A) A High Surface Area Silica-Supported Aldehyde as a Flow-Compatible Amine Scavenger

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A-1 Quantitative LC

A-1.1 Calibration curve of *N*-benzylamine

Benzylamine was made to six concentrations and was performed in triplicate as a precision measure for sample preparation. All calibration samples were prepared with an internal control to ensure instrumental precision.

In a 10.00 mL volumetric flask, 100.00 mg of the compound in question was dissolved in HPLC acetonitrile or ACN: MeOH (1:1) and filled to the calibration mark, producing a 10 $mg.mL^{-1}$ solution. A 2.00 mL fraction of sample A was transferred to a second 10 mL volumetric flask and filled to the calibration mark with HPLC acetonitrile, producing a 2 $mg.mL^{-1}$ solution. Two sub-dilutions were prepared from sample B. A 1.00 mL fraction of sample B was transferred into a third 10 mL volumetric flask and filled up to the calibration mark, resulting in a 0.2 $mg.mL^{-1}$ solution. A 2.00 mL fraction of sample B was transferred into a fourth 10 mL volumetric flask and filled up to the calibration mark, resulting in a 0.4 $mg.mL^{-1}$ solution.

Three fractions from Sample C were transferred into three separate vials; 40 μL into E (8 $\mu g.mL^{-1}$), 80 μL into F (16 $\mu g.mL^{-1}$) and 160 μL into G (32 $\mu g.mL^{-1}$). Samples E, F and G were prepared in triplicate. To each vial, 100 μL of a 0.2 $\mu g.mL^{-1}$ solution of anisole was added. The vials were filled up with the volume difference to make 1.0 mL LC samples.

Three fractions from Sample D were transferred into three separate vials; 120 μL into H (48 μg/mL), 160 μL into I (64 μg/mL) and 200 μL into J (80 μg/mL). Samples H, I and J were prepared in triplicate. To each vial, 100 μL of a 0.2 μg/mL solution of anisole was added. The vials were filled up with the volume difference to make 1.0 mL LC samples.

A-1.1.1 Method

A mixture of *N*-benzylamine and anisole was separated. A representative chromatogram is shown below (Figure A.1) which shows retention times for *N*-benzylamine as 1.529 min and anisole as 3.045 min.

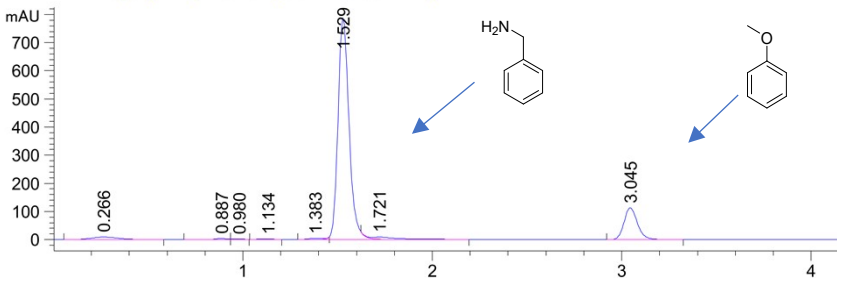


Figure A.1: Representative chromatogram of N-benzylamine and Anisole

The calibration curves for *N*-benzylamine and anisole were performed with the use of the solvent system described in table A.1. The column oven temperature was controlled at 40 $^{\circ}C$. The flowrate was set at 1.00 $mL.min^{-1}$ with a run time of 4.00 minutes and a sampling volume of 5.00 μL. Mass spectra were obtained for each peak during method development but was bypassed during the generation of the calibration curve because quantification was based on UV-VIS absorption and not on results from mass spectra. This was done due to the fact that quantification would be performed on crude reaction mixtures and we deemed it fit to bypass the MS for these samples for instrument preservation.

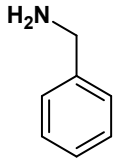
Table A.1: Solvent system and volumetric ratios used for method

	Solvent system	Volumetric ratio (%)
A	Organic (50:50 Acetonitrile: Methanol)	50
B	Aqueous Buffered (90:5:5 Aqueous phosphate buffer (10mM): Acetonitrile: Methanol)	40
C	Acetonitrile (100%)	0
D	Aqueous (90:5:5 Water: Acetonitrile: Methanol)	10

A-1.1.2 Calibration curve of *N*-benzylamine

The calibration curve of *N*-benzylamine was generated with method above. The samples were prepared in triplicate and a peak area was recorded for each sample. As an internal control, all samples were analyzed with Anisole. *N*-benzylamine was quantified at a wavelength of 210 nm and anisole at a wavelength of 250 nm.

The average area was calculated for each concentration manually (Table A.2). The area was plotted as a function of concentration. A line of best fit was included with a y-intercept set at zero. The slope of the line of best fit was found to be 38.833 with a regression of 0.9985 (Graph A.1). The slope of the line of best fit was used in the quantification calculations.

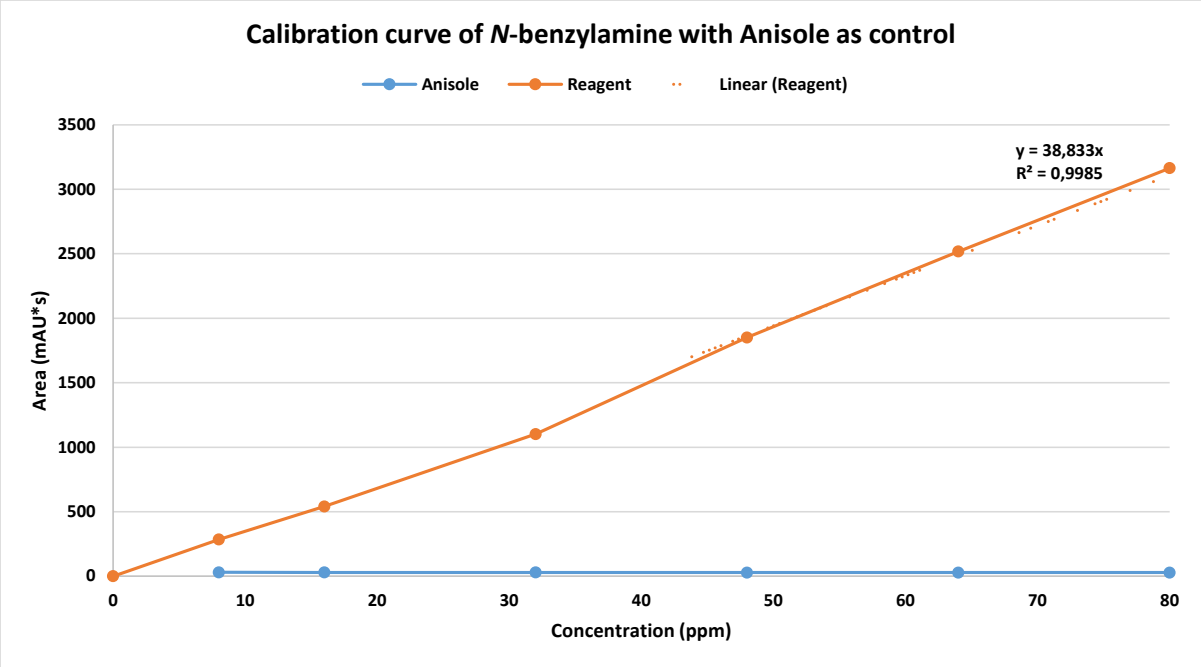


N-benzylamine
107,1531 g/mol

Scheme F.1: Structure of N-benzylamine with molar mass

Table A.2: Absorbance area data for each sample and average area for each concentration of N-benzylamine and Anisole control

		Area (mAU*s)	
Concentration	**Repeat**	***N*-Benzylamine (1.529 min) (210 nm)**	**Anisole control (3.045min) (250 nm)**
8 ppm (0.008 mg/mL)	A	290,62704	30,81436
	B	275,70724	30,43671
	C	288,02319	30,75514
	Average	284,7858233	30,66873667
16 ppm (0.016 mg/mL)	A	521,78662	28,49541
	B	513,45728	28,5079
	C	587,82275	31,41241
	Average	541,0222167	29,47190667
32 ppm (0.032 mg/mL)	A	1182,59167	31,54969
	B	1059,40552	28,24783
	C	1065,75537	28,66535
	Average	1102,584187	29,48762333
48 ppm (0.048 mg/mL)	A	1865,9563	28,0777
	B	1825,48547	27,56844
	C	1861,00989	28,81656
	Average	1850,81722	28,15423333
64 ppm (0.064 mg/mL)	A	2530,54248	28,36065
	B	2504,09912	28,21263
	C	2517,97192	28,38569
	Average	2517,53784	28,31965667
80 ppm (0.080 mg/mL)	A	3188,02783	28,36313
	B	3192,72534	28,24411
	C	3109,69067	28,84111
	Average	3163,48128	28,48278333



Graph A.1: Calibration curve of N-benzylamine (orange) and anisole (blue) as a control

A-1.2 Quantification of *N*-benzylamine

Table A.3: Dilutions and conversion calculations

Sample	Area	[LC sample] (ppm)	Dilution factor code	Dilution Factor	[Rxn sample]	[Rxn sample]	Volume of reaction sample	Total mass	Total moles	Collection scale	Absorbed moles	Percentage unabsorbed moles
	A	B	C	D	E	F	G	H	I	J	K	L
Unit	*mAU*s*	*ug/mL*	-	-	*ug/mL*	*mg/mL*	*mL*	*mg*	*mol*	*mol*	*mol*	*%*
Description	*Area given from LC chromatogram*	*Calculated concentration of analyte in LC sample based on area given by chromatogram*	*Concentration of reaction sample divided by the final diluted concentration of the analysed LC sample*		*Calculated concentration of analyte in original reaction solution based on area given by chromatogram*		*Volume of original reaction sample*	*Calculated Mass of analyte in original reaction sample*	*Calculated moles of analyte in original reaction sample*	*Theoretical Moles per reaction collection vial of limiting reagent (investment moles)*	*Moles that wast retained in polymer and was not eluted*	*Percentage moles that was not retained in polymer*
Formula	-	*A/38.833*	*From dilution factor table*		*B x D*	*E/1000*	-	*F x G*	*(H/1000)/107.1531*	*From dilution factor table*	*I - J*	*(I/J) x 100*
1 polymer test	767,04913	19,75250766	PDF001	20	395,0501532	0,395050153	25	9,87625383	9,21696E-05	0,0004	0,00030783	23,04238942
2 polymer test	908,43884	23,39347565	PDF001	20	467,869513	0,467869513	25	11,6967378	0,000109159	0,0004	0,000290841	27,28977936
3 polymer test	929,54144	23,93689491	PDF001	20	478,7378982	0,478737898	25	11,9684475	0,000111695	0,0004	0,000288305	27,92370789
4 polymer test	742,42902	19,11850797	PDF001	20	382,3701594	0,382370159	25	9,55925399	8,92112E-05	0,0004	0,000310789	22,30279382
Partition 1	54,19356	1,395554297	PDF002	267,3796791	373,1428601	0,37314286	1	0,37314286	3,48233E-06	0,0004	0,000396518	0,870583446
Partition 2	39,61137	1,020044035	PDF002	267,3796791	272,7390467	0,272739047	1	0,27273905	2,54532E-06	0,0004	0,000397455	0,636330276
Partition 3	43,3489	1,116290269	PDF002	267,3796791	298,4733338	0,298473334	1	0,29847333	2,78548E-06	0,0004	0,000397215	0,696371206
Partition 4	41,83158667	1,077217487	PDF002	267,3796791	288,026066	0,288026066	1	0,28802607	2,68799E-06	0,0004	0,000397312	0,671996578
Partition 5	43,93217333	1,131310312	PDF002	267,3796791	302,4893881	0,302489388	1	0,30248939	2,82296E-06	0,0004	0,000397177	0,705741103
Partition 6	40,44244333	1,041445248	PDF002	267,3796791	278,4612964	0,278461296	1	0,2784613	2,59872E-06	0,0004	0,000397401	0,649680915
Partition 7	41,28297	1,063089898	PDF002	267,3796791	284,2486358	0,284248636	1	0,28424864	2,65273E-06	0,0004	0,000397347	0,663183416
Loading cap 1	163,7425367	4,216582202	PDF003	134,0482574	565,2254963	0,565225496	1	0,5652255	5,27493E-06	0,0004	0,000394725	1,31873342
Loading cap 2	127,5750233	3,285221933	PDF003	134,0482574	440,3782752	0,440378275	1	0,44037828	4,1098E-06	0,0004	0,00039589	1,027451085
Loading cap 3	154,9674567	3,990612537	PDF003	134,0482574	534,9346565	0,534934656	1	0,53493466	4,99225E-06	0,0004	0,000395008	1,24806155
Loading cap 4	176,4804533	4,544600039	PDF003	134,0482574	609,1957157	0,609195716	1	0,60919572	5,68528E-06	0,0004	0,000394315	1,421320792
Loading cap 5	240,12392	6,183501661	PDF003	134,0482574	828,8876221	0,828887622	1	0,82888762	7,73554E-06	0,0004	0,000392264	1,933886239
Loading cap 6	221,9675833	5,715952497	PDF003	134,0482574	766,2134715	0,766213472	1	0,76621347	7,15064E-06	0,0004	0,000392849	1,787660533
Loading cap 7	263,2082967	6,777954231	PDF003	134,0482574	908,5729533	0,908572953	1	0,90857295	8,4792E-06	0,0004	0,000391521	2,119800905
Loading cap 8	264,1973233	6,803422948	PDF005	134,0482574	911,9869903	0,91198699	2	1,82397398	1,70221E-05	0,0004	0,000382978	4,255532459
Loading cap 9	346,7359433	8,928899218	PDF004	160,7717042	1435,514344	1,435514344	4	5,74205737	5,35874E-05	0,0004	0,000346413	13,39685314
DOE1-pol-N1	677,053955	17,43501545	PDF006	160,7717042	2803,057146	2,803057146	4	11,2122286	0,000104637	0,0004	0,000295363	26,15936586
DOE1-pol-N2	51,18441	1,31806479	PDF015	5	6,590323951	0,006590324	1	0,00659032	6,15038E-08	0,0004	0,000399938	0,015375953
DOE1-pol-N3	503,0621	12,95450004	PDF007	160,7717042	2082,717048	2,082717048	25	52,0679262	0,000485921	0,002	0,001514079	24,29604286
DOE1-pol-N4	3223,879635	83,01907231	PDF008	160,7717042	13347,11773	13,34711773	4	53,3884709	0,000498245	0,002	0,001501755	24,91223816
DOE1-pol-N5	101,627045	2,617027914	PDF009	100	261,7027914	0,261702791	1	0,26170279	2,44233E-06	0,0004	0,000397558	0,610581475
DOE1-pol-N6	45,233115	1,164811243	PDF009	100	116,4811243	0,116481124	1	0,11648112	1,08705E-06	0,0004	0,000398913	0,271763309
DOE1-pol-N7	38,89594	1,001620786	PDF010	100	100,1620786	0,100162079	1	0,10016208	9,34757E-07	0,002	0,001999065	0,046737835
DOE1-pol-N8	49,901265	1,285022146	PDF010	100	128,5022146	0,128502215	1	0,12850221	1,19924E-06	0,002	0,001998801	0,059961968
DOE1-pol-N9	6,287735	0,161917313	PDF009	20	3,238346252	0,003238346	1	0,00323835	3,02217E-08	0,0004	0,00039997	0,007555419
DOE1-pol-N10	101,652475	2,61768277	PDF009	20	52,3536554	0,052353655	1	0,05235366	4,88587E-07	0,0004	0,000399511	0,122146852
DOE1-pol-N11	114,336805	2,944320681	PDF010	20	58,88641362	0,058886414	1	0,05888641	5,49554E-07	0,002	0,00199945	0,027477699
DOE1-pol-N12	13,10226	0,337400149	PDF010	20	6,748002987	0,006748003	1	0,006748	6,29753E-08	0,002	0,001999937	0,003148767
DOE1-pol-N13	6,89546	0,177567018	PDF009	100	17,75670177	0,017756702	1	0,0177567	1,65713E-07	0,0004	0,000399834	0,041428344
DOE1-pol-N14	15,247185	0,392634744	PDF009	100	39,26347436	0,039263474	1	0,03926347	3,66424E-07	0,0004	0,000399634	0,091606016
DOE1-pol-N15	348,72255	8,98005691	PDF011	100	898,005691	0,898005691	4	3,59202276	3,35223E-05	0,002	0,001966478	1,676117053

DOE1-pol-N16	34,10644	0,878284964	PDF010	100	87,82849638	0,087828496	1	0,0878285	8,19654E-07	0,002	0,00199918	0,040982714
DOE1-pol-N17	3888,80615	100,1417905	PDF012	20	2002,83581	2,00283581	10	20,0283581	0,000186913	0,0012	0,001013087	15,57612278
DOE1-pol-N18	4472,891605	115,1827468	PDF013	20	2303,654935	2,303654935	10	23,0365494	0,000214987	0,002	0,001785013	10,74936206
DOE1-pol-N19	3198,91565	82,37621739	PDF014	20	1647,524348	1,647524348	10	16,4752435	0,000153754	0,0012	0,001046246	12,81285335
DOE1-pol-N20	2826,13672	72,77667757	PDF014	20	1455,533551	1,455533551	10	14,5553355	0,000135837	0,0012	0,001064163	11,31973434
DOE1-pol-N21	2816,791135	72,53601666	PDF014	20	1450,720333	1,450720333	10	14,5072033	0,000135388	0,0012	0,001064612	11,28230178
DOE1-pol-N22	3380,22607	87,04519532	PDF014	20	1740,903906	1,740903906	10	17,4090391	0,000162469	0,0012	0,001037531	13,53906938
Spent pol part 1	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 2	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 3	7029,897705	181,0289626	PDF016	50	9051,44813	9,05144813	1	9,05144813	8,44721E-05	0,0004	0,000315528	21,11802675
Spent pol part 4	5493,321045	141,4601253	PDF016	50	7073,006264	7,073006264	1	7,07300626	6,60084E-05	0,0004	0,000333992	16,50210368
Spent pol part 5	18,37477	0,473174104	PDF016	50	23,65870522	0,023658705	1	0,02365871	2,20793E-07	0,0004	0,000399779	0,055198369
Spent pol part 6	11,884465	0,306040352	PDF016	50	15,30201761	0,015302018	1	0,01530202	1,42805E-07	0,0004	0,000399857	0,035701295
Spent pol part 7	7,441235	0,19162143	PDF016	50	9,581071511	0,009581072	1	0,00958107	8,94148E-08	0,0004	0,000399911	0,022353697
Spent pol part 8	11,553965	0,29752955	PDF016	50	14,87647748	0,014876477	1	0,01487648	1,38834E-07	0,0004	0,000399861	0,034708463
Spent pol part 9	9,73908	0,250793912	PDF016	50	12,53969562	0,012539696	1	0,0125397	1,17026E-07	0,0004	0,000399883	0,029256493
Spent pol part 10	12,037585	0,30998339	PDF016	50	15,49916952	0,01549917	1	0,01549917	1,44645E-07	0,0004	0,000399855	0,036161272
Spent pol part 11	3,679685	0,09475665	PDF016	50	4,737832514	0,004737833	1	0,00473783	4,42155E-08	0,0004	0,000399956	0,011053886
Spent pol part 12	13,625635	0,350877733	PDF016	50	17,54388664	0,017543887	1	0,01754389	1,63727E-07	0,0004	0,000399836	0,040931822
Spent pol part 13	12,132515	0,312427961	PDF016	50	15,62139804	0,015621398	1	0,0156214	1,45786E-07	0,0004	0,000399854	0,036446444
Spent pol part 14	4,34986	0,112014524	PDF016	50	5,600726186	0,005600726	1	0,00560073	5,22684E-08	0,0004	0,000399948	0,013067112
Spent pol part 15	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 16	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 17	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 18	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 19	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Spent pol part 20	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Silica part 1	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Silica part 2	0	0	PDF016	50	0	0	1	0	0	0,0004	0,0004	0
Silica part 3	6,26719	0,161388252	PDF016	50	8,069412613	0,008069413	1	0,00806941	7,53073E-08	0,0004	0,000399925	0,01882683
Silica part 4	4,06414	0,104656864	PDF016	50	5,2328432	0,005232843	1	0,00523284	4,88352E-08	0,0004	0,000399951	0,0122088
Silica part 5	4,258515	0,109662272	PDF016	50	5,483113589	0,005483114	1	0,00548311	5,11708E-08	0,0004	0,000399949	0,012792709
Silica part 6	608,431275	15,66789264	PDF016	50	783,3946321	0,783394632	1	0,78339463	7,31098E-06	0,0004	0,000392689	1,827746076
Silica part 7	3386,14856	87,1977071	PDF016	50	4359,885355	4,359885355	1	4,35988536	4,06884E-05	0,0004	0,000359312	10,17209338
Silica part 8	3352,272095	86,32534429	PDF016	50	4316,267215	4,316267215	1	4,31626721	4,02813E-05	0,0004	0,000359719	10,07032744
Silica part 9	1875,064695	48,28534223	PDF016	50	2414,267112	2,414267112	1	2,41426711	2,2531E-05	0,0004	0,000377469	5,632751436
Silica part 10	805,648135	20,74648199	PDF016	50	1037,324099	1,037324099	1	1,0373241	9,68077E-06	0,0004	0,000390319	2,420191528
Silica part 11	349,438625	8,998496768	PDF016	50	449,9248384	0,449924838	1	0,44992484	4,1989E-06	0,0004	0,000395801	1,049724269
Silica part 12	58,909155	1,51698697	PDF016	50	75,84934849	0,075849348	1	0,07584935	7,0786E-07	0,0004	0,000399292	0,176964895
Silica part 13	20,451585	0,526654778	PDF016	50	26,33273891	0,026332739	1	0,02633274	2,45749E-07	0,0004	0,000399754	0,061437184
Silica part 14	10,371205	0,267071949	PDF016	50	13,35359746	0,013353597	1	0,0133536	1,24622E-07	0,0004	0,000399875	0,031155416
Silica part 15	12,924695	0,332827621	PDF016	50	16,64138104	0,016641381	1	0,01664138	1,55305E-07	0,0004	0,000399845	0,038826177
Silica part 16	5,69619	0,146684263	PDF016	50	7,334213169	0,007334213	1	0,00733421	6,84461E-08	0,0004	0,000399932	0,017111528
Silica part 17	14,584125	0,375560091	PDF016	50	18,77800453	0,018778005	1	0,018778	1,75245E-07	0,0004	0,000399825	0,043811156
Silica part 18	12,13399	0,312465944	PDF016	50	15,6232972	0,015623297	1	0,0156233	1,45804E-07	0,0004	0,000399854	0,036450875
Silica part 19	2,915645	0,075081632	PDF016	50	3,75408158	0,003754082	1	0,00375408	3,50347E-08	0,0004	0,000399965	0,008758686
Silica part 20	3,828675	0,098593336	PDF016	50	4,929666778	0,004929667	1	0,00492967	4,60058E-08	0,0004	0,000399954	0,011501456

A-1.7 LC dilution factors

Table A.4: Calculations of dilution factors

Flow reaction details											Additional Dilutions after collection				LC sample Details						Dilution factor
Code	**[Stock]**	**Rxn scale**	**Rxn scale**	**Rxn Scale**	**Pumps**	**Rxn plug**	**[Rxn plug]**	**Coll. Vol.**	**Coll. Scale**	**[Rxn plug]**	**Initial mol**	**final vol.**	**final []**	**final []**	**Vol. sln**	**Vol. sln.**	**Mass**	**Tot. vol**	**[LC sample]**	**[LC sample]**	
	A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*O*	*P*	*Q*	*R*	*S*	*T*	
Unit	*mol/L*	*mL*	*L*	*mol*	*number*	*mL*	*mol/mL*	*mL*	*mol*	*mg/mL*	*mol*	*mL*	*mol/mL*	*mg/mL*	*uL*	*mL*	*mg*	*mL*	*mg/mL*	*ug/mL*	
Specific dilution factor	*Concentration of stock solution*	*Size of sampling volume*	*Size of sampling volume*	*reaction scale in mol*	*Number of pumps (dilution factor)*	*Size of reaction plug after mixing point*	*Concentration of plug after mixing*	*Volume of collection per vial*	*Moles per collection vial*	*Concentration of reaction plug*	*initial mol of sample*	*Final volume after dilution*	*Final concentration*	*Final concentration*	*volume of reaction solution*	*volume of reaction solution*	*mass of reaction solution in LC sample*	*Total volume of LC sample*	*Concentration of LC sample*	*ppm*	*Initial concentration divided by the final concentration*
Formula	-	-	*B*/1000	*C* x *A*	-	-	*D*/*F*	-	*G* x *H*	*G* x MW x 1000 MW= 107.1531 g/mol	= *I*	-	*K*/*L*	*M* x MW x 1000 MW= 107.1531 g/mol	-	*O*/1000	*N* x *P*	-	*Q*/*R*	*S* x 1000	*N* / *S*
PDF001	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	25	0,000016	1,7144496	50	0,05	0,08572248	1	0,08572248	85,72248	20
PDF002	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	1	0,0004	42,86124	3,74	0,00374	0,160301038	1	0,160301038	160,3010376	267,3796791
PDF003	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	1	0,0004	42,86124	7,46	0,00746	0,31974485	1	0,31974485	319,7448504	134,0482574
PDF004	0,24	2	0,002	0,00048	1	2	0,00024	2	0,00048	25,716744	0,00048	4	0,00012	12,858372	6,22	0,00622	0,079979074	1	0,079979074	79,97907384	160,7717042
PDF005	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	2	0,0002	21,43062	7,46	0,00746	0,159872425	1	0,159872425	159,8724252	134,0482574
PDF006	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	4	0,0001	10,71531	6,22	0,00622	0,066649228	1	0,066649228	66,6492282	160,7717042
PDF007	1	2	0,002	0,002	1	2	0,001	2	0,002	107,1531	0,002	25	0,00008	8,572248	6,22	0,00622	0,053319383	1	0,053319383	53,31938256	160,7717042
PDF008	1	2	0,002	0,002	1	2	0,001	2	0,002	107,1531	0,002	1	0,002	214,3062	6,22	0,00622	1,332984564	1	1,332984564	1332,984564	160,7717042
PDF009	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	1	0,0004	42,86124	10	0,01	0,4286124	1	0,4286124	428,6124	100
PDF010	1	2	0,002	0,002	1	2	0,001	2	0,002	107,1531	0,002	1	0,002	214,3062	10	0,01	2,143062	1	2,143062	2143,062	100
PDF011	1	2	0,002	0,002	1	2	0,001	2	0,002	107,1531	0,002	4	0,0005	53,57655	10	0,01	0,5357655	1	0,5357655	535,7655	100
PDF012	0,6	2	0,002	0,0012	1	2	0,0006	2	0,0012	64,29186	0,0012	10	0,00012	12,858372	50	0,05	0,6429186	1	0,6429186	642,9186	20
PDF013	1	2	0,002	0,002	1	2	0,001	2	0,002	107,1531	0,002	10	0,0002	21,43062	50	0,05	1,071531	1	1,071531	1071,531	20
PDF014	0,6	2	0,002	0,0012	1	2	0,0006	2	0,0012	64,29186	0,0012	10	0,00012	12,858372	50	0,05	0,6429186	1	0,6429186	642,9186	20
PDF015	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	1	0,0004	42,86124	200	0,2	8,572248	1	8,572248	8572,248	5
PDF016	0,2	2	0,002	0,0004	1	2	0,0002	2	0,0004	21,43062	0,0004	1	0,0004	42,86124	20	0,02	0,8572248	1	0,8572248	857,2248	50

A-2 BET results: Isotherm, Particle size distribution and Pore Size vs Pore Volume

A-2.1 Silica

The duration of the analysis was 244.1 min with a cold zone of 3.04092 mL and a warm zone of 3.82125 mL.

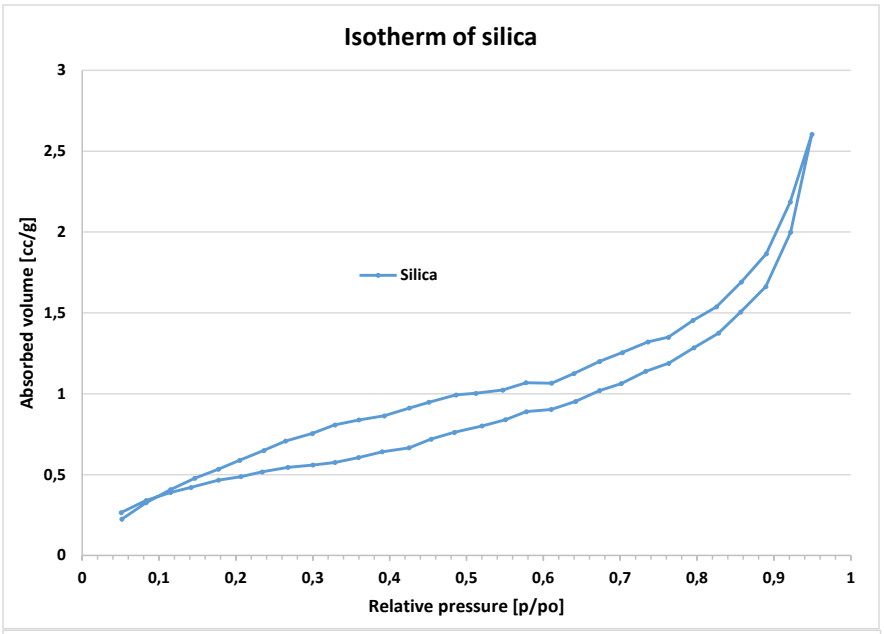
Table A.5: Summary of BET results for silica

BET Results	
Pore Volume	0.0032 cm^3/g
Surface area	1.2718 m^2/g
Lower confidence limit	0.8440 nm
Mode (Half pore width)	1.3236 nm
Fitting error	0.7242 %

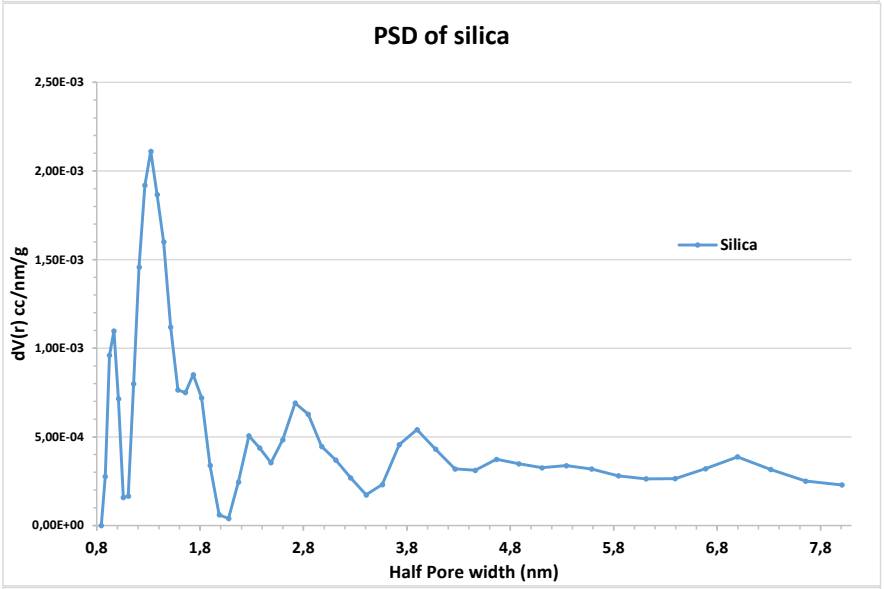
Table A.6: Raw data of BET isotherm, particle size distribution, pore size and pore volume for silica

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0505298	0,265828	0,84397	1,07E-05	0,00E+00	1,21E-02	0,00E+00
0,0829441	0,340377	0,882816	4,97E-05	2,76E-04	5,40E-02	3,13E-01
0,114767	0,389911	0,92345	9,64E-05	9,60E-04	1,02E-01	1,03E+00
0,14132	0,420922	0,965954	1,28E-04	1,10E-03	1,34E-01	1,14E+00
0,177057	0,46606	1,01041	1,35E-04	7,14E-04	1,42E-01	7,18E-01
0,206304	0,487714	1,05692	1,44E-04	1,58E-04	1,49E-01	1,57E-01
0,234136	0,517356	1,10557	1,84E-04	1,66E-04	1,83E-01	1,43E-01
0,267398	0,545281	1,15646	2,62E-04	7,99E-04	2,47E-01	6,80E-01
0,299859	0,559396	1,20969	3,69E-04	1,46E-03	3,31E-01	1,20E+00
0,328567	0,575014	1,26537	4,92E-04	1,92E-03	4,24E-01	1,51E+00
0,359282	0,605681	1,32361	6,05E-04	2,11E-03	5,07E-01	1,60E+00
0,390309	0,641351	1,38453	7,07E-04	1,87E-03	5,77E-01	1,35E+00
0,425084	0,665916	1,44826	7,82E-04	1,60E-03	6,27E-01	1,11E+00
0,453939	0,720119	1,51492	8,35E-04	1,12E-03	6,61E-01	7,46E-01
0,484015	0,761496	1,58465	8,90E-04	7,64E-04	6,94E-01	4,85E-01
0,519961	0,80132	1,65758	9,55E-04	7,50E-04	7,31E-01	4,51E-01
0,550581	0,840087	1,73388	1,01E-03	8,51E-04	7,63E-01	4,91E-01
0,577781	0,889607	1,81369	1,04E-03	7,20E-04	7,78E-01	4,00E-01
0,610075	0,9028	1,89717	1,05E-03	3,38E-04	7,81E-01	1,82E-01
0,641764	0,952467	1,98449	1,05E-03	5,96E-05	7,83E-01	3,14E-02
0,672824	1,01981	2,07583	1,07E-03	3,89E-05	7,93E-01	1,79E-02
0,701125	1,06301	2,17138	1,12E-03	2,45E-04	8,15E-01	1,10E-01
0,733096	1,13883	2,27132	1,17E-03	5,06E-04	8,35E-01	2,22E-01
0,762957	1,18873	2,37586	1,21E-03	4,37E-04	8,50E-01	1,85E-01
0,795672	1,28393	2,48522	1,26E-03	3,54E-04	8,71E-01	1,42E-01
0,82782	1,37452	2,59961	1,35E-03	4,83E-04	9,02E-01	1,84E-01
0,856476	1,50552	2,71926	1,42E-03	6,90E-04	9,29E-01	2,53E-01
0,889324	1,66187	2,84443	1,48E-03	6,28E-04	9,49E-01	2,22E-01
0,92155	1,9985	2,97535	1,53E-03	4,46E-04	9,65E-01	1,51E-01
0,949251	2,6046	3,1123	1,57E-03	3,69E-04	9,77E-01	1,19E-01
0,921017	2,18545	3,25555	1,60E-03	2,69E-04	9,85E-01	8,33E-02
0,889933	1,86519	3,4054	1,63E-03	1,73E-04	9,95E-01	5,11E-02
0,857518	1,69106	3,56214	1,71E-03	2,31E-04	1,01E+00	6,38E-02
0,825091	1,53739	3,7261	1,80E-03	4,56E-04	1,04E+00	1,22E-01
0,794637	1,45384	3,8976	1,88E-03	5,41E-04	1,06E+00	1,39E-01
0,762537	1,34975	4,077	1,94E-03	4,31E-04	1,07E+00	1,06E-01
0,73612	1,32053	4,26465	2,00E-03	3,19E-04	1,09E+00	7,51E-02
0,702591	1,25458	4,46095	2,08E-03	3,11E-04	1,10E+00	6,96E-02
0,673099	1,20031	4,66628	2,15E-03	3,73E-04	1,12E+00	7,99E-02
0,639685	1,12522	4,88105	2,22E-03	3,48E-04	1,13E+00	7,15E-02
0,610651	1,06568	5,10572	2,30E-03	3,25E-04	1,15E+00	6,37E-02
0,57732	1,0683	5,34072	2,38E-03	3,37E-04	1,16E+00	6,32E-02
0,547249	1,02284	5,58655	2,45E-03	3,18E-04	1,17E+00	5,71E-02
0,512085	1,0032	5,84368	2,52E-03	2,80E-04	1,18E+00	4,81E-02
0,48631	0,992688	6,11265	2,60E-03	2,63E-04	1,20E+00	4,31E-02
0,450965	0,947806	6,39401	2,69E-03	2,65E-04	1,21E+00	4,13E-02
0,425495	0,911467	6,68831	2,81E-03	3,20E-04	1,23E+00	4,76E-02
0,39288	0,863595	6,99616	2,91E-03	3,87E-04	1,24E+00	5,54E-02
0,360034	0,838652	7,31818	3,00E-03	3,16E-04	1,25E+00	4,34E-02
0,328682	0,807535	7,65502	3,08E-03	2,50E-04	1,26E+00	3,28E-02
0,299214	0,754101	8,00736	3,16E-03	2,28E-04	1,27E+00	2,85E-02
0,264428	0,707491					
0,236191	0,6496					
0,204748	0,589272					
0,177086	0,533694					
0,146191	0,477191					
0,11465	0,406827					
0,0829192	0,326427					

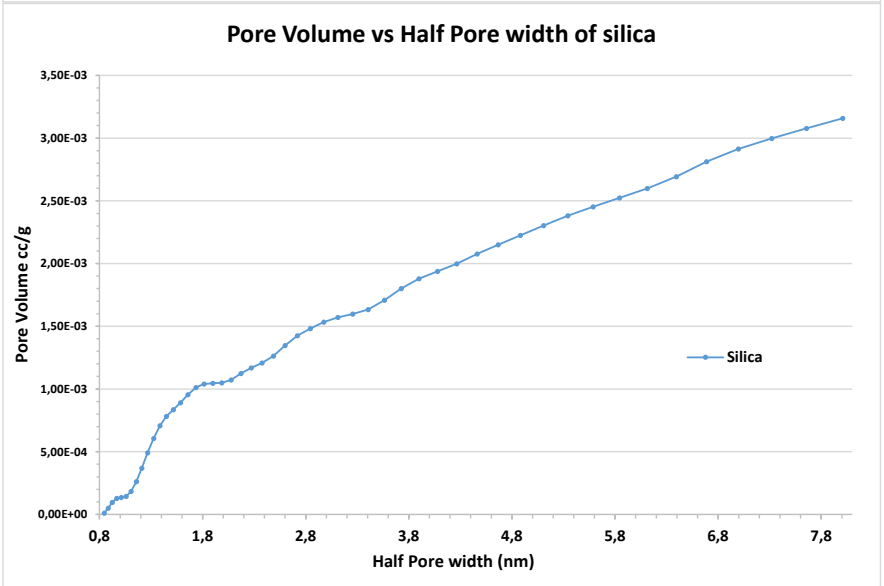
a)



b)



c)



Graph A.2: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of Silica

A-2.2 SSA-3

The duration of the analysis was 253.7 min with a cold zone of 23.6523 mL and a warm zone of 4.25158 mL.

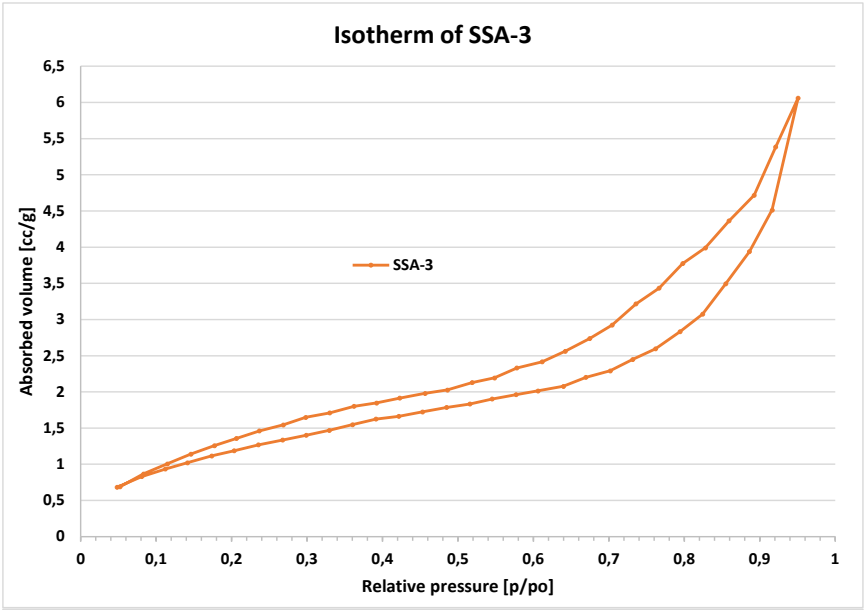
*Table A.7: Summary of BET results for **SSA-3***

Calculation Results	
Pore Volume	0.0079 cm^3/g
Surface area	3.0479 m^2/g
Lower confidence limit	0.8068 nm
Mode (Half pore width)	1.3845 nm
Fitting error	0.77 %

*Table A.8: Raw data of BET isotherm, particle size distribution, pore size and pore volume for **SSA-3***

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0479419	0,68239	0,806833	1,68E-04	4,54E-04	2,79E-01	5,62E-01
0,080914	0,830332	0,84397	2,42E-04	1,17E-03	3,62E-01	1,39E+00
0,112127	0,93484	0,882816	3,35E-04	1,90E-03	4,63E-01	2,14E+00
0,141422	1,02026	0,92345	4,14E-04	2,29E-03	5,45E-01	2,48E+00
0,173554	1,11626	0,965954	4,61E-04	1,86E-03	5,93E-01	1,94E+00
0,203154	1,18698	1,01041	4,72E-04	1,07E-03	6,04E-01	1,07E+00
0,235357	1,26787	1,05692	4,81E-04	2,32E-04	6,12E-01	2,29E-01
0,267475	1,33522	1,10557	5,28E-04	1,84E-04	6,52E-01	1,59E-01
0,298552	1,40055	1,15646	6,27E-04	9,35E-04	7,33E-01	7,94E-01
0,329366	1,46852	1,20969	7,68E-04	1,86E-03	8,44E-01	1,52E+00
0,360217	1,54714	1,26537	9,35E-04	2,53E-03	9,70E-01	1,99E+00
0,391153	1,62465	1,32361	1,11E-03	2,87E-03	1,10E+00	2,17E+00
0,421298	1,66252	1,38453	1,27E-03	2,89E-03	1,20E+00	2,09E+00
0,453071	1,72448	1,44826	1,39E-03	2,42E-03	1,29E+00	1,68E+00
0,484919	1,78493	1,51492	1,51E-03	1,94E-03	1,36E+00	1,29E+00
0,515649	1,83266	1,58465	1,60E-03	1,60E-03	1,42E+00	1,01E+00
0,54518	1,90132	1,65758	1,66E-03	1,22E-03	1,45E+00	7,42E-01
0,576754	1,96194	1,73388	1,70E-03	8,79E-04	1,47E+00	5,11E-01
0,605919	2,01314	1,81369	1,70E-03	4,26E-04	1,48E+00	2,40E-01
0,639607	2,07641	1,89717	1,71E-03	7,94E-05	1,48E+00	4,38E-02
0,66934	2,20075	1,98449	1,75E-03	7,20E-05	1,50E+00	3,47E-02
0,701637	2,29196	2,07583	1,86E-03	4,52E-04	1,55E+00	2,13E-01
0,731538	2,44943	2,17138	2,02E-03	1,16E-03	1,62E+00	5,27E-01
0,761689	2,59495	2,27132	2,18E-03	1,63E-03	1,69E+00	7,18E-01
0,79415	2,8315	2,37586	2,35E-03	1,46E-03	1,75E+00	6,18E-01
0,824053	3,0738	2,48522	2,55E-03	1,53E-03	1,83E+00	6,15E-01
0,854669	3,49301	2,59961	2,77E-03	1,75E-03	1,91E+00	6,74E-01
0,886066	3,93738	2,71926	2,99E-03	1,86E-03	1,99E+00	6,83E-01
0,916251	4,51379	2,84443	3,20E-03	1,78E-03	2,06E+00	6,28E-01
0,950705	6,06115	2,97535	3,44E-03	1,60E-03	2,14E+00	5,37E-01
0,920868	5,38502	3,1123	3,68E-03	1,75E-03	2,21E+00	5,61E-01
0,892399	4,71807	3,25555	3,89E-03	1,66E-03	2,27E+00	5,10E-01
0,85917	4,36399	3,4054	4,12E-03	1,43E-03	2,34E+00	4,20E-01
0,827803	3,99034	3,56214	4,41E-03	1,45E-03	2,41E+00	4,07E-01
0,797687	3,77406	3,7261	4,72E-03	1,75E-03	2,50E+00	4,69E-01
0,766347	3,43382	3,8976	4,97E-03	1,85E-03	2,56E+00	4,75E-01
0,735772	3,21625	4,077	5,15E-03	1,40E-03	2,60E+00	3,47E-01
0,704075	2,92277	4,26465	5,30E-03	9,13E-04	2,63E+00	2,15E-01
0,674474	2,7367	4,46095	5,48E-03	7,94E-04	2,67E+00	1,78E-01
0,642092	2,56195	4,66628	5,66E-03	8,71E-04	2,71E+00	1,86E-01
0,611402	2,41491	4,88105	5,85E-03	8,52E-04	2,75E+00	1,75E-01
0,577918	2,33055	5,10572	6,04E-03	8,23E-04	2,78E+00	1,61E-01
0,548296	2,1942	5,34072	6,21E-03	8,20E-04	2,81E+00	1,54E-01
0,518709	2,12836	5,58655	6,35E-03	6,89E-04	2,84E+00	1,24E-01
0,485969	2,02651	5,84368	6,49E-03	5,59E-04	2,86E+00	9,60E-02
0,45626	1,97901	6,11265	6,63E-03	5,16E-04	2,88E+00	8,46E-02
0,422667	1,91484	6,39401	6,81E-03	5,04E-04	2,91E+00	7,89E-02
0,391937	1,84736	6,68831	7,05E-03	5,91E-04	2,94E+00	8,78E-02
0,362114	1,80087	6,99616	7,27E-03	7,81E-04	2,97E+00	1,11E-01
0,329766	1,70978	7,31818	7,46E-03	6,96E-04	3,00E+00	9,56E-02
0,298126	1,64807	7,65502	7,65E-03	5,68E-04	3,02E+00	7,45E-02
0,268488	1,54459	8,00736	7,87E-03	5,20E-04	3,05E+00	6,49E-02
0,236678	1,46132					
0,206139	1,35619					
0,177272	1,2567					
0,145998	1,14055					
0,114596	1,00566					
0,0831815	0,86584					
0,0518673	0,688108					
0,0513587	0,224188					

a)



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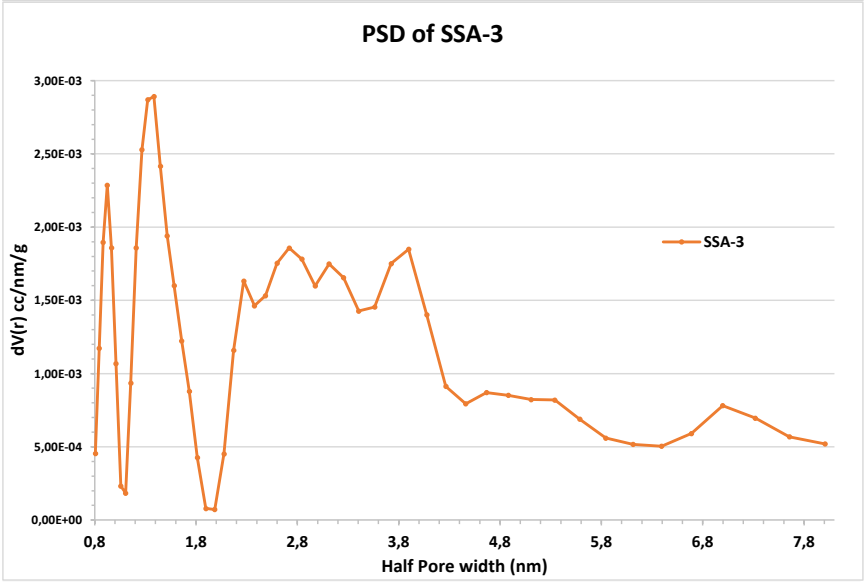
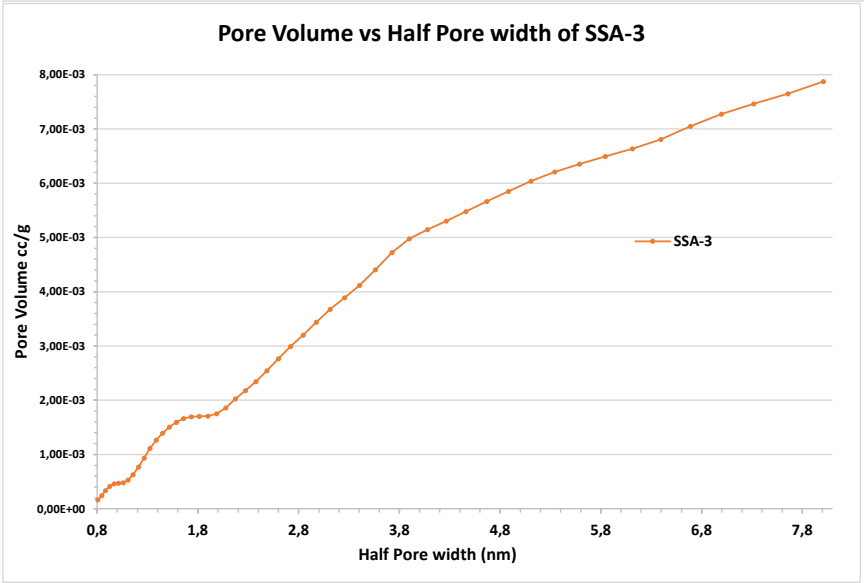


c)



*Graph A.3: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of **SSA-3***

A-2.3 SSA-4

The duration of the analysis was 1027.8 min with a cold zone of 24.3343 mL and a warm zone of 4.16389 mL.

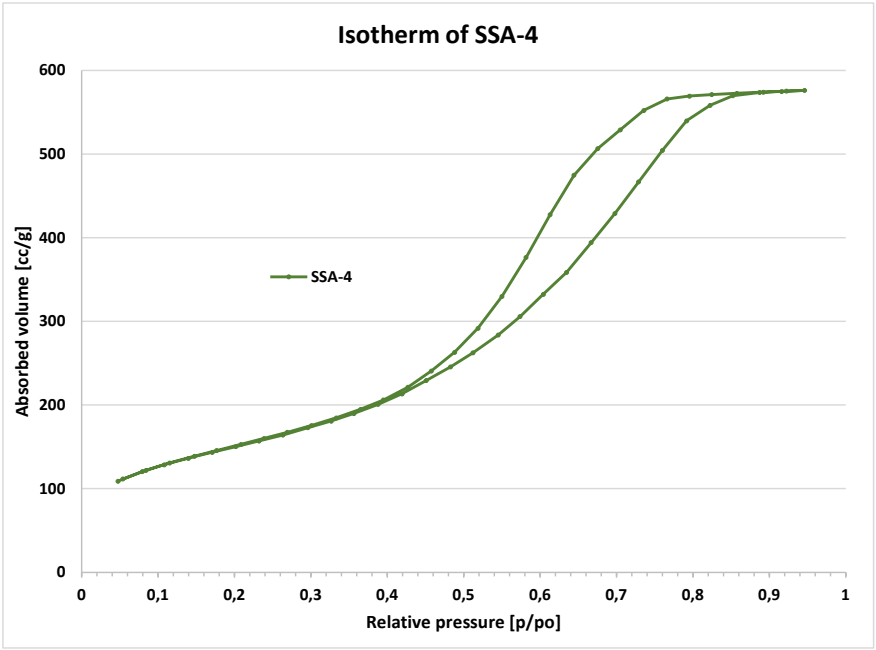
*Table A.9: Summary of BET results for **SSA-4***

Calculation Results	
Pore Volume	0.8493 cm^3/g
Surface area	424.2920 m^2/g
Lower confidence limit	0.8068 nm
Mode (Half pore width)	2.2713 nm
Fitting error	1.47 %

*Table A.10: Raw data of BET isotherm, particle size distribution, pore size and pore volume for **SSA-4***

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0476536	109,063	0,806833	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,0793329	120,434	0,84397	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,108218	128,595	0,882816	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,139705	136,412	0,92345	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,171085	143,56	0,965954	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,201967	150,392	1,01041	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,232241	157,085	1,05692	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,263298	164,19	1,10557	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,296264	172,951	1,15646	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,326676	180,885	1,20969	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,35649	189,954	1,26537	3,22E-02	0,00E+00	7,43E+01	0,00E+00
0,387949	200,897	1,32361	3,24E-02	0,00E+00	7,45E+01	0,00E+00
0,419358	213,453	1,38453	3,50E-02	3,49E-03	7,62E+01	2,41E+00
0,450836	229,268	1,44826	4,45E-02	4,19E-02	8,24E+01	2,80E+01
0,482723	245,577	1,51492	5,98E-02	1,42E-01	9,20E+01	9,25E+01
0,512113	262,453	1,58465	7,93E-02	2,19E-01	1,04E+02	1,37E+02
0,545172	283,702	1,65758	1,02E-01	2,67E-01	1,17E+02	1,61E+02
0,57383	305,838	1,73388	1,26E-01	2,92E-01	1,30E+02	1,69E+02
0,60425	332,477	1,81369	1,50E-01	3,06E-01	1,43E+02	1,69E+02
0,634693	358,771	1,89717	1,80E-01	2,84E-01	1,58E+02	1,50E+02
0,666794	394,233	1,98449	2,33E-01	3,44E-01	1,83E+02	1,72E+02
0,698005	429,228	2,07583	3,07E-01	5,88E-01	2,17E+02	2,81E+02
0,728979	466,9	2,17138	3,95E-01	7,74E-01	2,56E+02	3,55E+02
0,760094	504,412	2,27132	4,86E-01	8,78E-01	2,94E+02	3,86E+02
0,791892	539,858	2,37586	5,66E-01	8,65E-01	3,26E+02	3,65E+02
0,82266	558,44	2,48522	6,33E-01	7,32E-01	3,52E+02	2,96E+02
0,852227	569,834	2,59961	6,86E-01	5,92E-01	3,72E+02	2,29E+02
0,88729	573,75	2,71926	7,26E-01	4,44E-01	3,86E+02	1,64E+02
0,916062	575,059	2,84443	7,55E-01	3,18E-01	3,96E+02	1,13E+02
0,946027	576,251	2,97535	7,81E-01	2,19E-01	4,04E+02	7,41E+01
0,922496	575,444	3,1123	8,04E-01	1,88E-01	4,11E+02	6,06E+01
0,892332	574,204	3,25555	8,22E-01	1,62E-01	4,17E+02	5,00E+01
0,857804	572,762	3,4054	8,36E-01	1,23E-01	4,21E+02	3,62E+01
0,824748	571,318	3,56214	8,44E-01	8,72E-02	4,23E+02	2,47E+01
0,795625	569,525	3,7261	8,47E-01	4,86E-02	4,24E+02	1,32E+01
0,766176	565,97	3,8976	8,49E-01	1,99E-02	4,24E+02	5,20E+00
0,735781	552,306	4,077	8,49E-01	7,29E-03	4,24E+02	1,82E+00
0,705069	529,173	4,26465	8,50E-01	2,84E-03	4,24E+02	6,76E-01
0,675495	506,674	4,46095	8,50E-01	1,54E-03	4,24E+02	3,50E-01
0,644332	474,876	4,66628	8,50E-01	3,82E-04	4,24E+02	8,56E-02
0,613194	427,794	4,88105	8,50E-01	6,43E-05	4,24E+02	1,26E-02
0,581612	376,599	5,10572	8,50E-01	1,88E-04	4,24E+02	3,68E-02
0,550175	330,041	5,34072	8,50E-01	6,26E-05	4,24E+02	1,23E-02
0,518856	291,907	5,58655	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,488192	263,17	5,84368	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,457771	240,737	6,11265	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,427031	221,296	6,39401	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,39501	206,17	6,68831	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,365188	194,985	6,99616	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,333304	184,755	7,31818	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,301045	175,67	7,65502	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,269181	167,497	8,00736	8,50E-01	0,00E+00	4,24E+02	0,00E+00
0,238802	160,126					
0,208395	152,976					
0,176692	145,659					
0,147734	138,862					
0,115301	130,787					
0,0842931	122,072					
0,0540856	111,645					

a)



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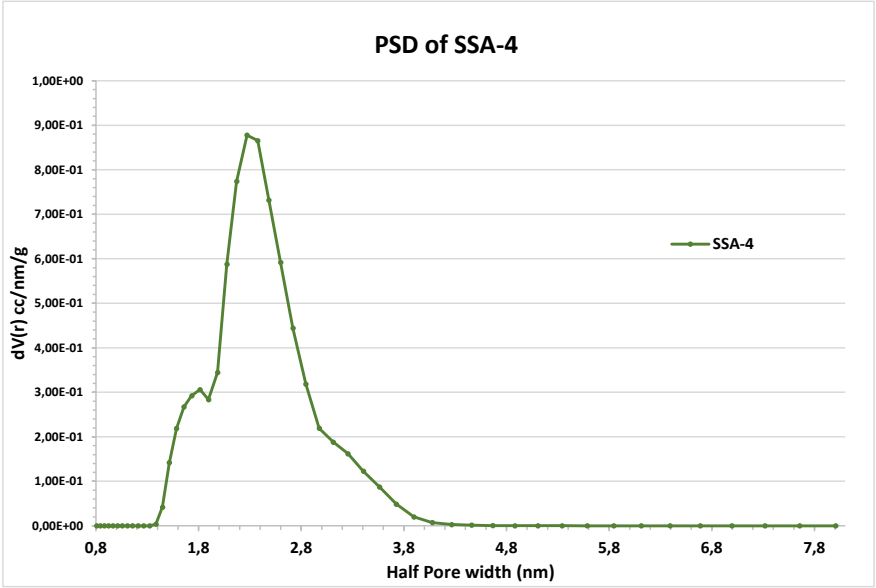

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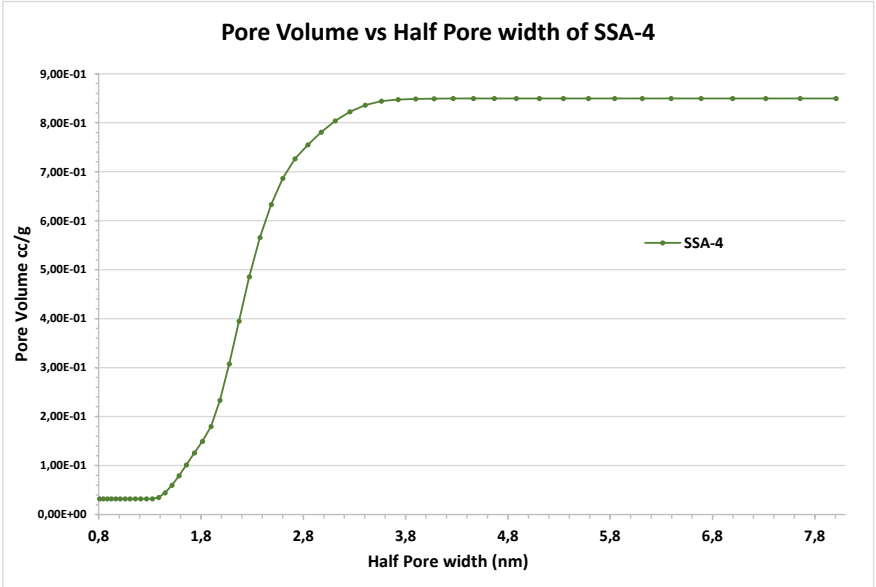


*Graph A.4: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of **SSA-4***

A-2.4 SSA-5

The duration of the analysis was 859.6 min with a cold zone of 23.8374 mL and a warm zone of 4.31597 mL.

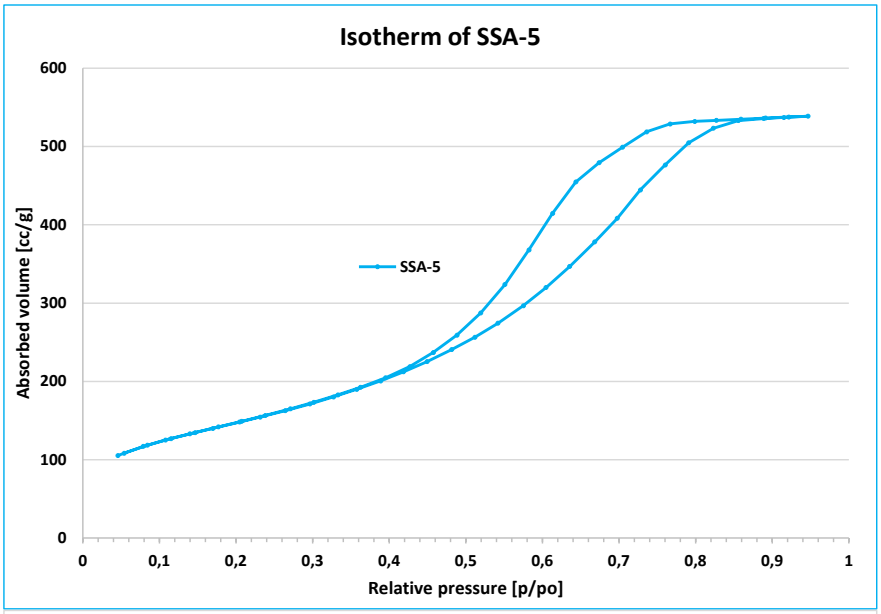
*Table A.11: Summary of BET results of **SSA-5***

Calculation Results	
Pore Volume	0.7920 cm^3/g
Surface area	412.7466 m^2/g
Lower confidence limit	0.7713 nm
Mode (Half pore width)	2.2713 nm
Fitting error	1.47 %

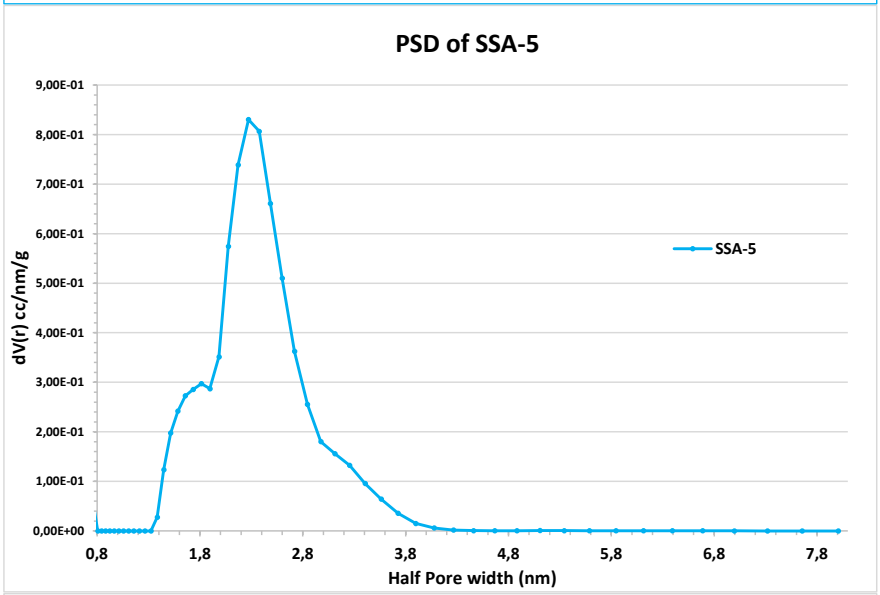
*Table A.12: Raw data of BET isotherm, particle size distribution, pore size and pore volume for **SSA-5***

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0458154	105,466	0,77133	3,68E-02	4,43E-02	8,18E+01	5,74E+01
0,0788931	117,139	0,806833	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,107978	125,261	0,84397	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,13969	133,119	0,882816	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,169566	140,055	0,92345	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,204572	148,136	0,965954	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,231494	154,512	1,01041	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,264162	162,603	1,05692	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,296376	171,202	1,10557	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,32723	180,178	1,15646	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,357725	190,003	1,20969	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,388762	200,665	1,26537	3,68E-02	0,00E+00	8,18E+01	0,00E+00
0,418576	212,23	1,32361	3,84E-02	0,00E+00	8,30E+01	0,00E+00
0,449397	225,266	1,38453	4,63E-02	2,76E-02	8,84E+01	1,91E+01
0,481441	240,702	1,44826	5,95E-02	1,23E-01	9,70E+01	8,40E+01
0,511954	256,534	1,51492	7,64E-02	1,98E-01	1,08E+02	1,30E+02
0,541954	274,435	1,58465	9,63E-02	2,42E-01	1,20E+02	1,52E+02
0,575169	296,709	1,65758	1,18E-01	2,73E-01	1,32E+02	1,65E+02
0,604652	319,909	1,73388	1,42E-01	2,86E-01	1,45E+02	1,65E+02
0,63549	346,813	1,81369	1,66E-01	2,97E-01	1,58E+02	1,64E+02
0,668328	378,094	1,89717	1,96E-01	2,87E-01	1,73E+02	1,51E+02
0,697655	408,309	1,98449	2,49E-01	3,52E-01	1,98E+02	1,76E+02
0,72786	444,55	2,07583	3,20E-01	5,74E-01	2,31E+02	2,75E+02
0,760293	476,394	2,17138	4,03E-01	7,39E-01	2,67E+02	3,39E+02
0,790942	504,717	2,27132	4,87E-01	8,30E-01	3,03E+02	3,65E+02
0,823182	523,242	2,37586	5,59E-01	8,07E-01	3,32E+02	3,40E+02
0,855809	533,03	2,48522	6,17E-01	6,61E-01	3,55E+02	2,67E+02
0,888979	535,761	2,59961	6,61E-01	5,10E-01	3,71E+02	1,97E+02
0,915128	537,028	2,71926	6,93E-01	3,63E-01	3,82E+02	1,34E+02
0,946618	538,638	2,84443	7,16E-01	2,55E-01	3,90E+02	9,04E+01
0,921606	537,563	2,97535	7,38E-01	1,80E-01	3,97E+02	6,09E+01
0,891219	536,244	3,1123	7,57E-01	1,56E-01	4,03E+02	5,02E+01
0,85921	534,773	3,25555	7,71E-01	1,32E-01	4,07E+02	4,09E+01
0,827126	533,29	3,4054	7,81E-01	9,59E-02	4,10E+02	2,84E+01
0,79896	531,943	3,56214	7,87E-01	6,42E-02	4,11E+02	1,82E+01
0,766607	528,766	3,7261	7,90E-01	3,57E-02	4,12E+02	9,72E+00
0,736048	518,625	3,8976	7,91E-01	1,51E-02	4,12E+02	3,95E+00
0,704535	499,007	4,077	7,91E-01	6,14E-03	4,13E+02	1,53E+00
0,673928	479,251	4,26465	7,91E-01	1,86E-03	4,13E+02	4,48E-01
0,643524	454,646	4,46095	7,91E-01	7,12E-04	4,13E+02	1,60E-01
0,613263	414,578	4,66628	7,91E-01	4,16E-04	4,13E+02	9,06E-02
0,582335	367,866	4,88105	7,92E-01	2,97E-04	4,13E+02	5,97E-02
0,551	323,671	5,10572	7,92E-01	7,77E-04	4,13E+02	1,51E-01
0,51948	287,561	5,34072	7,92E-01	7,13E-04	4,13E+02	1,35E-01
0,48838	259,213	5,58655	7,92E-01	3,83E-04	4,13E+02	6,92E-02
0,457518	236,954	5,84368	7,92E-01	4,02E-04	4,13E+02	6,84E-02
0,426915	218,866	6,11265	7,92E-01	4,73E-04	4,13E+02	7,74E-02
0,395108	204,638	6,39401	7,92E-01	4,09E-04	4,13E+02	6,42E-02
0,362332	192,457	6,68831	7,92E-01	3,21E-04	4,13E+02	4,83E-02
0,333068	182,797	6,99616	7,92E-01	1,64E-04	4,13E+02	2,39E-02
0,301647	173,34	7,31818	7,92E-01	3,12E-05	4,13E+02	4,46E-03
0,27079	164,999	7,65502	7,92E-01	0,00E+00	4,13E+02	0,00E+00
0,238196	156,599	8,00736	7,92E-01	0,00E+00	4,13E+02	0,00E+00
0,207124	149,077					
0,176935	141,918					
0,14662	134,752					
0,115039	127,008					
0,0843003	118,571					
0,0539059	108,4					

a)



b)



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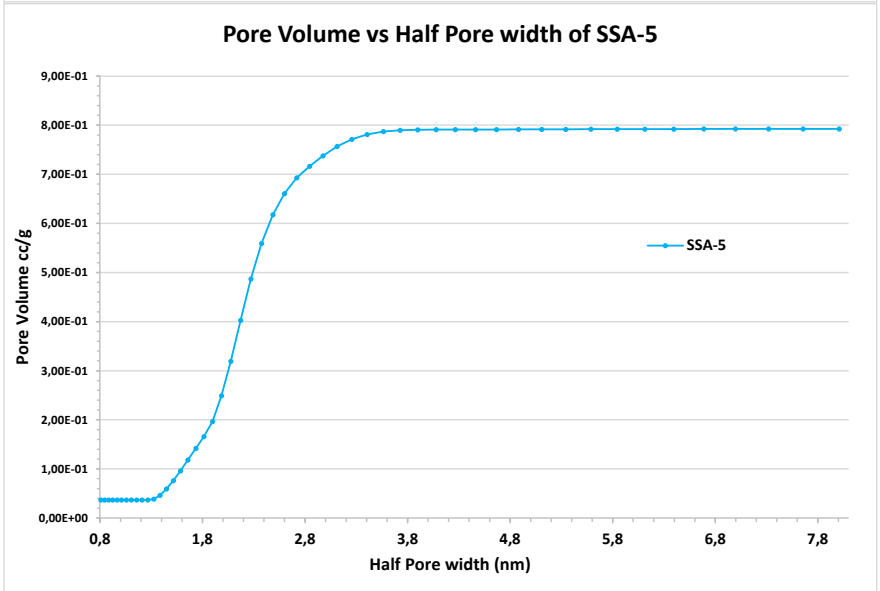


*Graph A.5: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of **SSA-5***

A-2.5 SSA-6

The duration of the analysis was 299.7 min with a cold zone of 2.93766 mL and a warm zone of 3.85875 mL.

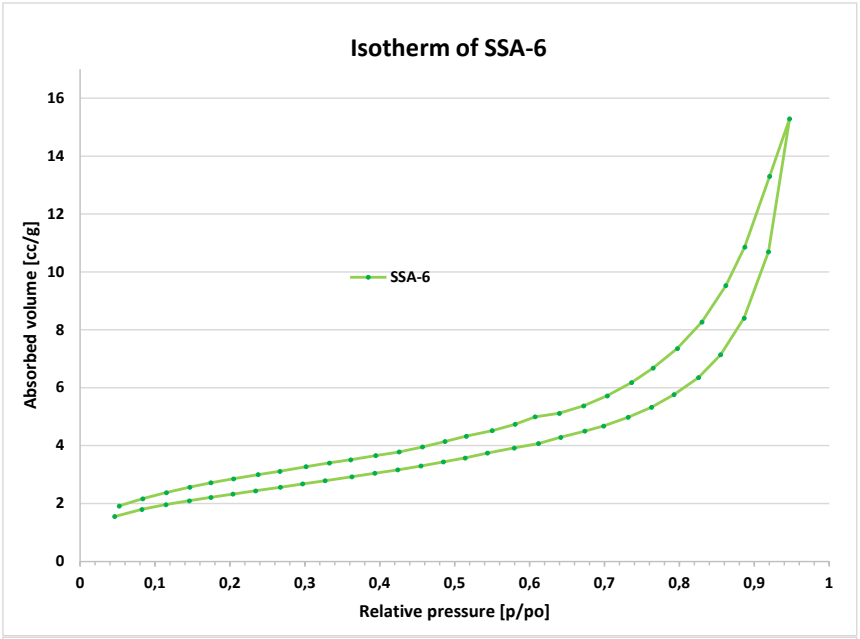
*Table A.13: Summary of BET results for **SSA-6***

Calculation Results	
Pore Volume	0.0194 cm^3/g
Surface area	7.2252 m^2/g
Lower confidence limit	0.7713 nm
Mode (Half pore width)	3.8976 nm
Fitting error	0.95 %

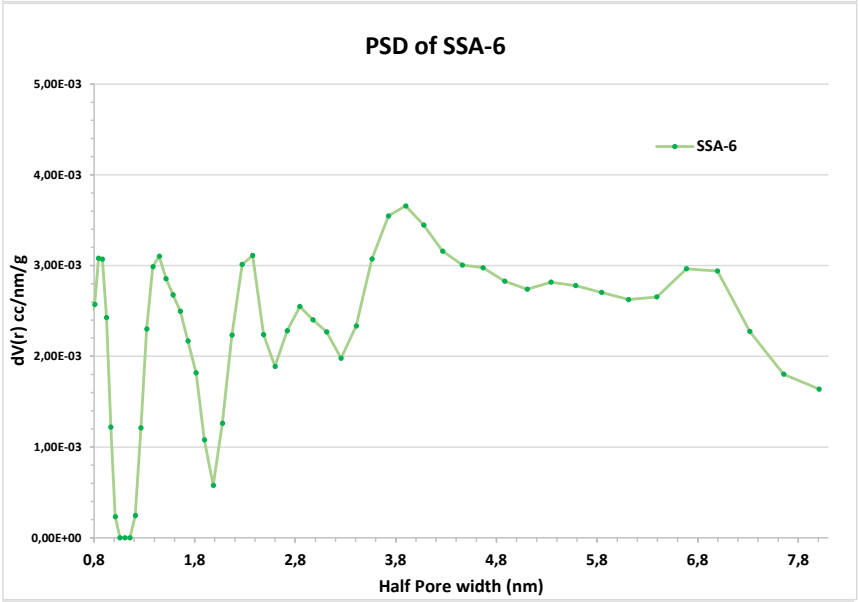
*Table A.14: Raw data of BET isotherm, particle size distribution, pore size and pore volume for **SSA-6***

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0458737	1,54993	0,77133	1,07E-03	2,47E-03	2,11E+00	3,21E+00
0,0824556	1,79758	0,806833	1,19E-03	2,57E-03	2,24E+00	3,19E+00
0,11441	1,96111	0,84397	1,30E-03	3,08E-03	2,38E+00	3,64E+00
0,145609	2,09355	0,882816	1,40E-03	3,07E-03	2,48E+00	3,49E+00
0,174585	2,21119	0,92345	1,46E-03	2,43E-03	2,54E+00	2,65E+00
0,20378	2,32437	0,965954	1,47E-03	1,22E-03	2,55E+00	1,29E+00
0,234017	2,4385	1,01041	1,47E-03	2,33E-04	2,55E+00	2,41E-01
0,267112	2,55925	1,05692	1,47E-03	0,00E+00	2,55E+00	0,00E+00
0,296987	2,67653	1,10557	1,47E-03	0,00E+00	2,55E+00	0,00E+00
0,326967	2,78875	1,15646	1,48E-03	0,00E+00	2,56E+00	0,00E+00
0,362725	2,92637	1,20969	1,55E-03	2,45E-04	2,61E+00	1,94E-01
0,393196	3,04435	1,26537	1,68E-03	1,21E-03	2,71E+00	9,42E-01
0,423864	3,16542	1,32361	1,86E-03	2,30E-03	2,84E+00	1,73E+00
0,454662	3,29802	1,38453	2,06E-03	2,99E-03	2,98E+00	2,15E+00
0,484739	3,43606	1,44826	2,25E-03	3,10E-03	3,11E+00	2,15E+00
0,513895	3,57365	1,51492	2,44E-03	2,86E-03	3,22E+00	1,89E+00
0,543552	3,74324	1,58465	2,62E-03	2,68E-03	3,33E+00	1,69E+00
0,579275	3,91855	1,65758	2,78E-03	2,50E-03	3,43E+00	1,51E+00
0,611739	4,07027	1,73388	2,93E-03	2,17E-03	3,51E+00	1,25E+00
0,641425	4,28581	1,81369	3,02E-03	1,82E-03	3,56E+00	1,01E+00
0,673641	4,50207	1,89717	3,07E-03	1,08E-03	3,58E+00	5,78E-01
0,69883	4,67833	1,98449	3,19E-03	5,78E-04	3,64E+00	2,90E-01
0,73132	4,98103	2,07583	3,40E-03	1,26E-03	3,74E+00	5,98E-01
0,762659	5,3237	2,17138	3,70E-03	2,23E-03	3,87E+00	1,02E+00
0,792581	5,76145	2,27132	4,02E-03	3,01E-03	4,01E+00	1,32E+00
0,825336	6,34732	2,37586	4,27E-03	3,11E-03	4,10E+00	1,31E+00
0,854935	7,14058	2,48522	4,49E-03	2,24E-03	4,19E+00	9,07E-01
0,886316	8,40371	2,59961	4,76E-03	1,89E-03	4,29E+00	7,26E-01
0,918866	10,6951	2,71926	5,08E-03	2,28E-03	4,40E+00	8,36E-01
0,946976	15,2918	2,84443	5,39E-03	2,55E-03	4,51E+00	8,97E-01
0,920303	13,3031	2,97535	5,70E-03	2,40E-03	4,61E+00	8,09E-01
0,88717	10,8592	3,1123	5,99E-03	2,27E-03	4,69E+00	7,31E-01
0,86182	9,52726	3,25555	6,34E-03	1,98E-03	4,80E+00	6,08E-01
0,829899	8,26797	3,4054	6,82E-03	2,33E-03	4,93E+00	6,82E-01
0,797076	7,35451	3,56214	7,40E-03	3,07E-03	5,09E+00	8,59E-01
0,764875	6,68067	3,7261	8,03E-03	3,55E-03	5,25E+00	9,51E-01
0,735971	6,17541	3,8976	8,64E-03	3,66E-03	5,40E+00	9,39E-01
0,70348	5,7194	4,077	9,24E-03	3,45E-03	5,54E+00	8,47E-01
0,672067	5,37437	4,26465	9,83E-03	3,16E-03	5,67E+00	7,42E-01
0,639552	5,1171	4,46095	1,04E-02	3,01E-03	5,80E+00	6,74E-01
0,607212	4,99357	4,66628	1,10E-02	2,98E-03	5,93E+00	6,38E-01
0,580477	4,73499	4,88105	1,17E-02	2,83E-03	6,05E+00	5,80E-01
0,54998	4,51878	5,10572	1,23E-02	2,74E-03	6,17E+00	5,37E-01
0,515367	4,32604	5,34072	1,30E-02	2,82E-03	6,29E+00	5,28E-01
0,486836	4,14327	5,58655	1,37E-02	2,78E-03	6,41E+00	4,98E-01
0,456802	3,95254	5,84368	1,44E-02	2,70E-03	6,53E+00	4,63E-01
0,425746	3,78157	6,11265	1,52E-02	2,62E-03	6,64E+00	4,30E-01
0,394573	3,65716	6,39401	1,60E-02	2,65E-03	6,77E+00	4,15E-01
0,361179	3,51279	6,68831	1,69E-02	2,96E-03	6,90E+00	4,43E-01
0,332509	3,40189	6,99616	1,77E-02	2,94E-03	7,01E+00	4,21E-01
0,301422	3,27201	7,31818	1,83E-02	2,27E-03	7,08E+00	3,12E-01
0,266619	3,11278	7,65502	1,88E-02	1,80E-03	7,16E+00	2,36E-01
0,237619	3,00019	8,00736	1,94E-02	1,64E-03	7,23E+00	2,05E-01
0,204594	2,8559					
0,174318	2,71846					
0,146391	2,56545					
0,11502	2,37785					
0,0834649	2,16773					
0,0519184	1,91631					

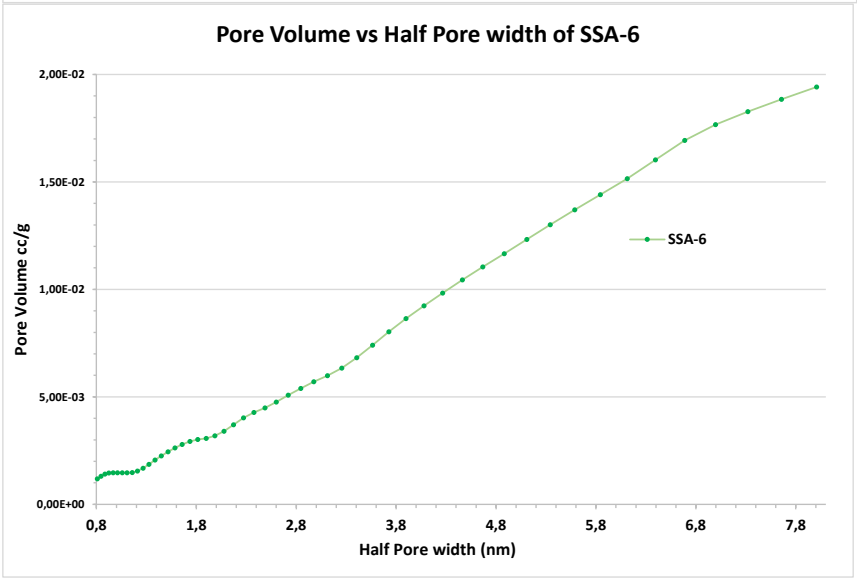
a)



b)



c)



*Graph A.6: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of **SSA-6***

A-2.6 SSA-7

The duration of the analysis was 240.2 min with a cold zone of 24.3789 mL and a warm zone of 4.25787 mL.

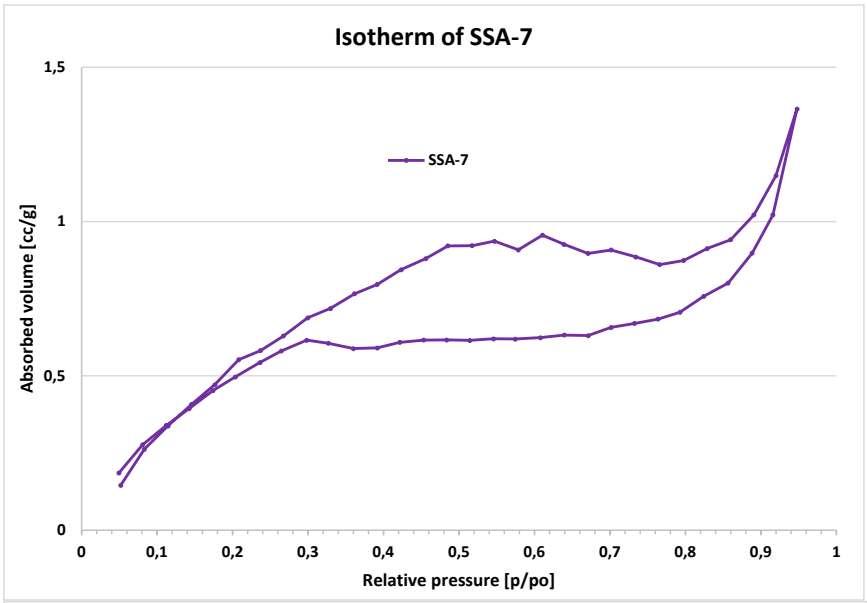
*Table A.15: Summary of BET results of **SSA-7***

Calculation Results	
Pore Volume	0.0016 cm^3/g
Surface area	1.0381 m^2/g
Lower confidence limit	0.8068 nm
Mode (Half pore width)	1.2097 nm
Fitting error	0.77 %

*Table A.16: Raw data of BET isotherm, particle size distribution, pore size and pore volume for **SSA-7***

Isotherm		*PSD and Pore Size vs Pore Volume*			*Surface area*	
Relative pressure [p/po]	***Absorbed volume [cm^3/g]***	***Half Pore width (nm)***	***Pore Volume cm^3/g***	***dV(r) $cm^3/nm/g$***	***Cumulative surface area m^2/g***	***dS(r) $m^2/nm/g$***
0,0492318	0,185249	0,806833	0,00E+00	0,00E+00	0,00E+00	0,00E+00
0,0808098	0,276768	0,84397	6,99E-06	0,00E+00	7,57E-03	0,00E+00
0,112174	0,339523	0,882816	4,09E-05	1,80E-04	4,37E-02	1,95E-01
0,142538	0,393921	0,92345	9,70E-05	8,34E-04	1,02E-01	8,89E-01
0,173968	0,452256	0,965954	1,45E-04	1,32E-03	1,49E-01	1,36E+00
0,203683	0,496598	1,01041	1,62E-04	1,07E-03	1,66E-01	1,08E+00
0,236312	0,543214	1,05692	2,00E-04	3,70E-04	1,99E-01	3,56E-01
0,26445	0,580432	1,10557	2,97E-04	7,75E-04	2,83E-01	6,83E-01
0,298312	0,615403	1,15646	4,10E-04	1,91E-03	3,77E-01	1,64E+00
0,32684	0,605626	1,20969	5,06E-04	2,13E-03	4,52E-01	1,77E+00
0,360082	0,58831	1,26537	6,09E-04	1,71E-03	5,31E-01	1,36E+00
0,391815	0,59058	1,32361	7,26E-04	1,78E-03	6,15E-01	1,34E+00
0,421443	0,608455	1,38453	8,24E-04	1,91E-03	6,83E-01	1,38E+00
0,453122	0,615829	1,44826	9,05E-04	1,54E-03	7,37E-01	1,07E+00
0,483764	0,616309	1,51492	9,83E-04	1,22E-03	7,86E-01	8,08E-01
0,514218	0,614795	1,58465	1,06E-03	1,12E-03	8,34E-01	7,09E-01
0,545765	0,619897	1,65758	1,14E-03	1,09E-03	8,80E-01	6,59E-01
0,574562	0,61919	1,73388	1,21E-03	1,03E-03	9,18E-01	5,94E-01
0,60799	0,623618	1,81369	1,27E-03	8,66E-04	9,49E-01	4,79E-01
0,63931	0,632387	1,89717	1,30E-03	7,15E-04	9,65E-01	3,79E-01
0,671136	0,630379	1,98449	1,31E-03	3,40E-04	9,70E-01	1,75E-01
0,70158	0,657027	2,07583	1,32E-03	1,18E-04	9,76E-01	5,70E-02
0,732566	0,66976	2,17138	1,34E-03	1,49E-04	9,82E-01	6,84E-02
0,763793	0,684054	2,27132	1,35E-03	1,36E-04	9,87E-01	6,04E-02
0,792705	0,70611	2,37586	1,36E-03	1,08E-04	9,91E-01	4,58E-02
0,824197	0,757736	2,48522	1,36E-03	7,58E-05	9,93E-01	3,07E-02
0,856534	0,800852	2,59961	1,37E-03	5,81E-05	9,96E-01	2,24E-02
0,888253	0,897431	2,71926	1,38E-03	5,30E-05	9,98E-01	1,95E-02
0,915842	1,02179	2,84443	1,38E-03	4,66E-05	9,99E-01	1,65E-02
0,947933	1,36488	2,97535	1,39E-03	3,54E-05	1,00E+00	1,20E-02
0,91994	1,14897	3,1123	1,39E-03	2,78E-05	1,00E+00	8,98E-03
0,890786	1,02153	3,25555	1,39E-03	1,73E-05	1,00E+00	5,36E-03
0,859782	0,940966	3,4054	1,39E-03	1,79E-05	1,00E+00	5,24E-03
0,828973	0,912619	3,56214	1,40E-03	2,41E-05	1,00E+00	6,75E-03
0,797666	0,873942	3,7261	1,40E-03	2,68E-05	1,01E+00	7,19E-03
0,765916	0,860467	3,8976	1,41E-03	2,62E-05	1,01E+00	6,74E-03
0,734319	0,885329	4,077	1,41E-03	2,18E-05	1,01E+00	5,38E-03
0,701462	0,907805	4,26465	1,41E-03	1,75E-05	1,01E+00	4,12E-03
0,670944	0,896701	4,46095	1,42E-03	1,57E-05	1,01E+00	3,52E-03
0,639188	0,926158	4,66628	1,42E-03	1,36E-05	1,01E+00	2,92E-03
0,610625	0,95595	4,88105	1,42E-03	1,03E-05	1,01E+00	2,12E-03
0,57863	0,908149	5,10572	1,42E-03	8,05E-06	1,01E+00	1,58E-03
0,546874	0,936371	5,34072	1,42E-03	4,98E-06	1,01E+00	9,46E-04
0,517368	0,92197	5,58655	1,42E-03	2,06E-06	1,01E+00	3,70E-04
0,485257	0,921174	5,84368	1,42E-03	3,66E-06	1,01E+00	6,18E-04
0,456108	0,880133	6,11265	1,43E-03	5,39E-06	1,01E+00	8,79E-04
0,423239	0,84388	6,39401	1,45E-03	1,32E-05	1,01E+00	2,02E-03
0,391654	0,796117	6,68831	1,49E-03	6,27E-05	1,02E+00	9,14E-03
0,361632	0,765956	6,99616	1,53E-03	1,41E-04	1,03E+00	2,00E-02
0,329696	0,718458	7,31818	1,57E-03	1,32E-04	1,03E+00	1,81E-02
0,299671	0,687989	7,65502	1,60E-03	1,06E-04	1,03E+00	1,39E-02
0,267322	0,629072	8,00736	1,64E-03	9,69E-05	1,04E+00	1,21E-02
0,237017	0,581979					
0,208117	0,552334					
0,176512	0,471604					
0,145796	0,407784					
0,114468	0,337844					
0,0830192	0,262134					
0,051671	0,145195					

a)



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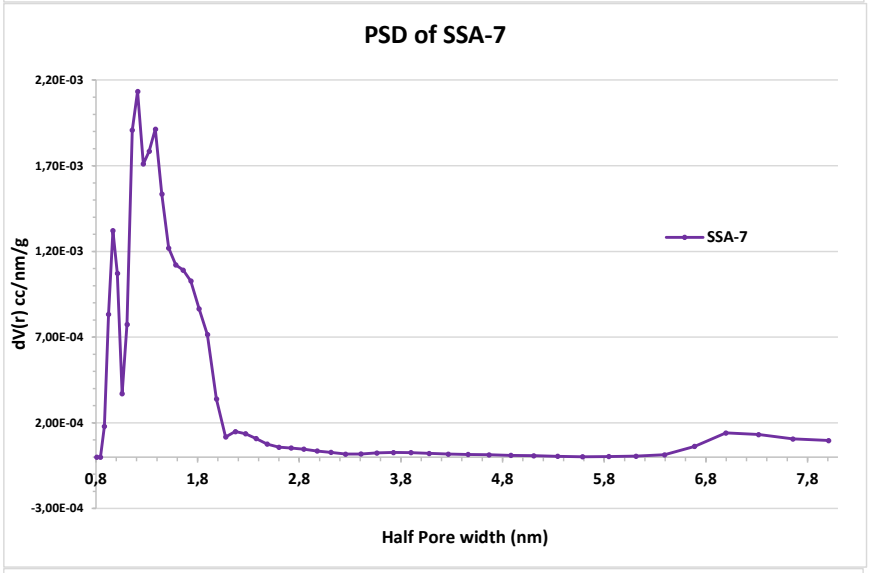

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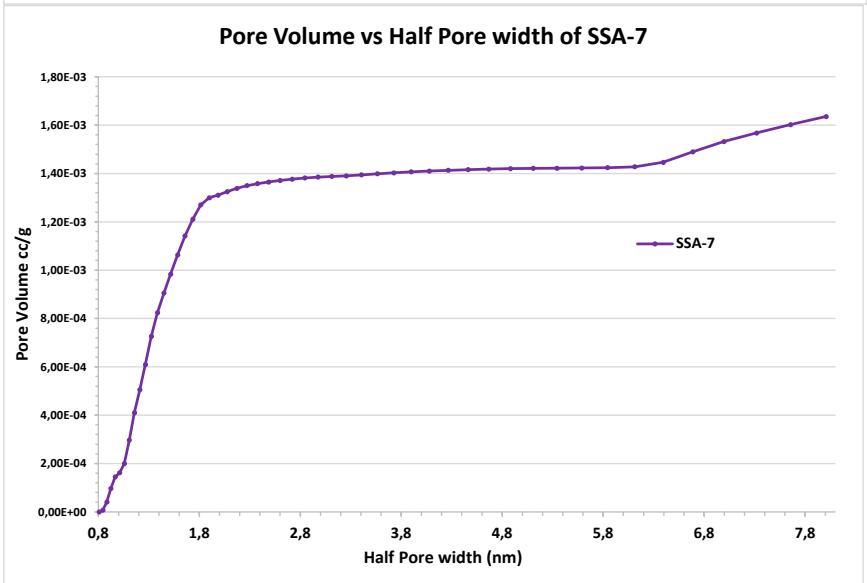
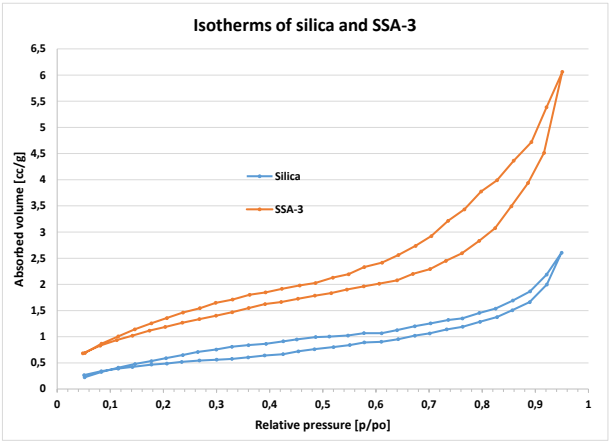


*Graph A.7: BET Isotherm (a), Particle size distribution (b) and Pore volume vs Half pore width (c) of **SSA-7***

A-2.7 Combinations

a)



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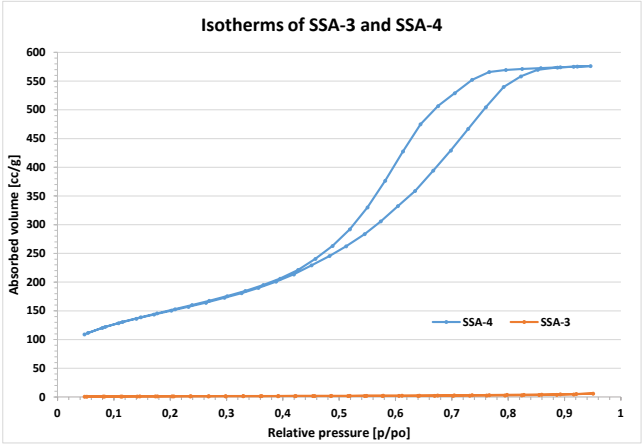

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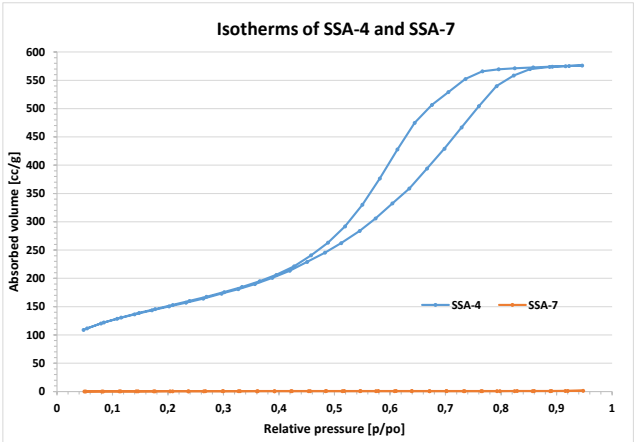

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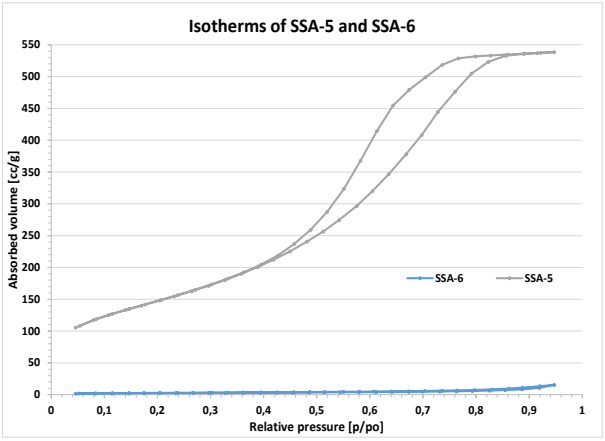

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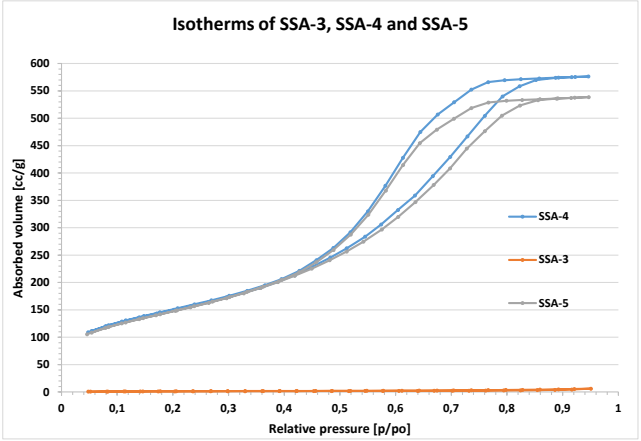

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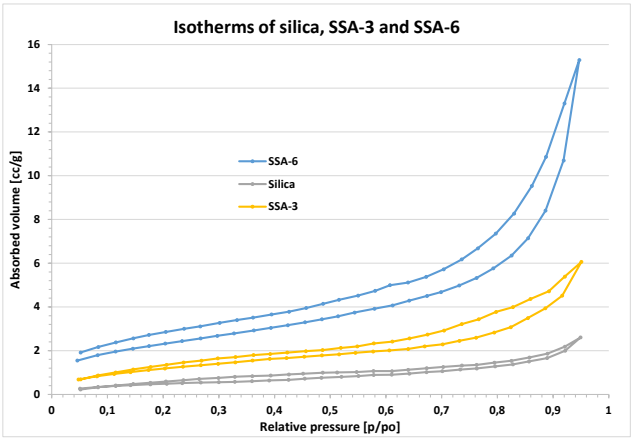
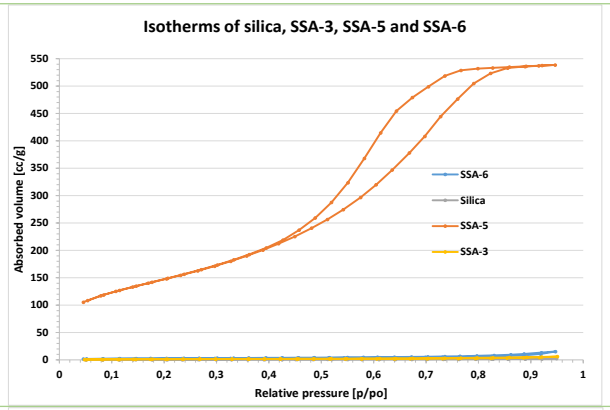
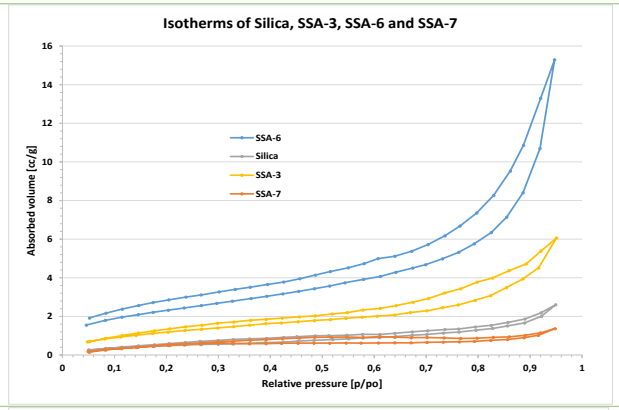


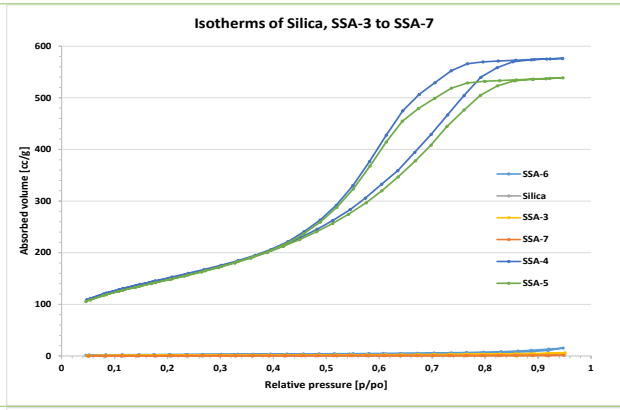
g)


Isotherms of silica, SSA-3, SSA-5 and SSA-6
Absorbed volume [cc/g]
Relative pressure [p/po]
SSA-6
Silica
SSA-5
SSA-3

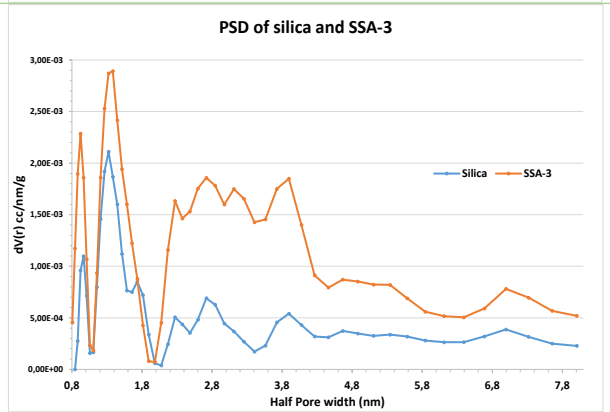
h)


Isotherms of Silica, SSA-3, SSA-6 and SSA-7
Absorbed volume [cc/g]
Relative pressure [p/po]
SSA-6
Silica
SSA-3
SSA-7

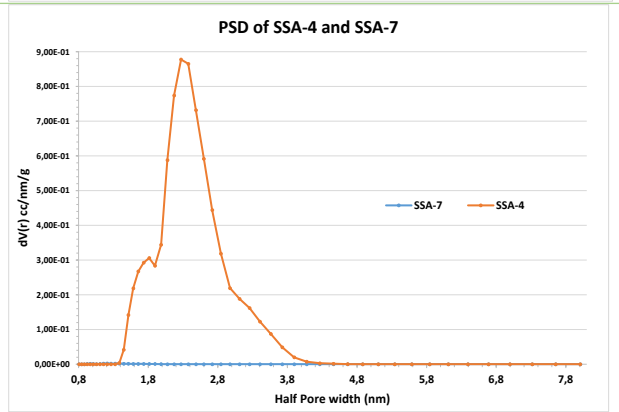
i)


Isotherms of Silica, SSA-3 to SSA-7
Absorbed volume [cc/g]
Relative pressure [p/po]
SSA-6
Silica
SSA-3
SSA-7
SSA-4
SSA-5

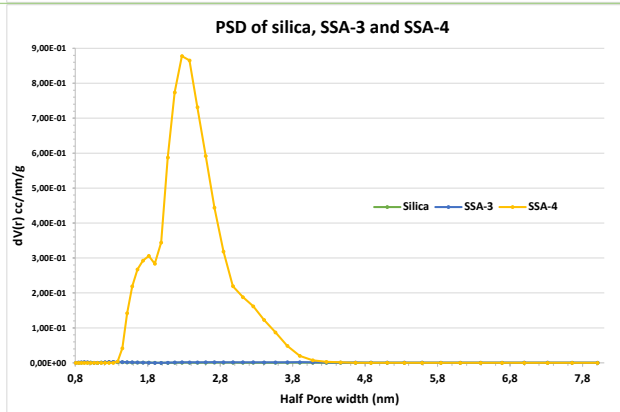
j)


PSD of silica and SSA-3
dV(r) cc/nm/g
Half Pore width (nm)
Silica
SSA-3

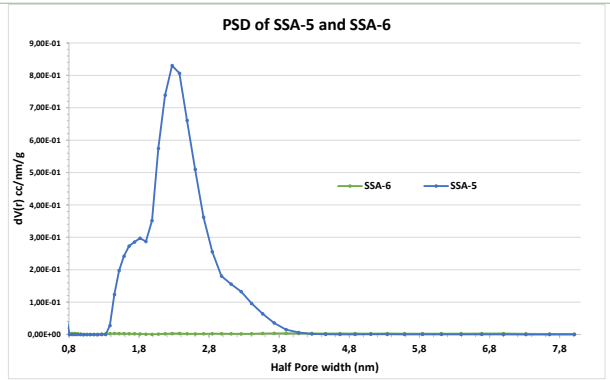
k)


PSD of SSA-4 and SSA-7
dV(r) cc/nm/g
Half Pore width (nm)
SSA-7
SSA-4

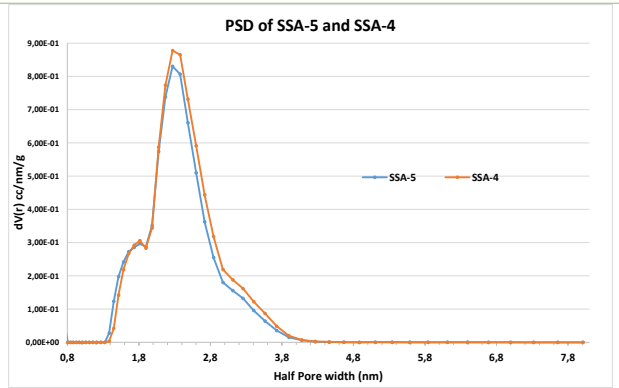
l)


PSD of silica, SSA-3 and SSA-4
dV(r) cc/nm/g
Half Pore width (nm)
Silica
SSA-3
SSA-4

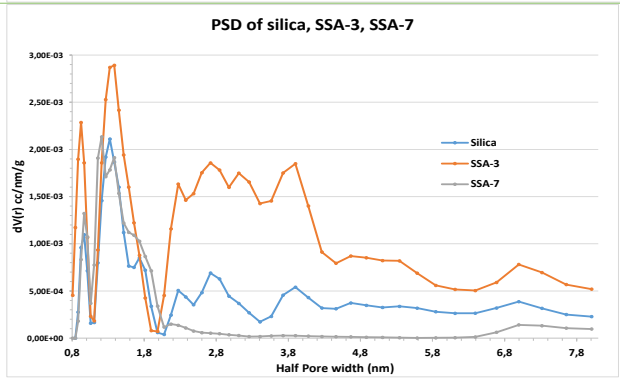
m)


PSD of SSA-5 and SSA-6
dV(r) cc/nm/g
Half Pore width (nm)
SSA-6
SSA-5

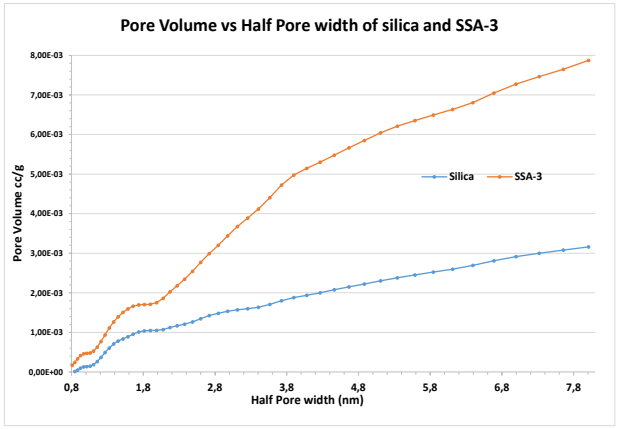
n)


PSD of SSA-5 and SSA-4
dV(r) cc/nm/g
Half Pore width (nm)
SSA-5
SSA-4

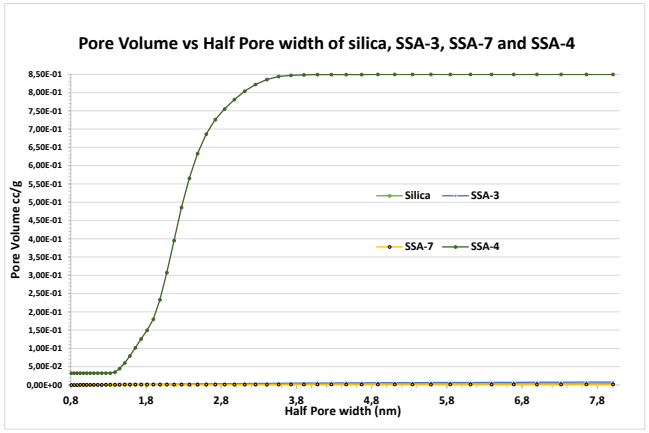
o)


PSD of silica, SSA-3, SSA-7
dV(r) cc/nm/g
Half Pore width (nm)
Silica
SSA-3
SSA-7

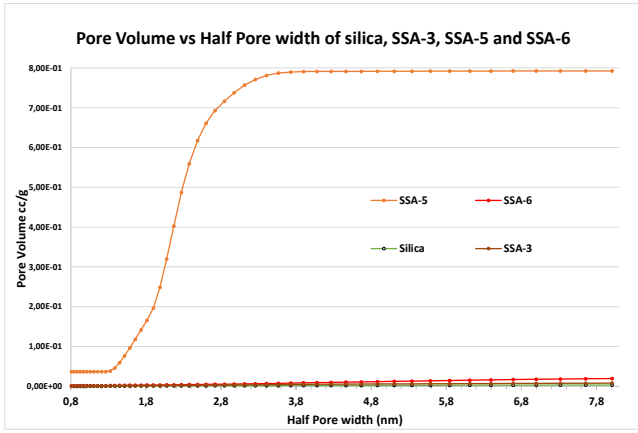
p)


Pore Volume vs Half Pore width of silica and SSA-3
Pore Volume cc/g
Half Pore width (nm)
Silica
SSA-3

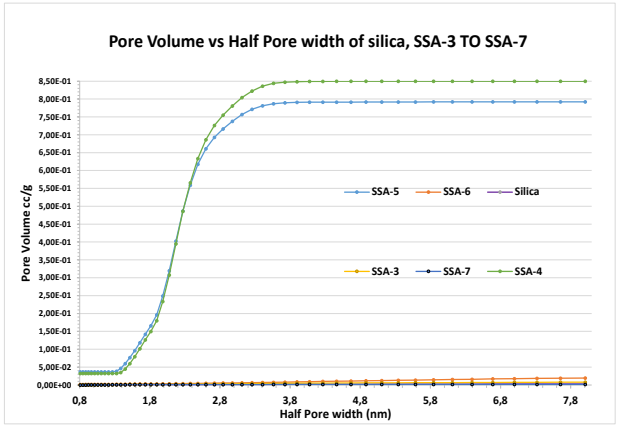
q)


Pore Volume vs Half Pore width of silica, SSA-3, SSA-7 and SSA-4
Pore Volume cc/g
Half Pore width (nm)
Silica
SSA-3
SSA-7
SSA-4

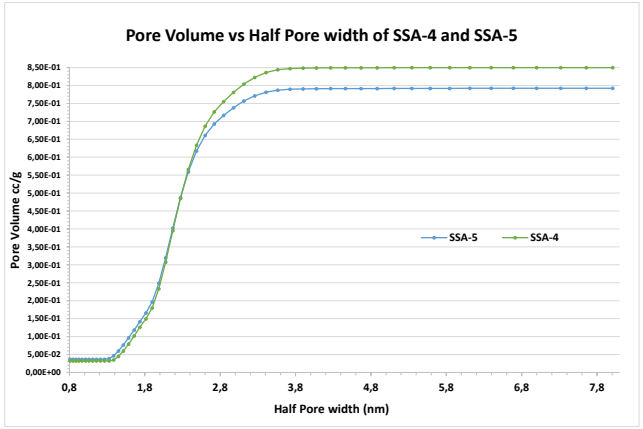
r)


Pore Volume vs Half Pore width of silica, SSA-3, SSA-5 and SSA-6
Pore Volume cc/g
Half Pore width (nm)
SSA-5
SSA-6
Silica
SSA-3

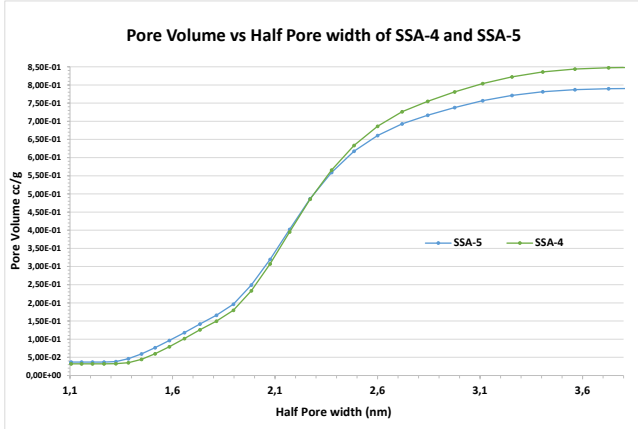
s)


Pore Volume vs Half Pore width of silica, SSA-3 TO SSA-7
Pore Volume cc/g
Half Pore width (nm)
SSA-5
SSA-6
Silica
SSA-3
SSA-7
SSA-4

t)

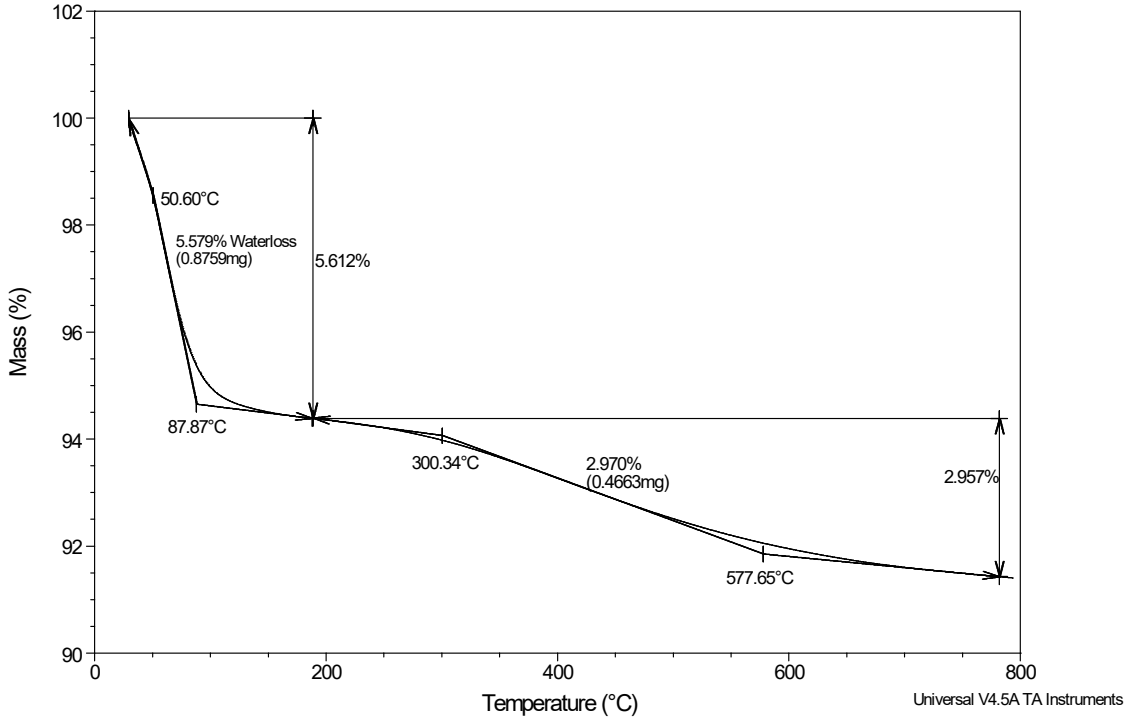

Pore Volume vs Half Pore width of SSA-4 and SSA-5
Pore Volume cc/g
Half Pore width (nm)
SSA-5
SSA-4

u)

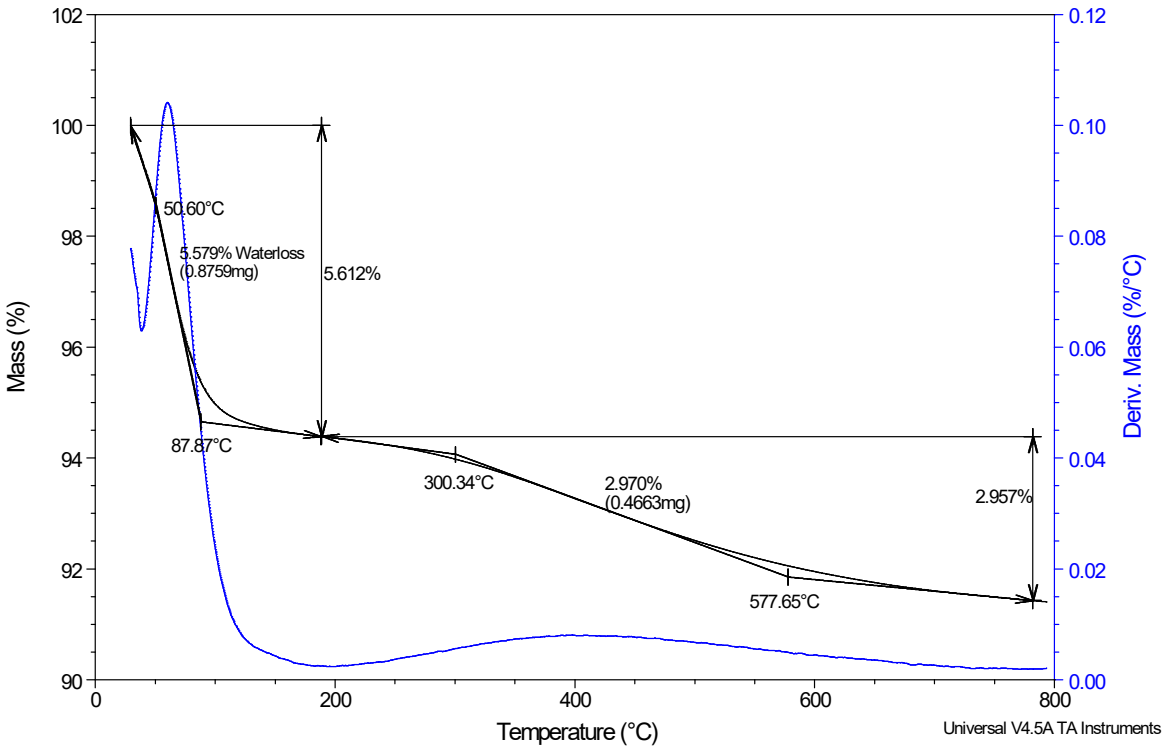

Pore Volume vs Half Pore width of SSA-4 and SSA-5
Pore Volume cc/g
Half Pore width (nm)
SSA-5
SSA-4

A-3 TGA and DSC results

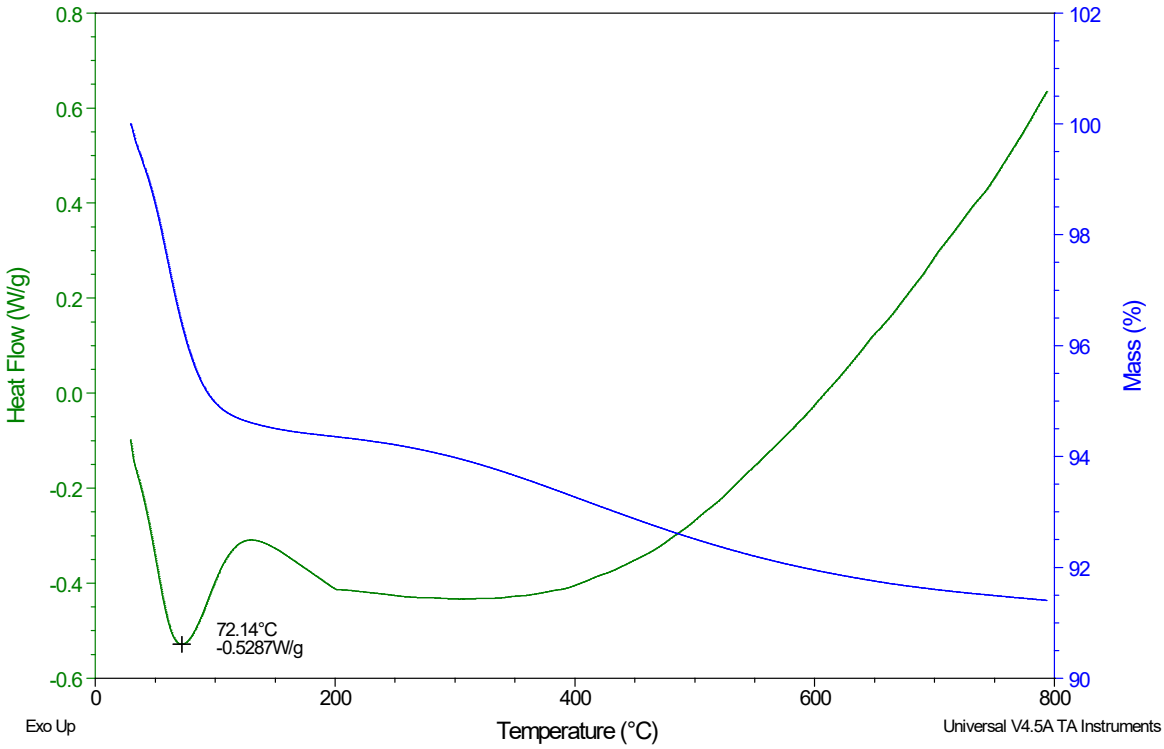
A-3.1 Silica



Graph A.8: TGA graph of silica

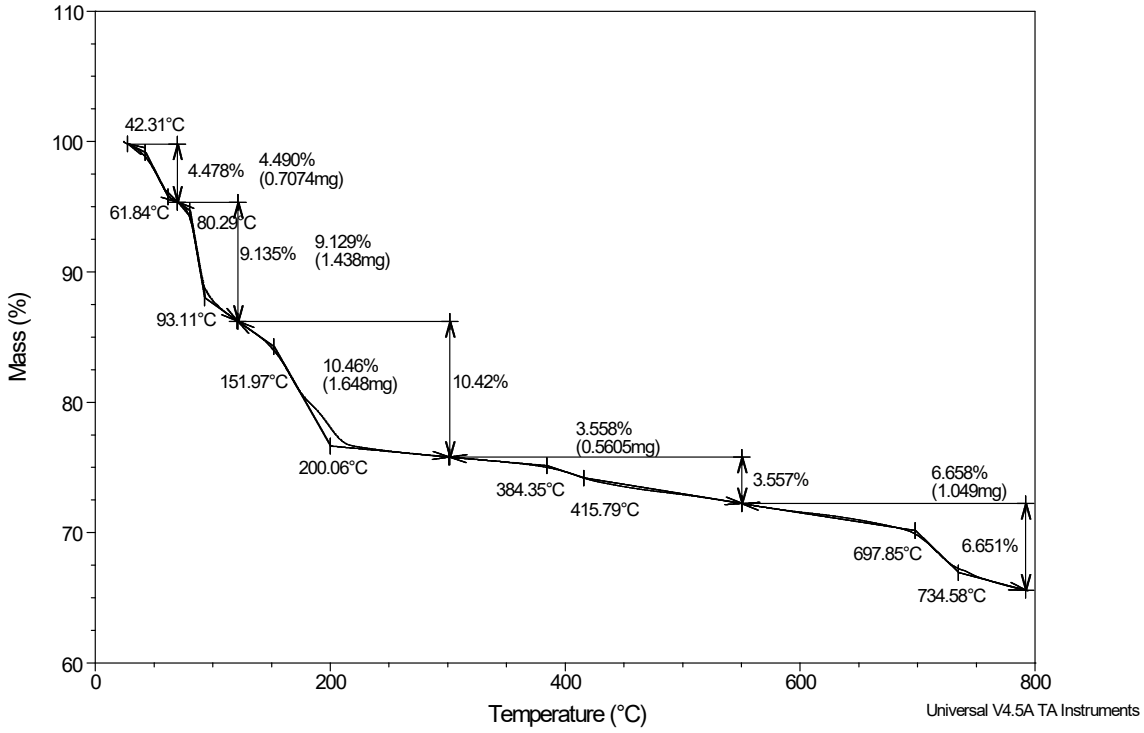


Graph A.9: TGA (black) and DTA (blue) of silica

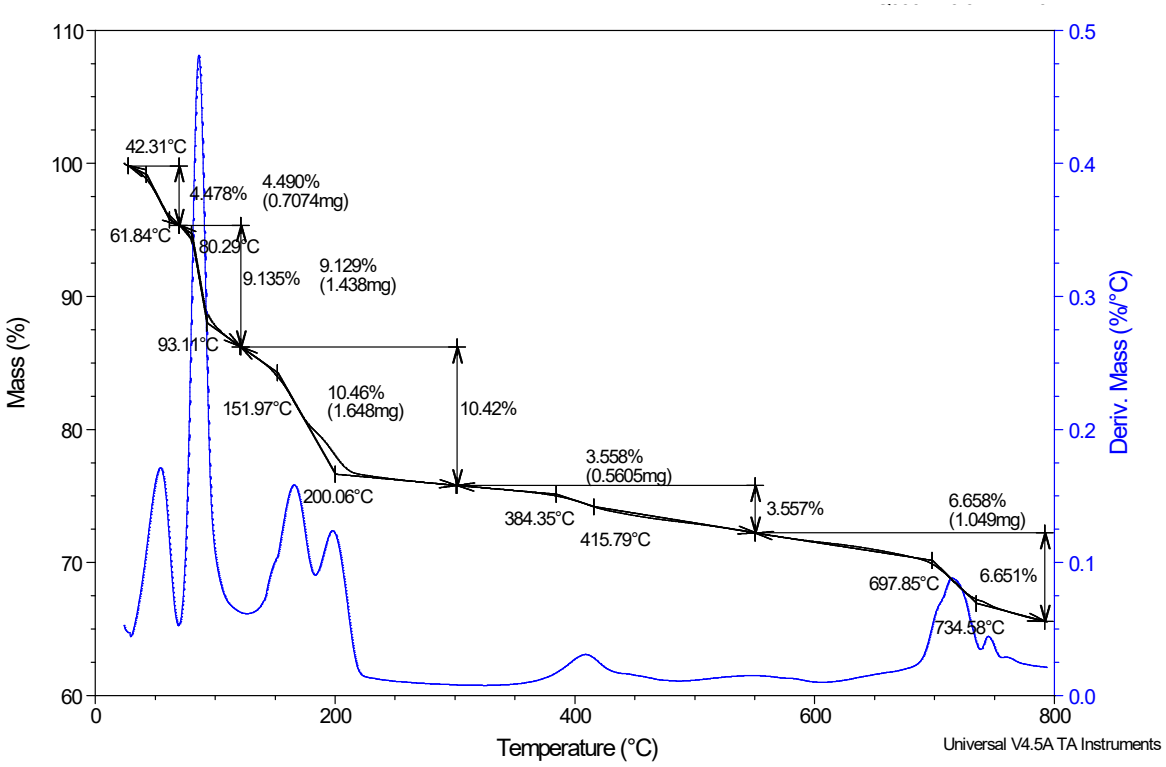


Graph A.10: DSC (green) and TGA (blue) graphs of silica

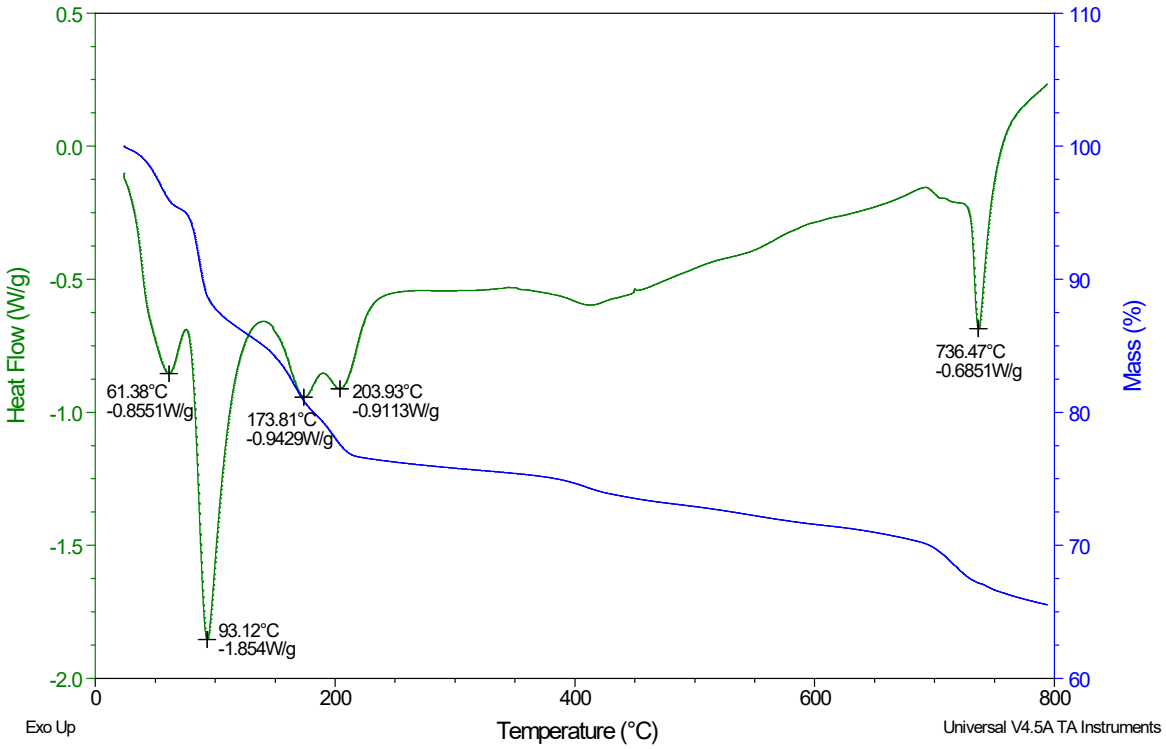
A-3.2 SSA-3



*Graph A.11: TGA graph of oxidized silica **SSA-3***

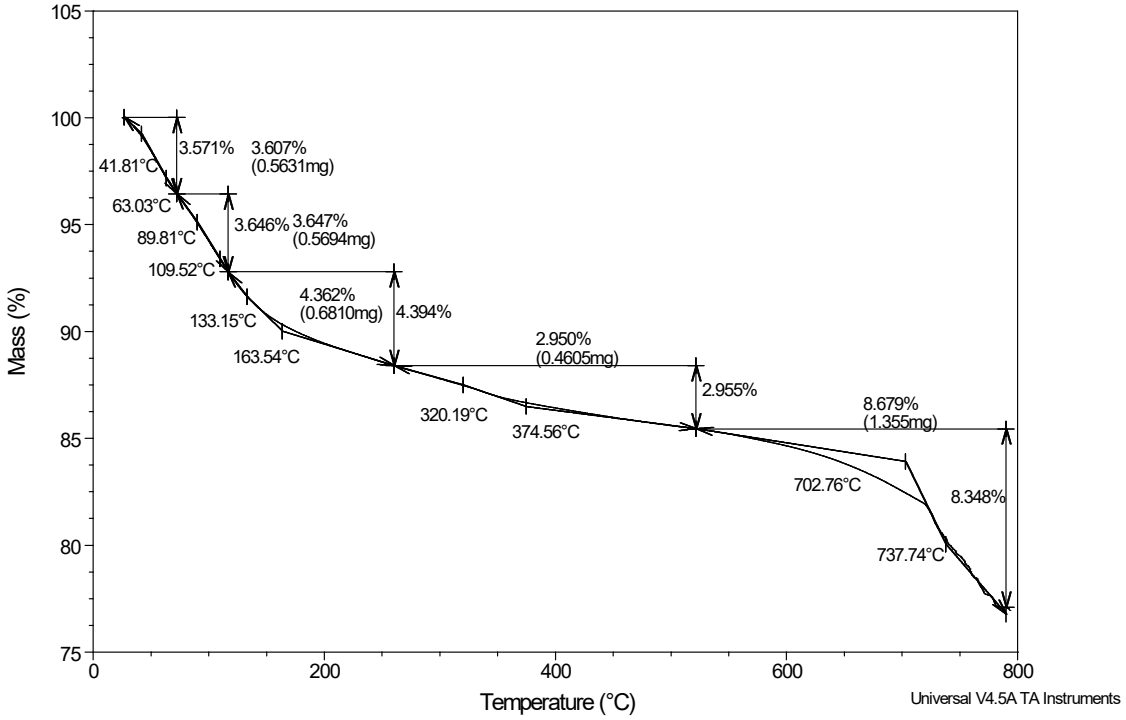


*Graph A.12: TGA (black) and DTG (blue) of **SSA-3***

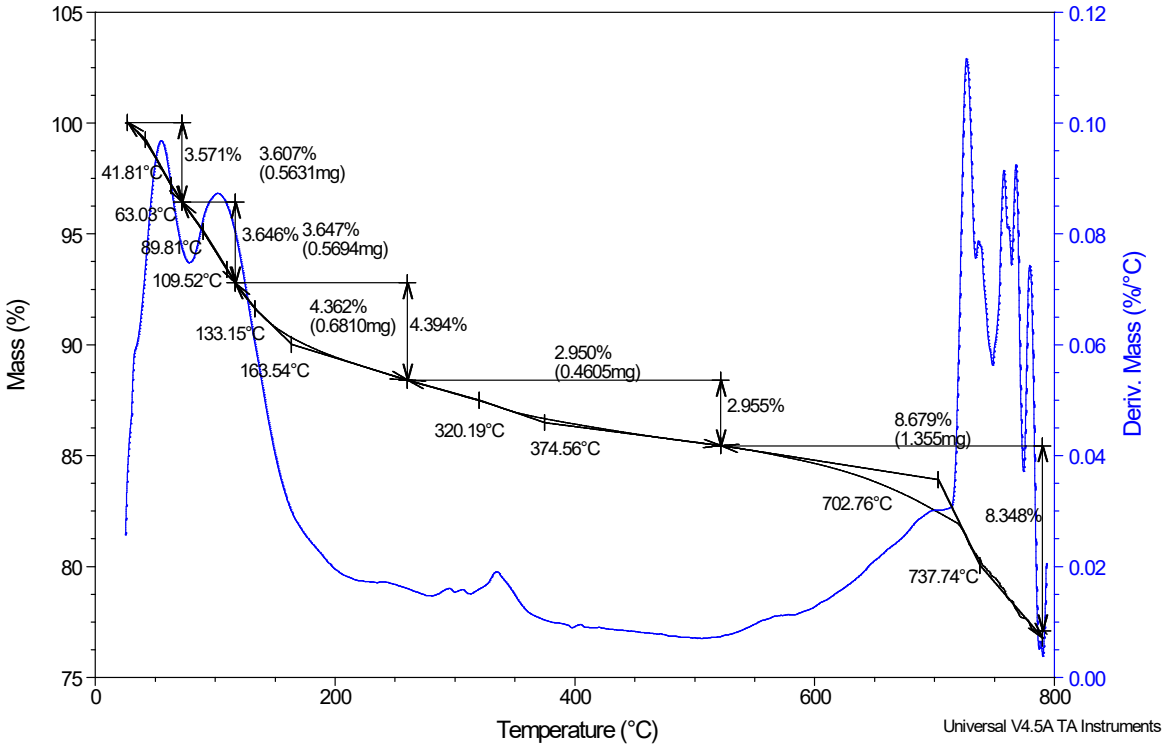


*Graph A.13: DSC (green) and TGA (blue) of oxidized silica **SSA-3***

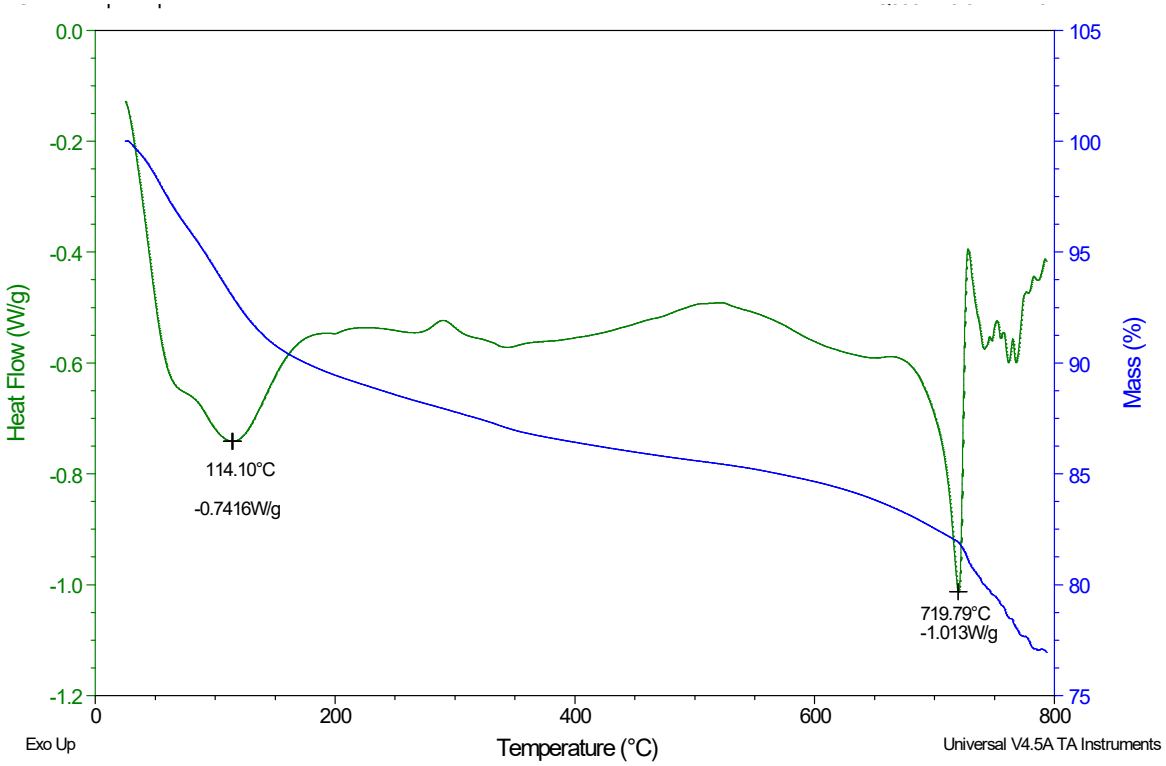
A-3.3 SSA-4



*Graph A.14: TGA graph of oxidized silica-DNPH **SSA-4***

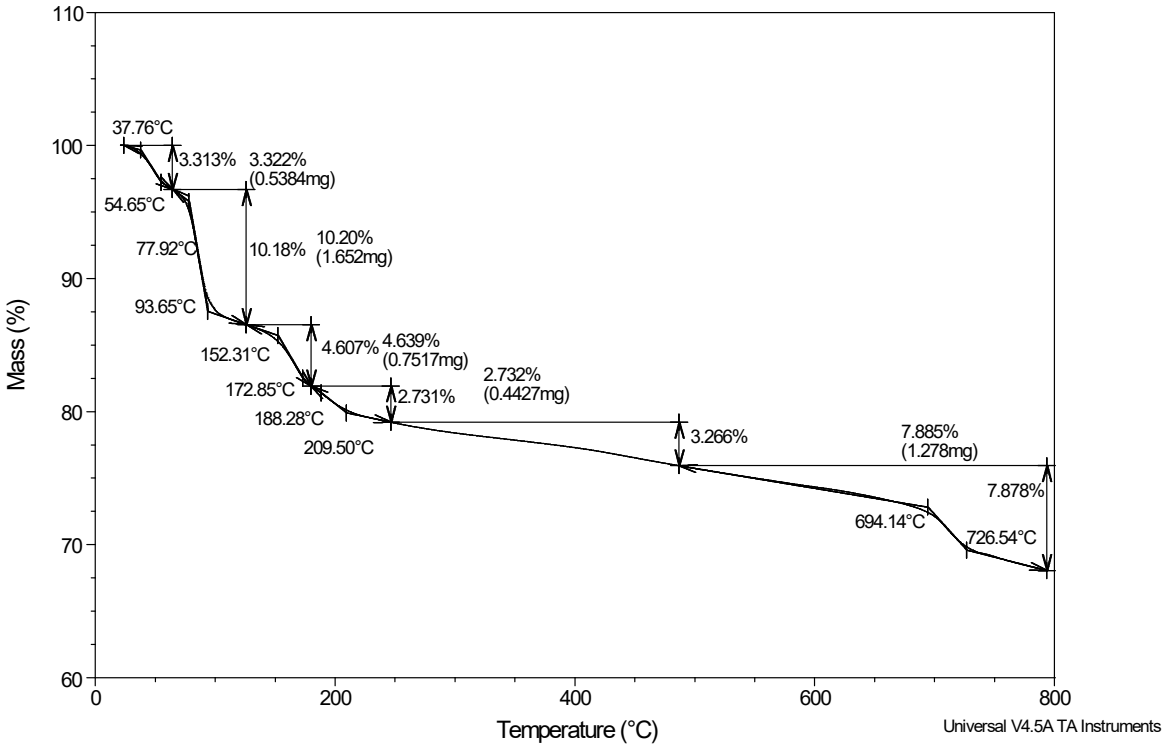


*Graph A.15: TGA (black) and DTG (blue) of oxidized silica-DNPH **SSA-4***

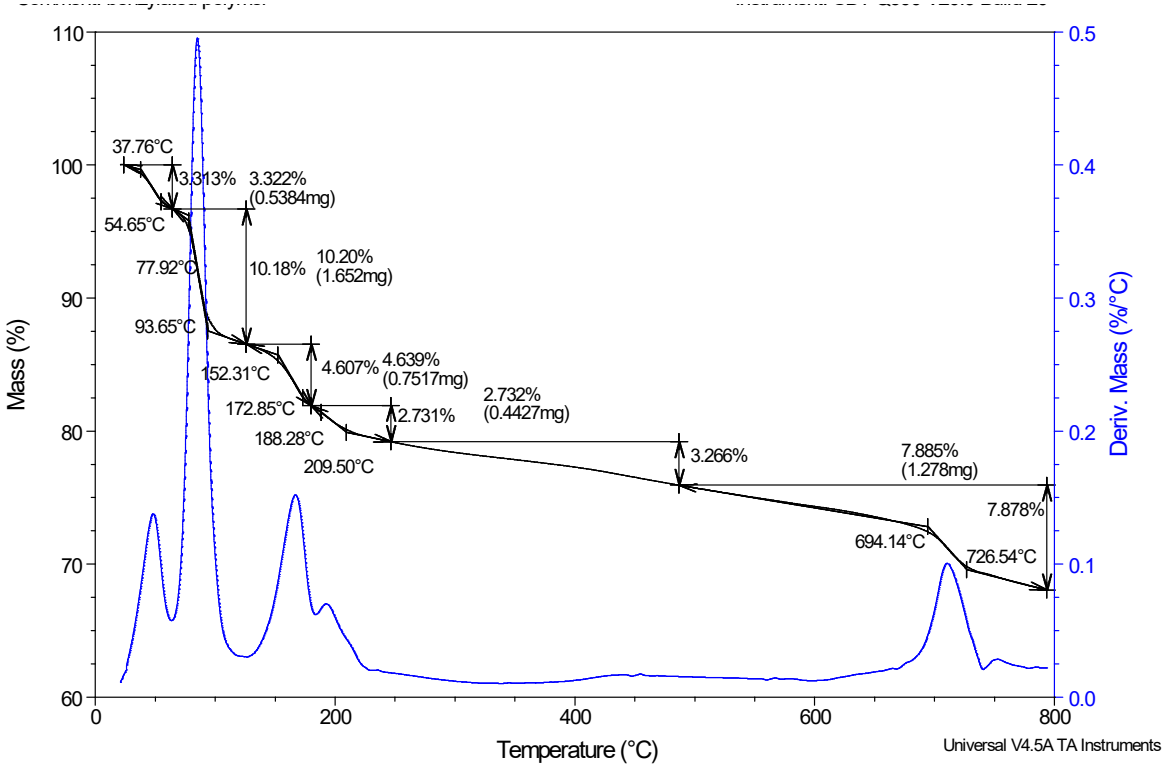


*Graph A.16: DSC (green) and TGA (blue) of oxidized silica-DNPH **SSA-4***

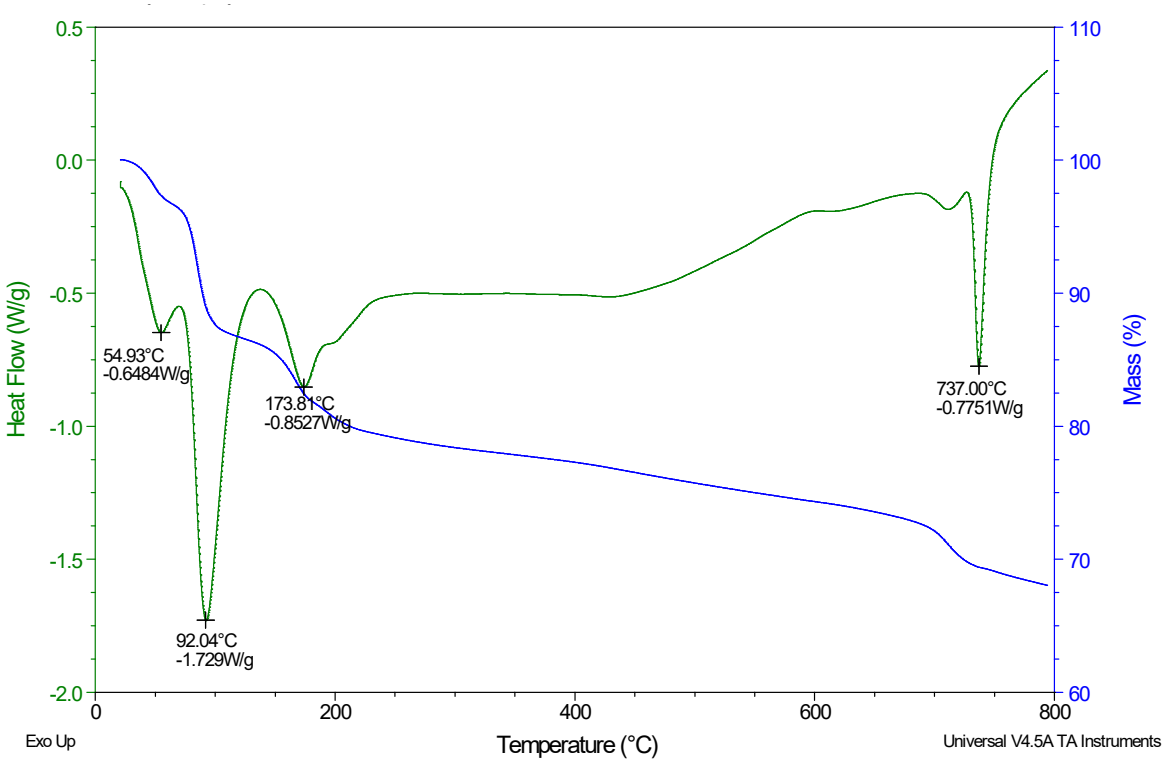
A-3.4 SSA-5



*Graph A.17: TGA graph of oxidized silica-benzylated **SSA-5***

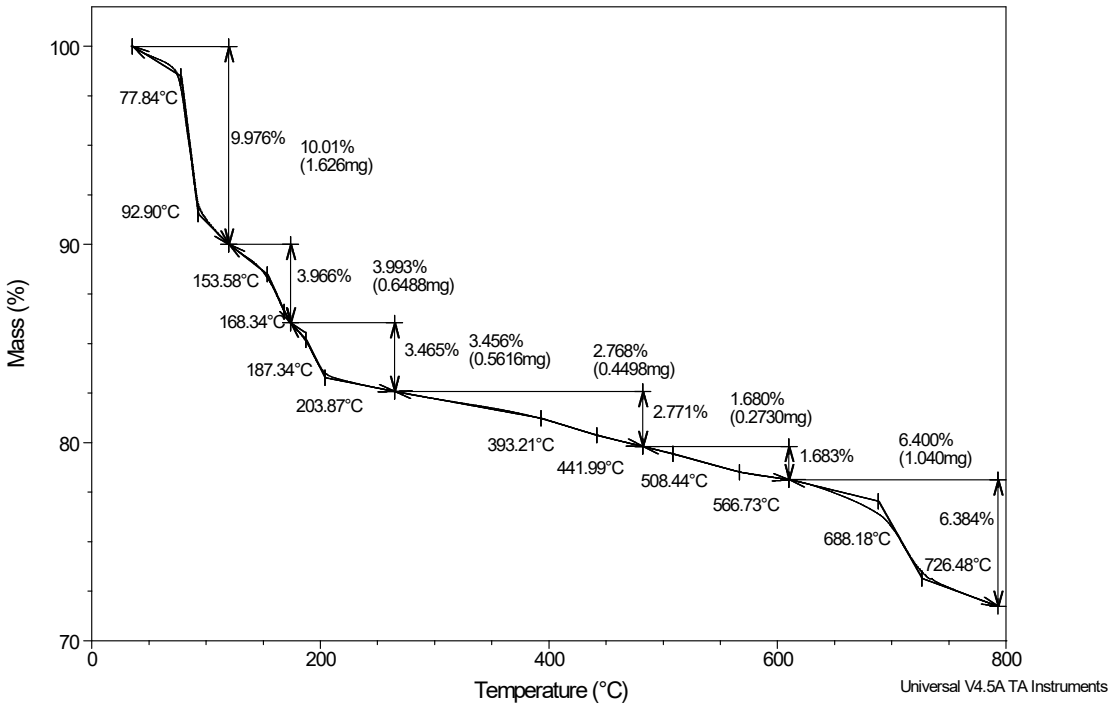


*Graph A.18: TGA (black) and DTA (blue) of oxidized silica-benzylated **SSA-5***

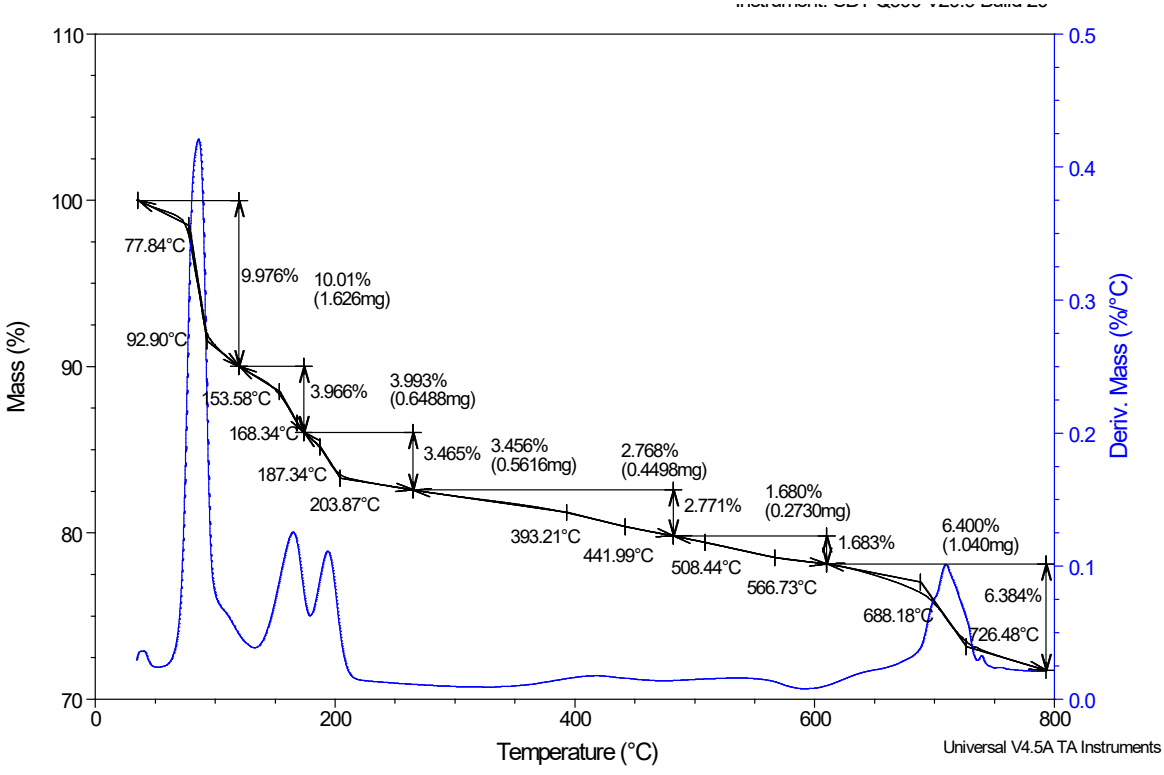


*Graph A.19: DSC (green) and TGA (blue) of oxidized silica-benzylated **SSA-5***

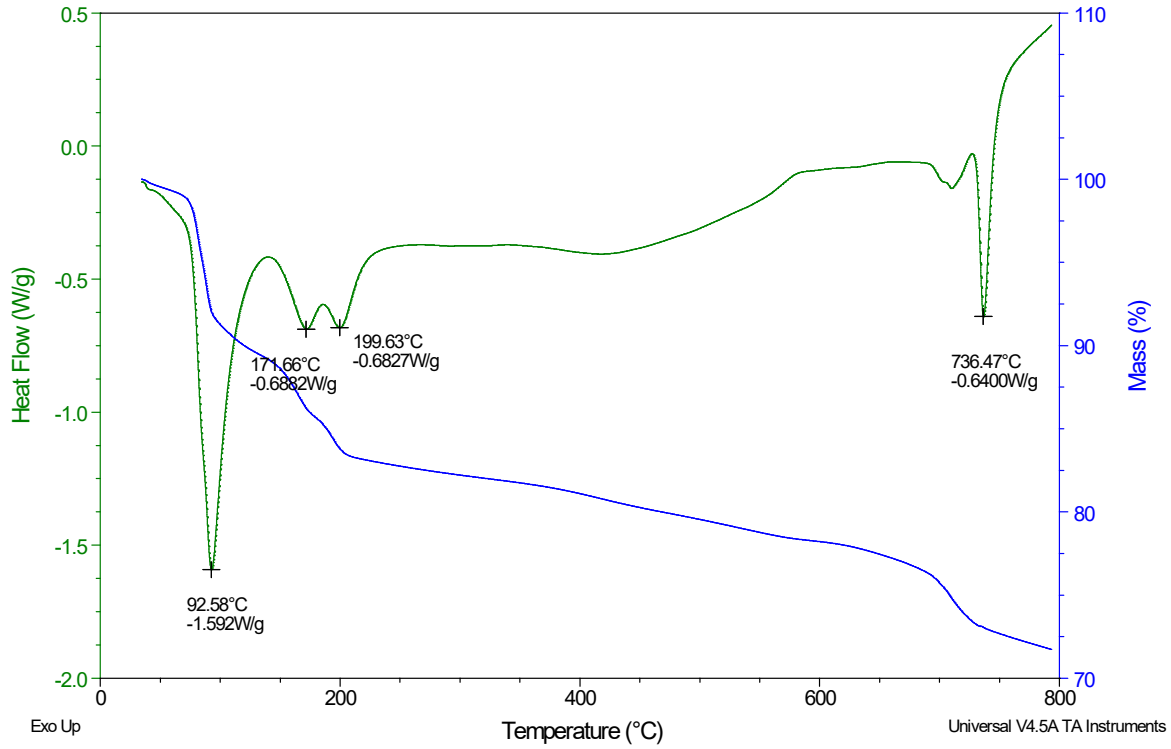
A-3.5 SSA-6



*Graph A.20: TGA graph of silica-benzylated **SSA-6***

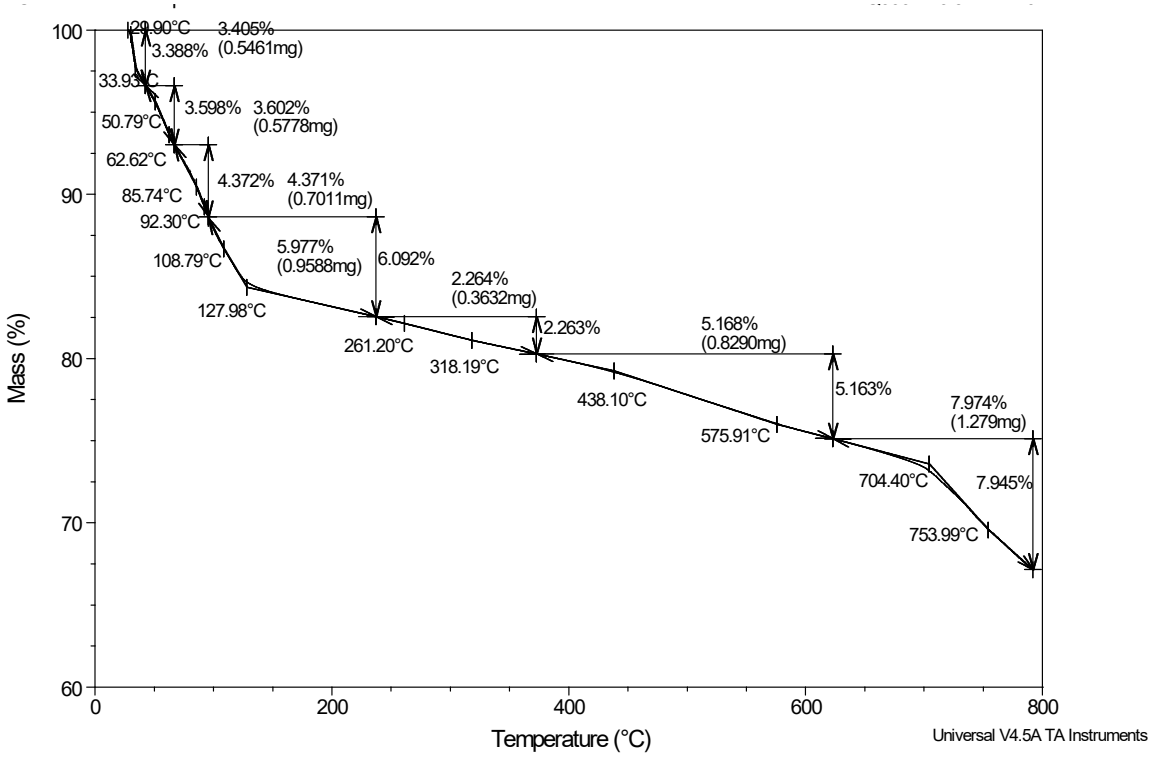


*Graph A.21: TGA (black) and DTA (blue) graphs of silica-benzylated **SSA-6***

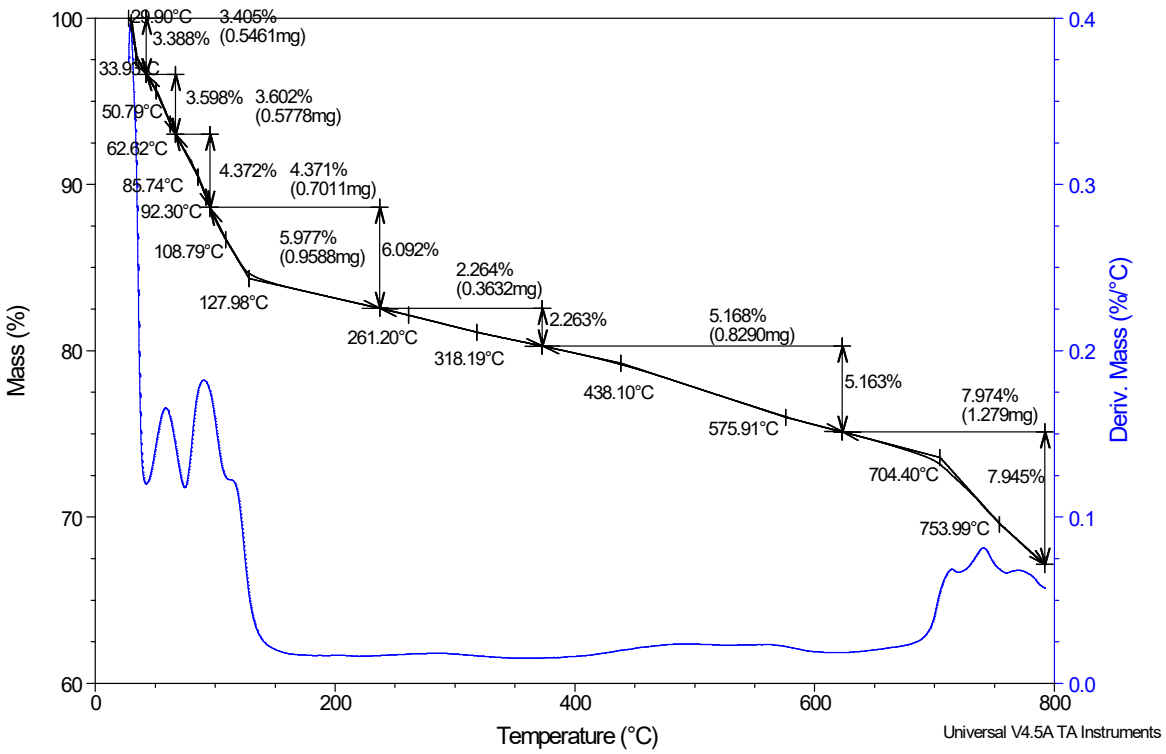


*Graph A.22: DSC (green) and TGA (blue) of silica-benzylated **SSA-6***

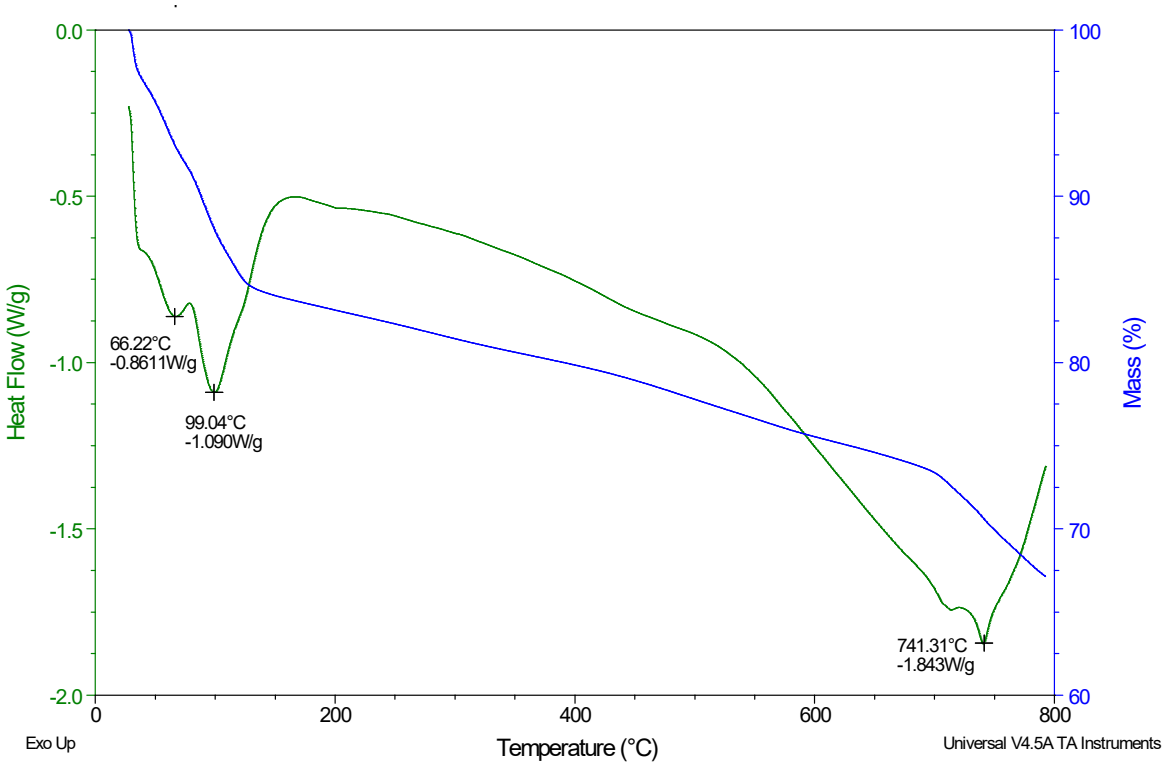
A-3.6 SSA-7



*Graph A.23: TGA graph of silica-DNPH **SSA-7***



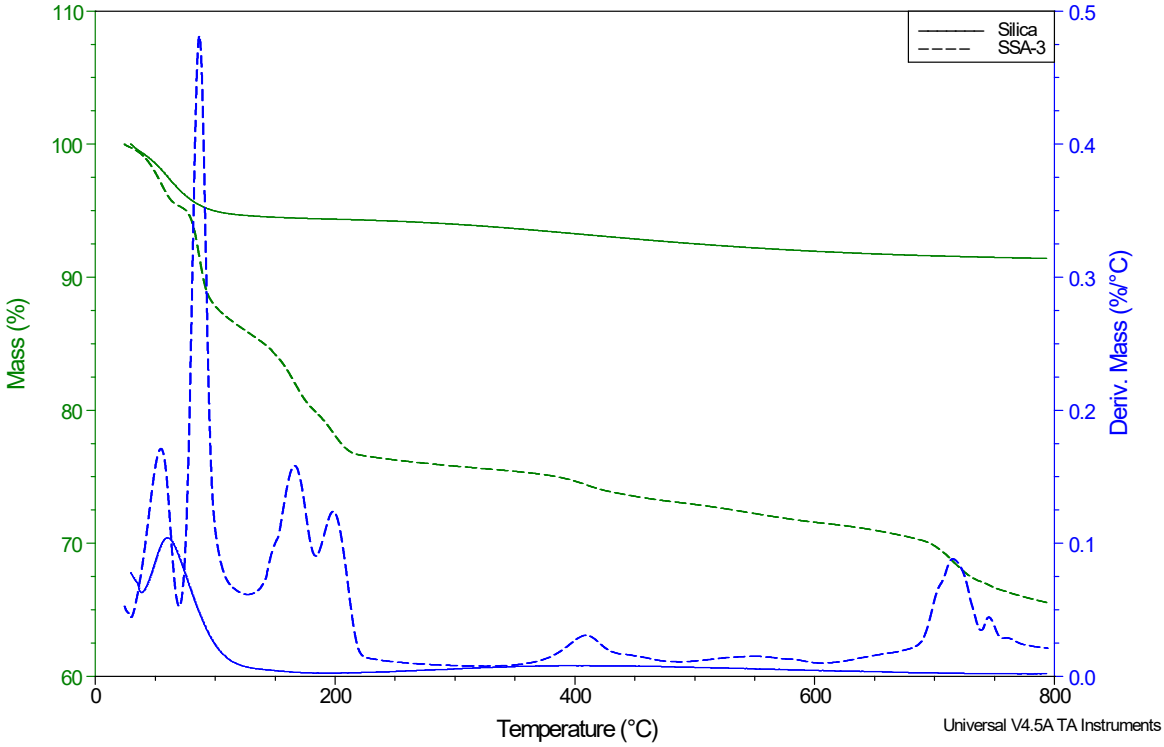
*Graph A.24: TGA (black) and DTA (blue) of silica-DNPH **SSA-7***



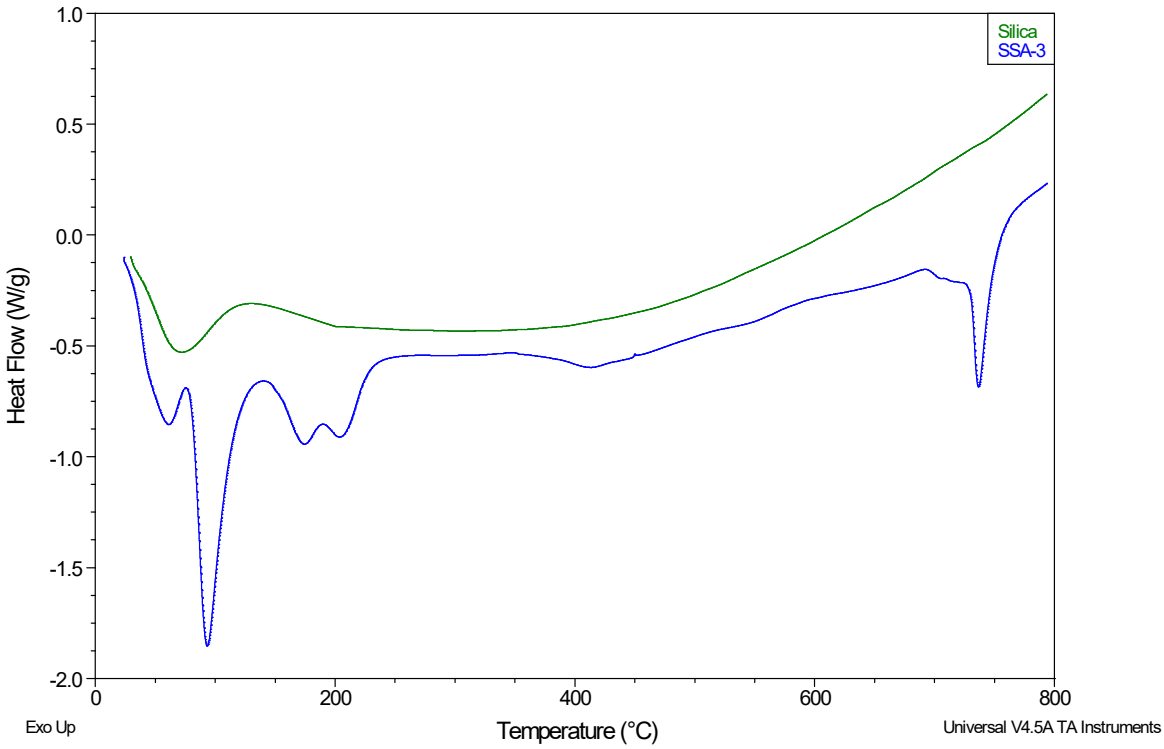
*Graph A.25: DSC (green) and TGA (blue) of silica-DNPH **SSA-7***

A-3.7 Combinations

Silica and SSA-3

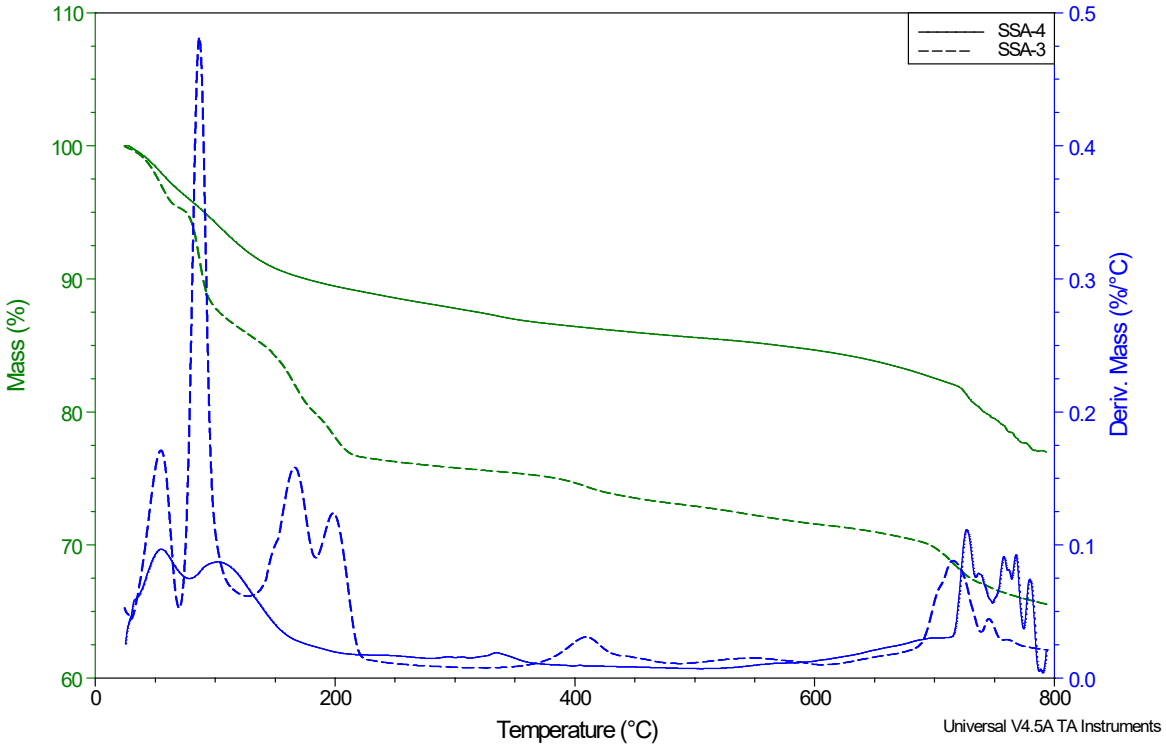


*Graph A.26: Overlay of TGA (green) and DTA (blue) graphs of silica (solid line) and oxidized silica **SSA-3** (dashed line)*

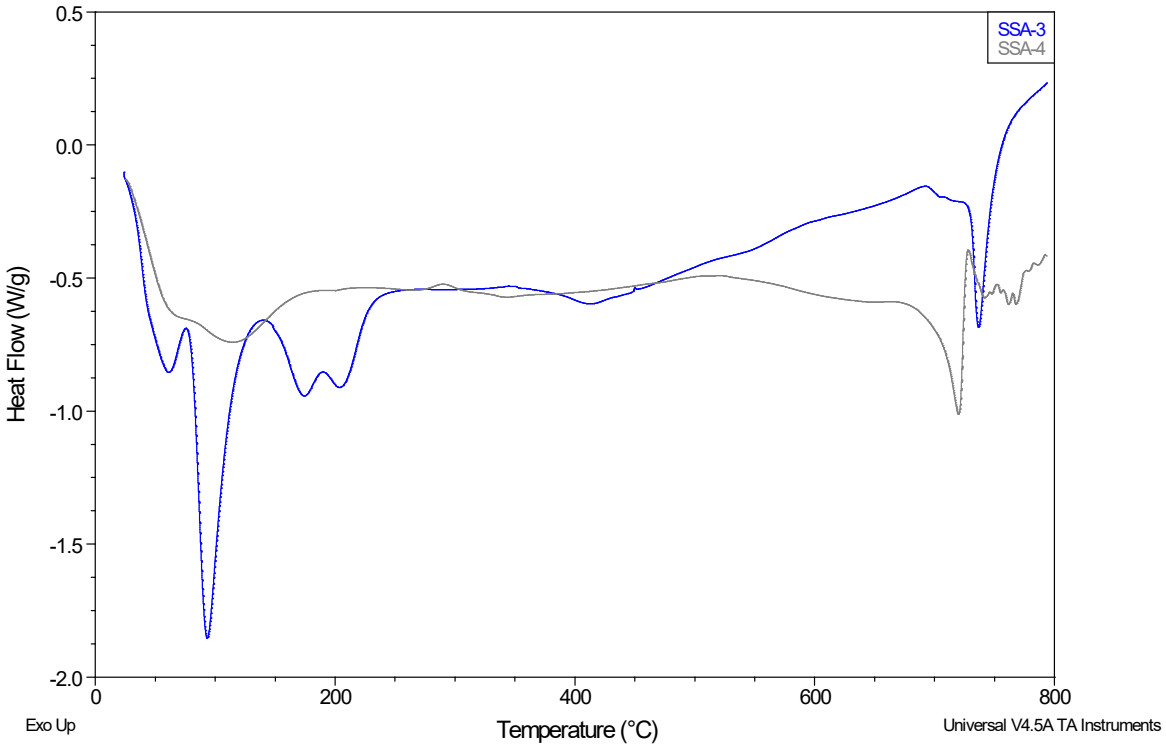


*Graph A.27: Overlay of DSC graphs of silica (green) and oxidized silica **SSA-3** (blue)*

SSA-3 and SSA-4

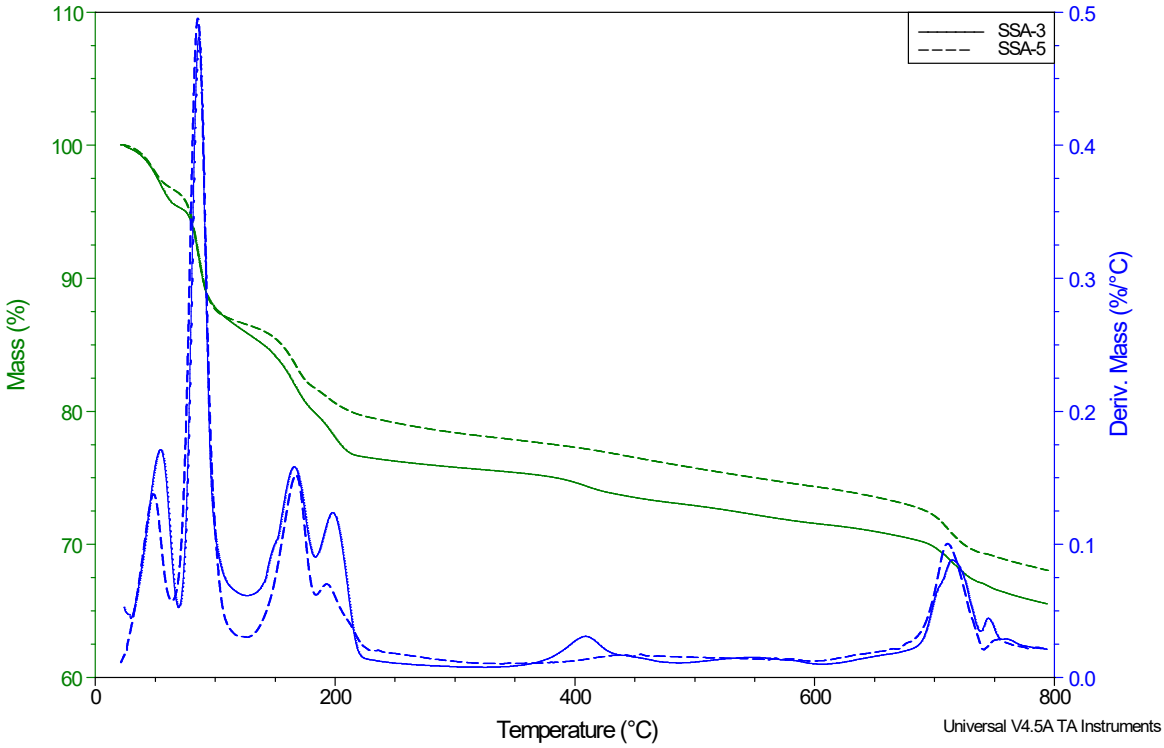


*Graph A.28: Overlay of TGA (green) and DTA (blue) graphs of oxidized silica-DNPH **SSA-4** (solid line) and oxidized silica **SSA-3 (**dashed line)*

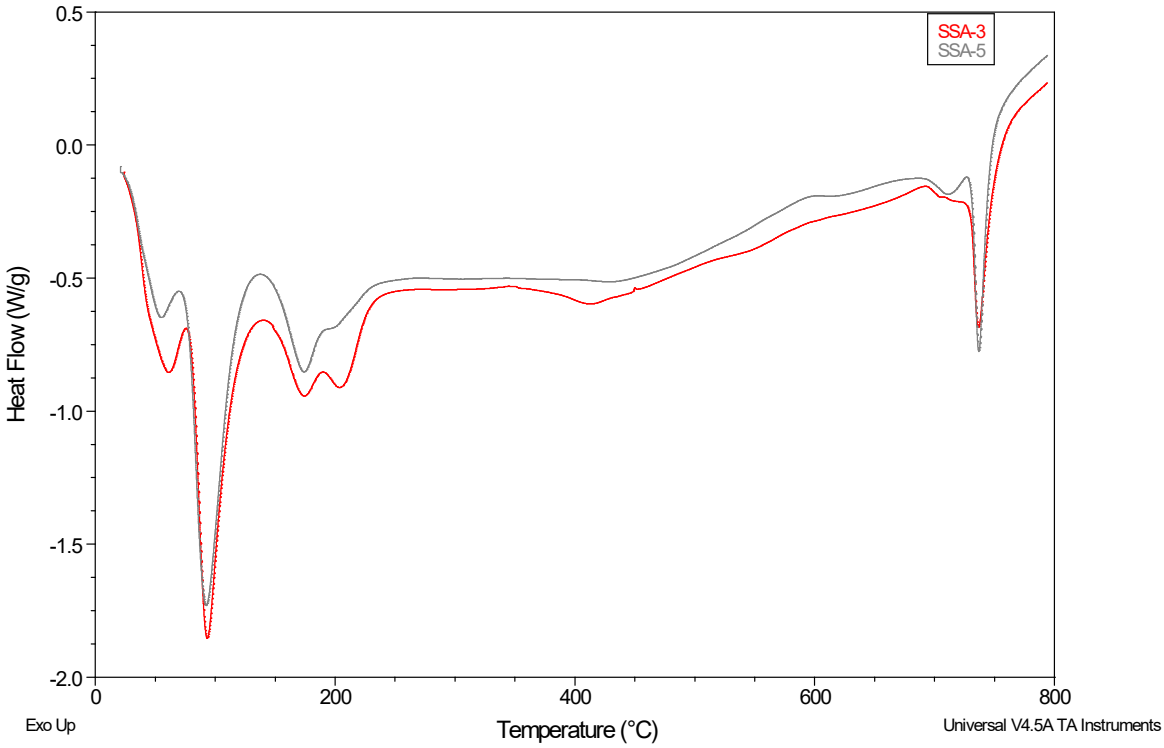


*Graph A.29: Overlay of DSC graphs of oxidized silica-DNPH **SSA-4** (grey) and oxidized silica **SSA-3** (blue)*

SSA-3 and SSA-5

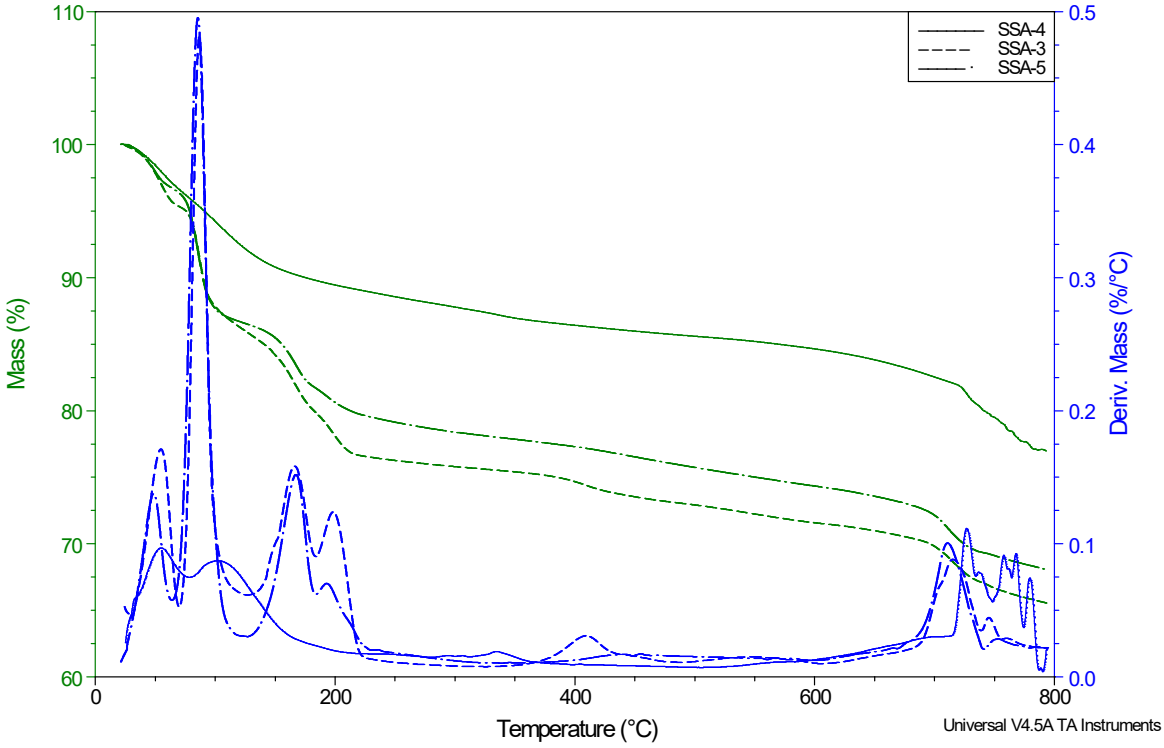


*Graph A.30: Overlay of TGA (green) and DTA (blue) graphs of oxidized silica **SSA-3** (solid line) and oxidized silica-benzylated **SSA-5** (dashed line)*

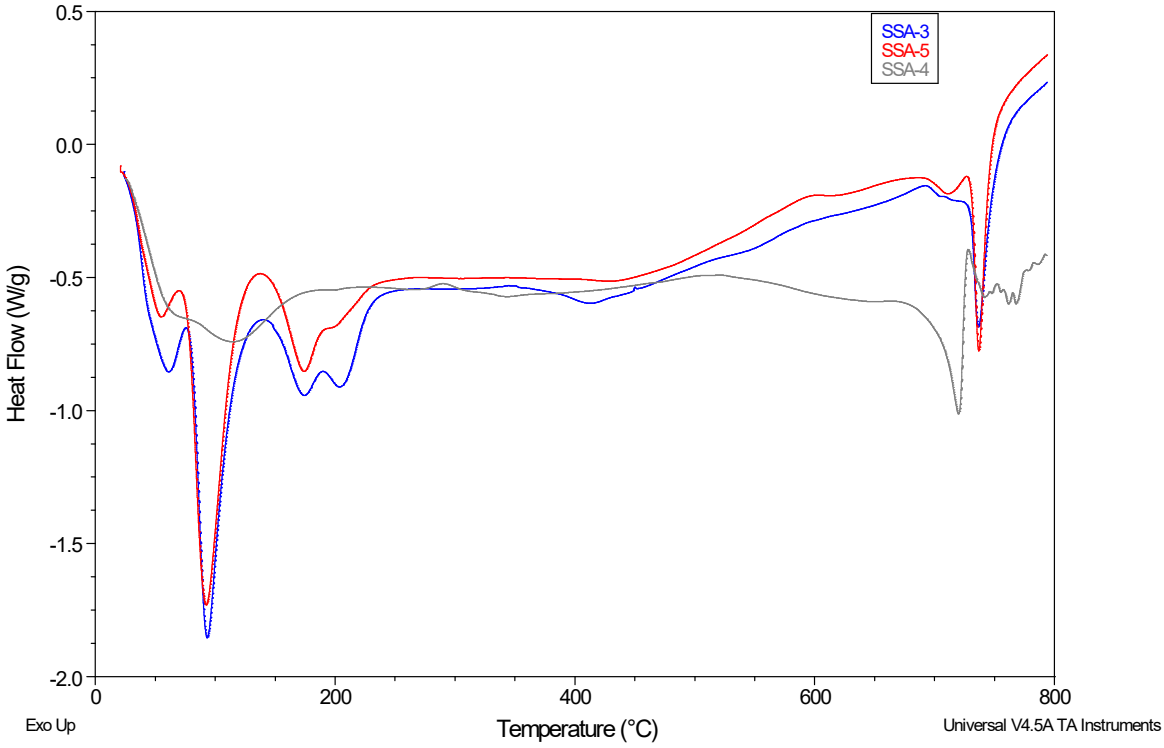


*Graph A.31: Overlay of DSC graphs of oxidized silica **SSA-3** (red) and oxidized silica-benzylated **SSA-5** (grey)*

SSA-3, SSA-4 and SSA-5

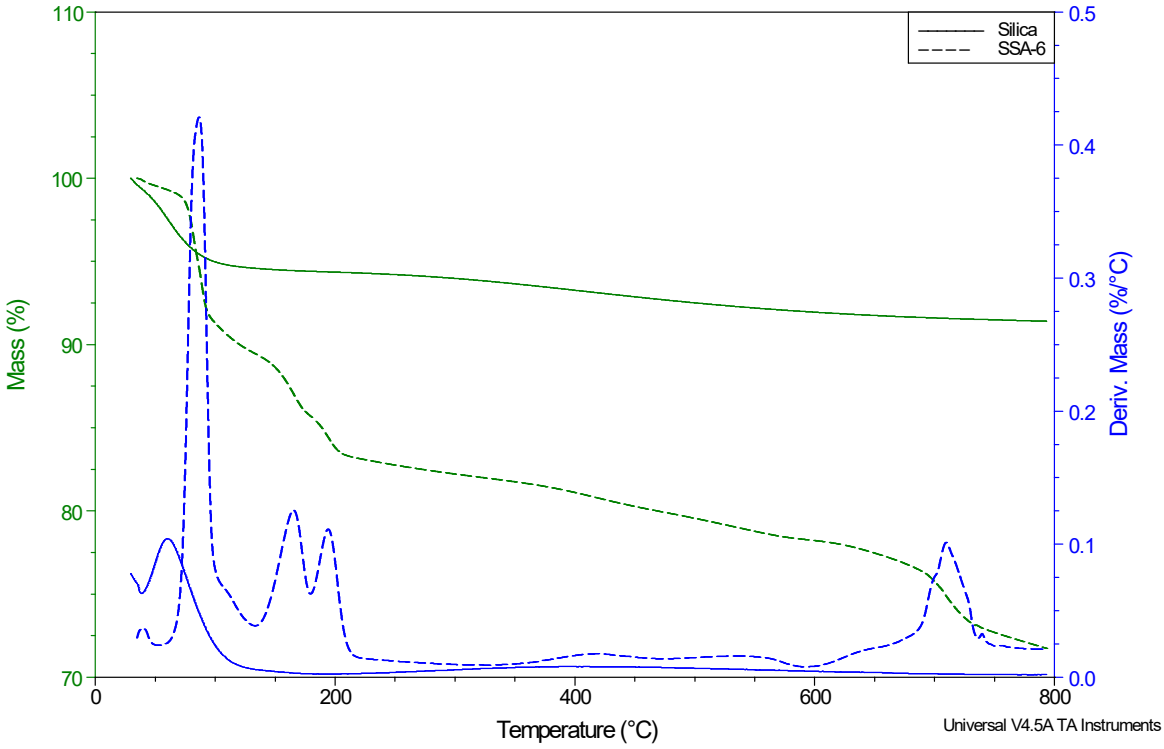


*Graph A.32: Overlay of TGA (green) and DTA (blue) graphs of oxidized silica **SSA-3** (dashed line), oxidized silica-DNPH **SSA-4** (solid line) and oxidized silica-benzylated **SSA-5** (dashed-dot line)*

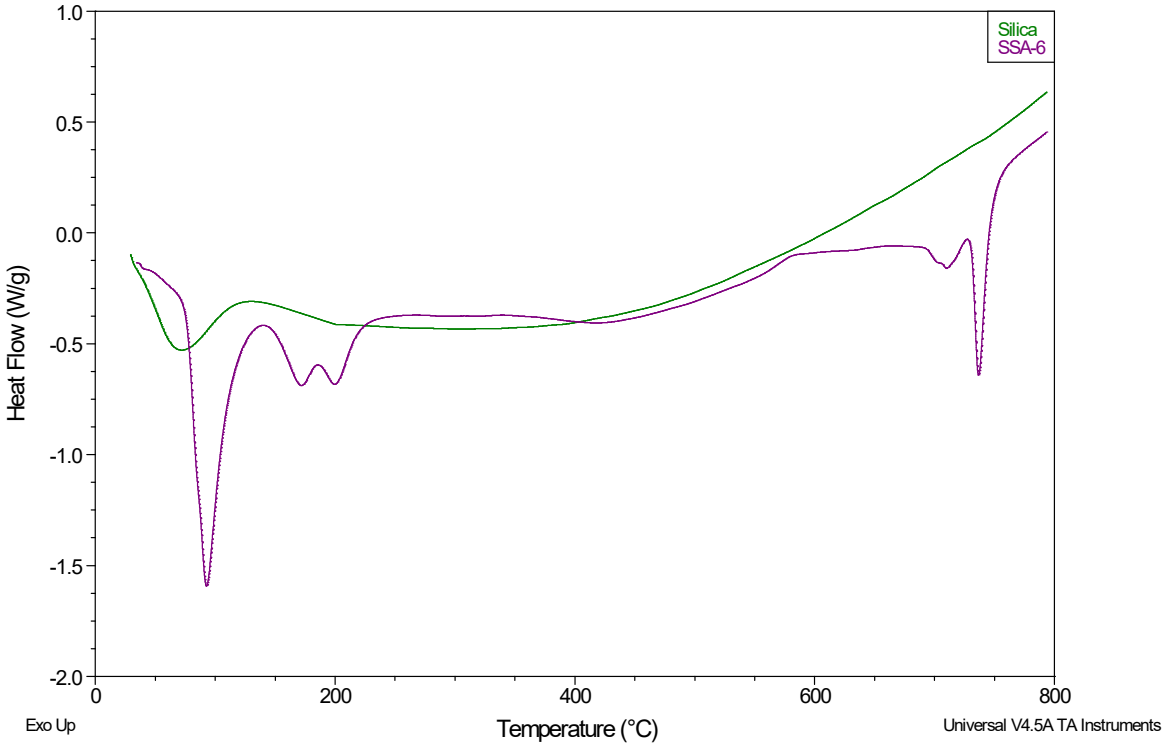


*Graph A.33: Overlay of DSC graphs of oxidized silica **SSA-3** (blue), oxidized silica-DNPH **SSA-4** (grey) and oxidized silica-benzylated **SSA-5** (red)*

Silica and SSA-6

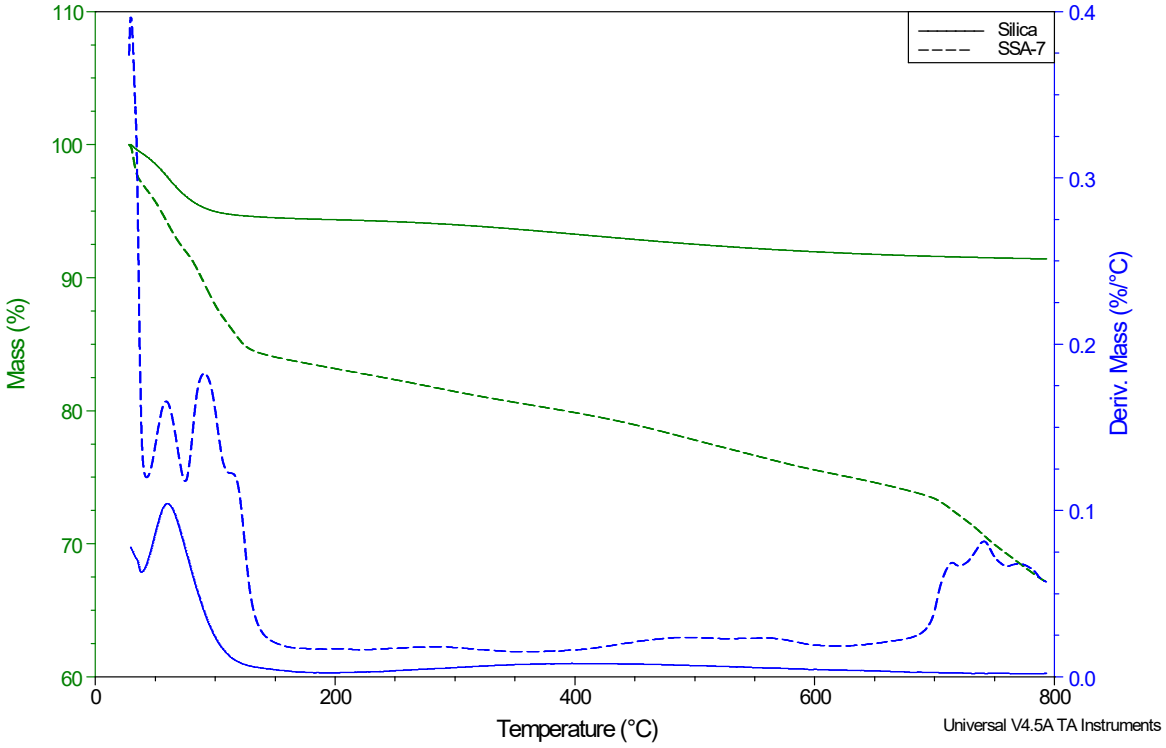


*Graph A.34: Overlay of TGA (green) and DTA (blue) graphs of silica (solid line) and silica-benzylated **SSA-6** (dashed line)*

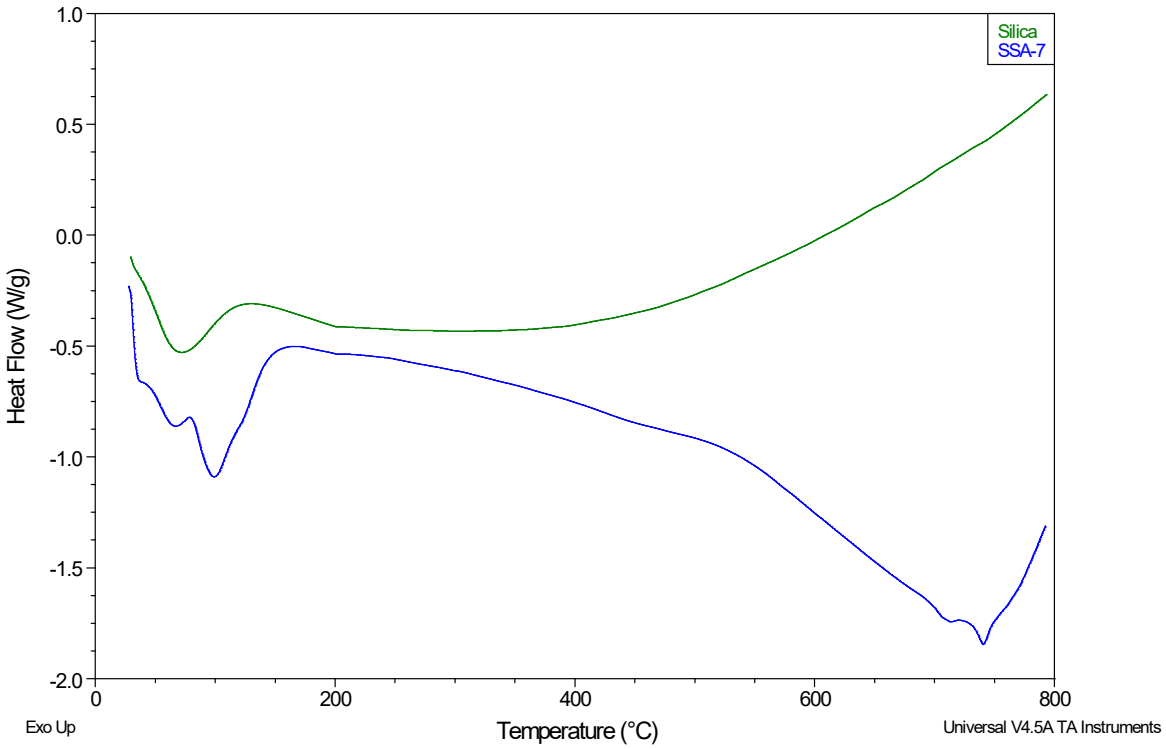


*Graph A.35: Overlay of DSC graphs of silica (green) and silica-benzylated **SSA-6** (purple)*

Silica and SSA-7

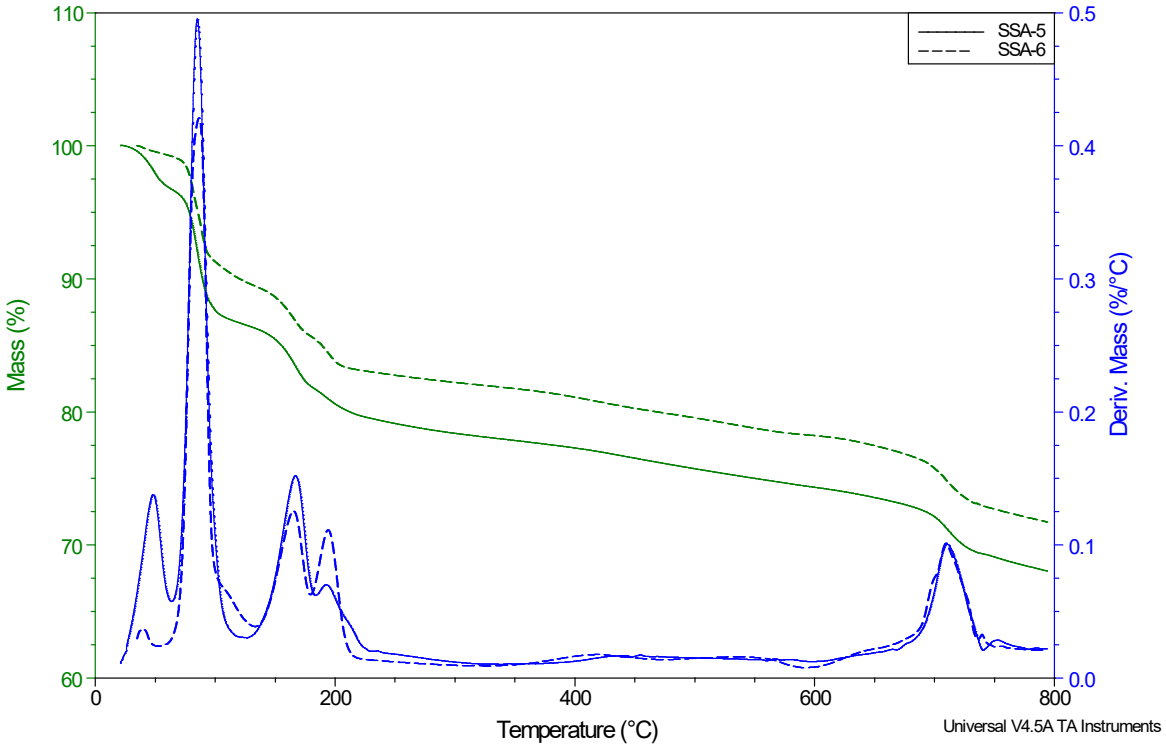


*Graph A.36: Overlay of TGA (green) and DTA (blue) graphs of silica (solid line) and silica-DNPH **SSA-7** (dashed line)*

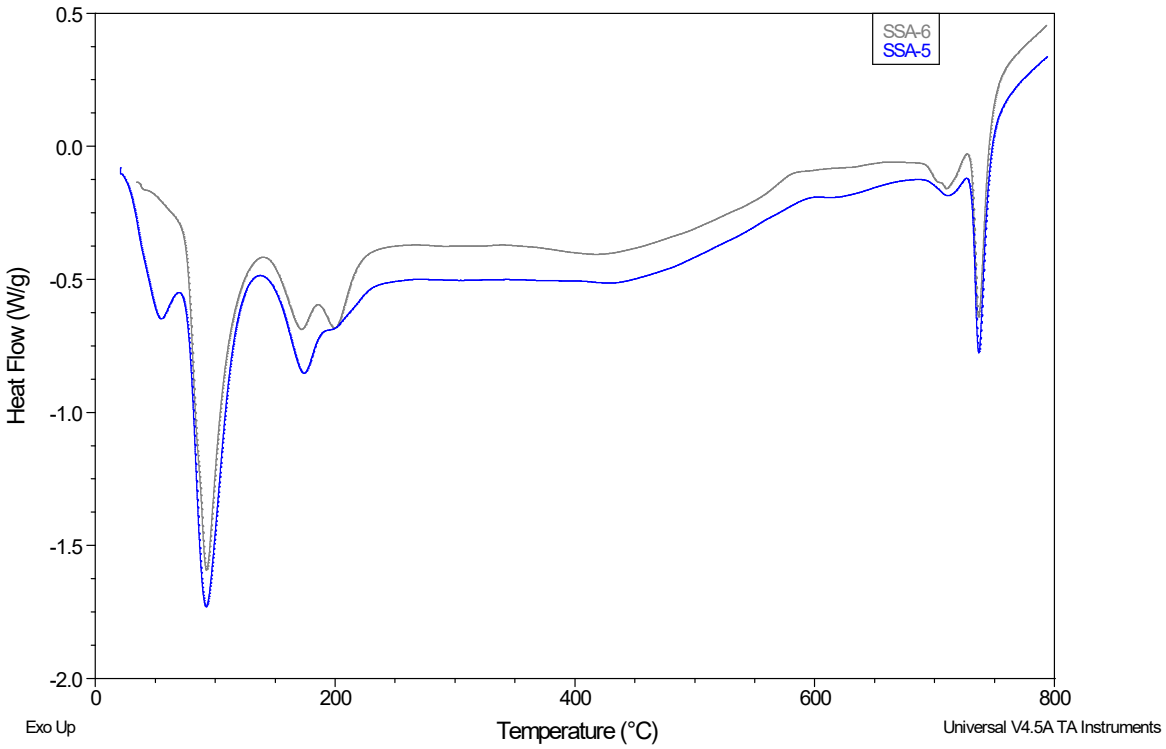


*Graph A.37: Overlay of DSC graphs of silica (green) and silica-DNPH **SSA-7** (blue)*

SSA-5 and SSA-6

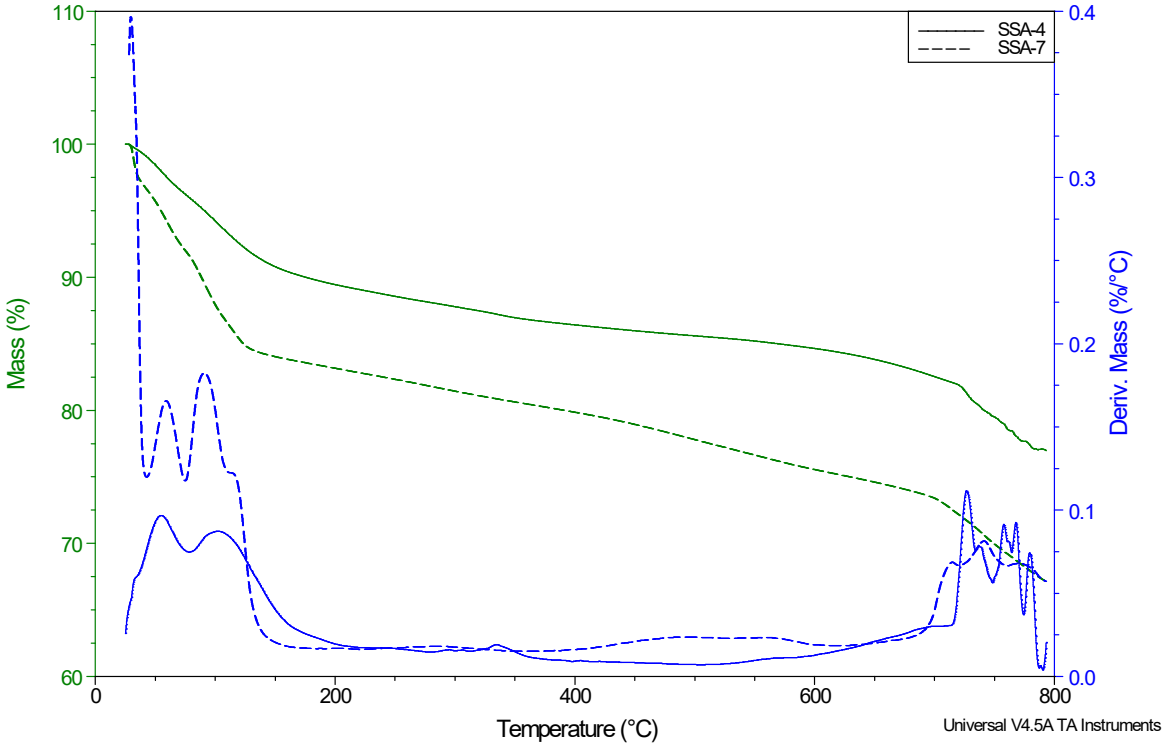


*Graph A.38: Overlay of TGA (green) and DTA (blue) graphs of oxidized silica-benzylated **SSA-5** (solid line) and silica-benzylated **SSA-6** (dashed line)*

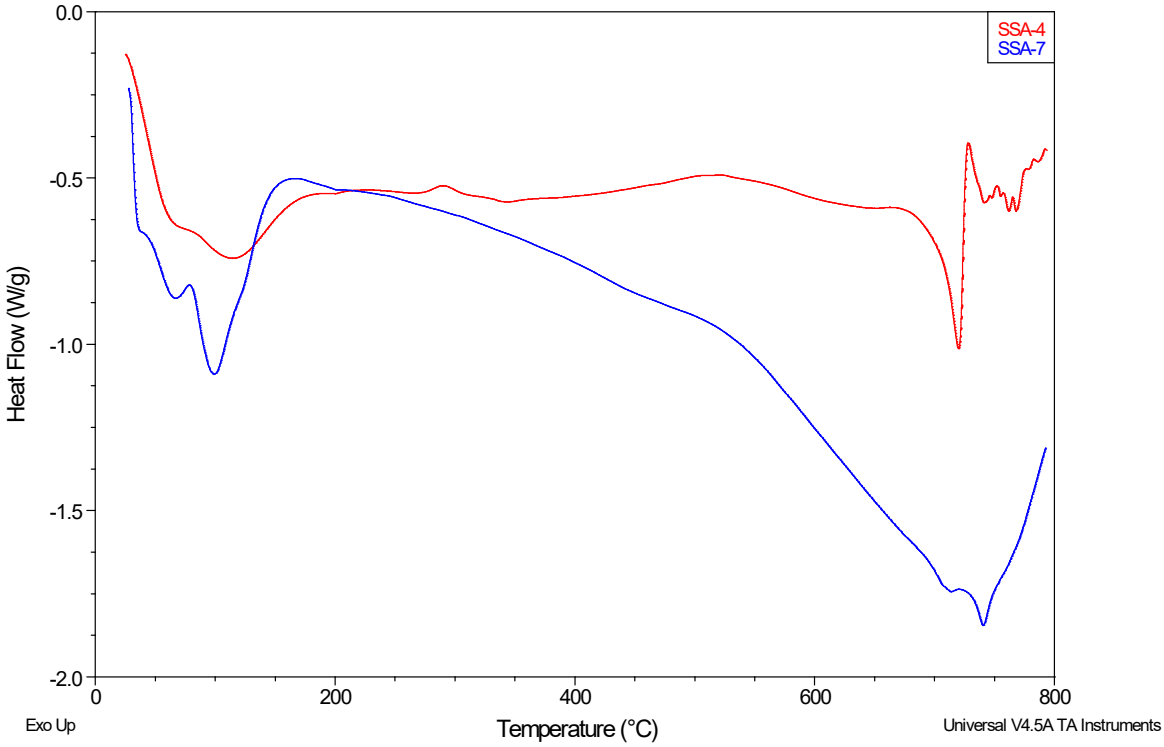


*Graph A.39: Overlay of DSC graphs of oxidized silica-benzylated **SSA-5** (blue) and silica-benzylated **SSA-6** (grey)*

SSA-4 and SSA-7



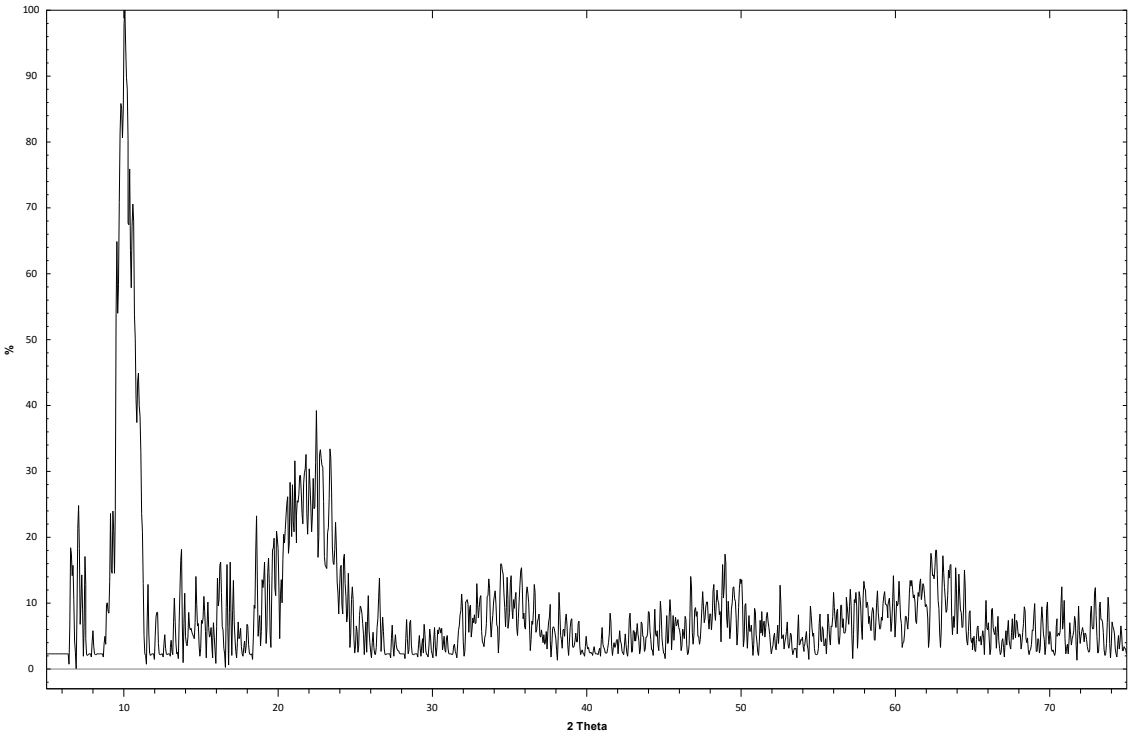
*Graph A.40: Overlay of TGA (green) and DTA (blue) graphs of oxidized silica-DNPH **SSA-4** (solid line) and silica-DNP **SSA-7** (dashed line)*



*Graph A.41: Overlay of DSC graphs of oxidized silica-DNPH **SSA-4** (red) and silica-DNP **SSA-7** (blue)*

A-4 PXRD results

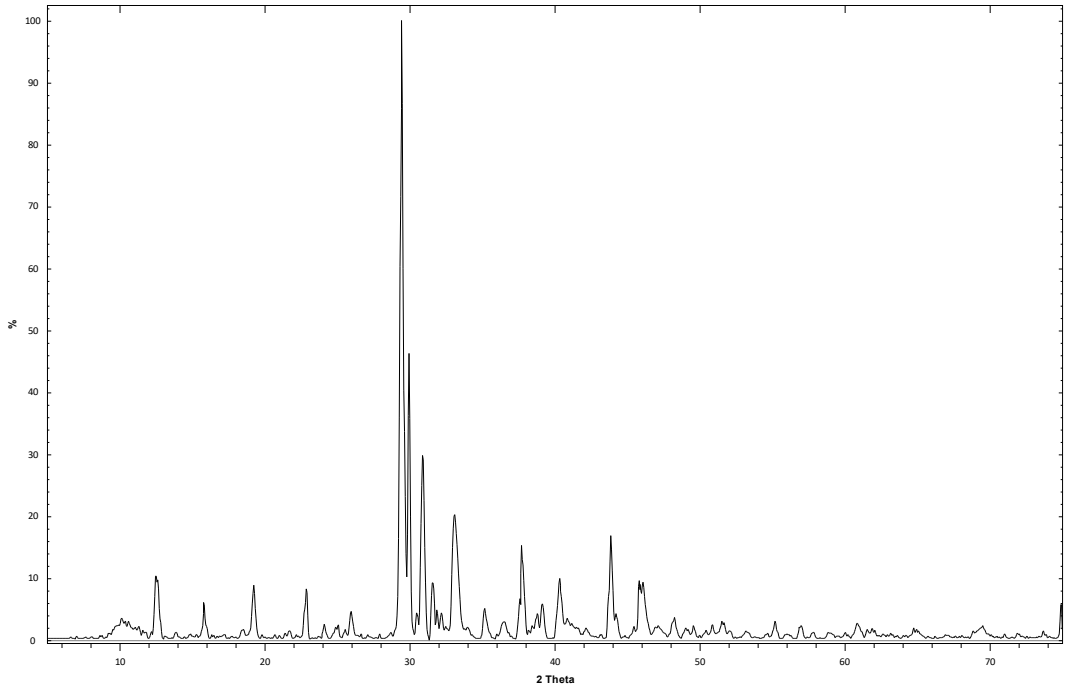
A-4.1 Silica



Graph A.42: PXRD of Silica

2 theta	***Percentage intensity***	***d-spacing***
7,07947	28,3	12,47636531
10,1249	53,12	8,729452571
21,4944	100	4,130825951
62,5568	24,53	1,48363737

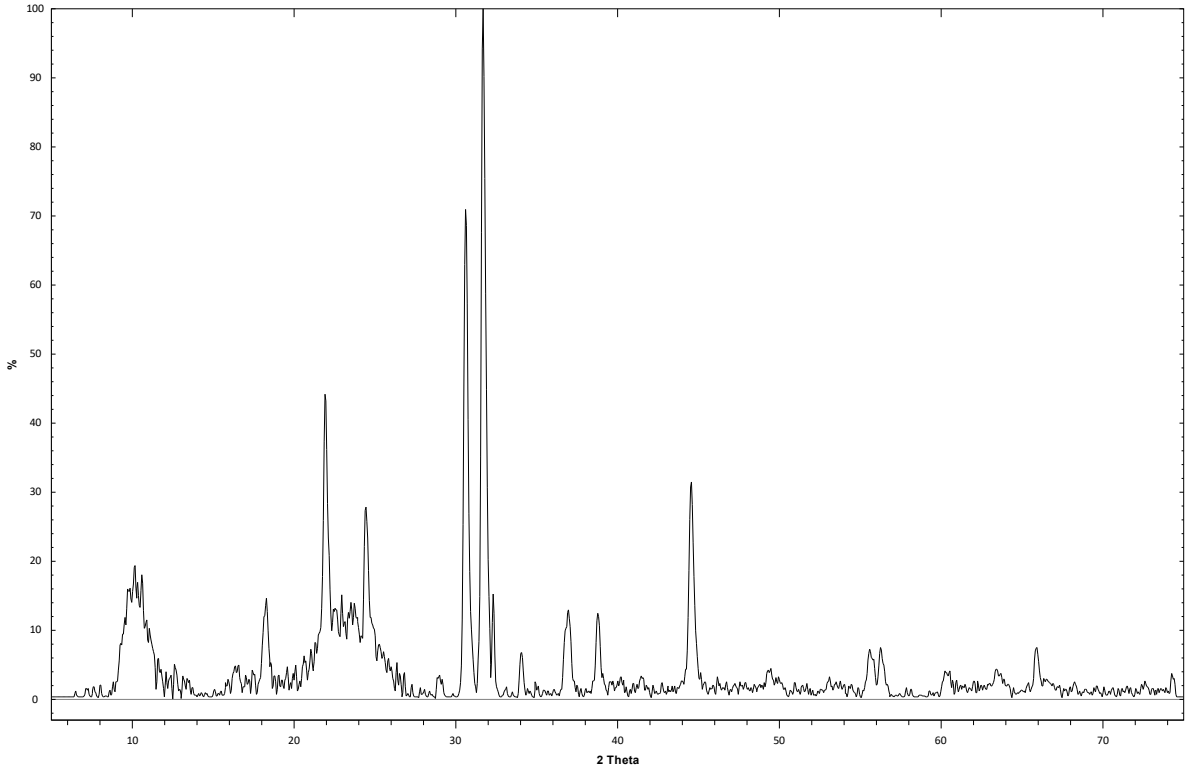
A-4.2 SSA-3



*Graph A.43: PXRD of oxidized Silica **SSA-3***

2 theta	***Percentage intensity***	***d-spacing***
12,54736	12,67	*7,049013464*
19,24955	10,25	*4,607192958*
15,84567	7,64	*5,588391755*
22,84111	8,95	*3,890227166*
29,45318	100	*3,030209933*
29,96609	37	*2,97950132*
30,89258	32,33	*2,892222898*
31,79323	11,88	*2,812315637*
33,15102	25,84	*2,700166308*
37,76793	15,63	*2,380020821*
40,3661	11,92	*2,23262066*
43,89955	17,19	*2,06076246*
46,02096	12,55	*1,970583272*

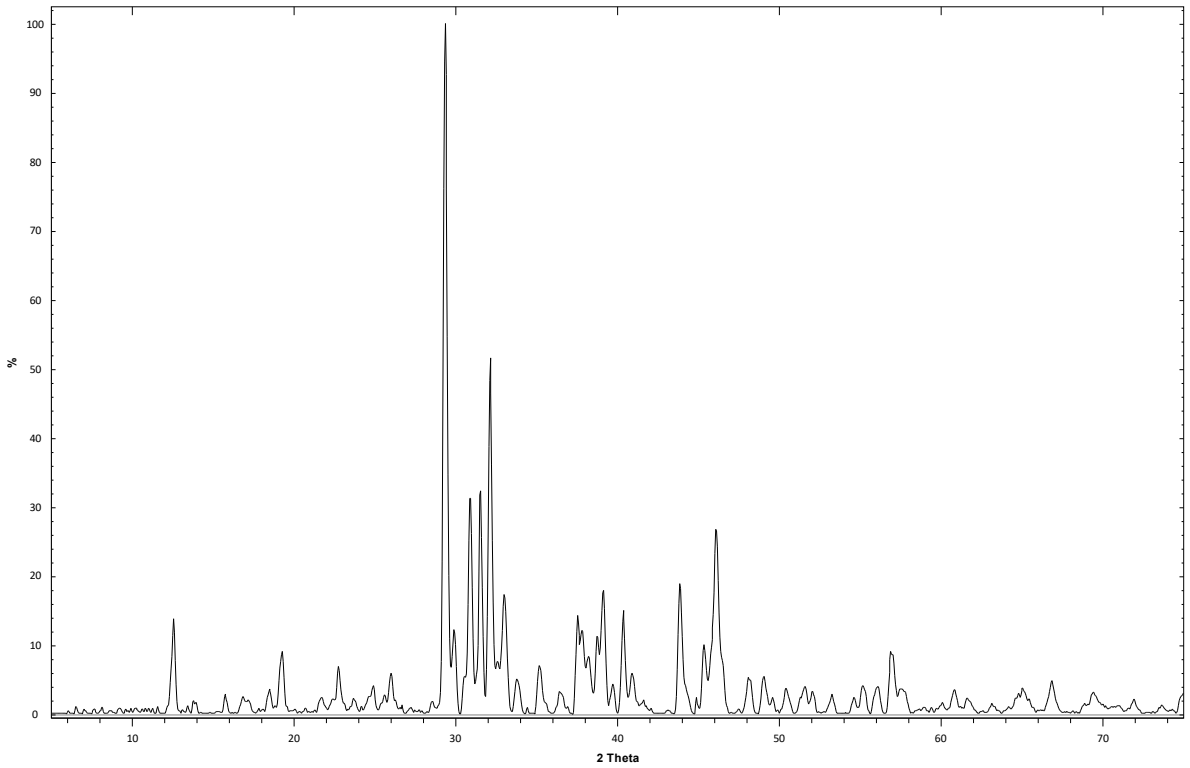
A-4.3 SSA-4



*Graph A.44: PXRD of oxidized Silica-DNPH **SSA-4***

2 theta	***Percentage intensity***	***d-spacing***
6,97796	9,15	*12,65763*
10,2264	21	*8,643037*
18,246	13,76	*4,858269*
21,95	47,71	*4,046104*
23,5247	23,41	*3,778707*
24,5399	37,04	*3,624635*
30,6815	72,6	*2,911638*
31,7473	100	*2,816279*
36,9246	13,67	*2,432419*
38,8533	12,21	*2,315996*
44,5889	30,91	*2,03049*
55,7046	8,38	*1,64878*
56,3645	8,1	*1,631032*
65,9575	7,69	*1,41514*

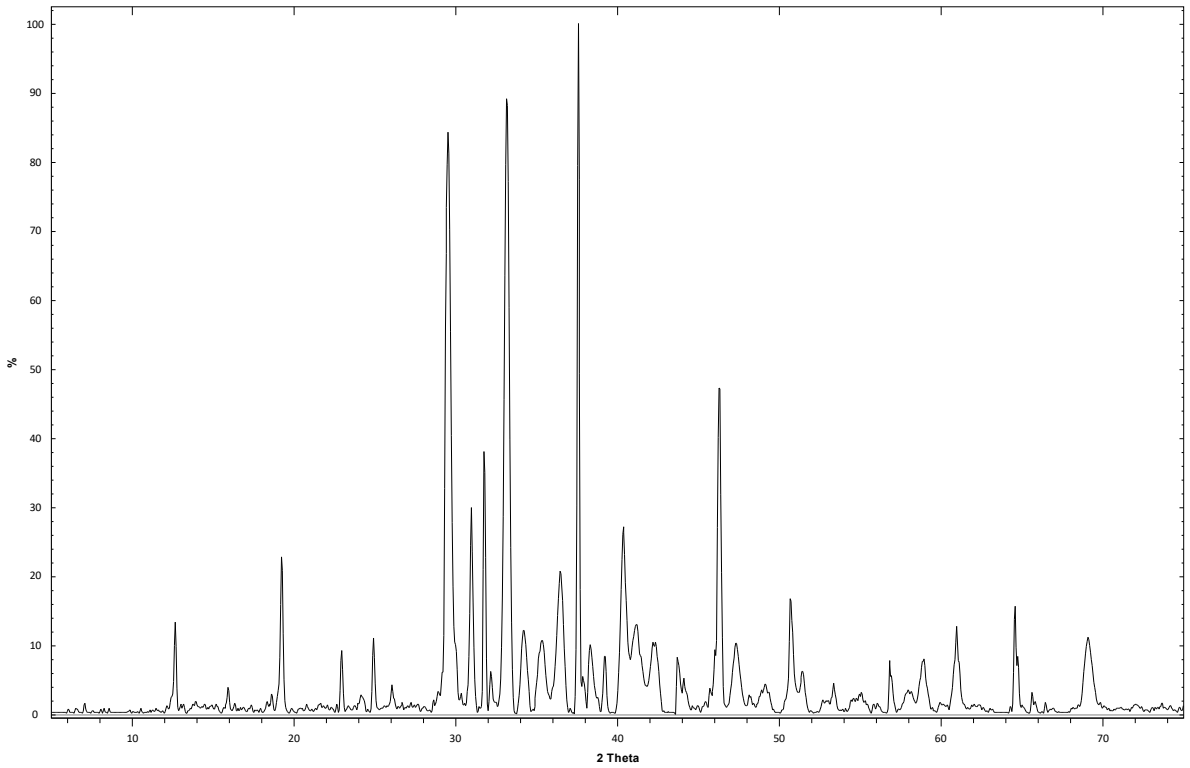
A-4.4 SSA-5



*Graph A.45: PXRD of oxidized Silica- benzylated **SSA-5***

2 theta	***Percentage intensity***	***d-spacing***
12,515	11,94	*7,067167272*
19,2611	9,03	*4,604456279*
29,3618	100	*3,039432314*
30,8845	28,91	*2,892961143*
31,4936	26,48	*2,838385271*
32,1534	49,11	*2,781630438*
33,067	16,53	*2,706834941*
37,5844	14,85	*2,391219983*
39,1071	17,44	*2,301548382*
40,376	14,34	*2,232096068*
43,929	18,47	*2,059449206*
46,1623	26,21	*1,964878196*
56,9736	11,32	*1,615032715*

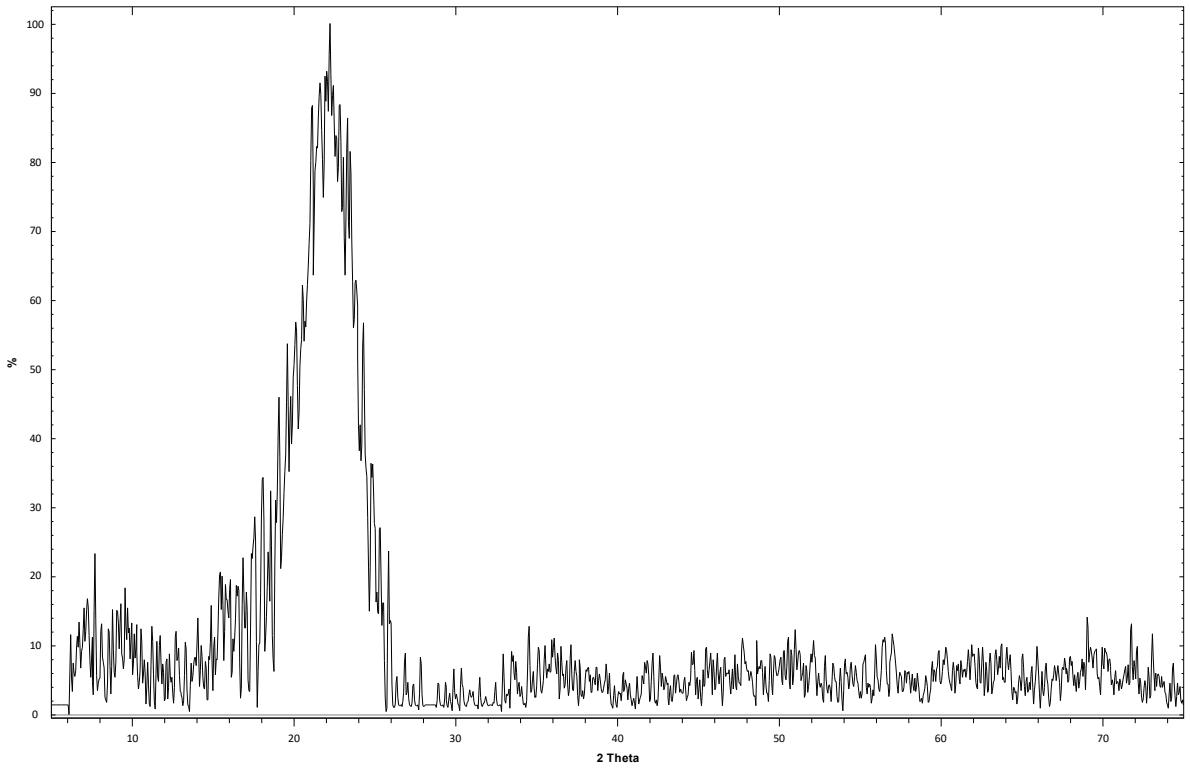
A-4.5 SSA-6



Graph A.46: PXRD of Silica-benzylated SSA-6

2 theta	***Percentage intensity***	***d-spacing***
12,6627	11,61	*6,985065*
19,2611	21,47	*4,604456*
22,9156	9,03	*3,87775*
24,9459	11,05	*3,566556*
29,5648	97,3	*3,019023*
30,986	30,66	*2,883716*
31,7981	32,97	*2,811896*
33,1685	100	*2,698783*
34,2344	19,72	*2,617155*
35,3511	19,7	*2,536999*
36,5185	30,17	*2,458531*
37,5844	83,5	*2,39122*
38,3458	16,35	*2,345473*
40,376	33,38	*2,232096*
41,1374	19,18	*2,192524*
42,3556	16,63	*2,13224*
43,7767	10,99	*2,06626*
46,3146	46,94	*1,958771*
47,3805	13,72	*1,917161*
50,7304	19,05	*1,798143*
56,872	10,09	*1,617676*
58,9023	10,92	*1,566665*
60,9834	14,33	*1,518091*
64,6379	16,52	*1,440804*
69,0537	15,2	*1,359051*

A-4.6 SSA-7

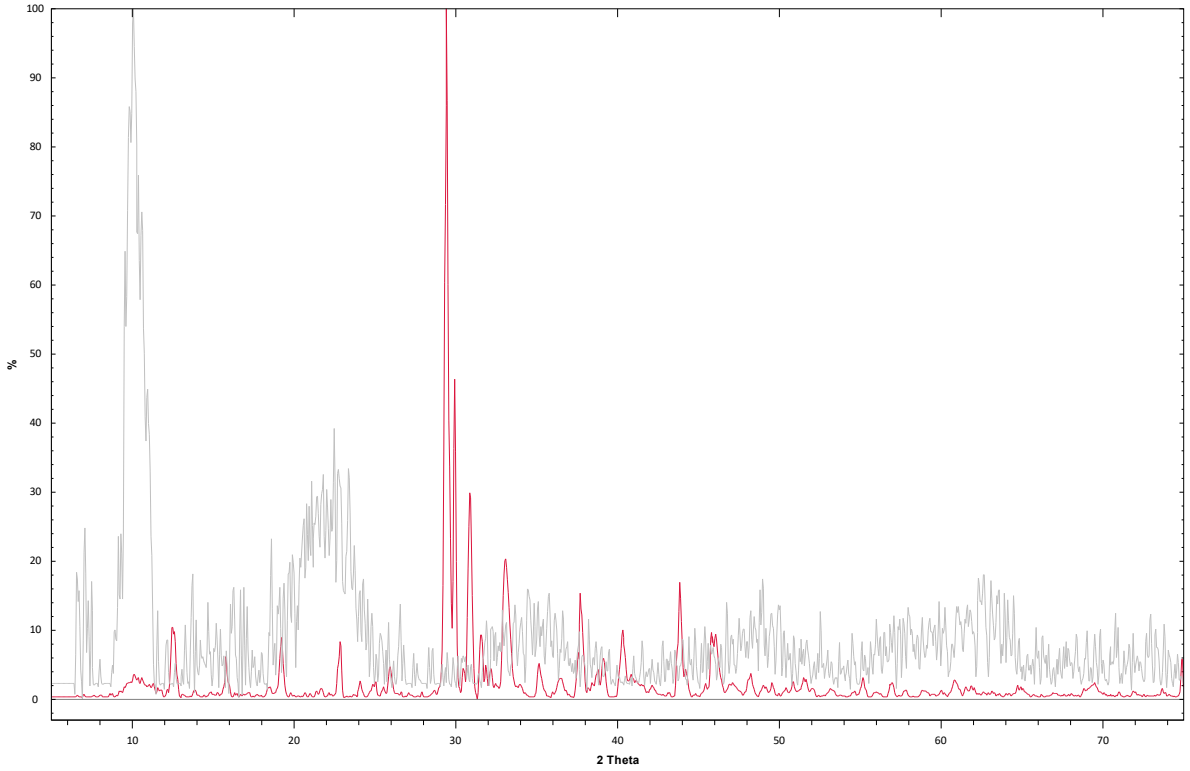


*Graph A.47: PXRD of Silica-DNPH **SSA-7***

2 theta	***Percentage intensity***	***d-spacing***
9,41429	11,06	*9,386714455*
22,2558	100	*3,991196237*

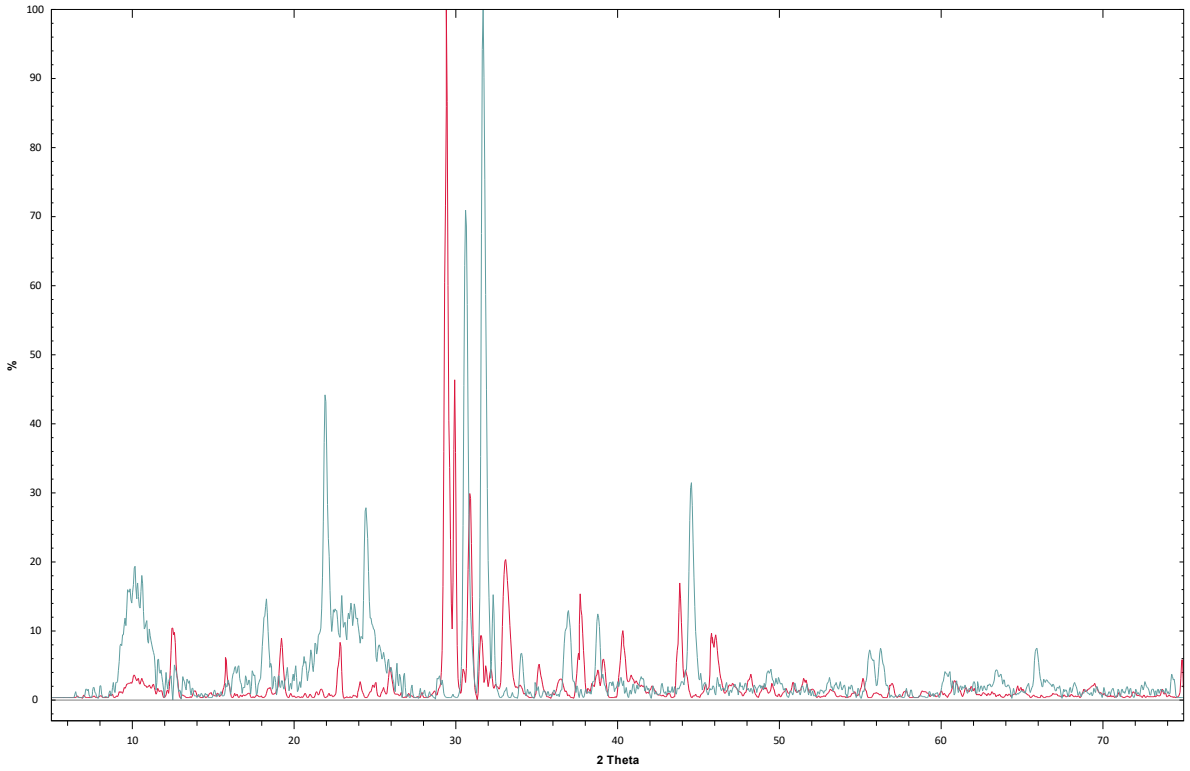
A-4.7 Combinations

Silica and SSA-3

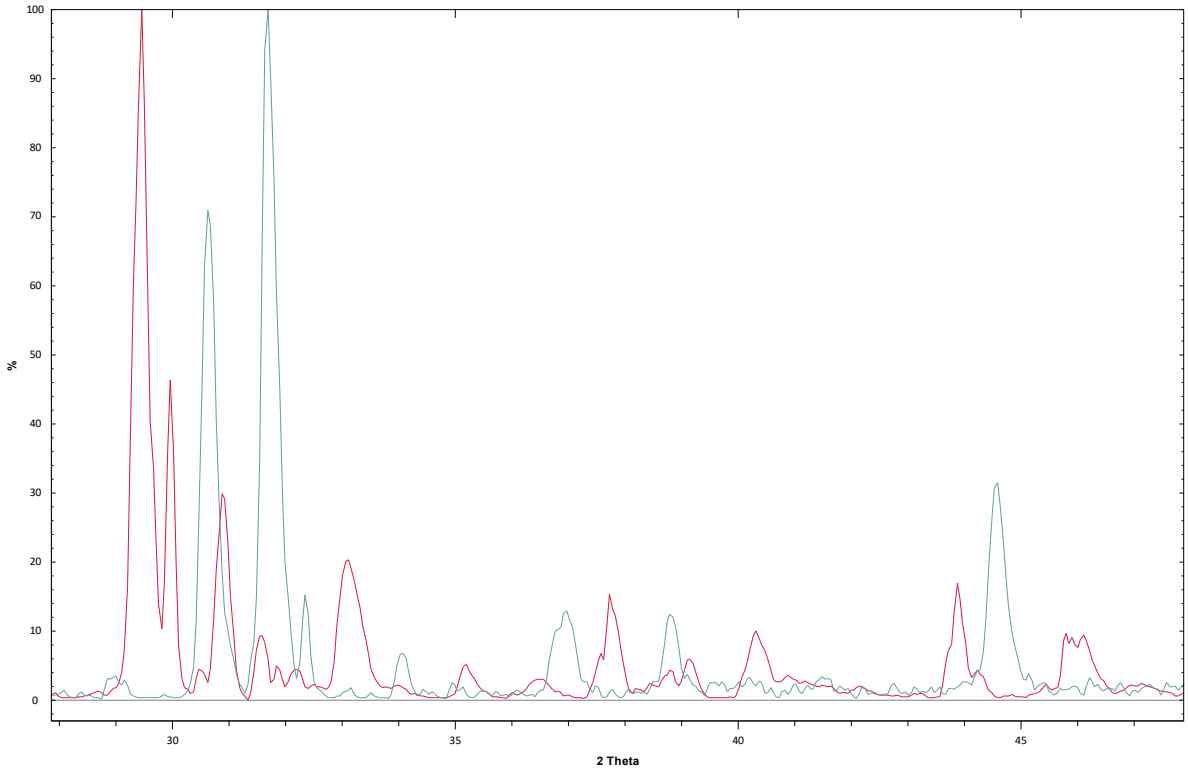


*Graph A.48: PXRD overlay of Silica (grey) and oxidized silica **SSA-3** (red)*

SSA-3 and SSA-4

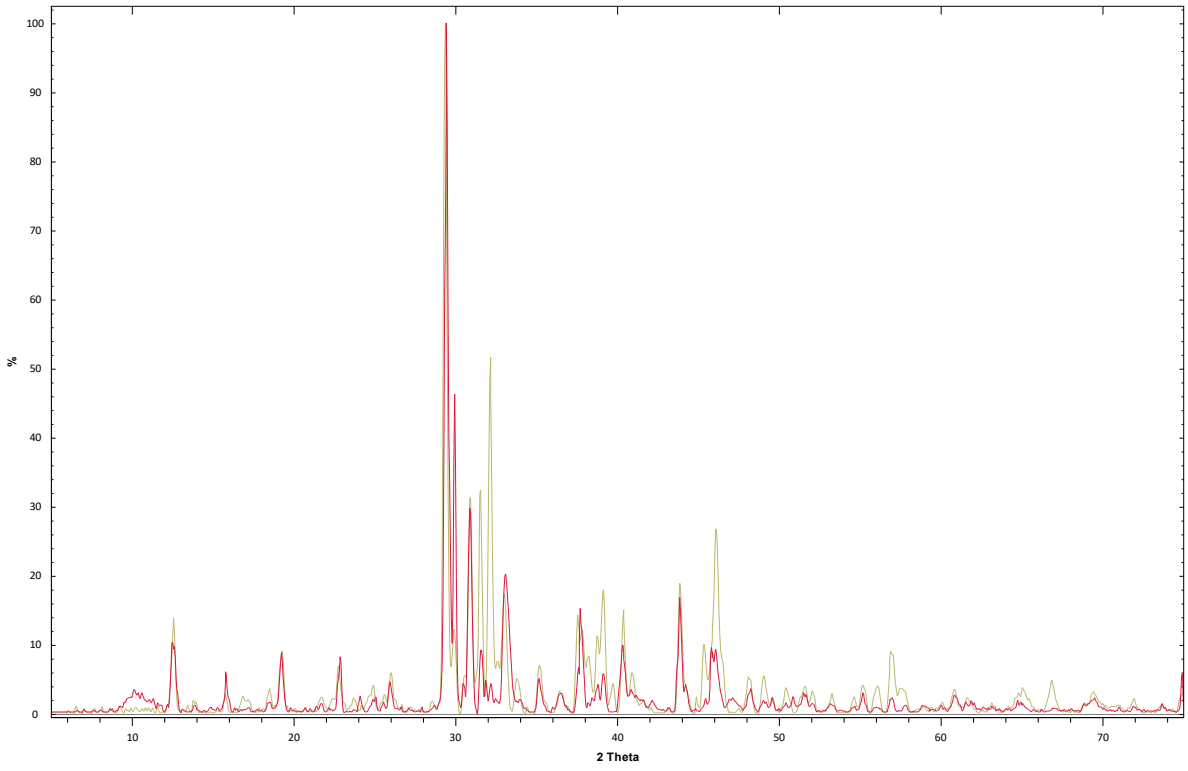


*Graph A.49: PXRD overlay of oxidized silica **SSA-3** (red) and oxidized silica-DNPH **SSA-4** (blue)*

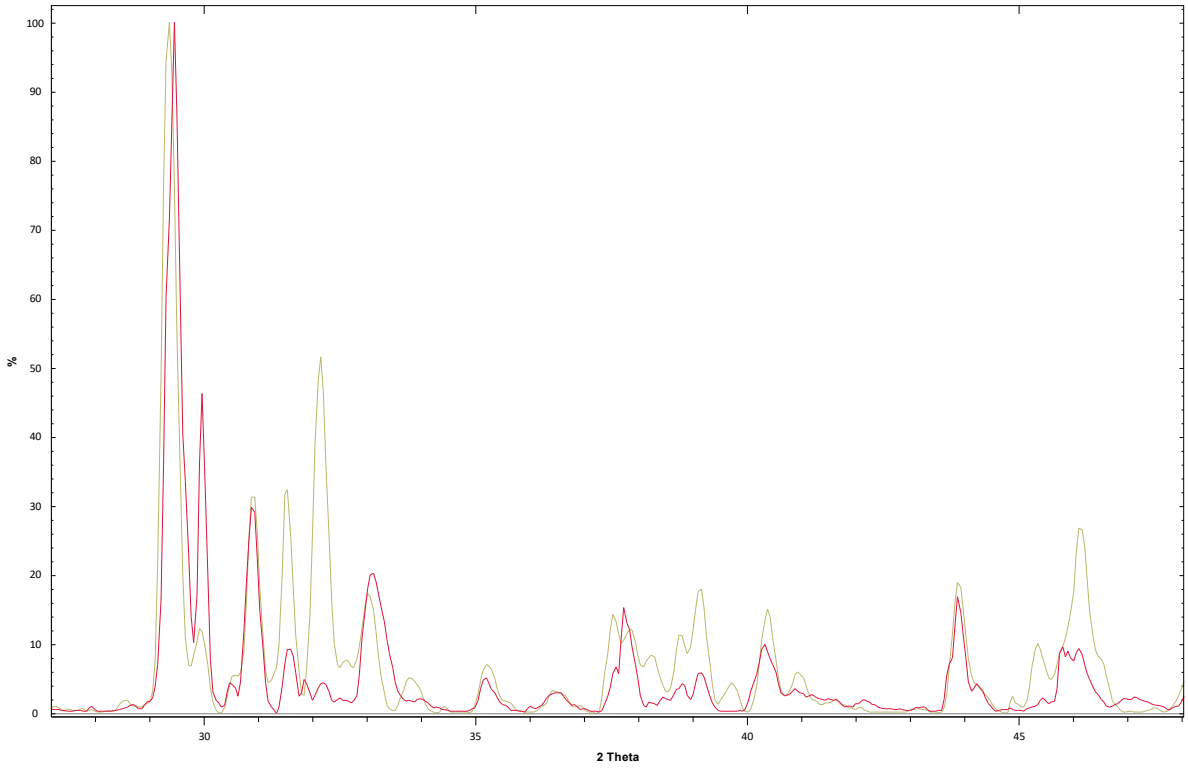


*Graph A.50: Expansion of PXRD overlay of oxidized silica **SSA-3** (red) and oxidized silica-DNPH **SSA-4** (blue)*

SSA-3 and SSA-5

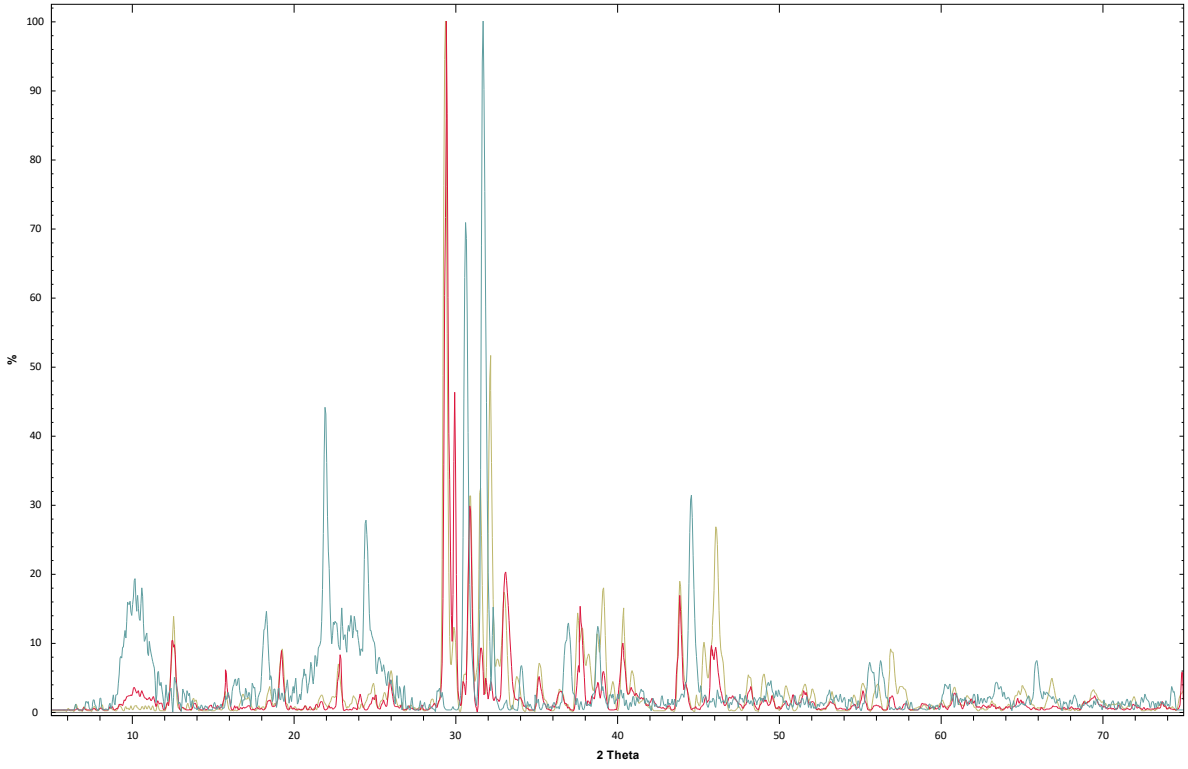


*Graph A.51: PXRD overlay of oxidized silica **SSA-3** (red) and oxidized silica-benzylated **SSA-5** (green)*

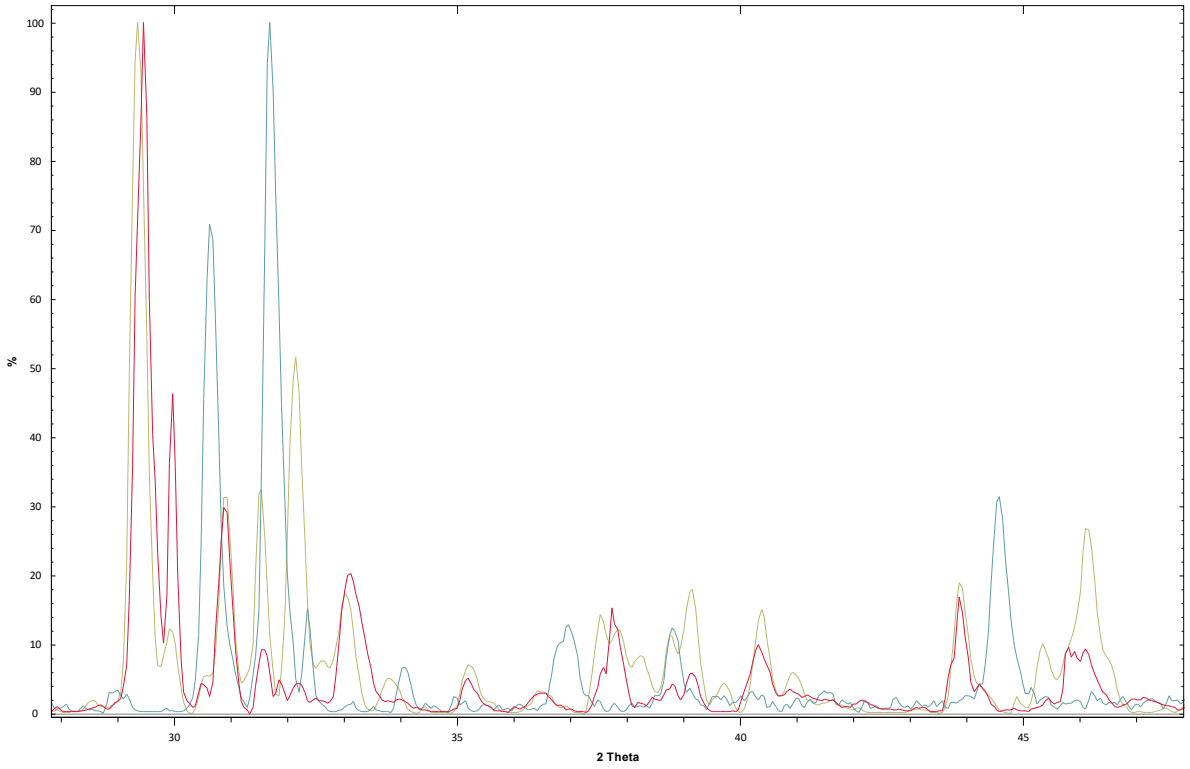


*Graph A.52: Expansion of PXRD overlay of oxidized silica **SSA-3** (red) and oxidized silica-benzylated **SSA-5** (green)*

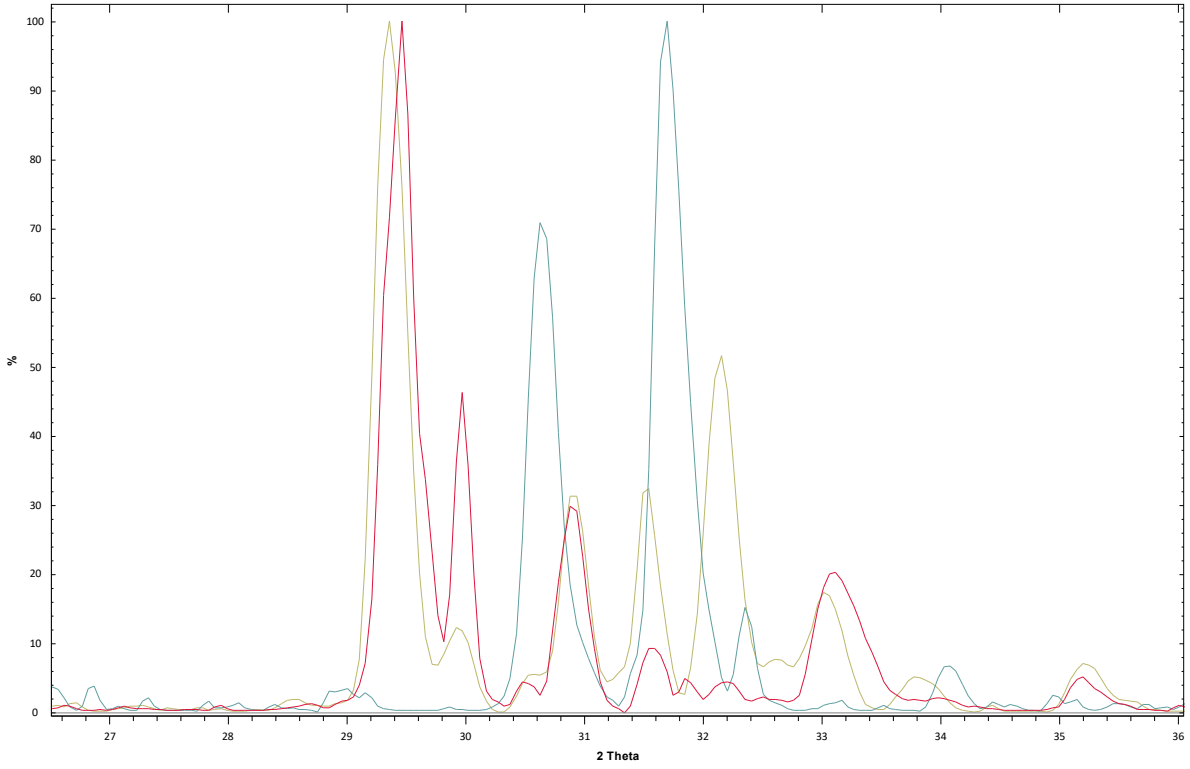
SSA-3, SSA-4 and SSA-5



*Graph A.53: PXRD overlay of oxidized silica **SSA-3** (red), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (green)*

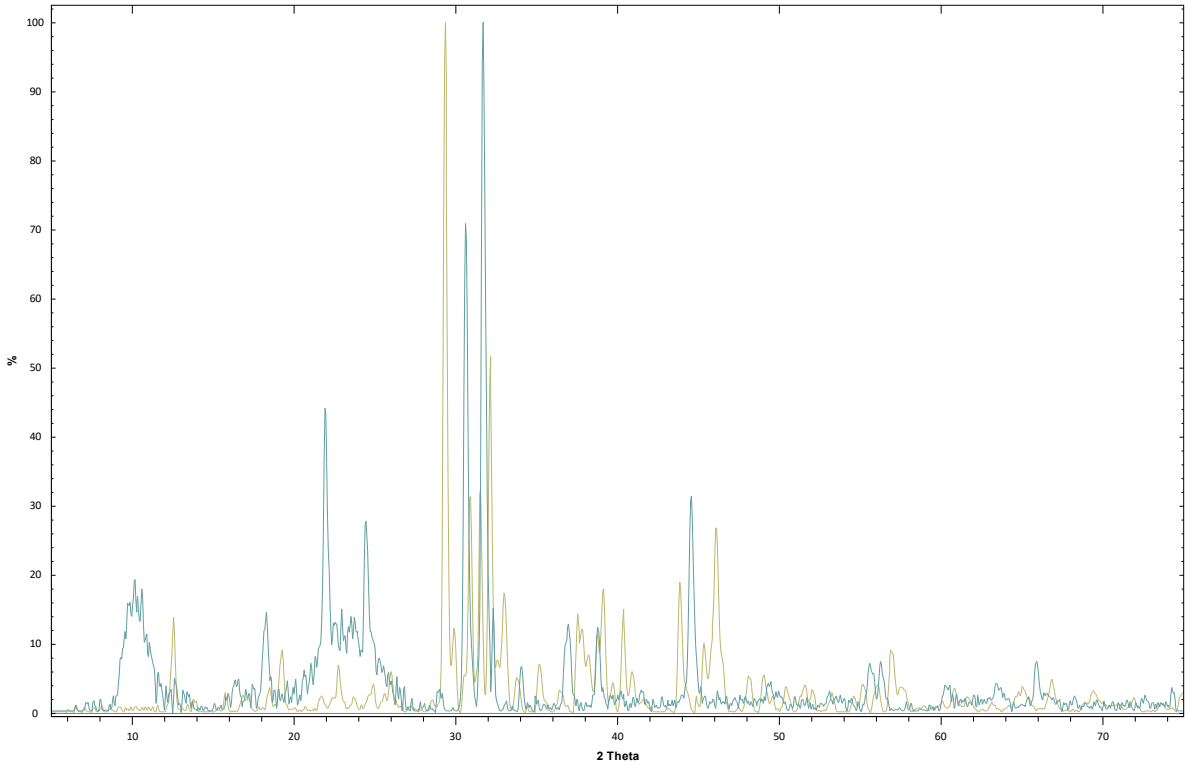


*Graph A.54: Expansion of PXRD overlay of oxidized silica **SSA-3** (red), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (green)*

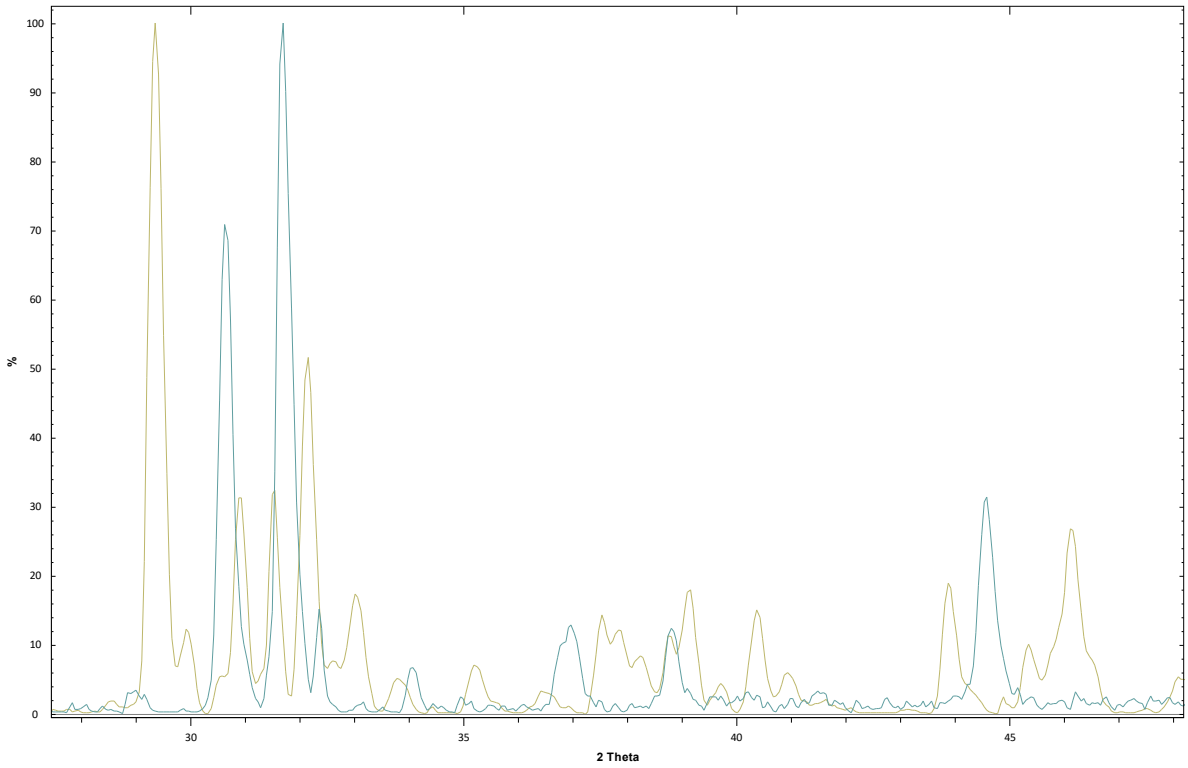


*Graph A.55: Expansion of PXRD overlay of oxidized silica **SSA-3** (red), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (green)*

SSA-4 and SSA-5

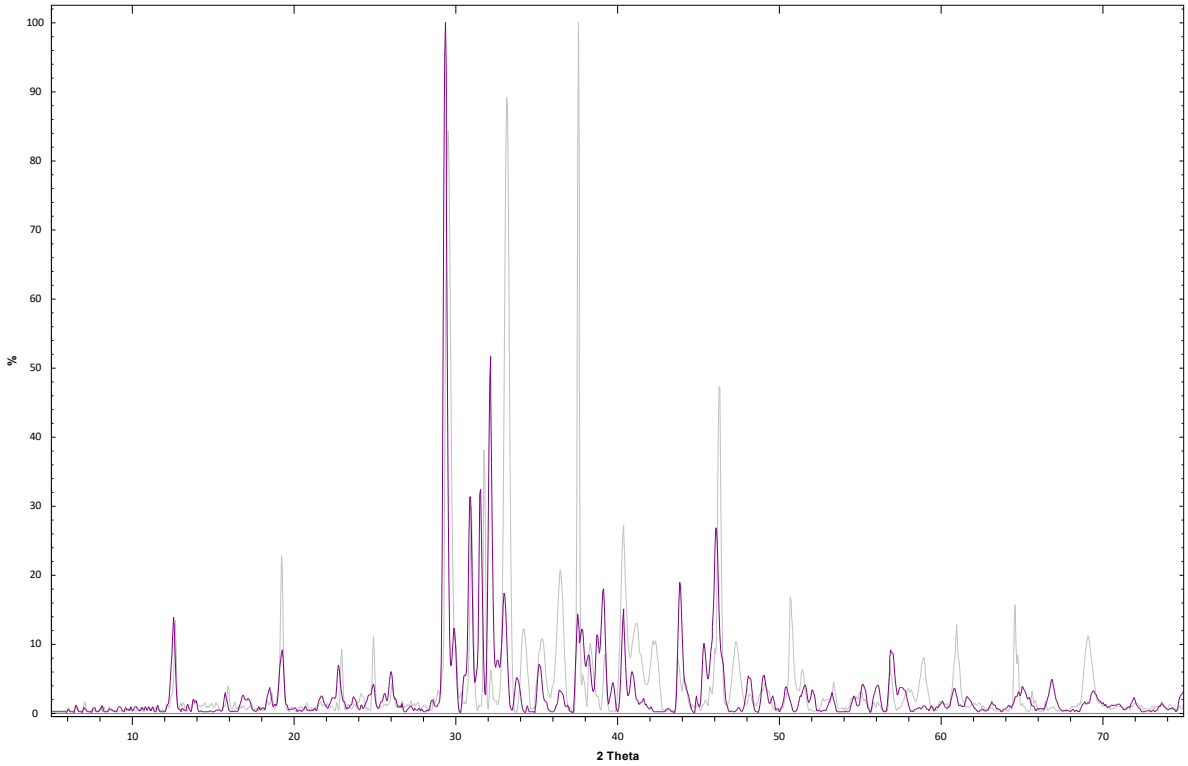


*Graph A.56: PXRD overlay of oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (green)*

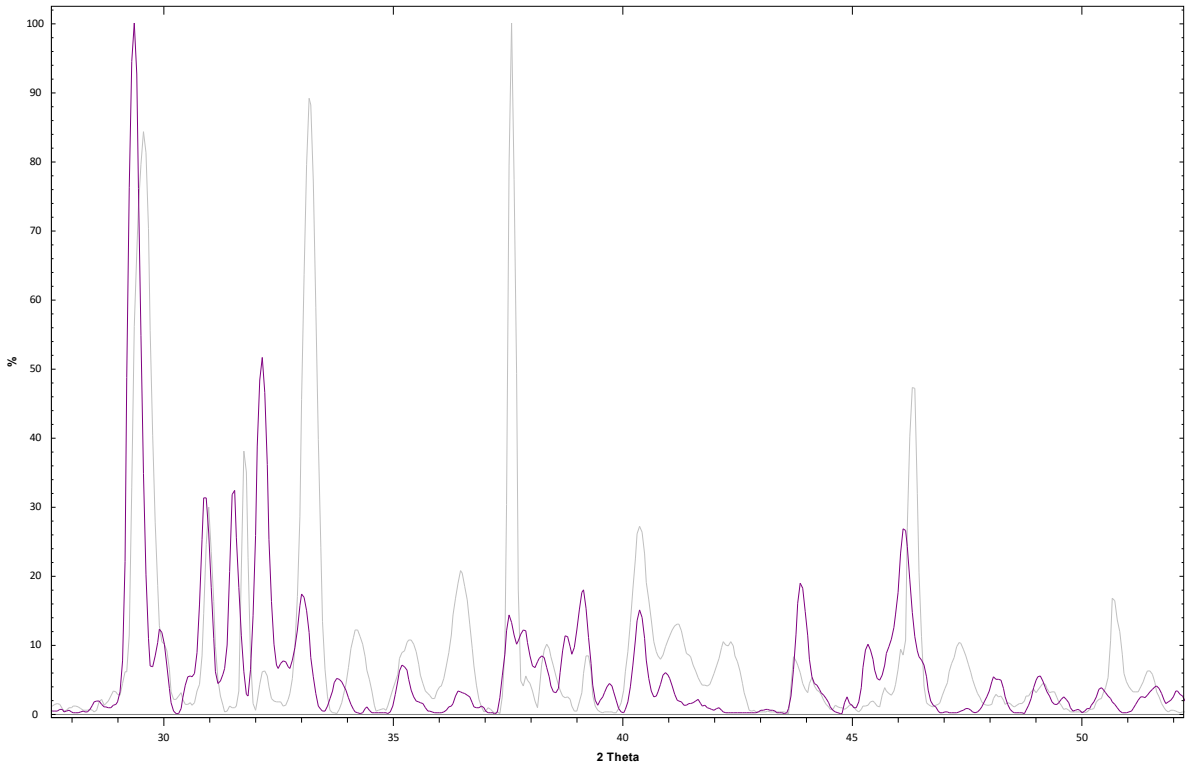


*Graph A.57: Expansion of PXRD overlay of oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (green)*

SSA-5 and SSA-6

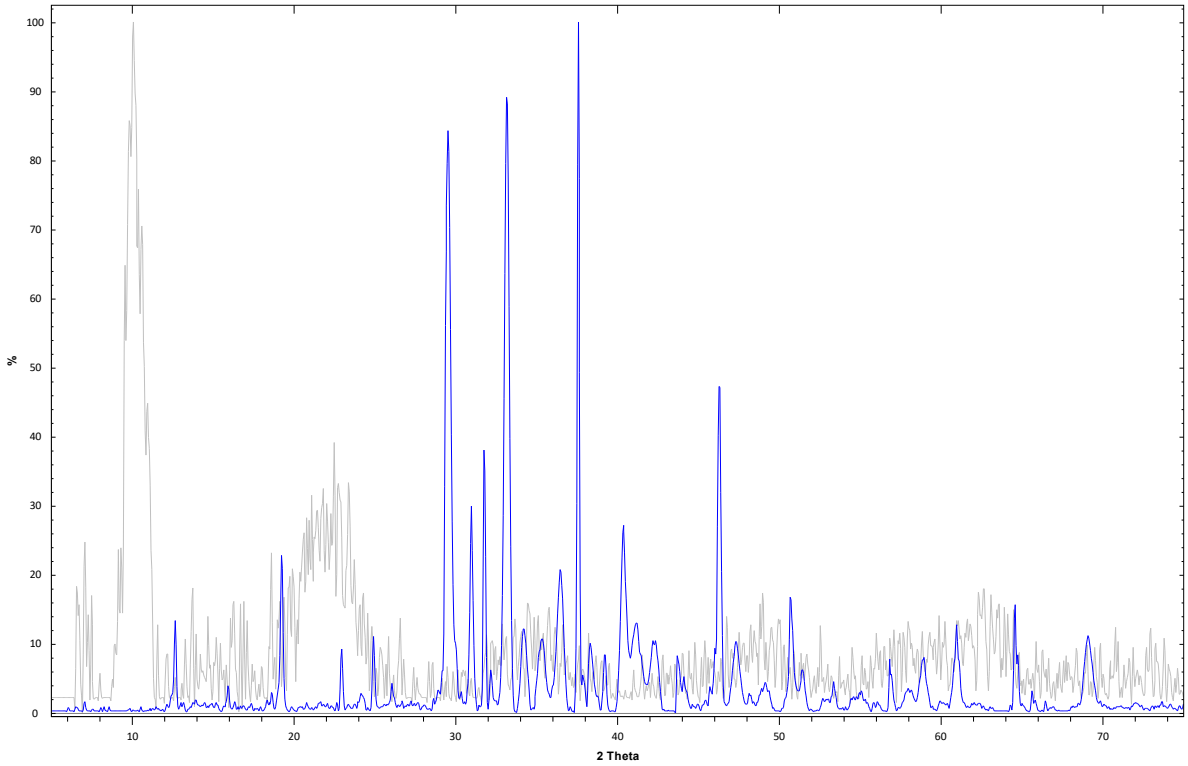


*Graph A.58: PXRD overlay of silica-benzylated **SSA-6** (grey) and oxidized silica-benzylated **SSA-5** (purple)*



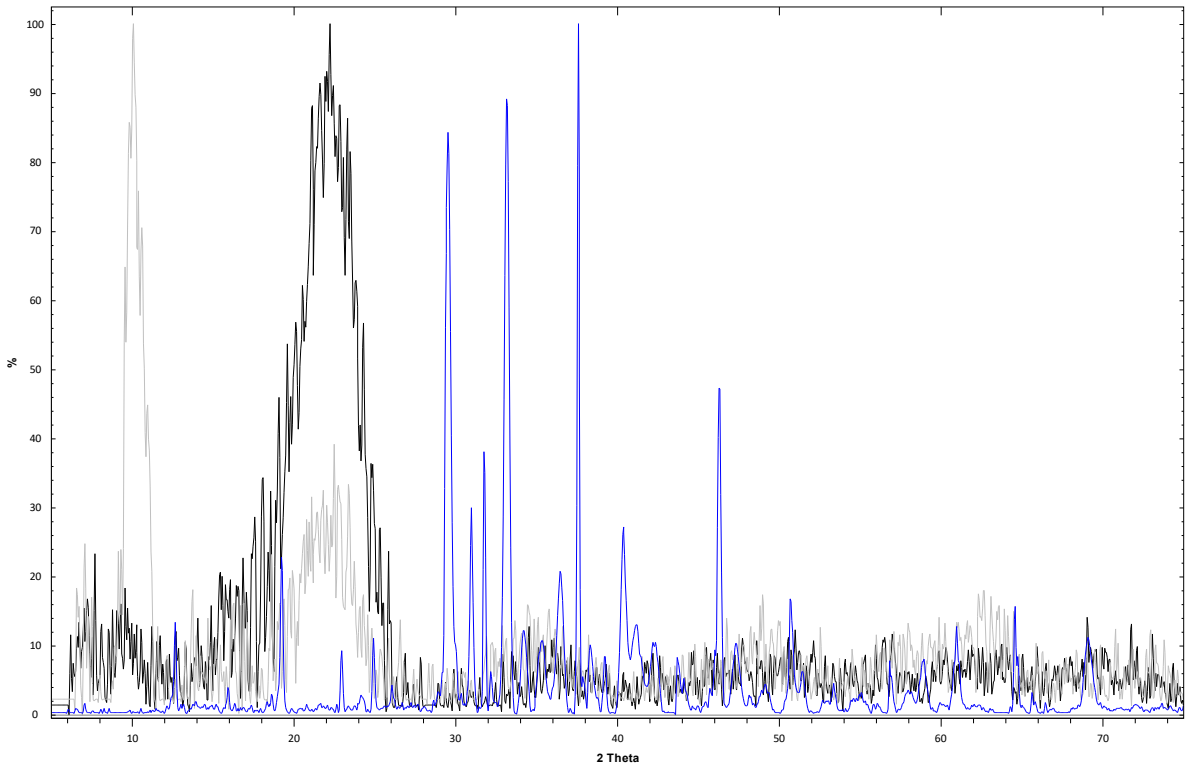
*Graph A.59: Expansion of PXRD overlay of silica-benzylated **SSA-6** (grey) and oxidized silica-benzylated **SSA-5** (purple)*

SSA-6 and Silica



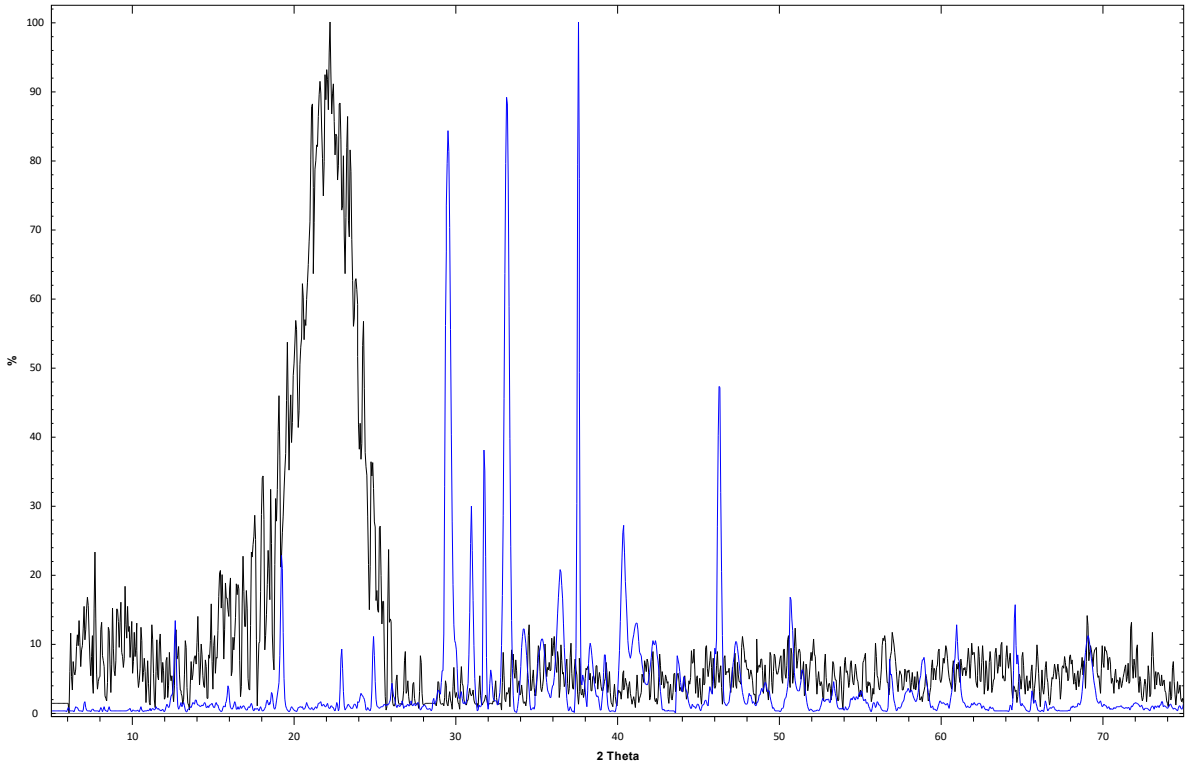
*Graph A.60: PXRD overlay of silica-benzylated **SSA-6** (blue) and silica (grey)*

Silica, SSA-6 and SSA-7



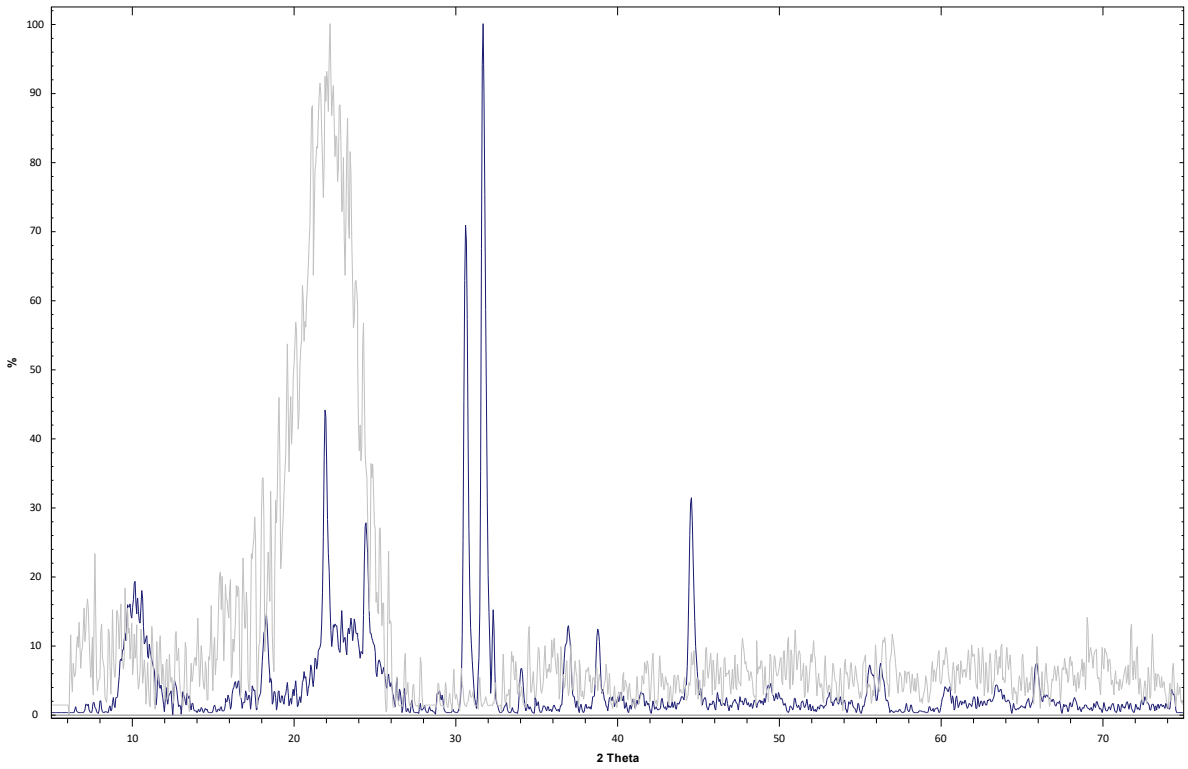
*Graph A.61: PXRD overlay of silica-benzylated **SSA-6** (blue), silica-DNPH **SSA-7** (black) and silica (grey)*

SSA-6 and SSA-7

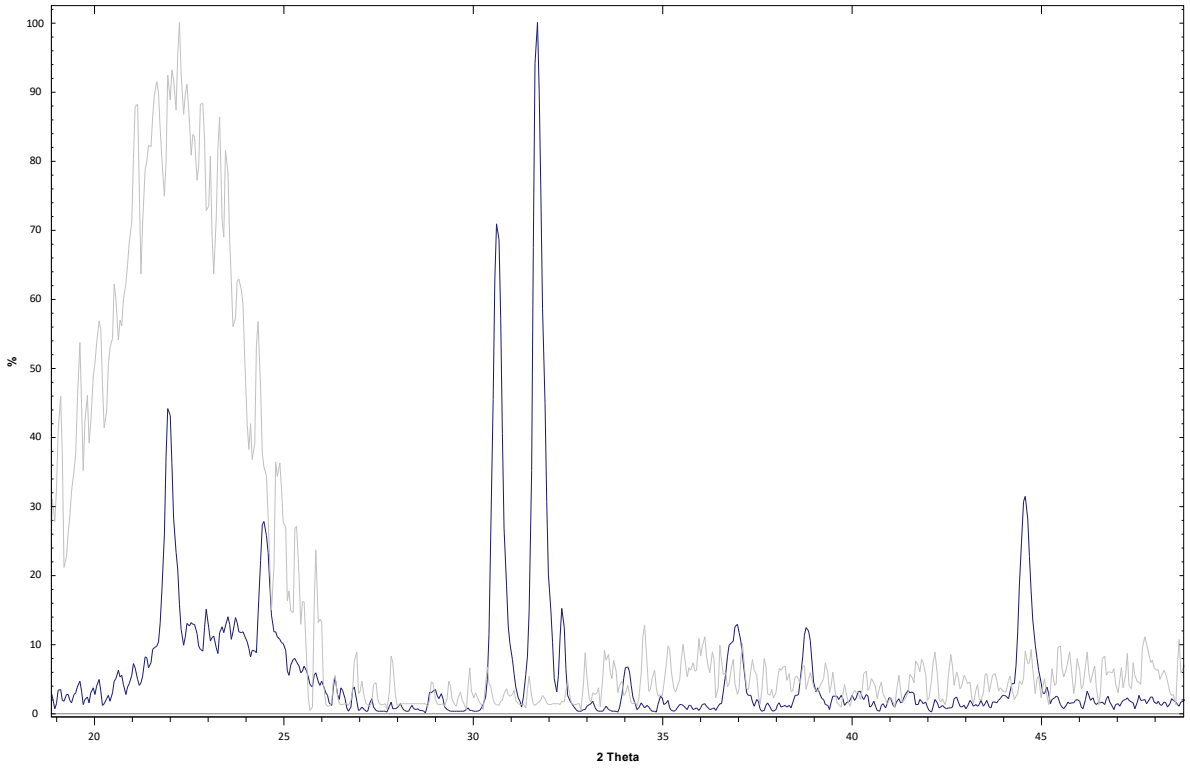


*Graph A.62: PXRD overlay of silica-benzylated **SSA-6** (blue) and silica-DNPH **SSA-7** (black)*

SSA-4 and SSA-7



*Graph A.63: PXRD overlay of silica-DNP **SSA-7** (grey) and oxidized silica-DNPH **SSA-4** (navy)*



*Graph A.64: Expansion of PXRD overlay of silica-DNPH **SSA-7** (grey) and oxidized silica-DNP **SSA-4** (navy)*

A-5 SEM results

A-5.1 Silica

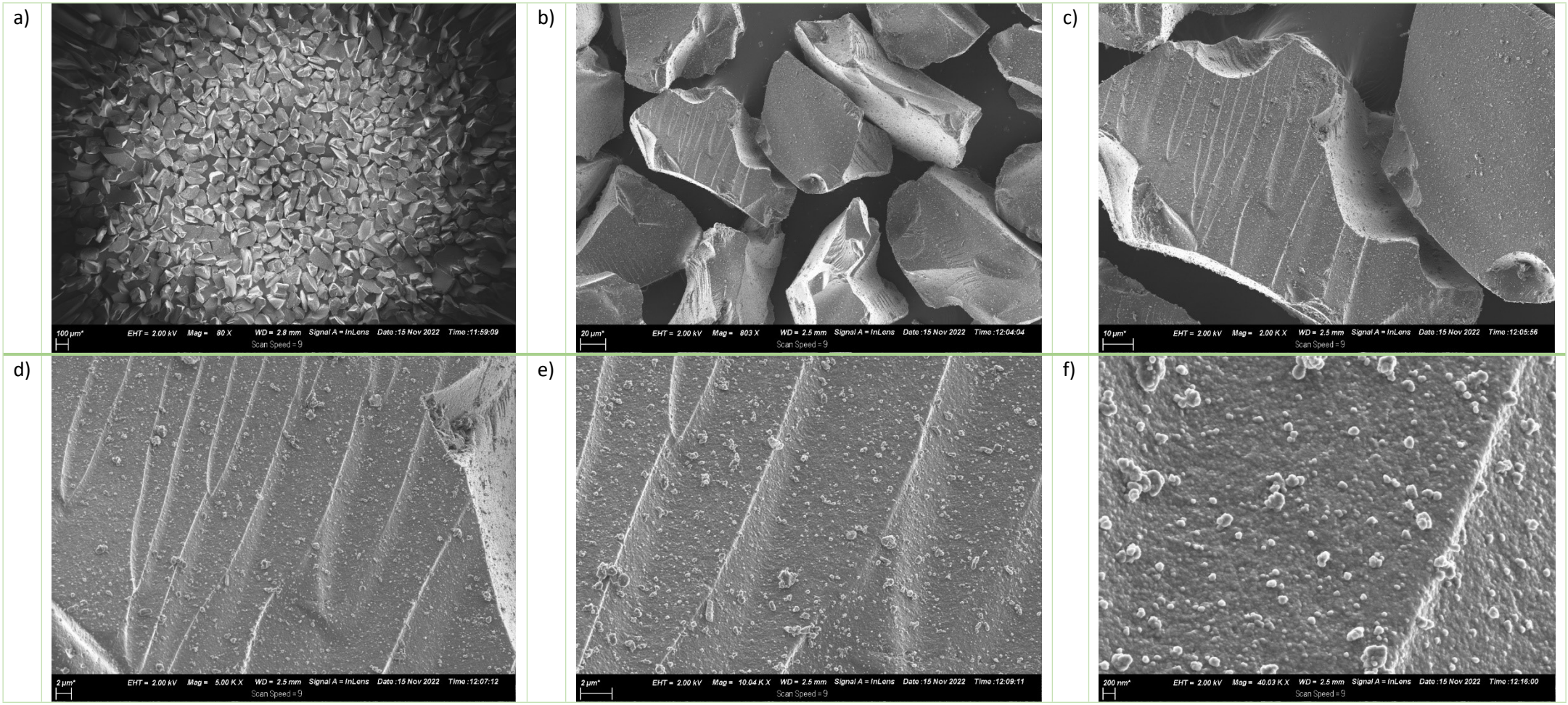


Figure A.2: Various SEM magnifications of Silica

A-5.2 SSA-3

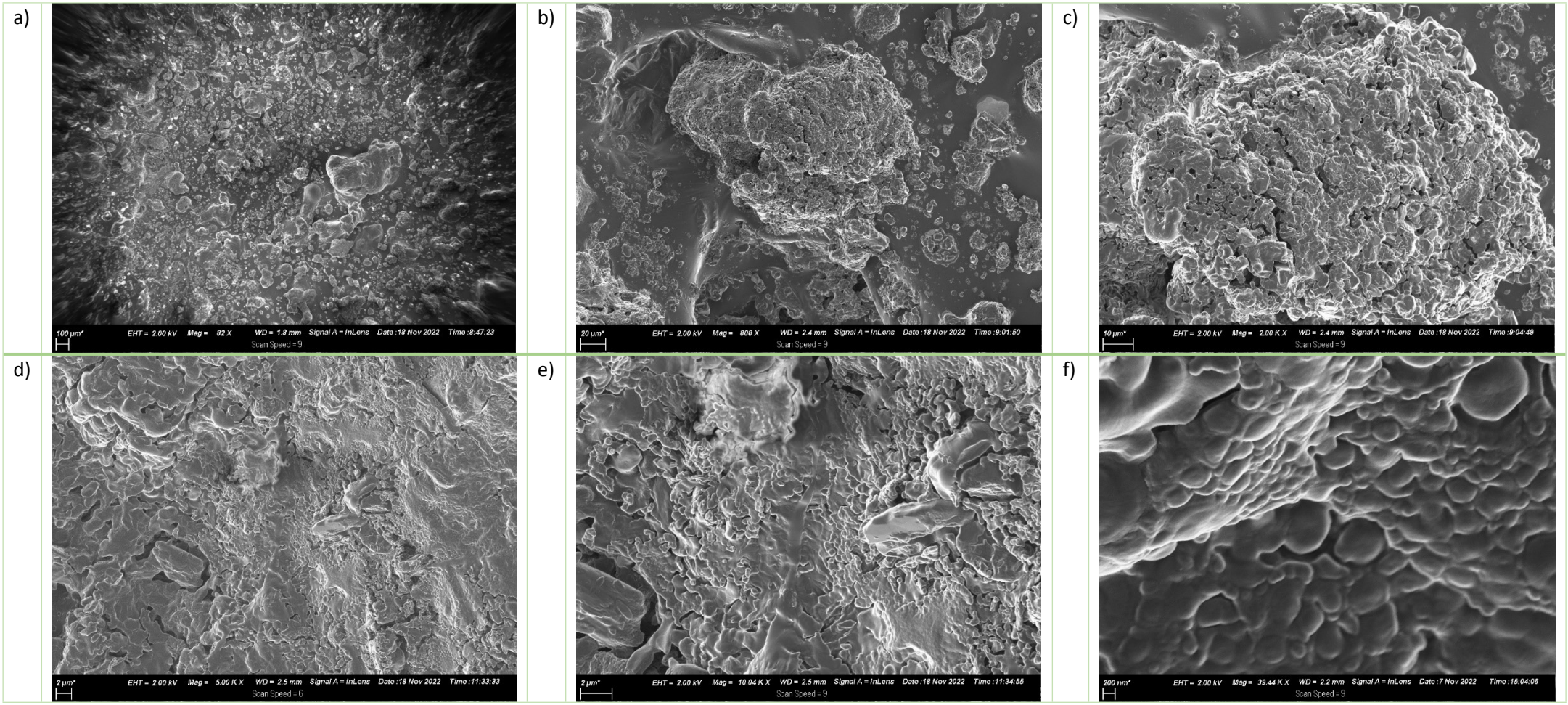


*Figure A.3: Various SEM magnifications of **SSA-3***

A-5.3 SSA-4

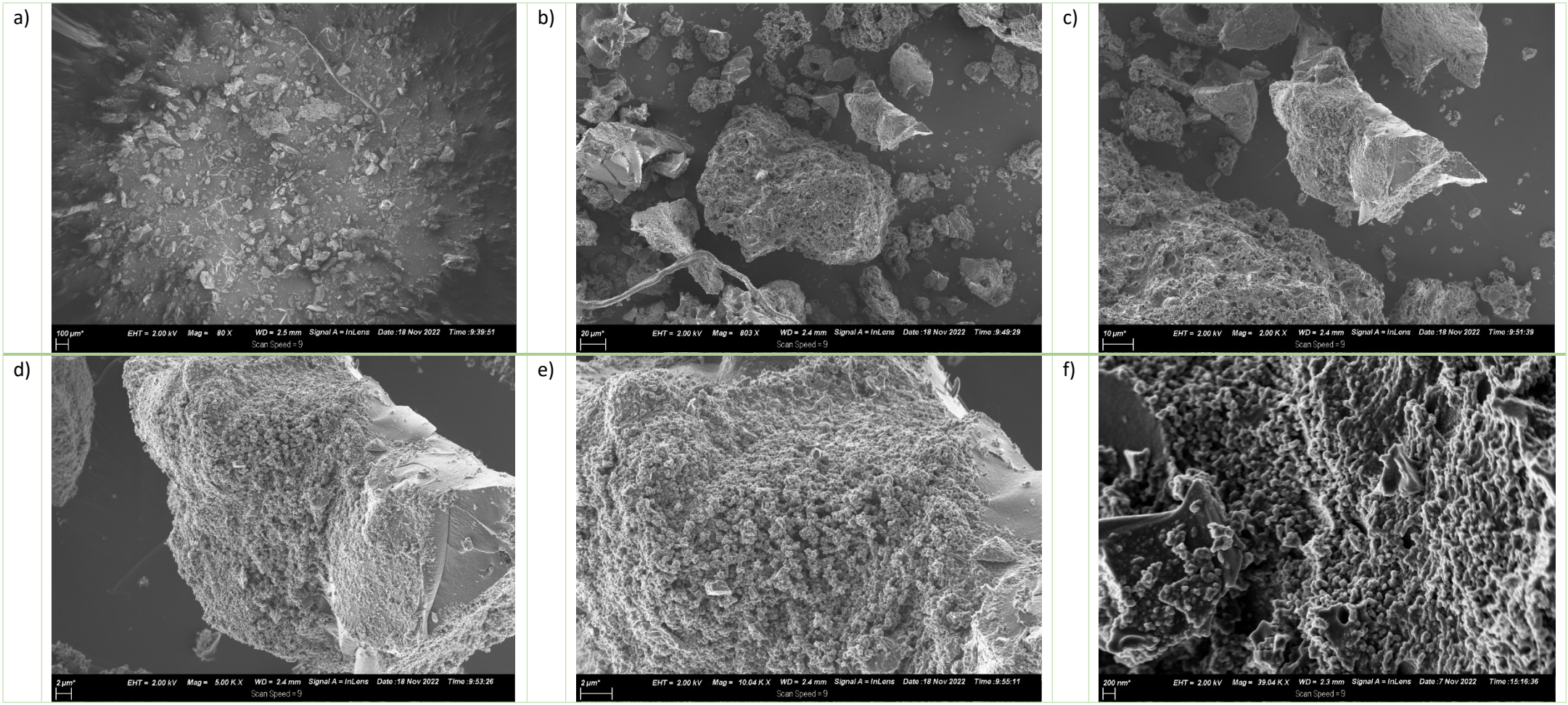


*Figure A.4: Various SEM magnifications of **SSA-4***

A-5.4 SSA-5

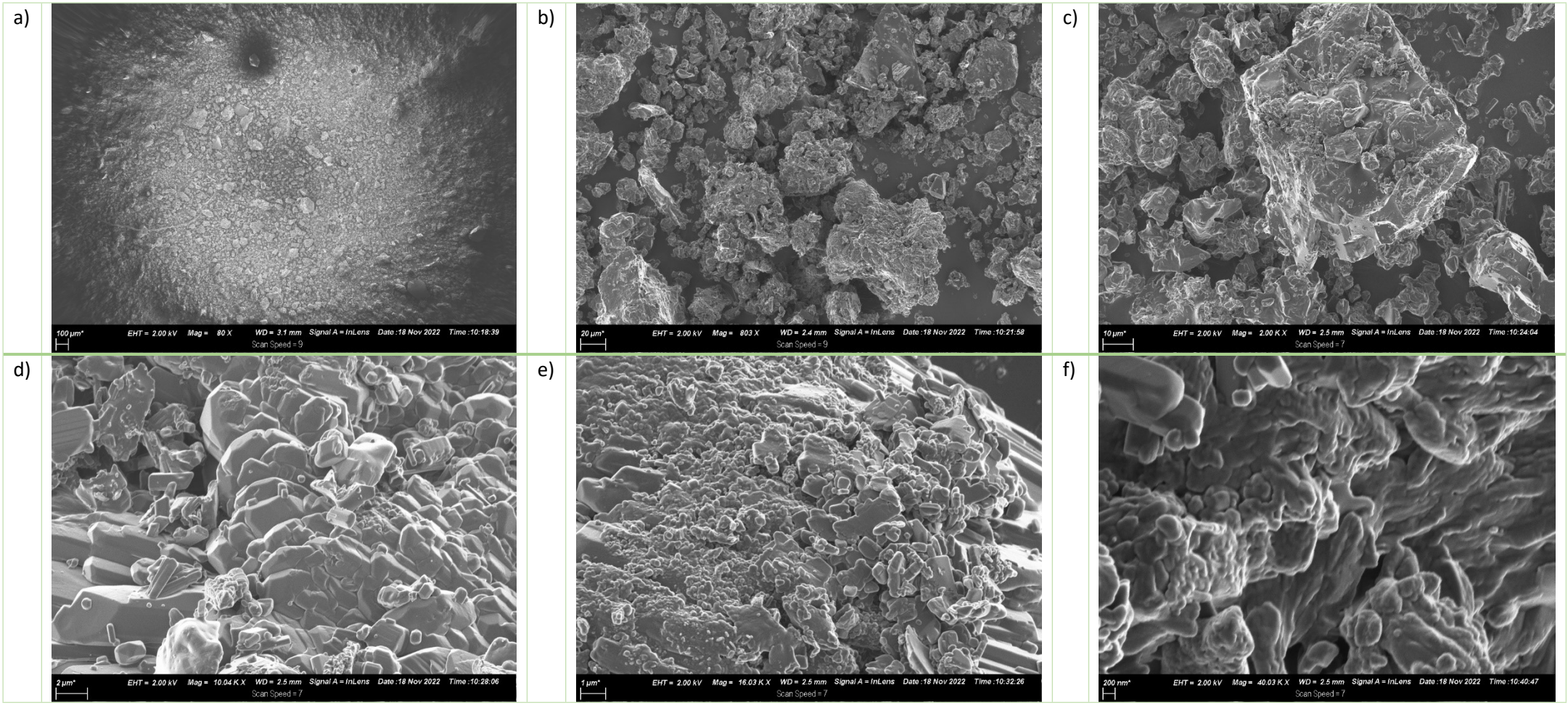


*Figure A.5: Various SEM magnifications of **SSA-5***

A-5.5 SSA-6

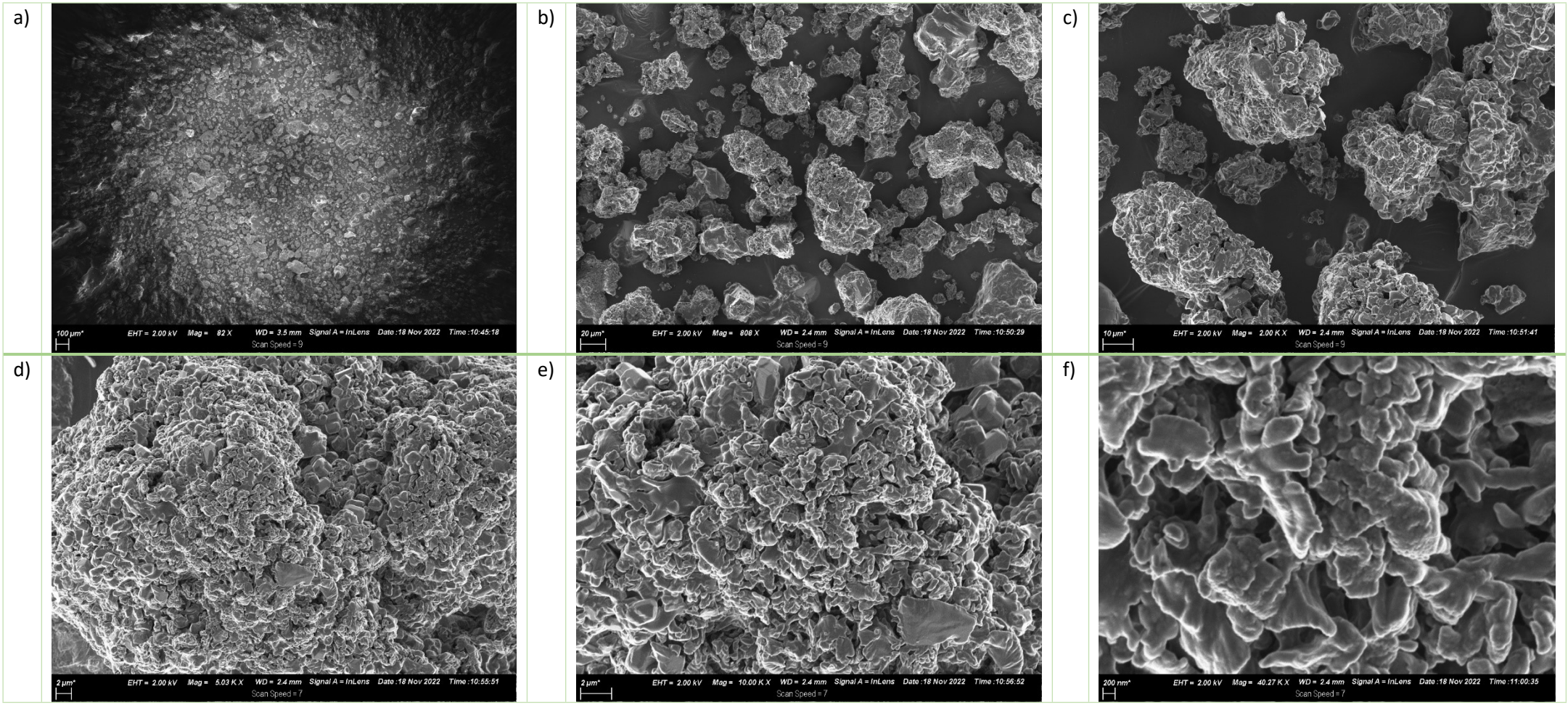


*Figure A.6: Various SEM magnifications of **SSA-6***

A-5.6 SSA-7

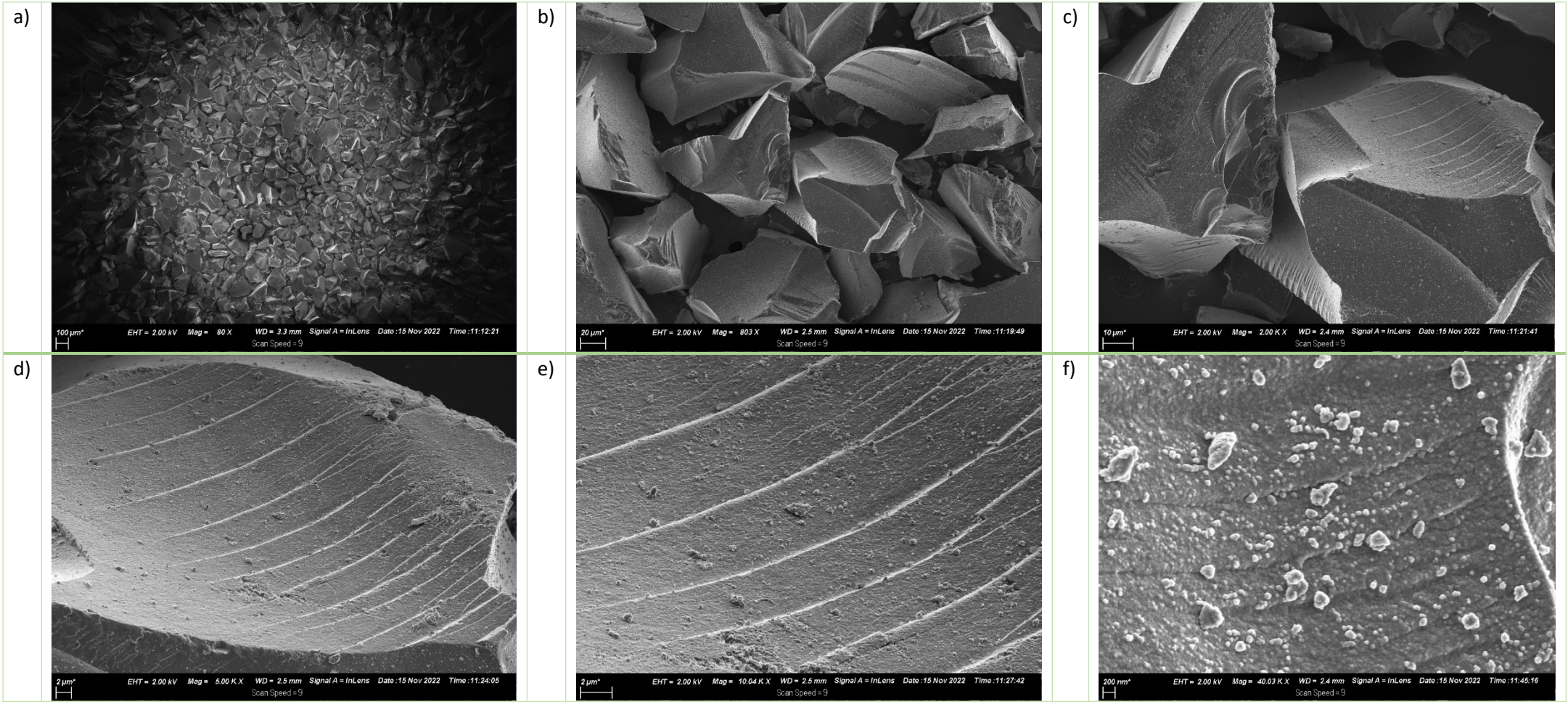


*Figure A.7: Various SEM magnifications of **SSA-7***

A-6 IR results

A-6.1 Silica

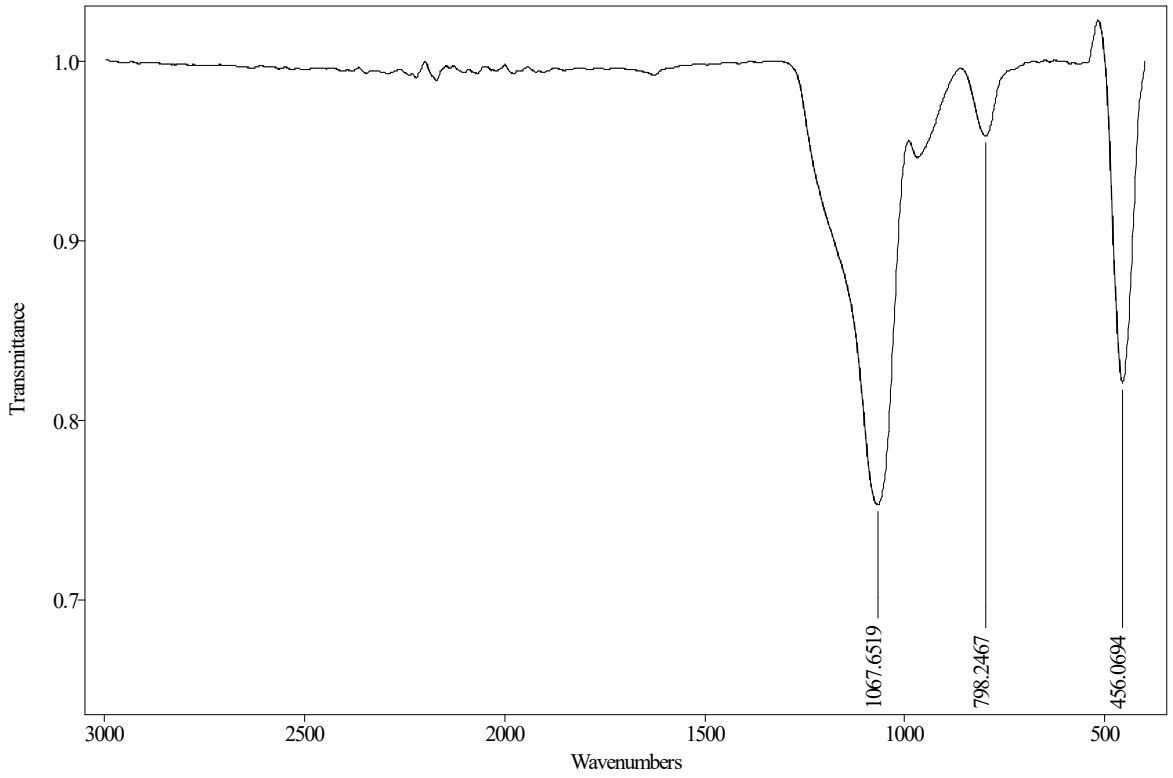


Figure A.8: FTIR spectrum of silica

A-6.2 SSA-3

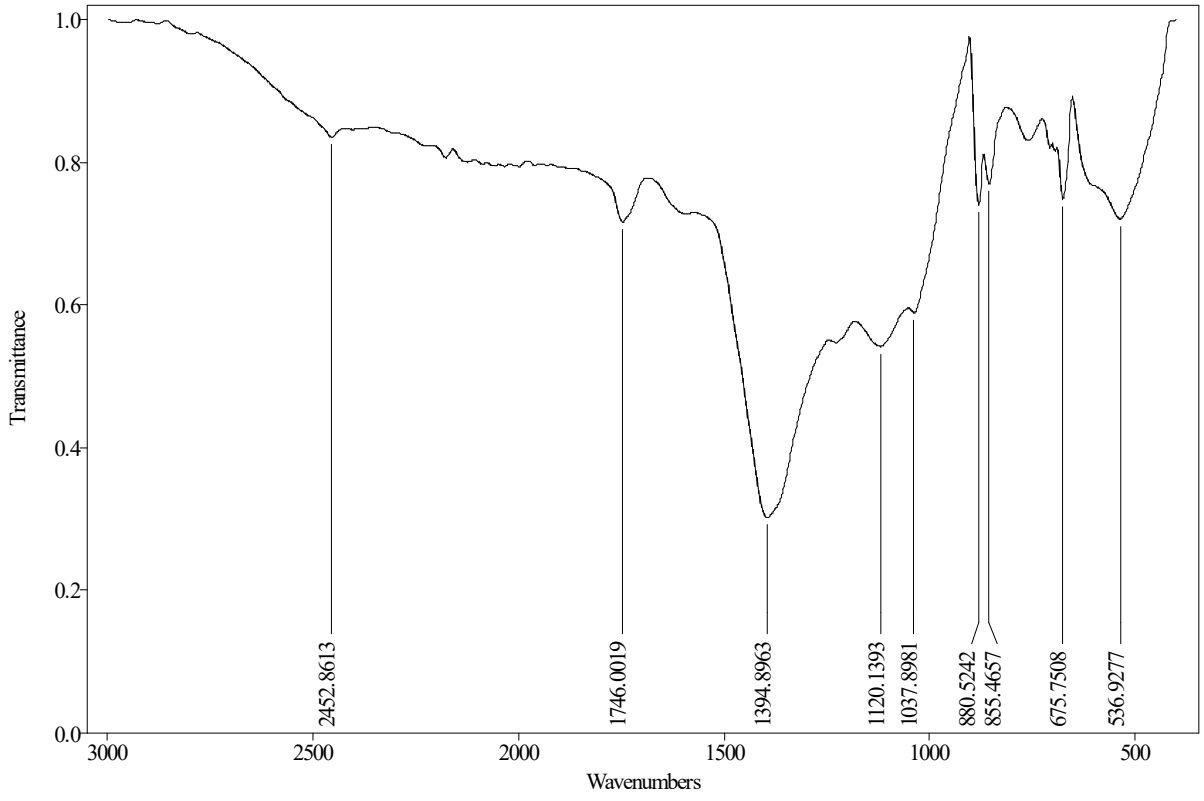


*Figure A.9: FTIR spectrum of oxidized silica **SSA-3***

A-6.3 SSA-4

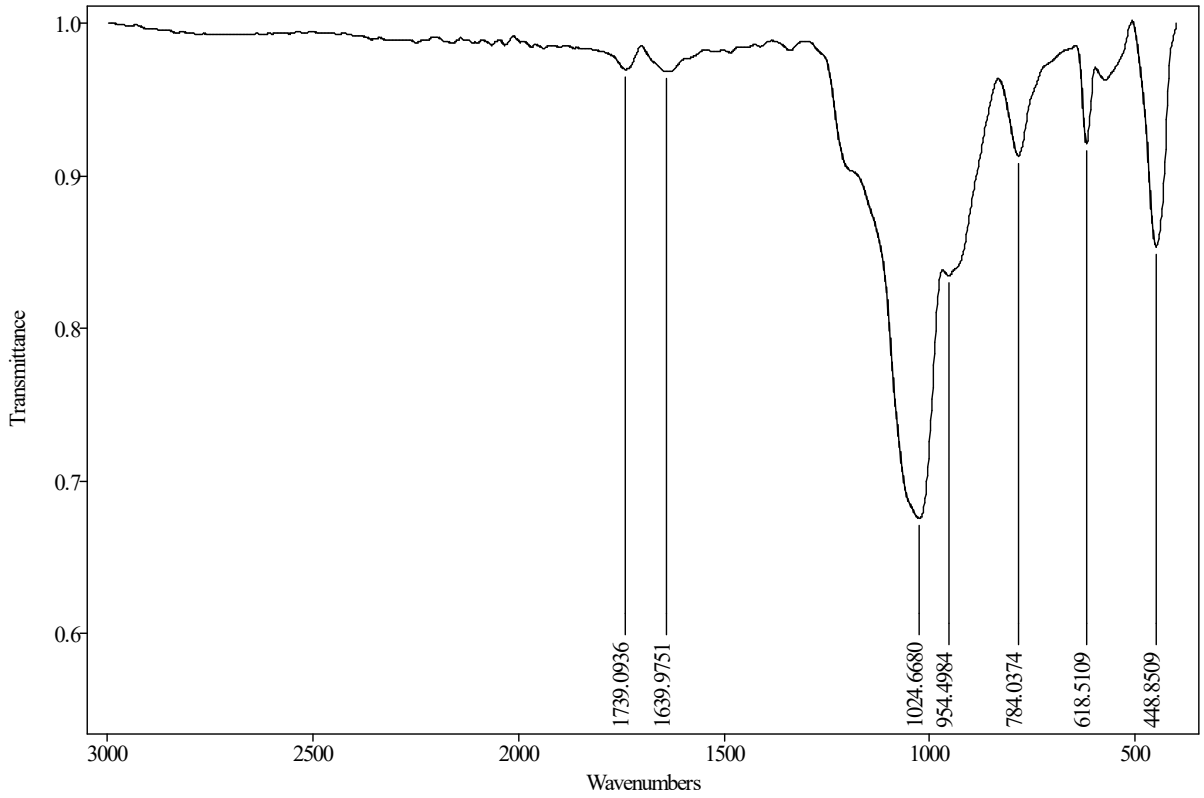


*Figure A.10: FTIR spectrum of oxidized silica-DNPH **SSA-4***

A-6.4 SSA-5

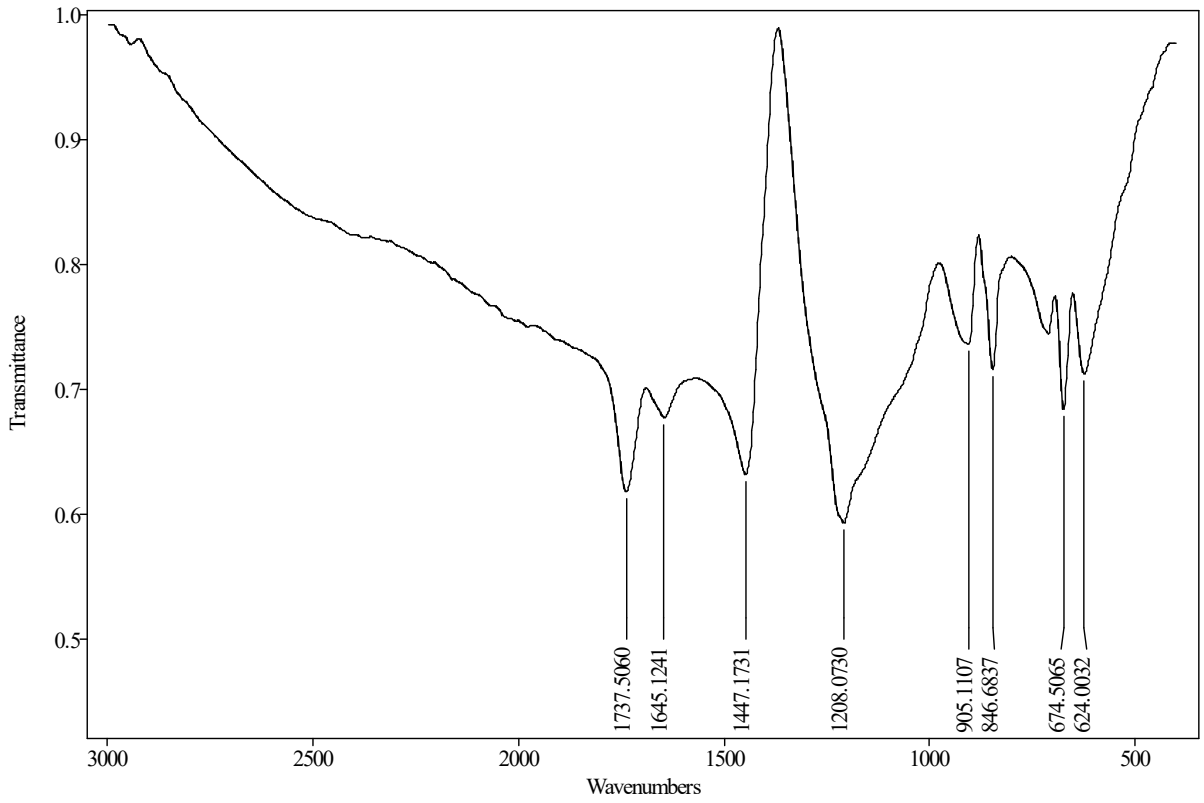


*Figure A.11: FTIR spectrum of oxidized silica- benzylated **SSA-5***

A-6.5 SSA-6

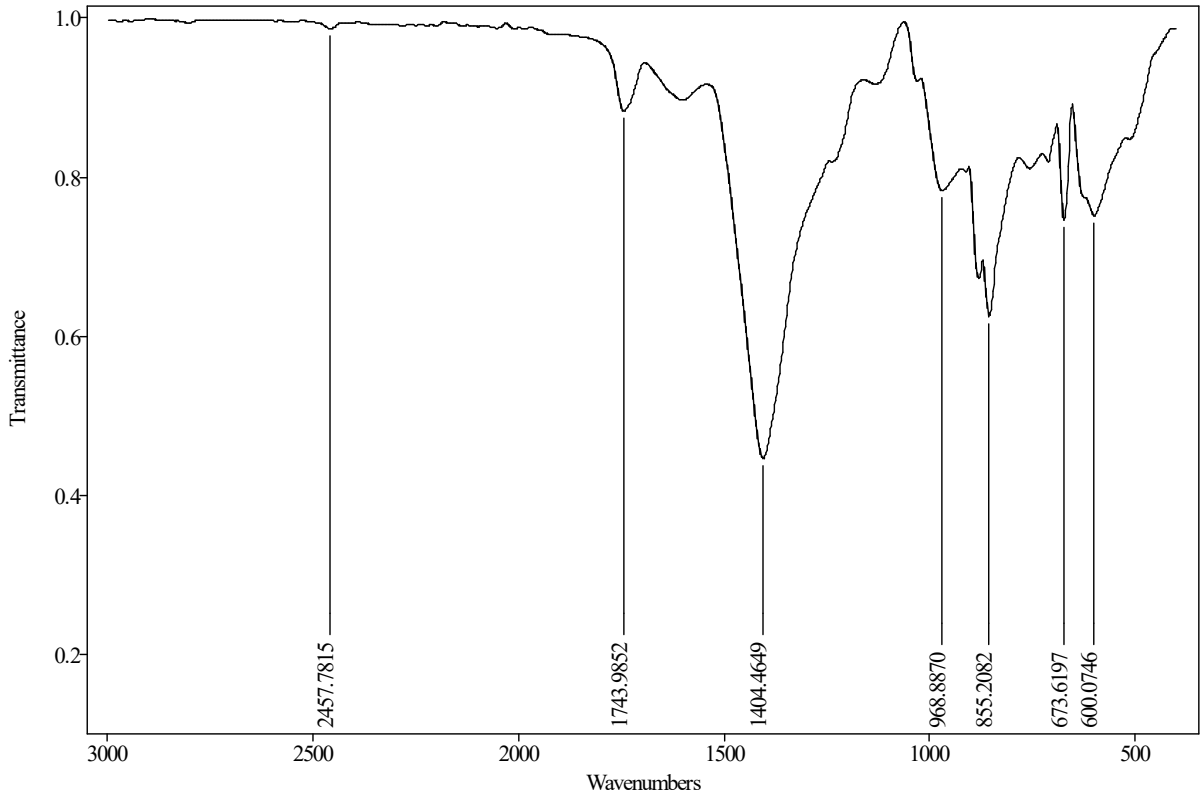


*Figure A.12: FTIR spectrum of silica-benzylated **SSA-6***

A-6.6 SSA-7

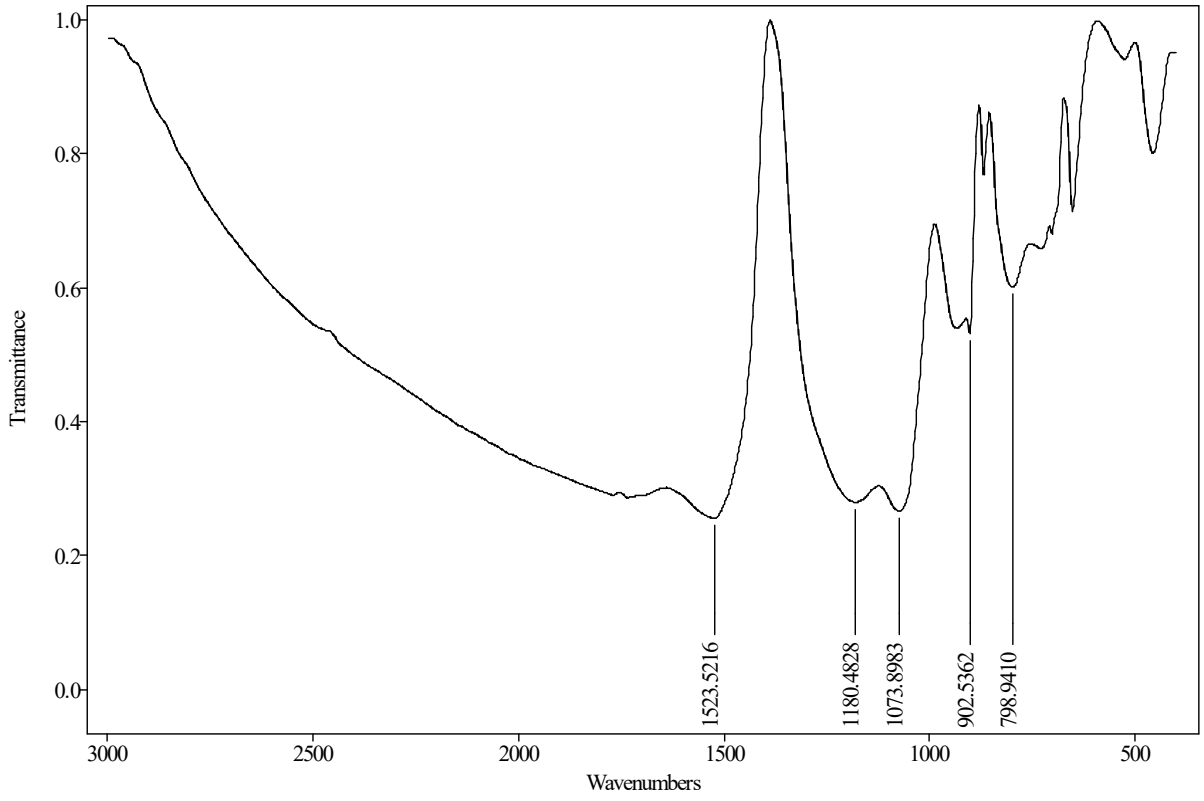


*Figure A.13: FTIR spectrum of silica-DNPH **SSA-7***

A-6.7 Combinations

Silica and SSA-3

*Figure A.14: FTIR overlay of silica (black) and oxidized silica **SSA-3** (red)*

SSA-3 and SSA-4

*Figure A.15: FTIR overlay of oxidized silica **SSA-3** (black) and oxidized silica-DNPH **SSA-4** (blue)*

SSA-3 and SSA-5

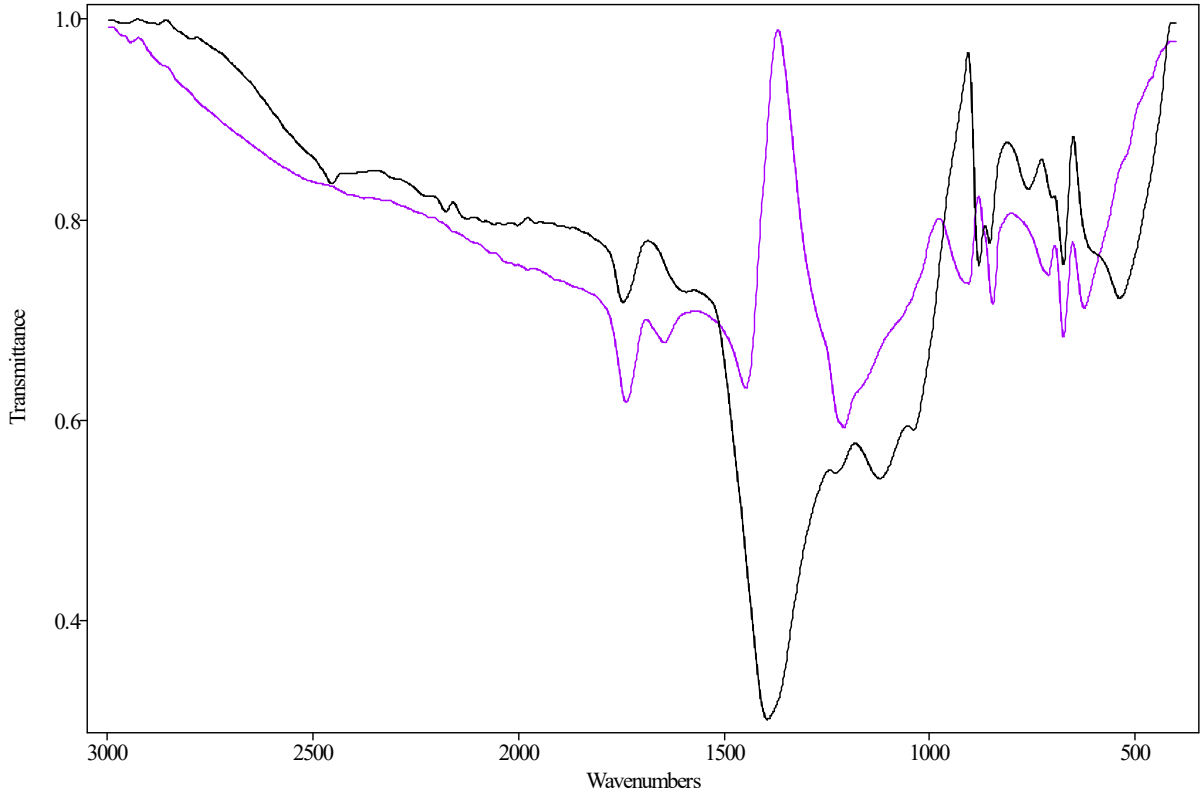


*Figure A.16: FTIR overlay of oxidized silica **SSA-3** (black) and oxidized silica-benzylated **SSA-5** (purple)*

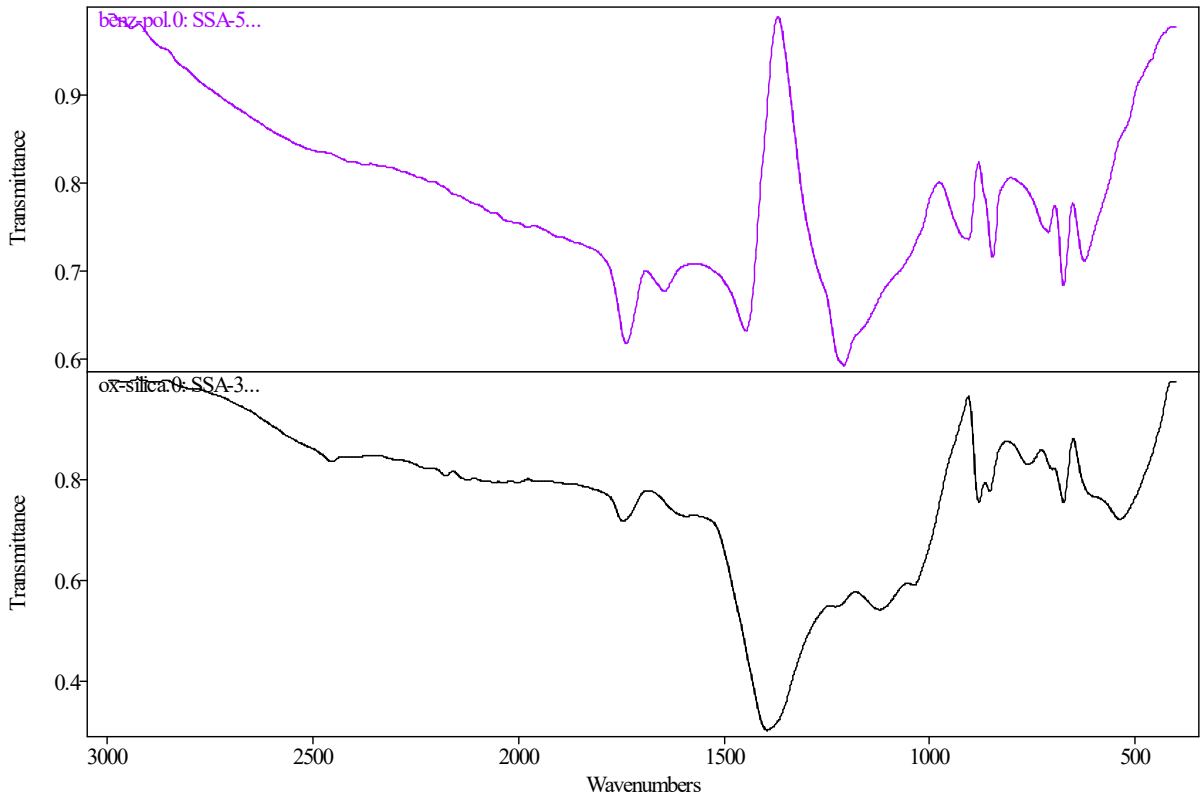


*Figure A.17: FTIR stacked of oxidized silica **SSA-3** (black) and oxidized silica-benzylated **SSA-5** (purple)*

SSA-3, SSA-4 and SSA-5

*Figure A.18: FTIR overlay of oxidized silica **SSA-3** (black), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (purple)*

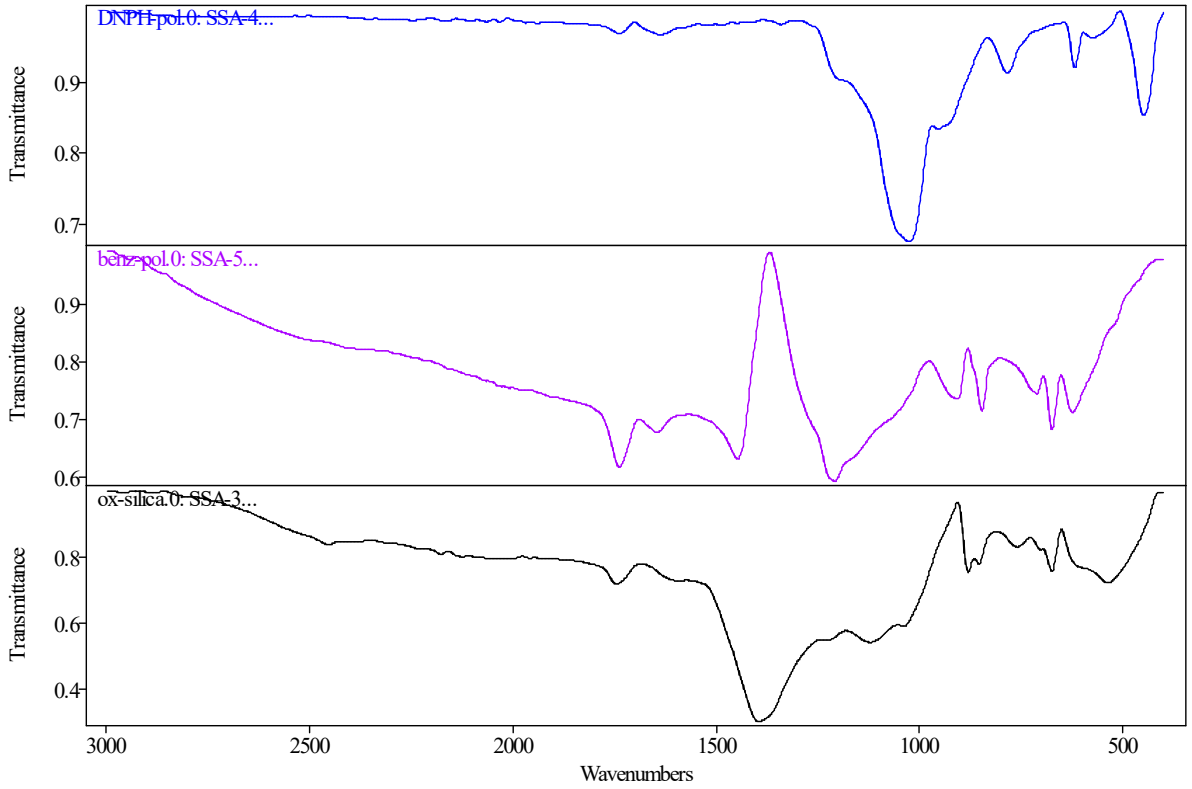


*Figure A.19: FTIR stacked of oxidized silica **SSA-3** (black), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica-benzylated **SSA-5** (purple)*

Silica and SSA-6

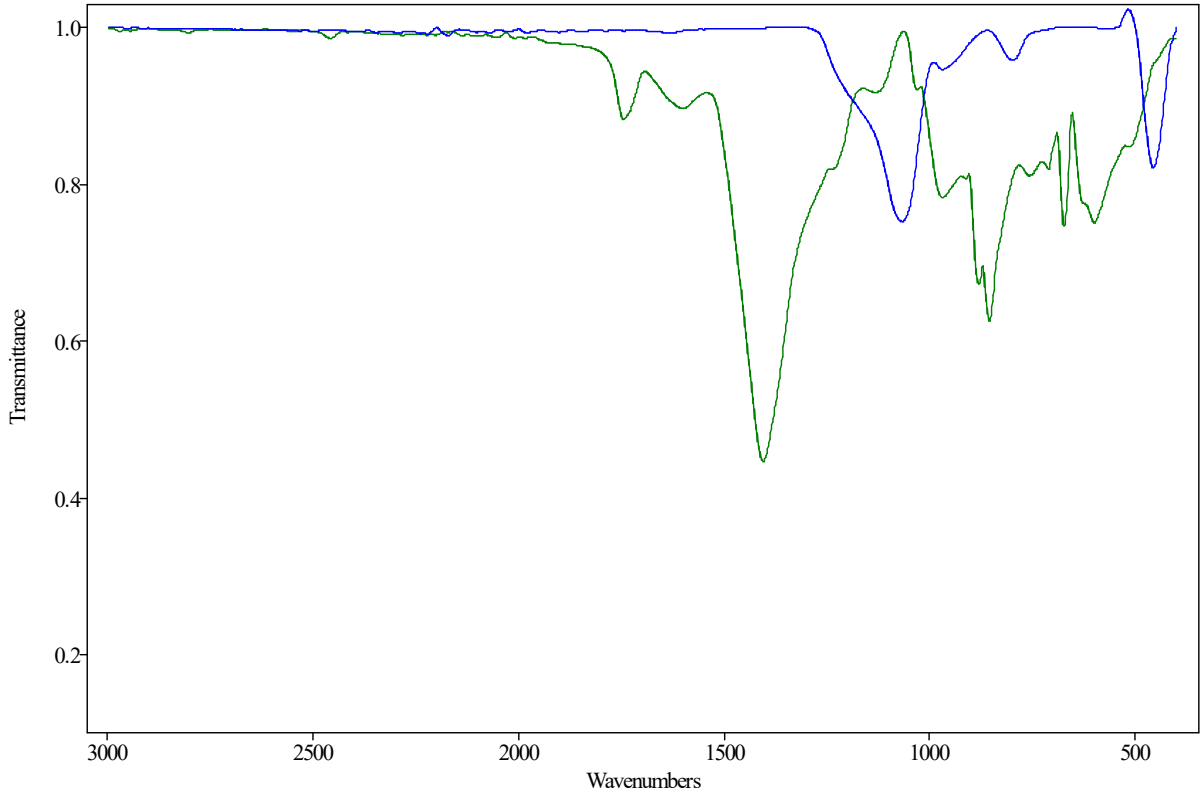


*Figure A.20: FTIR overlay of silica (blue) and silica-benzylated **SSA-6** (green)*

Silica and SSA-7

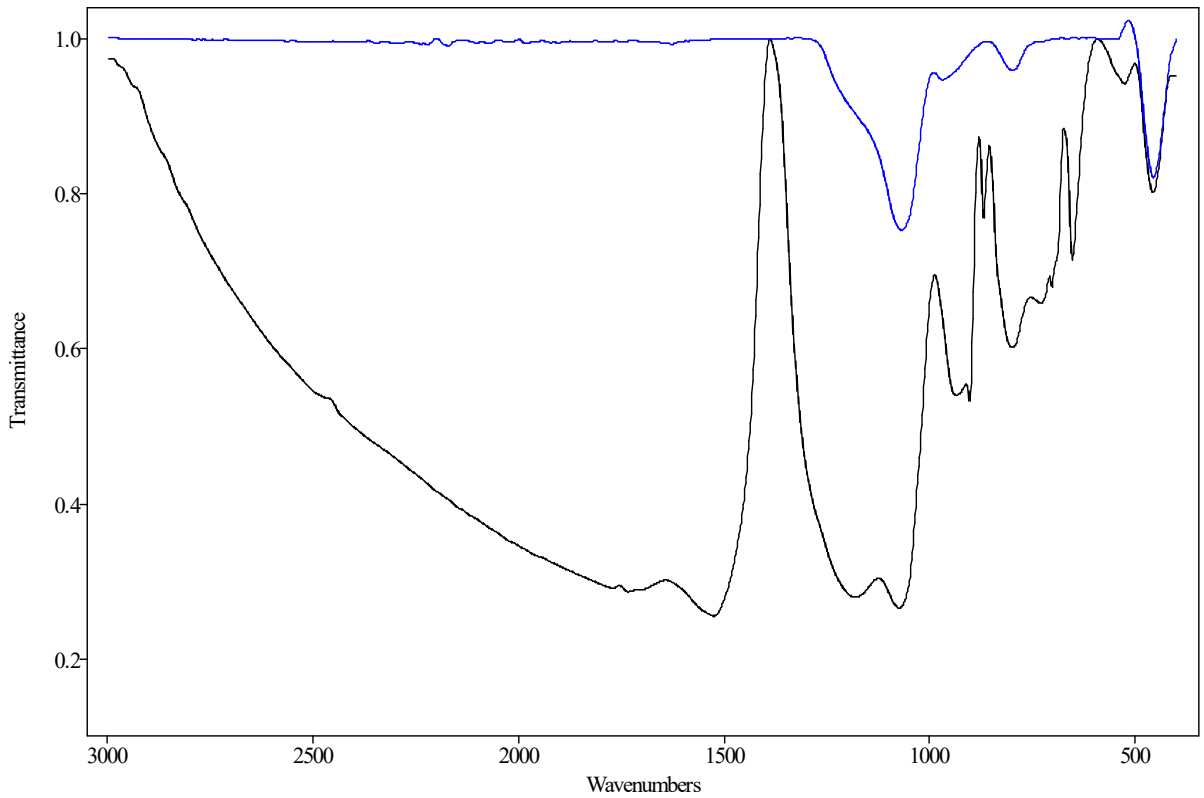


*Figure A.21: FTIR overlay of silica (blue) and silica-DNPH **SSA-7** (black)*

Silica, SSA-6 and SSA-7

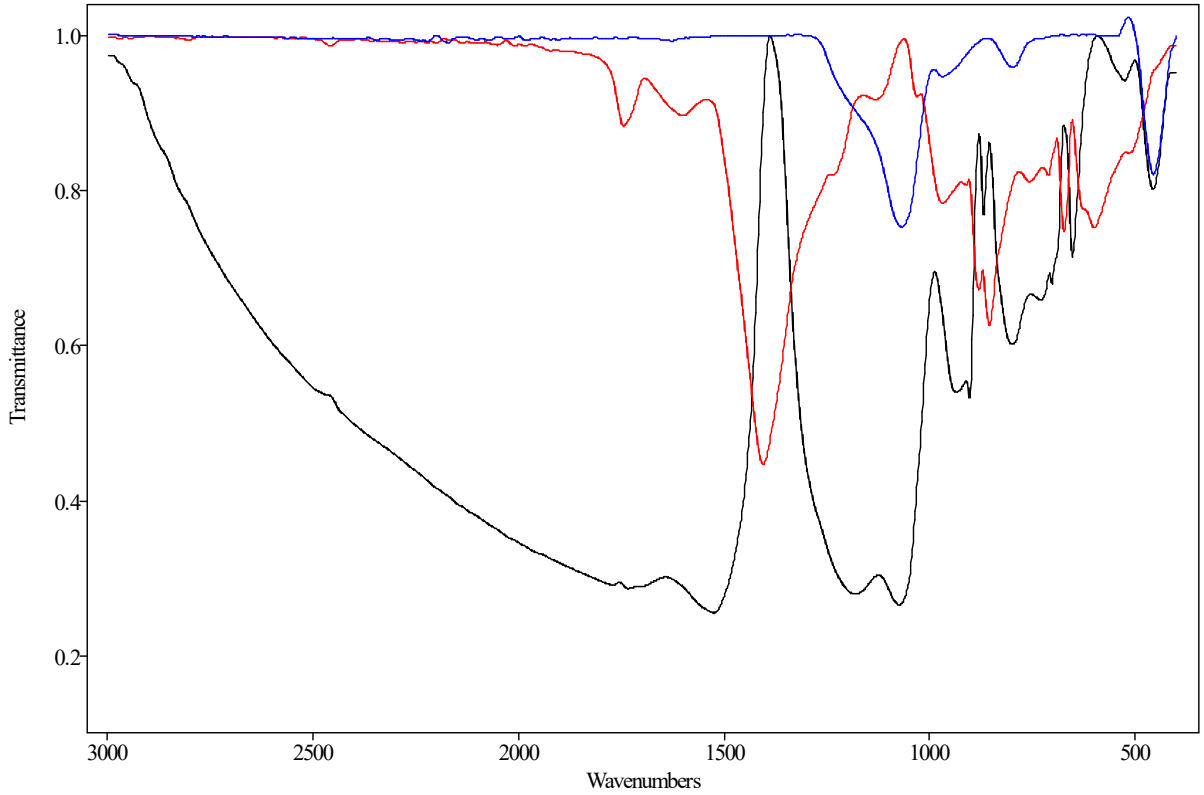


*Figure A.22: FTIR overlay of silica (blue), silica-benzylated **SSA-6** (red) and silica-DNPH **SSA-7** (black)*

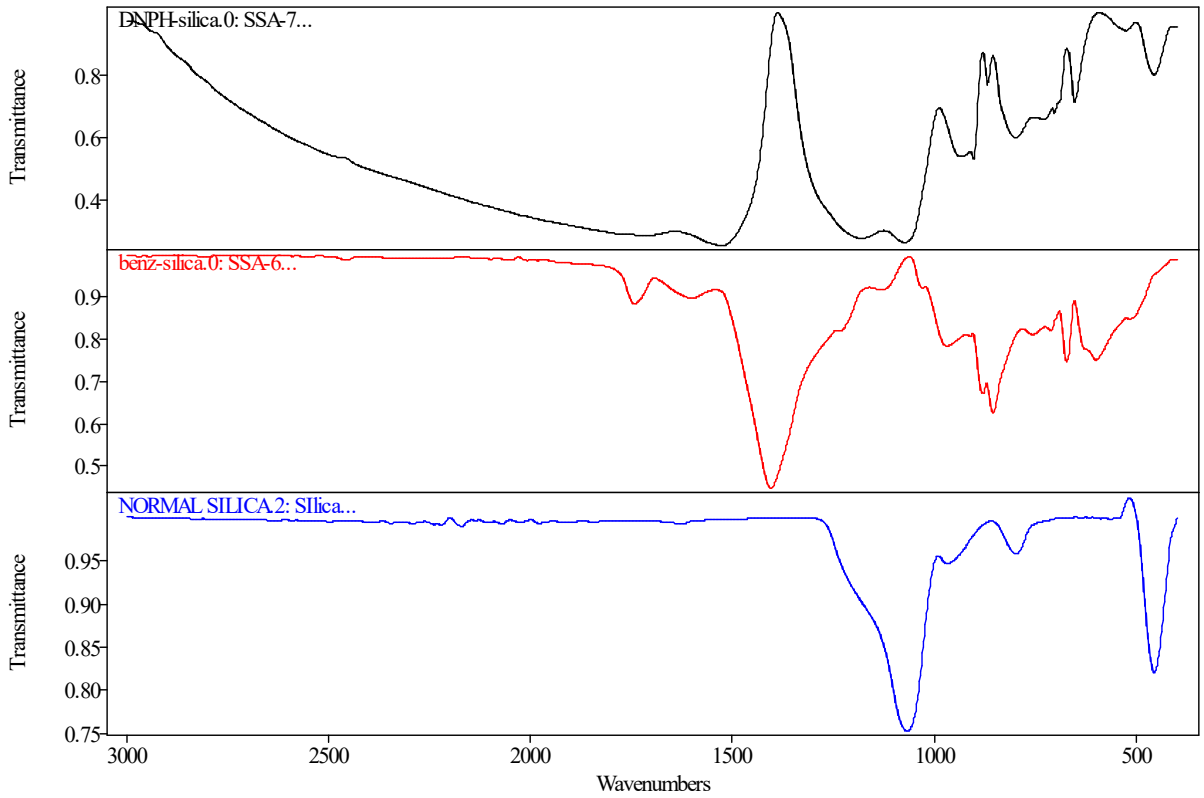


*Figure A.23: FTIR stacked of silica (blue), silica-benzylated **SSA-6** (red) and silica-DNPH **SSA-7** (black)*

SSA-4 and SSA-7

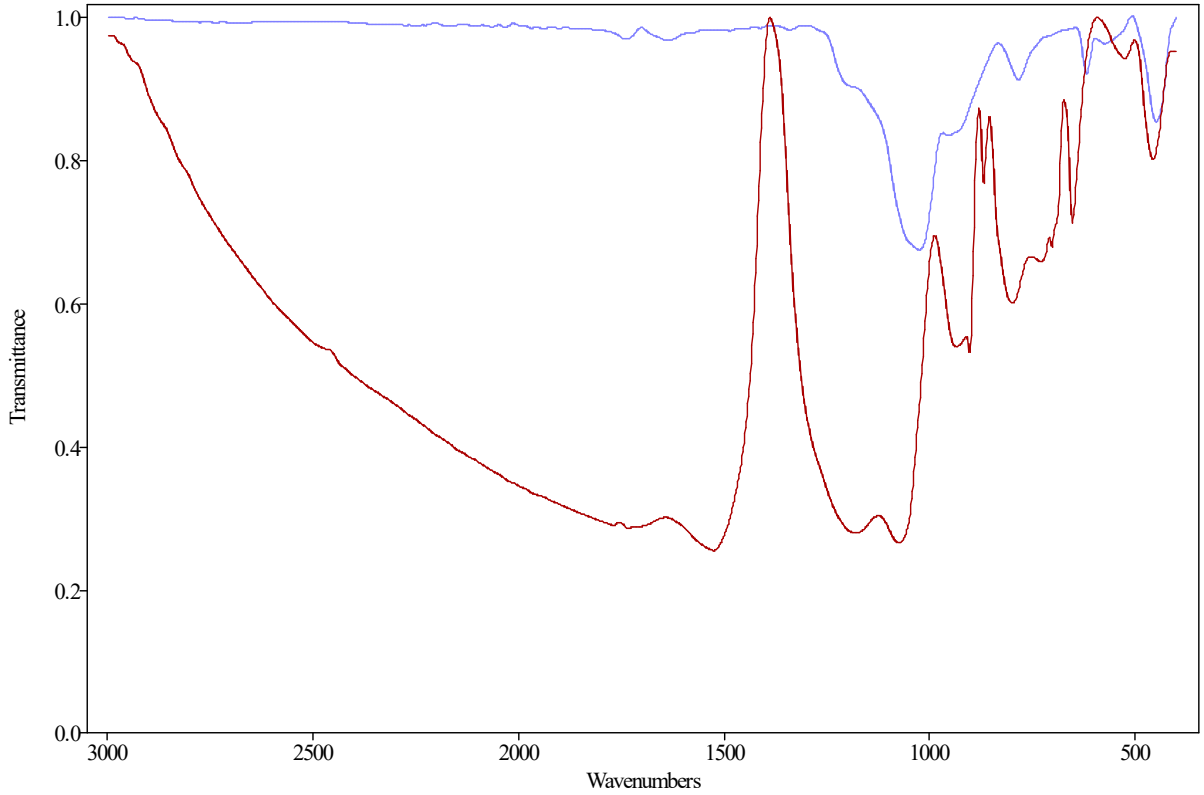


*Figure A.24: FTIR overlay of oxidized silica-DNP **SSA-4** (blue) and silica-DNPH **SSA-7** (brown)*

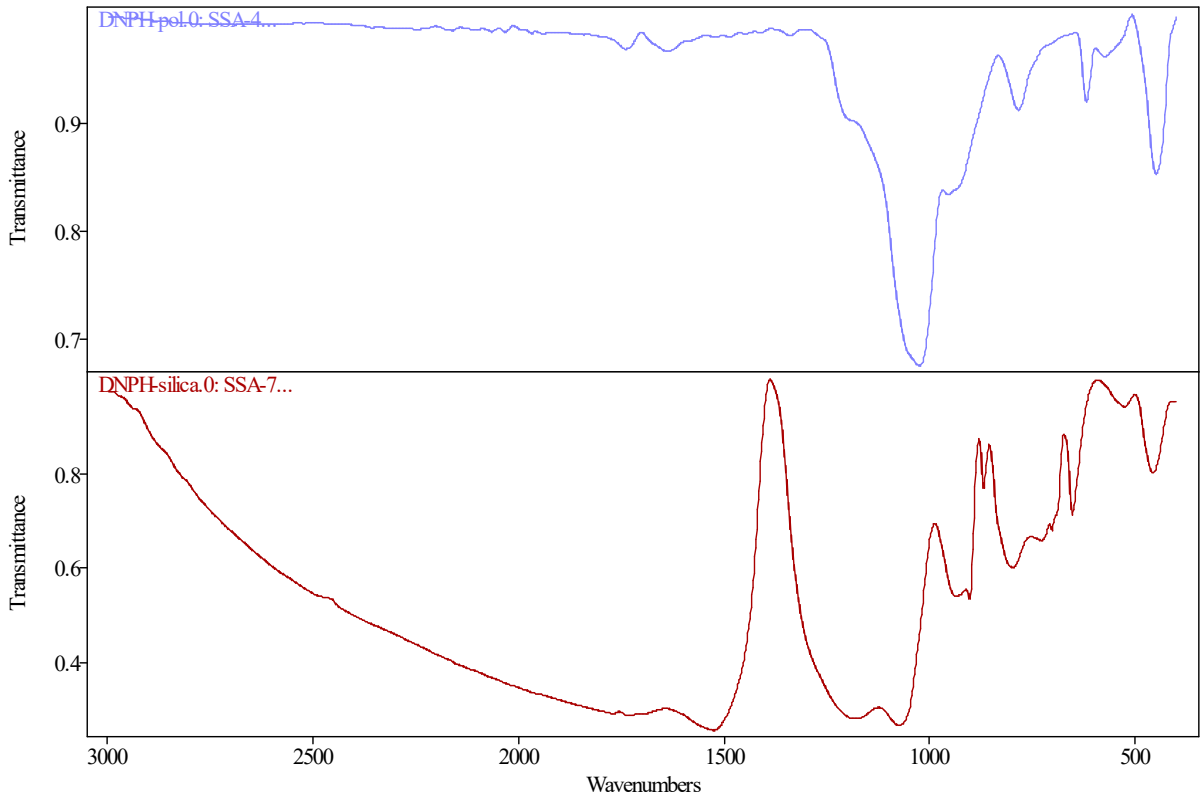


*Figure A.25: FTIR stacked of oxidized silica-DNP **SSA-4** (blue) and silica-DNPH **SSA-7** (brown)*

SSA-5 and SSA-6

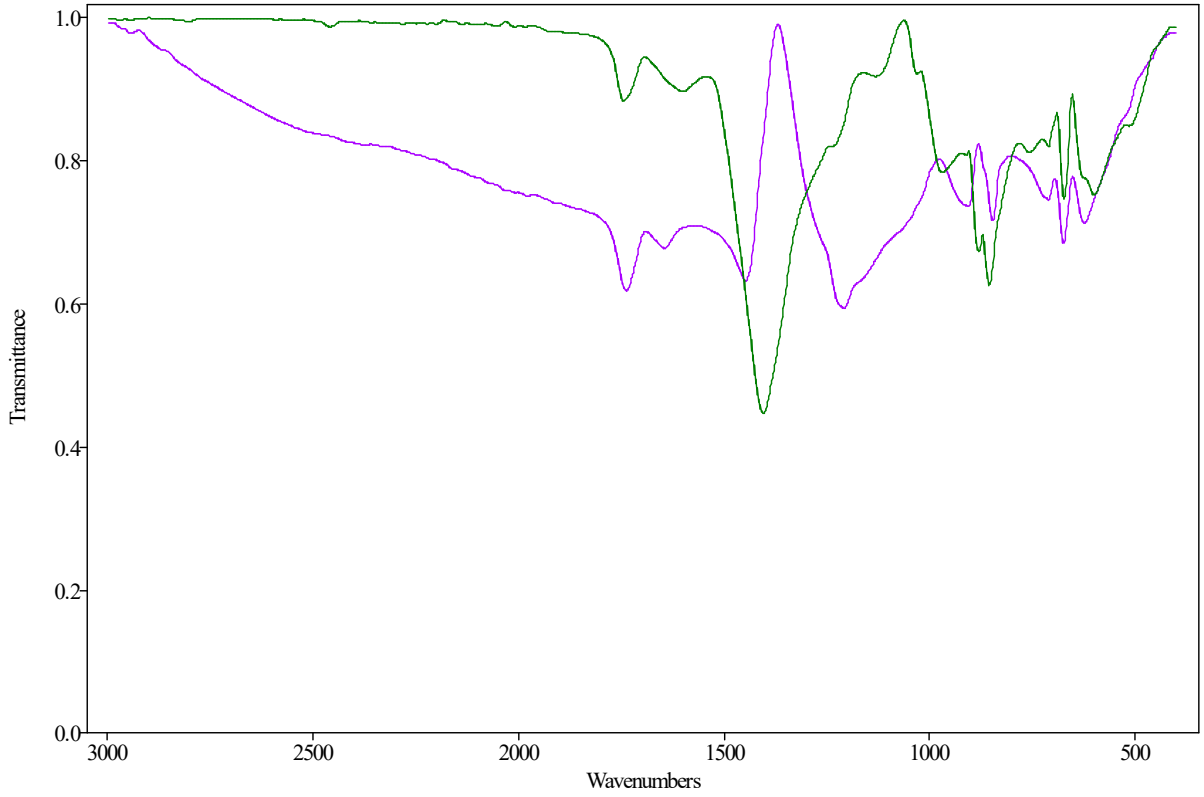


*Figure A.26: FTIR overlay of oxidized silica-benzylated **SSA-5** (purple) and silica-benzylated **SSA-6** (green)*

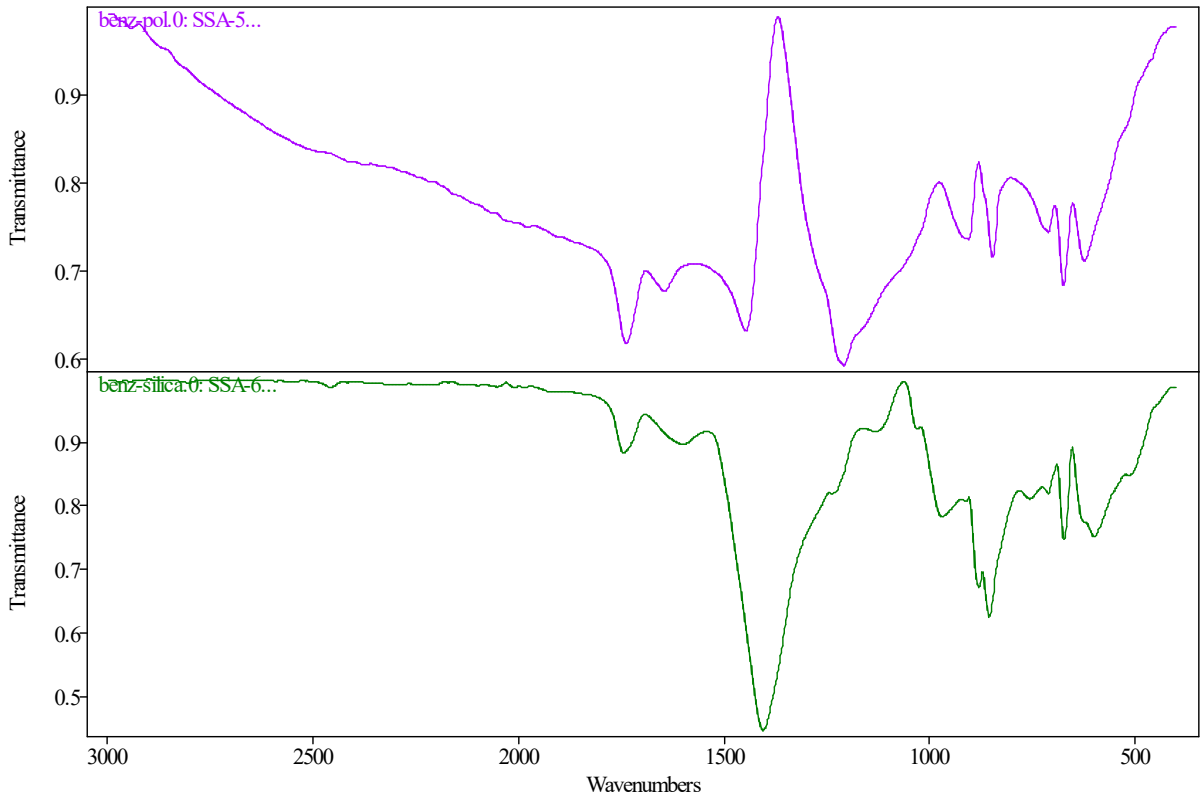


*Figure A.27: FTIR stacked of oxidized silica-benzylated **SSA-5** (purple) and silica-benzylated **SSA-6** (green)*

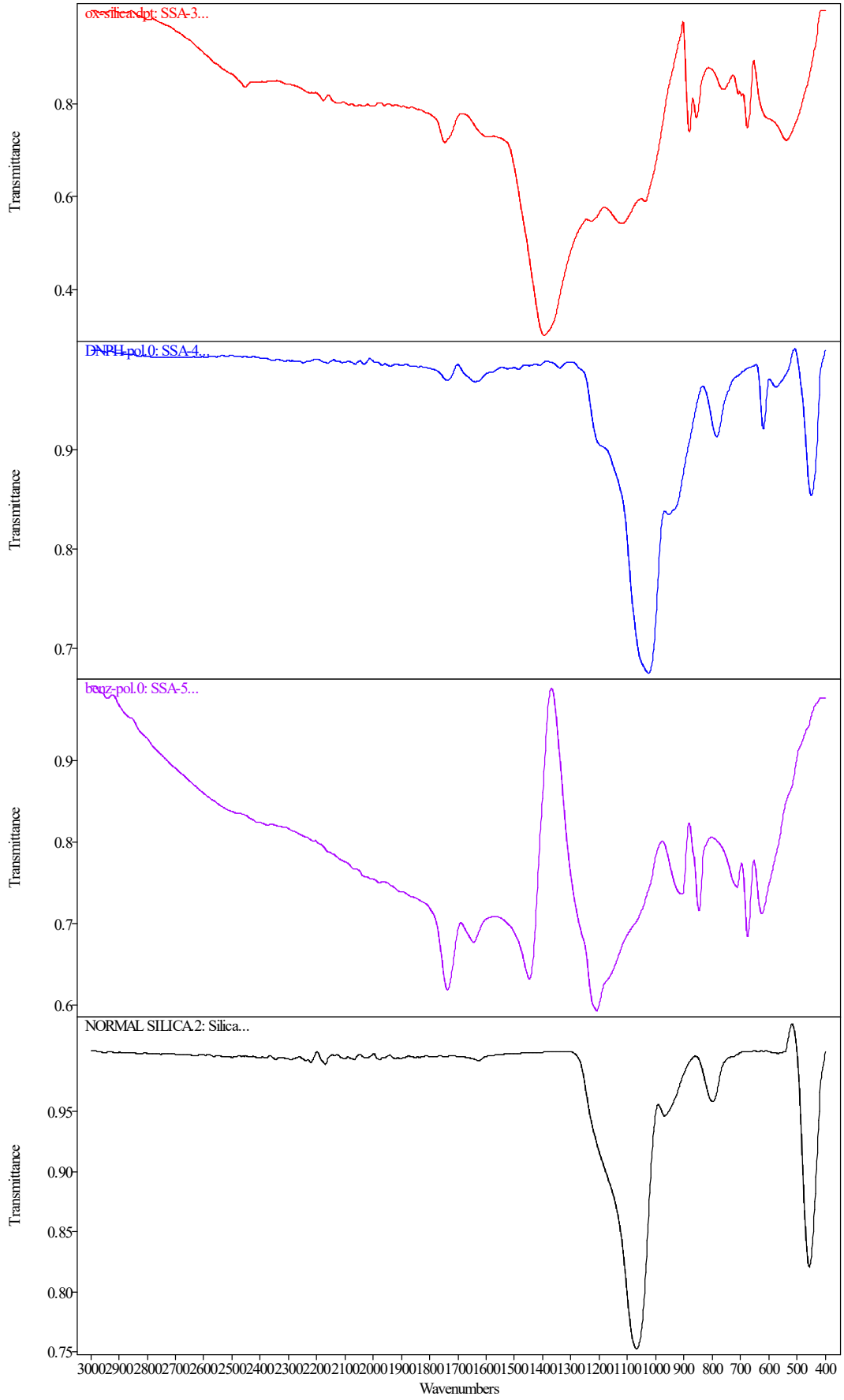


*Figure A.28: FTIR stacked of silica (black), oxidized silica-benzylated **SSA-5** (purple), oxidized silica-DNPH **SSA-4** (blue) and oxidized silica **SSA-3** (red)*

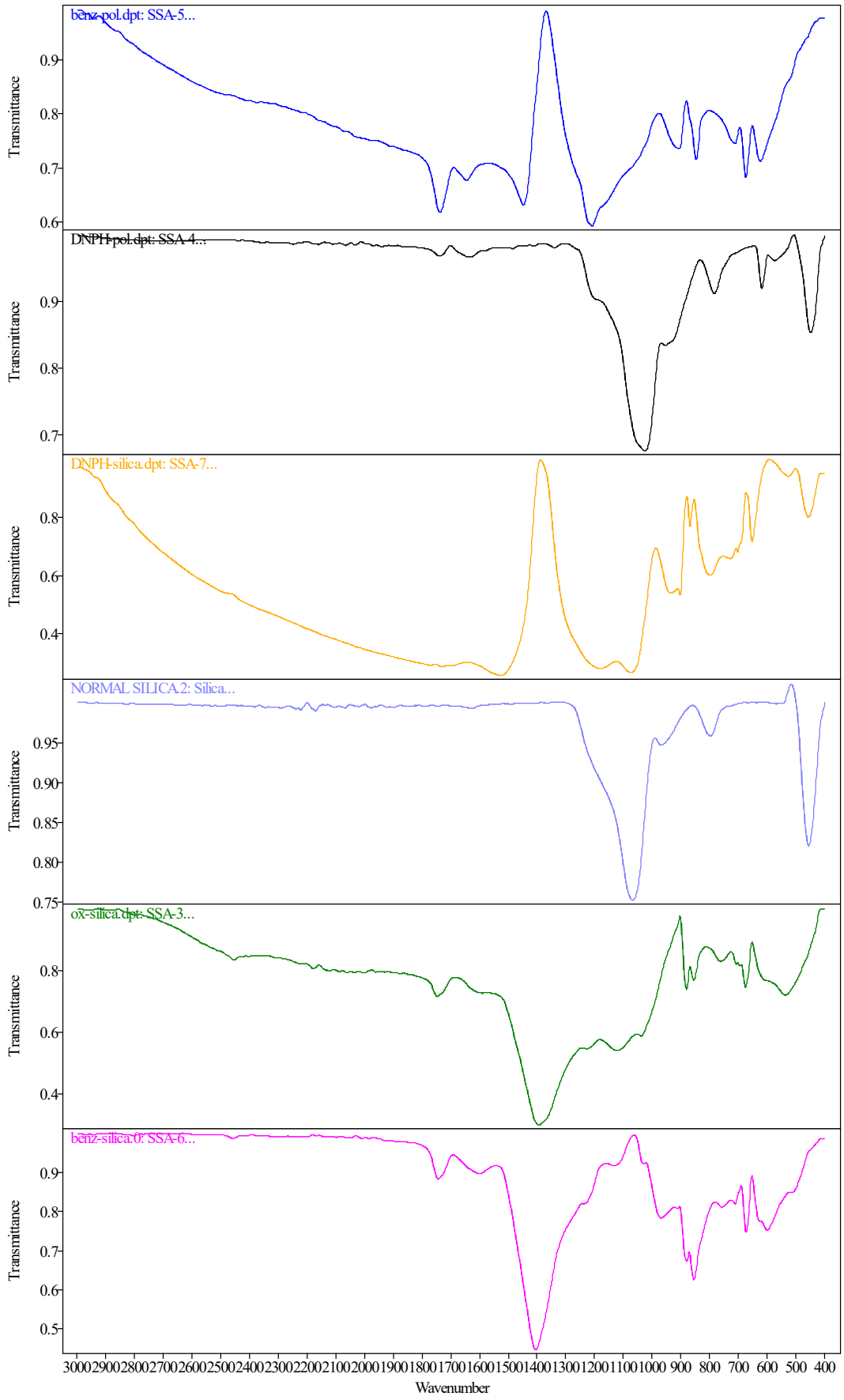


*Figure A.29: FTIR stacked of silica (light blue), oxidized silica-benzylated **SSA-5** (blue), oxidized silica-DNPH **SSA-4** (black), silica-DNPH **SSA-7** (orange), silica-benzylated **SSA-6** (pink) and oxidized silica **SSA-3** (green)*

A-7 Qualitative results

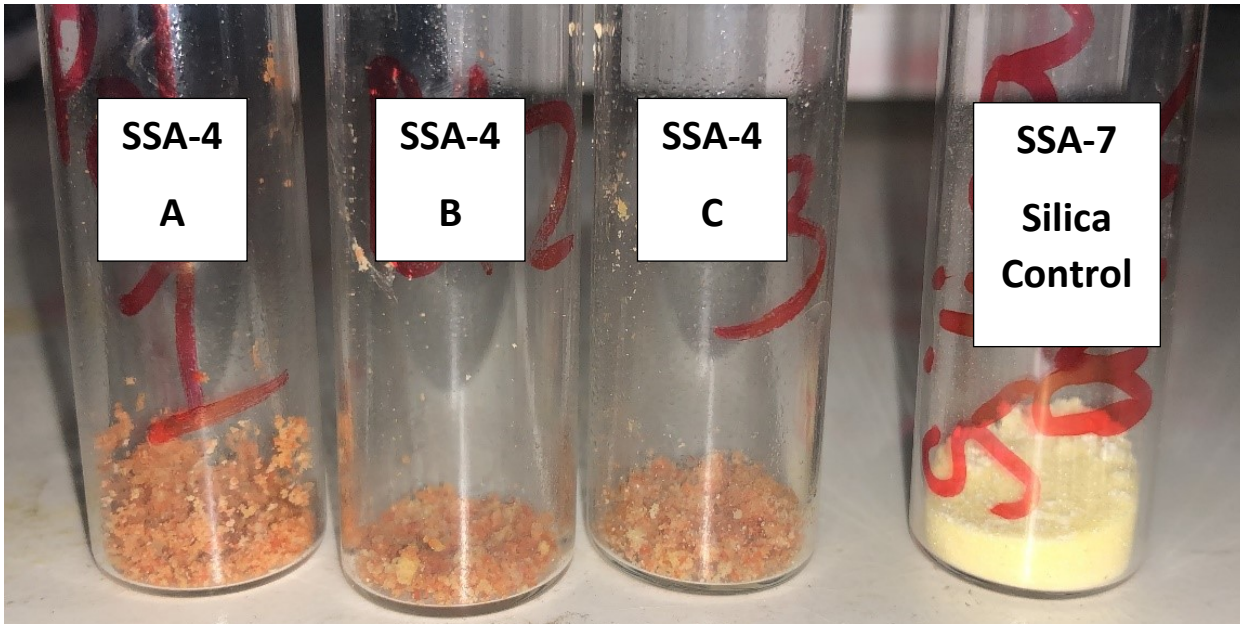


*Figure A.30: Photograph of qualitative DNP test with oxidized silica **SSA-4** (repeats A-C) with the silica-DNPH **SSA-7** (control)*

A-8 DoE

*Table A.17: D-optimal design set of experiments and calculated N-benzylamine **25** percentage unabsorbed*

Exp	F.R.	Temp	Conc	PC1	PC2	Q	Solvent	Run order	Column number	% unabsorbed
N1	1	30	0,2	-1	-1	3	**ACN**	1	1	26,16
N2	0,1	90	0,2	-1	-1	3	**ACN**	2	1	0,02
N3	0,1	30	1	-1	-1	3	**ACN**	4	1	24,30
N4	1	90	1	-1	-1	3	**ACN**	3	1	24,91
N5	0,1	30	0,2	1	-1	4	**EtOAc**	1	2	0,61
N6	1	90	0,2	1	-1	4	**EtOAc**	3	2	0,27
N7	1	30	1	1	-1	4	**EtOAc**	2	2	0,05
N8	0,1	90	1	1	-1	4	**EtOAc**	4	2	0,06
N9	0,1	30	0,2	-1	1	2	**DMA**	1	5	0,01
N10	1	90	0,2	-1	1	2	**DMA**	3	5	0,12
N11	1	30	1	-1	1	2	**DMA**	2	5	0,03
N12	0,1	90	1	-1	1	2	**DMA**	4	5	0,003
N13	1	30	0,2	1	1	1	**Anisole**	2	3	0,04
N14	0,1	90	0,2	1	1	1	**Anisole**	4	3	0,09
N15	0,1	30	1	1	1	1	**Anisole**	1	3	1,68
N16	1	90	1	1	1	1	**Anisole**	3	3	0,04
N17	0,55	90	0,6	0	0	0,0	**DCM**	4A	4	15,58
N18	0,55	60	1	0	0	0,0	**DCM**	1B	6	10,75
N19	0,55	60	0,6	1	0	(1;0)	**Cyclo-Hex**	1C	7	12,81
N20	0,55	60	0,6	0	0	0,0	**DCM**	1A	4	11,32
N21	0,55	60	0,6	0	0	0,0	**DCM**	2A	4	11,28
N22	0,55	60	0,6	0	0	0,0	**DCM**	3A	4	13,54

Table A.18: Individual column details for DOE experiments

Column number	Polymer mass (g)	Polymer height (cm)	Column dry mass (g)	Column wet mass (g)	Mass difference (g)	Solvent	Density (g/mL)	Wet volume (mL)
1	4.5055	4.60	63.6555	65.8886	2.2331	ACN	0.786	2.84
2	4.5029	4.62	63.8170	66.1497	2.3327	EtOAc	0.902	2.59
3	4.5039	4.55	63.5983	65.7533	2.1550	Anisole	0.995	2.17
4	4.5089	4.75	63.6634	68.0806	4.4172	DCM	1.33	3.32
5	4.5085	4.65	63.5525	68.7288	5.1763	DMA	0.940	5.51
6	4.5043	4.80	63.6820	68.2705	4.5885	DCM	1.33	3.45
7	4.5009	4.65	63.8465	65.8909	2.0444	Cyclohex	0.779	2.62
Average	4,5050	4,66	63,6879					
STD Dev	0,0027	0,08	0,0999					

A-9 DoE data

Factors and Responses

Table A.19: Summary of factors

Name	Abbreviation	Units	Type	Settings
Flow Rate	FR	mL/min	Quantitative	0,1 to 1
Temperature	Temp	Deg C	Quantitative	30 to 90
Concentration	Conc	M	Quantitative	0,2 to 1
Solvent PC1	S.PC1		Quantitative	-1 to 1
Solvent PC2	S.PC2		Quantitative	-1 to 1

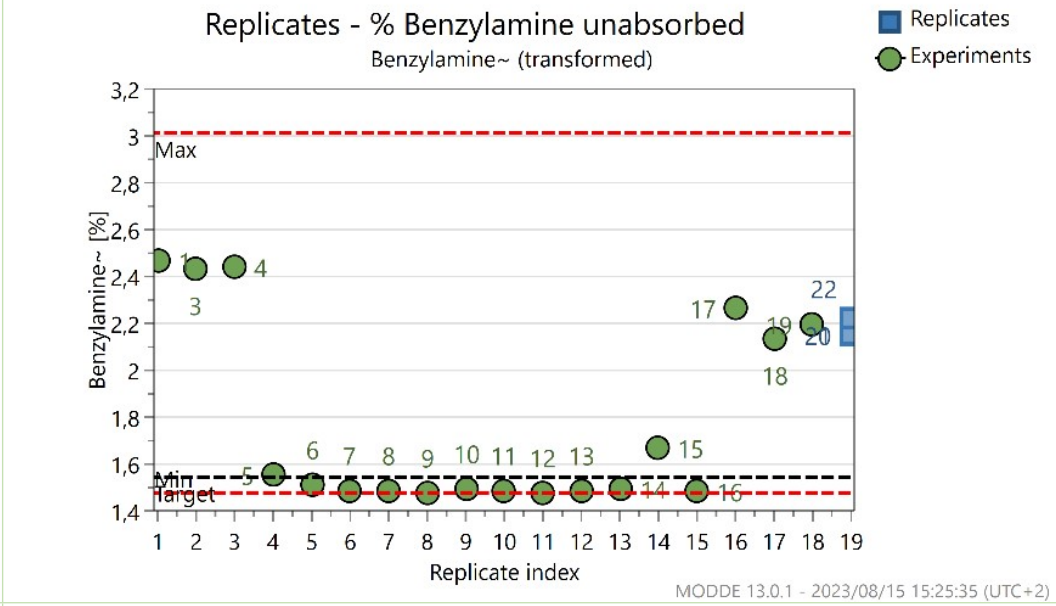
Table A.20: Summary of responses

Name	Abbr.	Units	Transform	Condition	Objective	Min	Target	Max
Benzylamine	%BnNh	%	Log: 10Log(10* Y+30)	Required	Minimize	0	0,5	100

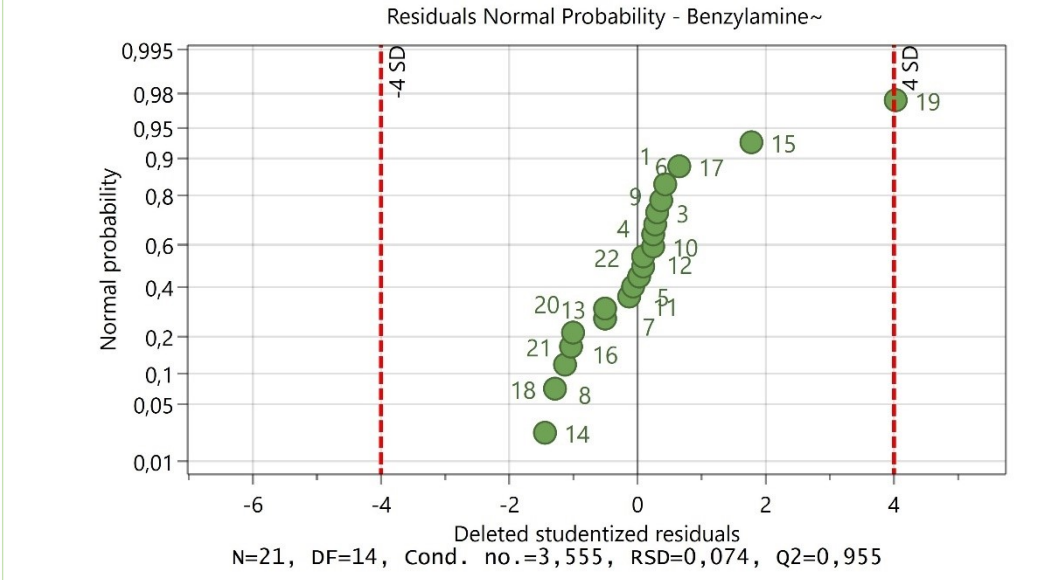
Replicates and Residuals

*Table A.21: Plots of replicates (a), residuals (b), distribution histogram (c), main effects for flow rate (d), solvent PC1 dimension (e), solvent PC2 dimension (f), Summary of fit (g), and interaction plots of FR*S.PC1 in terms of flow rate (h), Interaction plot S.PC1*S.PC2 in terms of solvent PC1 dimension (i) and solvent PC2 dimension (j)*

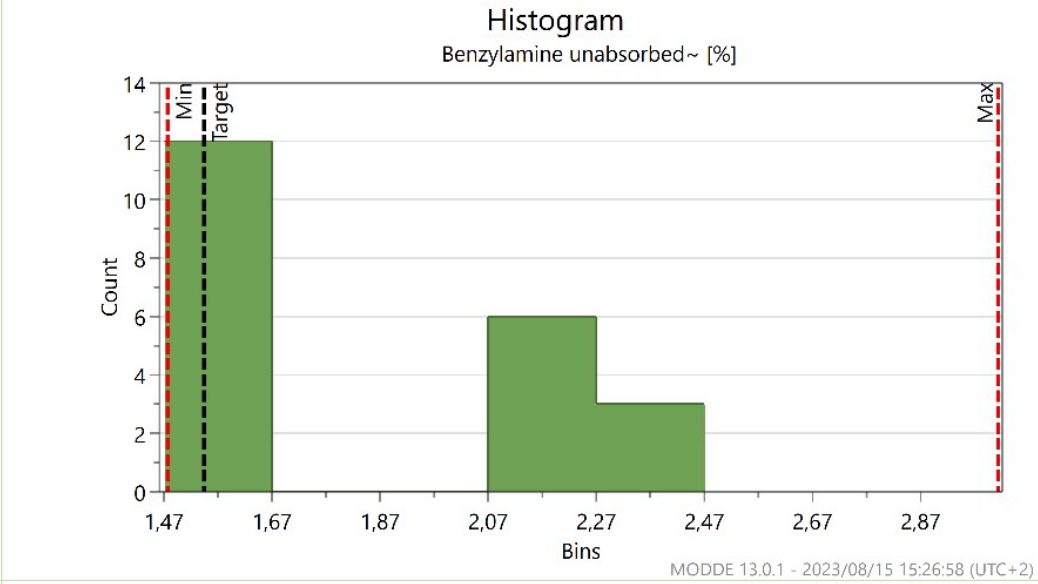
a)



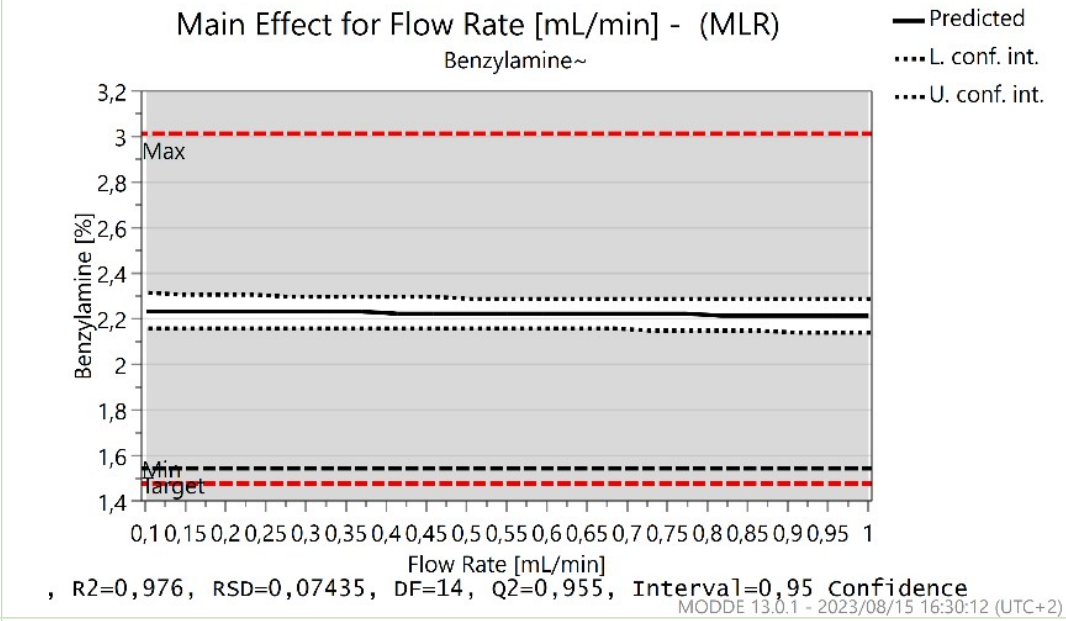
b)



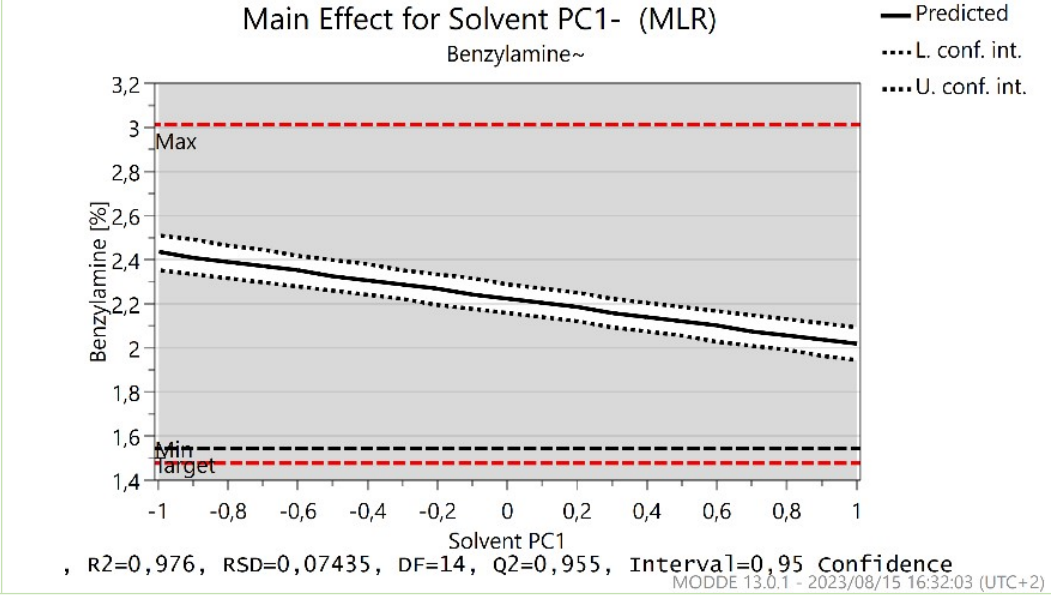
c)


Histogram
Benzylamine unabsorbed~ [%]
Min
Target
Max
Count
Bins
1,47
1,67
1,87
2,07
2,27
2,47
2,67
2,87
MODDE 13.0.1 - 2023/08/15 15:26:58 (UTC+2)

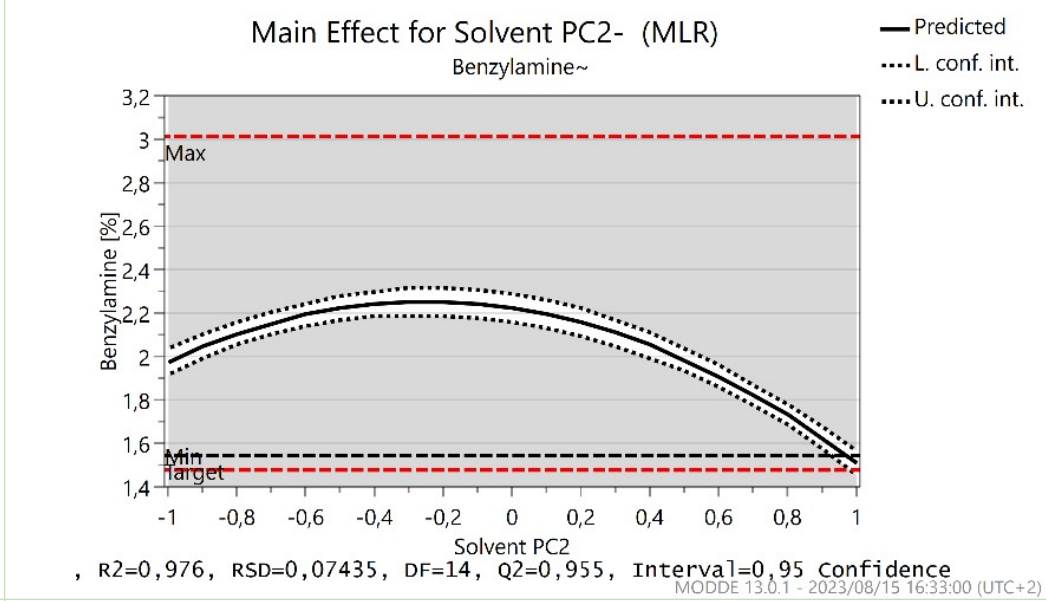
d)


Main Effect for Flow Rate [mL/min] - (MLR)
Benzylamine~
Predicted
L. conf. int.
U. conf. int.
Max
Min
Target
Benzylamine [%]
Flow Rate [mL/min]
, R2=0,976, RSD=0,07435, DF=14, Q2=0,955, Interval=0,95 Confidence
MODDE 13.0.1 - 2023/08/15 16:30:12 (UTC+2)

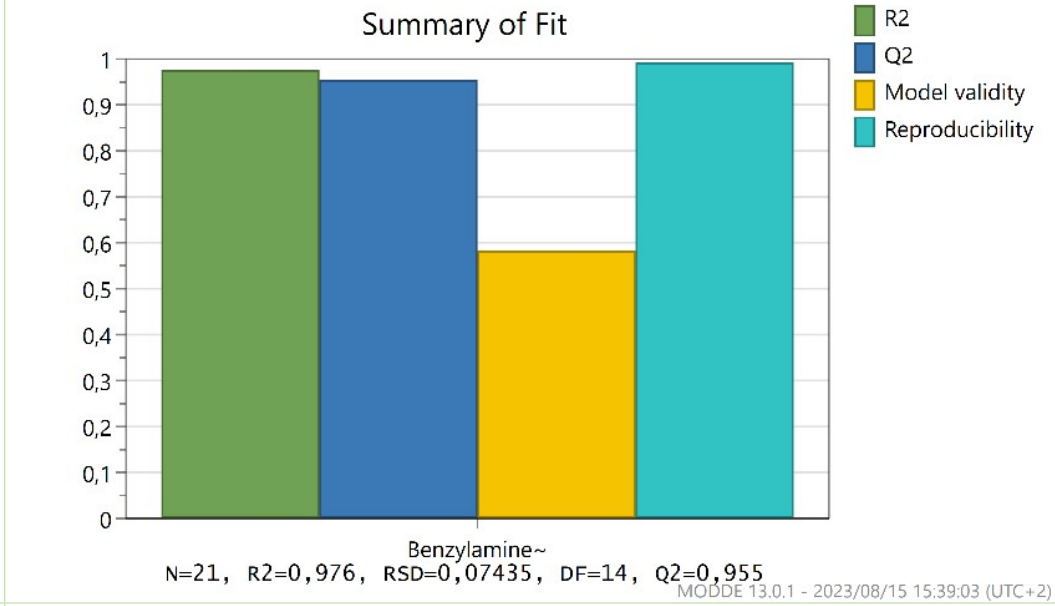
e)


Main Effect for Solvent PC1- (MLR)
Benzylamine~
Predicted
L. conf. int.
U. conf. int.
Max
Min
Target
Benzylamine [%]
Solvent PC1
, R2=0,976, RSD=0,07435, DF=14, Q2=0,955, Interval=0,95 Confidence
MODDE 13.0.1 - 2023/08/15 16:32:03 (UTC+2)

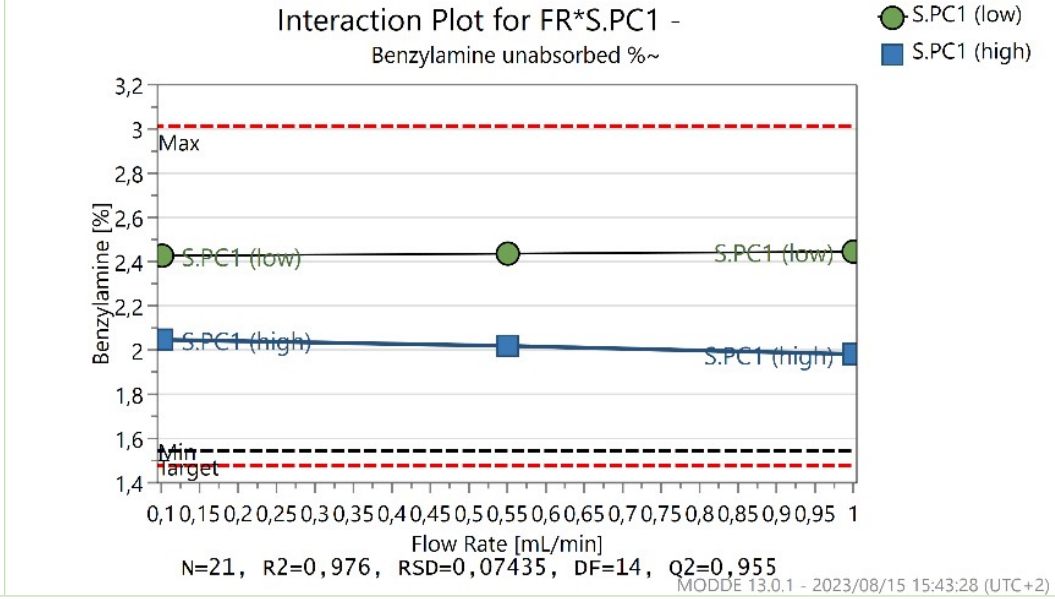
f)


Main Effect for Solvent PC2- (MLR)
Benzylamine~
Predicted
L. conf. int.
U. conf. int.
Max
Min
Target
Benzylamine [%]
Solvent PC2
, R2=0,976, RSD=0,07435, DF=14, Q2=0,955, Interval=0,95 Confidence
MODDE 13.0.1 - 2023/08/15 16:33:00 (UTC+2)

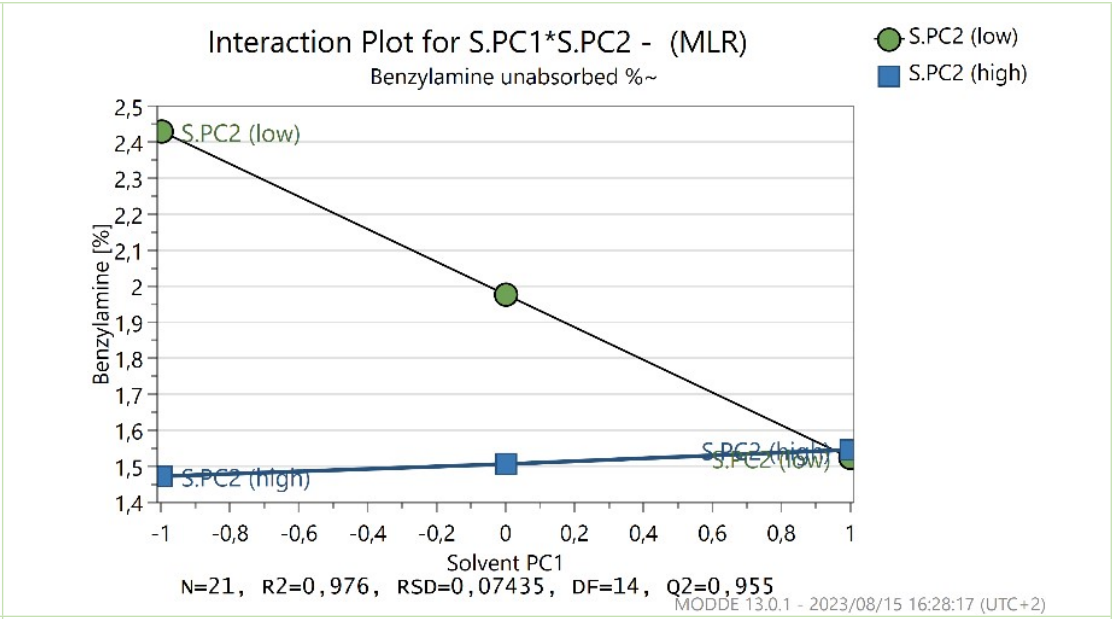
g)


Summary of Fit
R2
Q2
Model validity
Reproducibility
Benzylamine~
N=21, R2=0,976, RSD=0,07435, DF=14, Q2=0,955
MODDE 13.0.1 - 2023/08/15 15:39:03 (UTC+2)

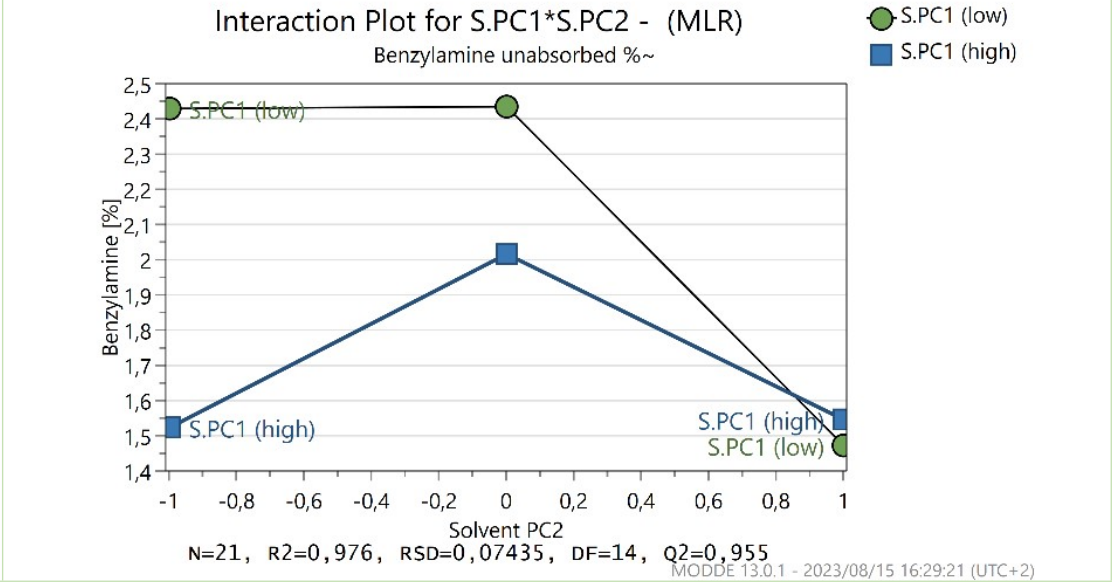
h)


Interaction Plot for FR*S.PC1 -
Benzylamine unabsorbed %~
S.PC1 (low)
S.PC1 (high)
Max
Min
Target
Benzylamine [%]
Flow Rate [mL/min]
N=21, R2=0,976, RSD=0,07435, DF=14, Q2=0,955
MODDE 13.0.1 - 2023/08/15 15:43:28 (UTC+2)

i)



j)



Coefficients

Table A.22: Summary of coefficients

Benzylamine	Coeff. SC	Std. Err.	P	Conf. int(±)
Constant	2,22412	0,0305158	1,81829e-19	0,0654505
Flow Rate	-0,0103658	0,0194894	0,603156	0,041801
Solvent PC1	-0,209203	0,0189583	2,72256e-08	0,0406618
Solvent PC2	-0,234532	0,0194894	9,02145e-09	0,041801
S.PC2*S.PC2	-0,482399	0,0360577	2,28886e-09	0,0773368
FR*S.PC1	-0,019466	0,0194894	0,334842	0,041801
S.PC1*S.PC2	0,245063	0,0194894	5,12186e-09	0,041801
N = 21	Q2 =	0,955	Cond. no. =	3,555
DF = 14	R2 =	0,976	RSD =	0,07435
	R2 adj. =	0,966		
			Confidence =	0,95

Effects

Table A.23: Summary of effects

Benzylamine	Effect	Conf. int(±)		
S.PC2*S.PC2	-0,964797	0,154674		
S.PC1*S.PC2	0,490127	0,083602		
Solvent PC2	-0,469064	0,083602		
Solvent PC1	-0,418405	0,0813236		
FR*S.PC1	-0,0389321	0,083602		
Flow Rate	-0,0207315	0,083602		
N = 21	Q2 =	0,955	Cond. no. =	3,555
DF = 14	R2 =	0,976	RSD =	0,07435
	R2 adj. =	0,966		
			Confidence =	0,95

Summary of fit

Table A.24: Summary of fit

	R2	R2 Adj.	Q2	SDY	RSD	N	Model Validity	Reproducibility
Benzylamine	0,975901	0,965573	0,954751	0,400691	0,074346 3	21	0,583223	0,99172
N = 21	Cond. no. =	3,555						
DF = 14								

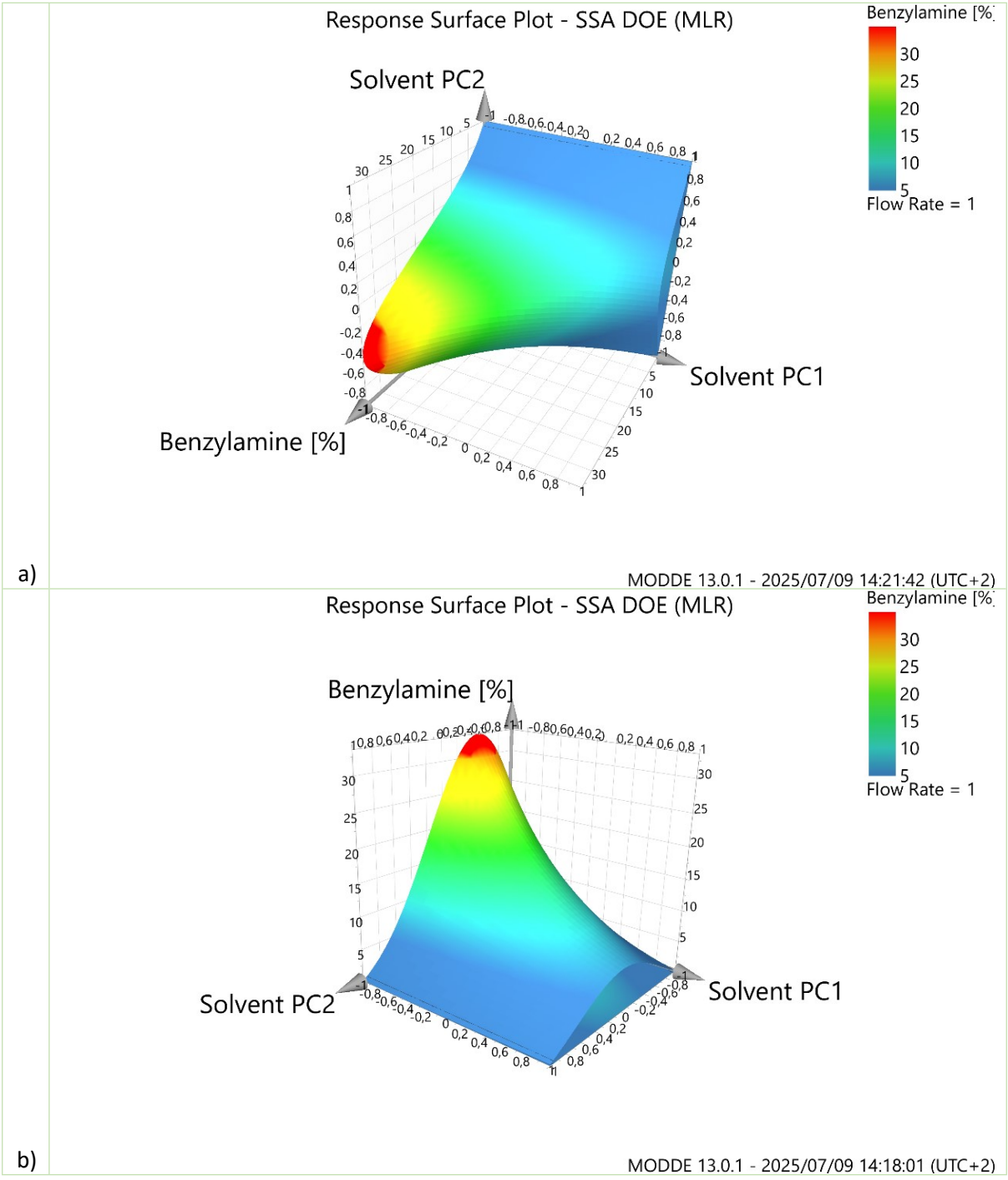
ANOVA

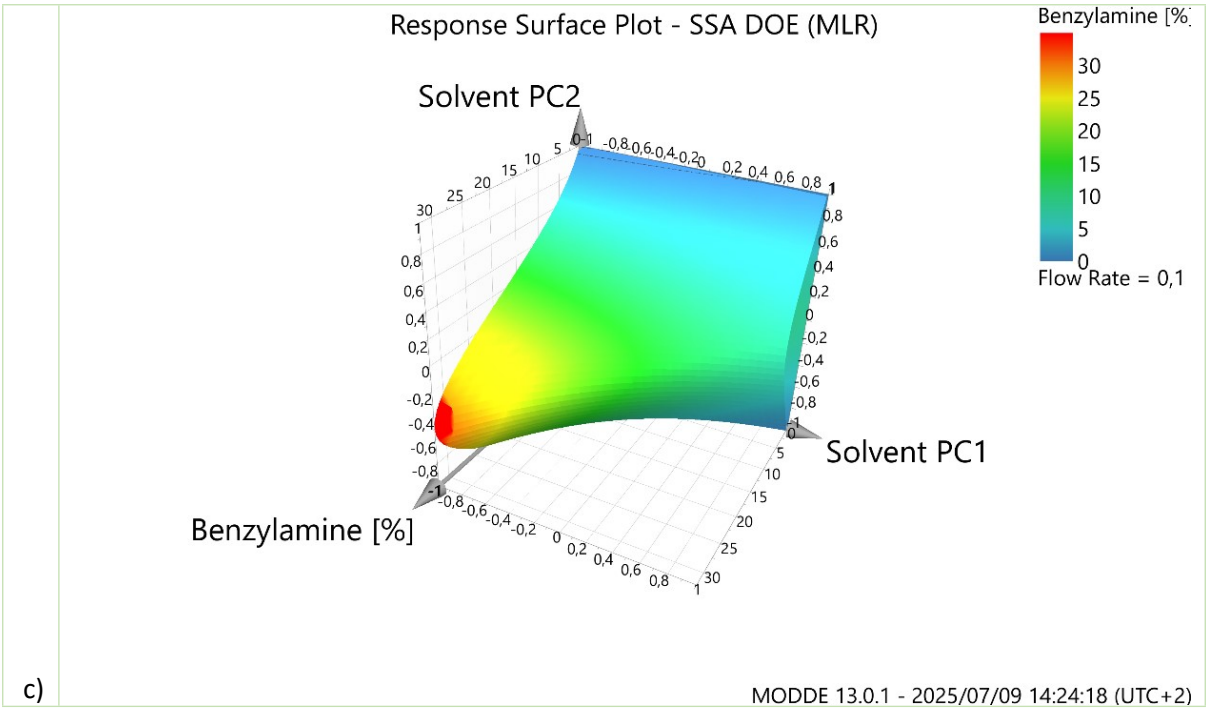
Table A.25: Analysis of variance

Benzylamine	DF	SS	MS (variance)	F	p	SD
Total	21	74,0938	3,52827			
Constant	1	70,8827	70,8827			
Total corrected	20	3,21106	0,160553			0,400691
Regression	6	3,13368	0,52228	94,4896	**0,000**	0,722689
Residual	14	0,0773833	0,00552738			0,0743463
Lack of Fit (Model error)	12	0,0747244	0,00622703	4,68391	**0,189**	0,0789116
Pure error (Replicate error)	2	0,0026589	0,00132945			0,0364616
	N = 21	Q2 =	0,955	Cond. no. =	3,555	
	DF = 14	R2 =	0,976	RSD =	0,07435	
		R2 adj. =	0,966			

Response surface plots

Table A.26: Response surface plots




Response Surface Plot - SSA DOE (MLR)
Solvent PC2
Solvent PC1
Benzylamine [%]
Benzylamine [%]
30
25
20
15
10
5
0
Flow Rate = 0,1
MODDE 13.0.1 - 2025/07/09 14:24:18 (UTC+2)

c)