618.8	**average**		18.8	1745.4
Std. dev.		2.19	55.5	**Std. dev.**		1.75	944.3
%RSD		14.3	8.97	**%RSD**		9.32	54.1
		HLB80				**Car80**	
filmn2_4s1	1.11	52.9	537.8	**Car_n_2_4**	2.41	63.3	
filmn2_4s2		68.6	648.7	**Car_n_2_4**		95.7	
filmn2_4s3		81.5	653.7	**Car_n_2_4**		85.3	
average		67.7	613.4	**average**		81.5	
Std. dev.		14.3	65.5	**Std. dev.**		16.5	
%RSD		21.2	10.7	**%RSD**		20.3	
		HLBOT				**CarOT**	
film1	0.509			**film1**	1.28		

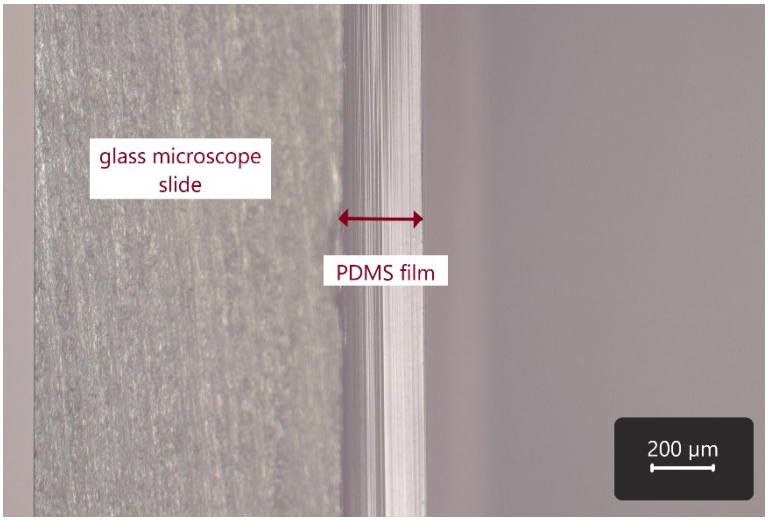


Figure S11 - Light micrograph of the side view of a PDMS film adhering to a glass microscope slide to measure the film thickness. Lines visible in the film stem from the layered approach of the synthesis process and are due to the light reflecting and refracting from the cut edge of the film.

Table S6: Summary of the p-values for the single factor ANOVA (95% confidence level), between the means of the two types of control groups (EPA and EPA_ON).

	MCAA	MBAA	DCAA	DBAA	TCAA	TBAA	BCAA	BDCAA	CDBAA
EPA & EPA_ON	0.285	0.279	0.258	0.203	0.865	0.073	0.515	0.029	0.087