LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036196.D
Acq On : 10 Aug 2022 17:31
Operator : CG/JU
Sample : N3972-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-9

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.234	190	195	198	rBV	199634	244364	2.09%	0.404%
2	4.281	198	203	216	rVB	1435208	2133641	18.21%	3.528%
3	4.922	306	312	320	rBV2	400528	608880	5.20%	1.007%
4	5.416	390	396	404	rBV	2184762	3077542	26.26%	5.089%
5	6.304	542	547	555	rVB	109205	162995	1.39%	0.270%
6	6.475	571	576	586	rBV	421303	601291	5.13%	0.994%
7	6.798	626	631	638	rVB	154344	225275	1.92%	0.372%
8	7.028	664	670	684	rBV	1202864	1944032	16.59%	3.215%
9	7.828	799	806	813	rBV	954292	1493575	12.74%	2.470%
10	7.898	813	818	833	rVB	170028	306239	2.61%	0.506%
11	8.198	863	869	876	rVB	252036	386340	3.30%	0.639%
12	8.457	906	913	920	rBV	96264	184193	1.57%	0.305%
13	9.004	999	1006	1017	rVV	2653562	4311908	36.79%	7.130%
14	9.569	1095	1102	1109	rVB	152417	244091	2.08%	0.404%
15	9.992	1166	1174	1177	rBV2	83189	138110	1.18%	0.228%
16	10.633	1276	1283	1290	rBV	1231881	2057696	17.56%	3.402%
17	11.598	1440	1447	1465	rVB	424670	850512	7.26%	1.406%
18	13.104	1693	1703	1716	rBV	6084989	9097061	77.62%	15.042%
19	13.333	1736	1742	1755	rVB	1942718	2661959	22.71%	4.402%
20	14.474	1929	1936	1945	rBV	1763839	2479380	21.16%	4.100%
21	15.962	2183	2189	2206	rBV	4304119	6353360	54.21%	10.505%
22	17.215	2396	2402	2411	rBV	1893719	2652369	22.63%	4.386%
23	17.886	2512	2516	2520	rVB2	140299	172264	1.47%	0.285%
24	18.115	2550	2555	2564	rBV2	85633	144399	1.23%	0.239%
25	19.845	2843	2849	2856	rBV	9548160	11720028	100.00%	19.379%
26	20.603	2975	2978	2982	rBV	117645	137053	1.17%	0.227%
27	21.397	3108	3113	3120	rBV	2364927	2958439	25.24%	4.892%
28	23.744	3506	3512	3520	rVB2	1578800	3129799	26.70%	5.175%

Sum of corrected areas: 60476795

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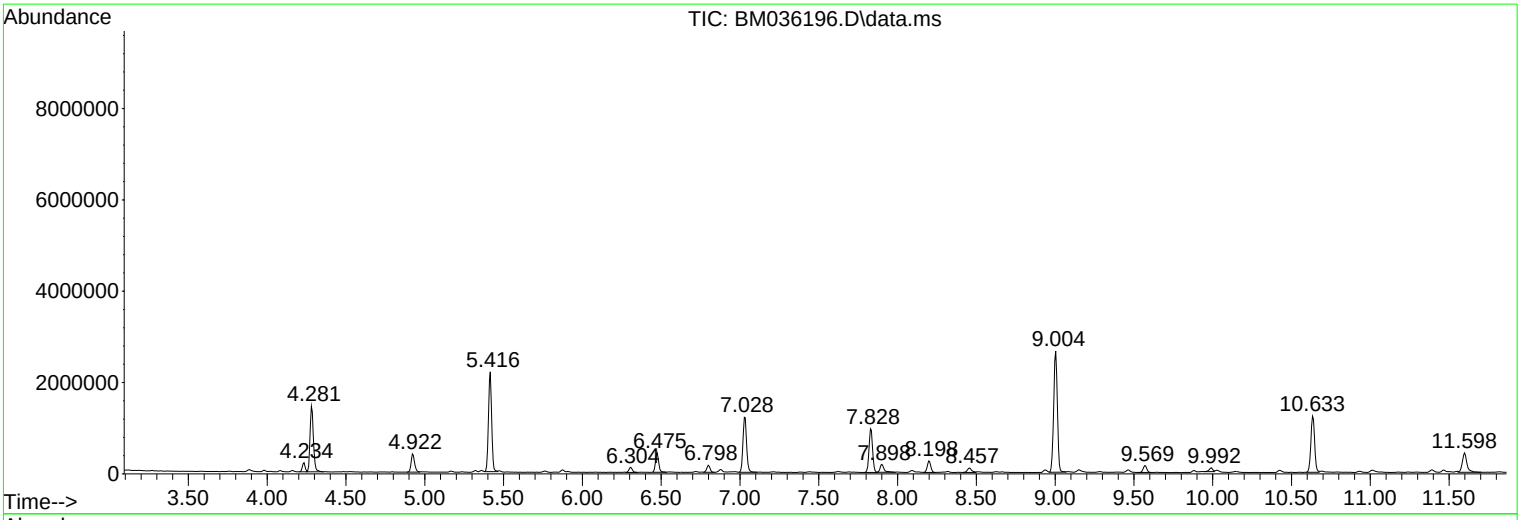
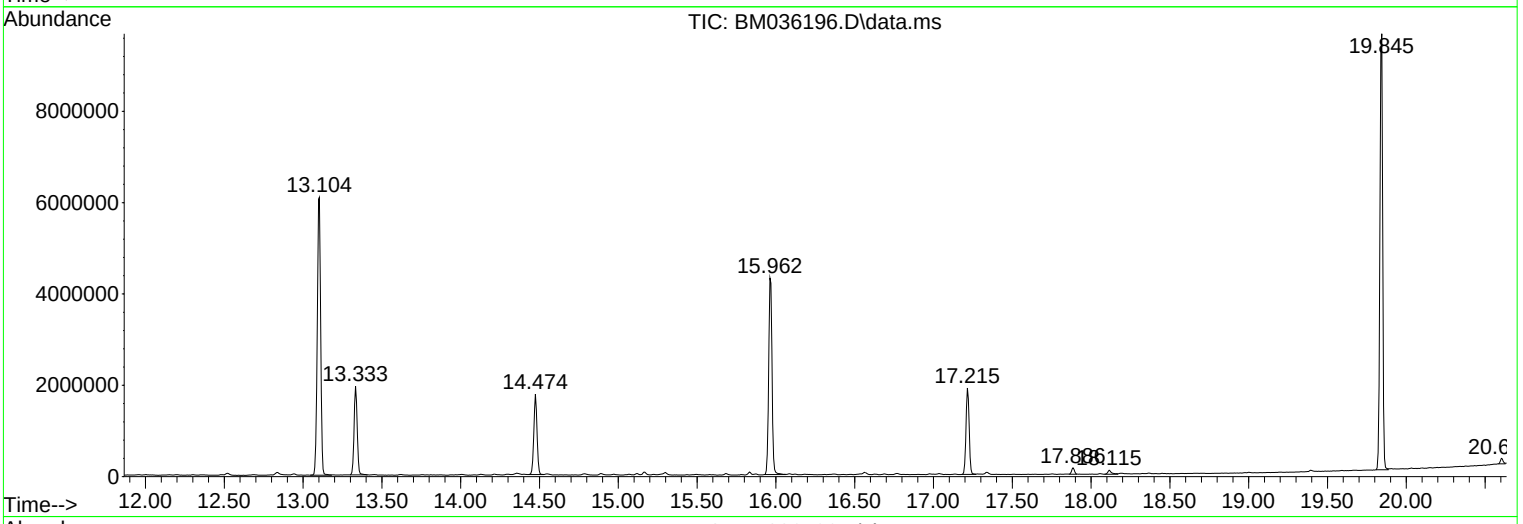
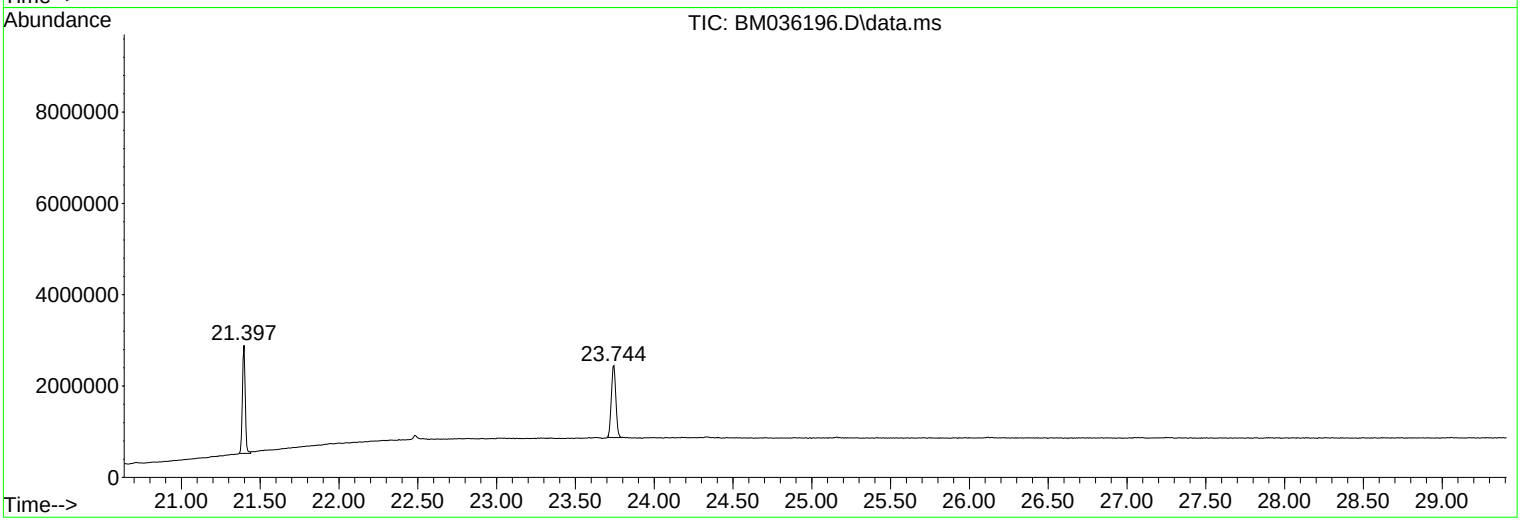
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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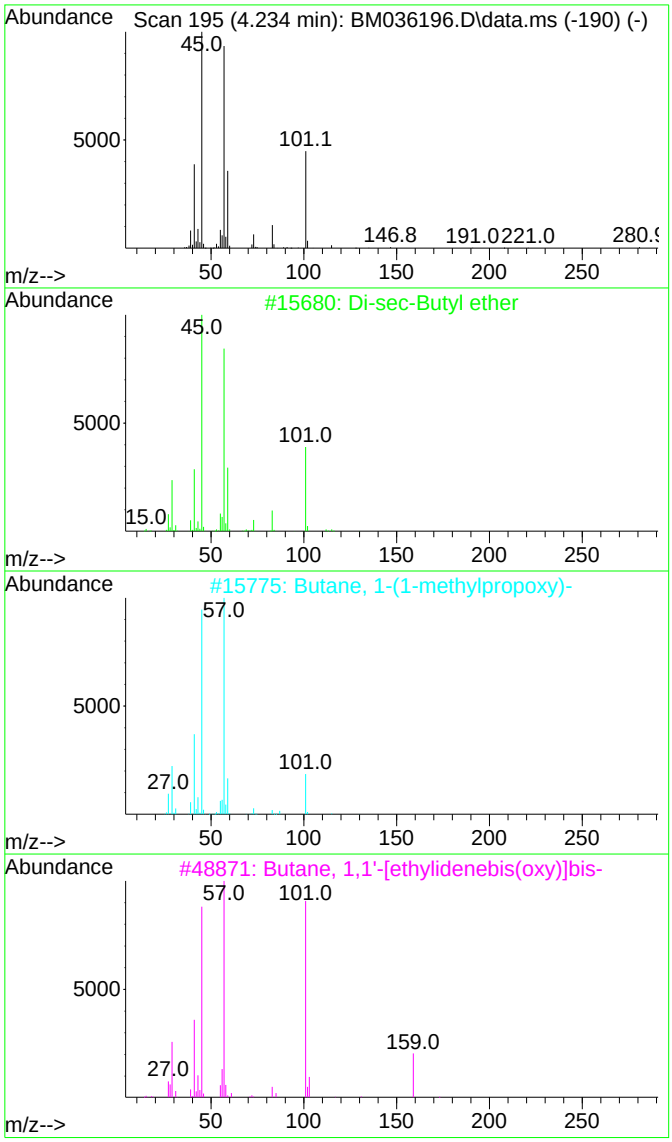
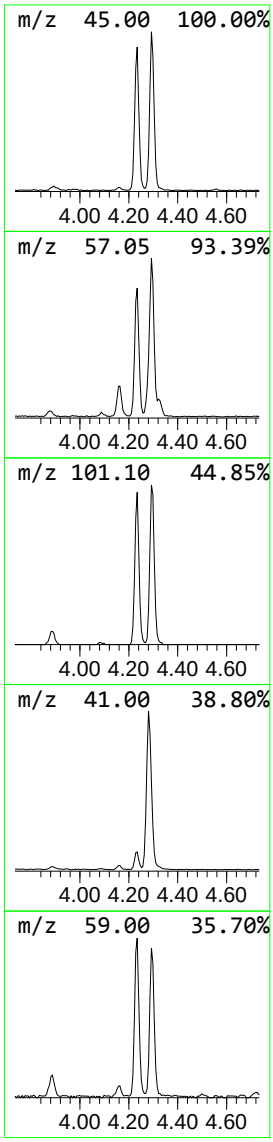
Peak Number 1 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.234	3.27 ng	244364	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	39
4	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39
5	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	36





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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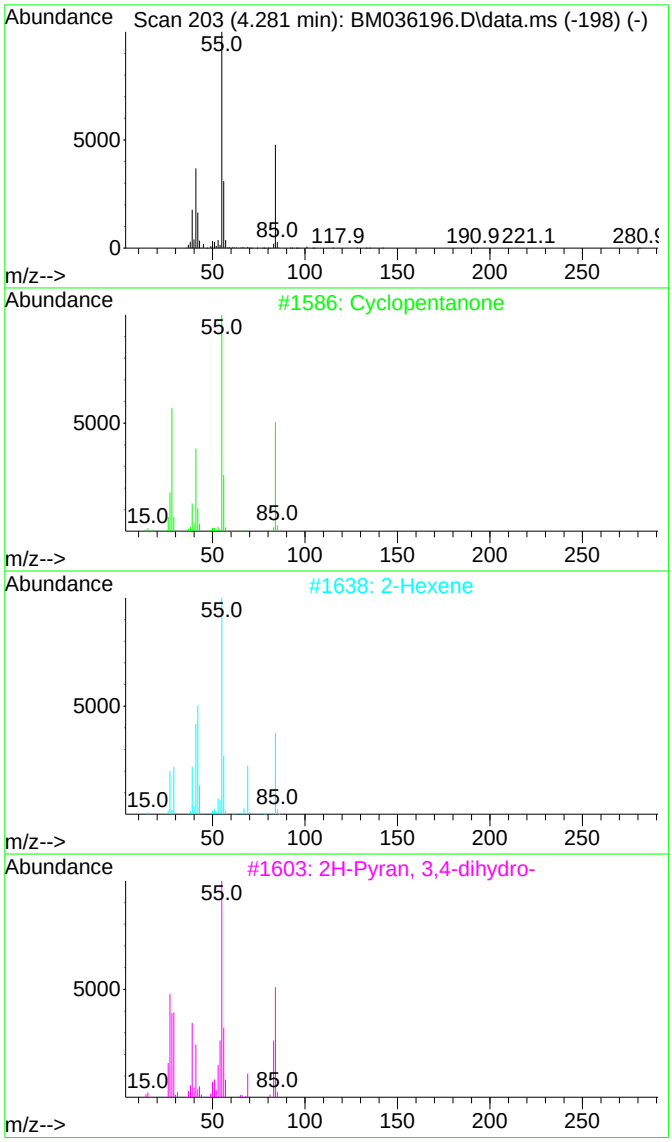
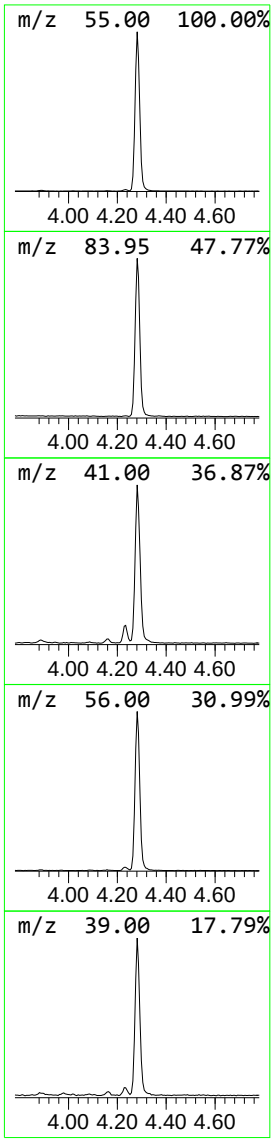
Peak Number 2 Cyclopentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	28.57 ng	2133640	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene	84	C6H12	000592-43-8	59
3	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	45
5	3-Hexene	84	C6H12	000592-47-2	38





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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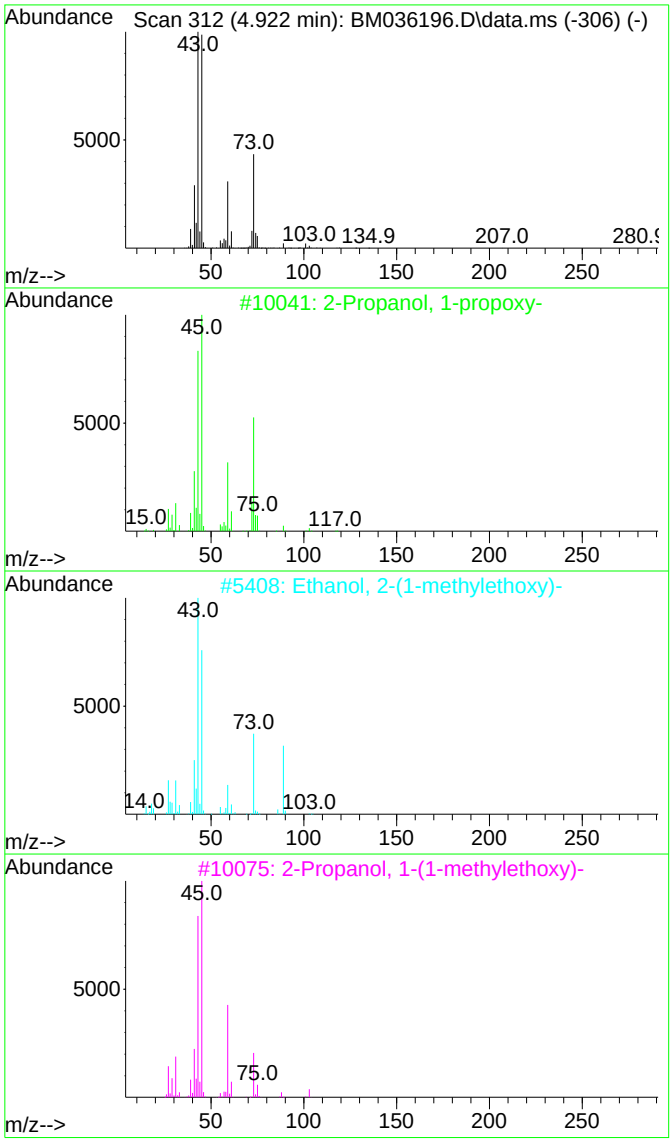
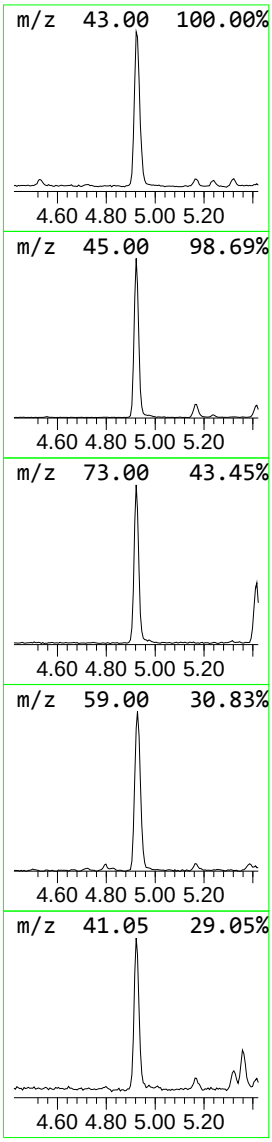
Peak Number 3 2-Propanol, 1-propoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	8.15 ng	608880	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	78
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
4	Monomethyl oxalate	104	C3H4O4	000600-23-7	50
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	47





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Sample : N3972-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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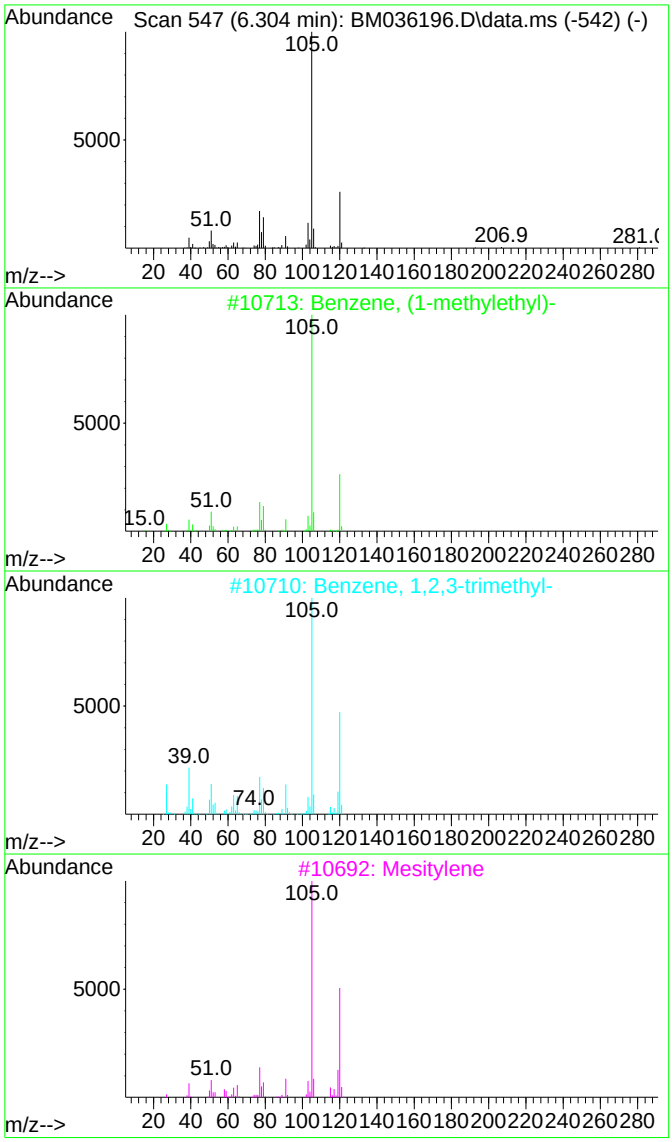
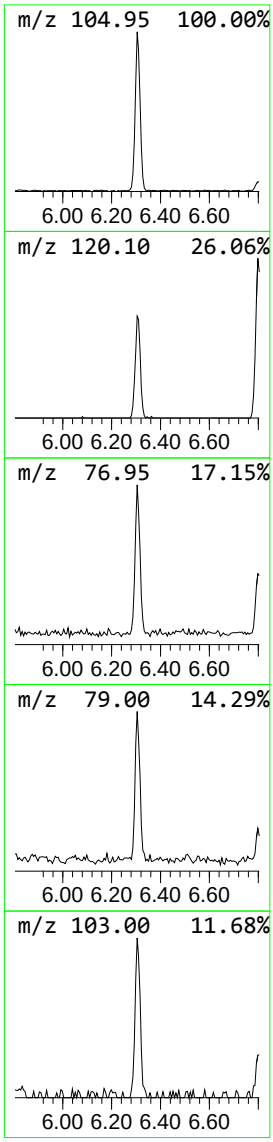
Peak Number 4 Benzene, (1-methylethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.304	2.18 ng	162995	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87





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Sample : N3972-05
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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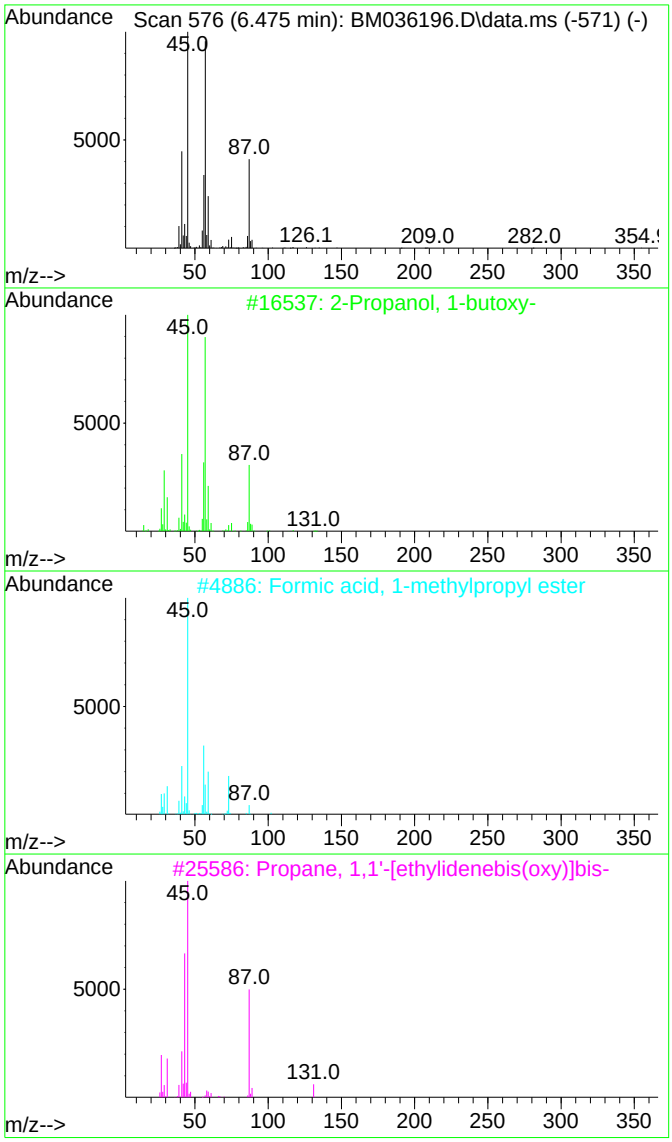
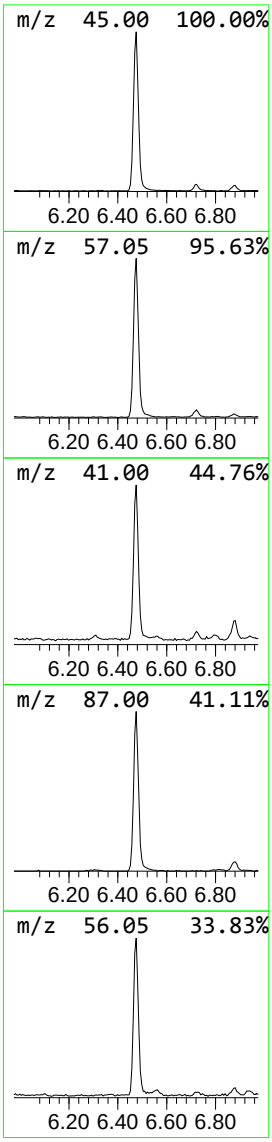
Peak Number 5 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	8.05 ng	601291	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	50
3	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	50
4	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	45
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42





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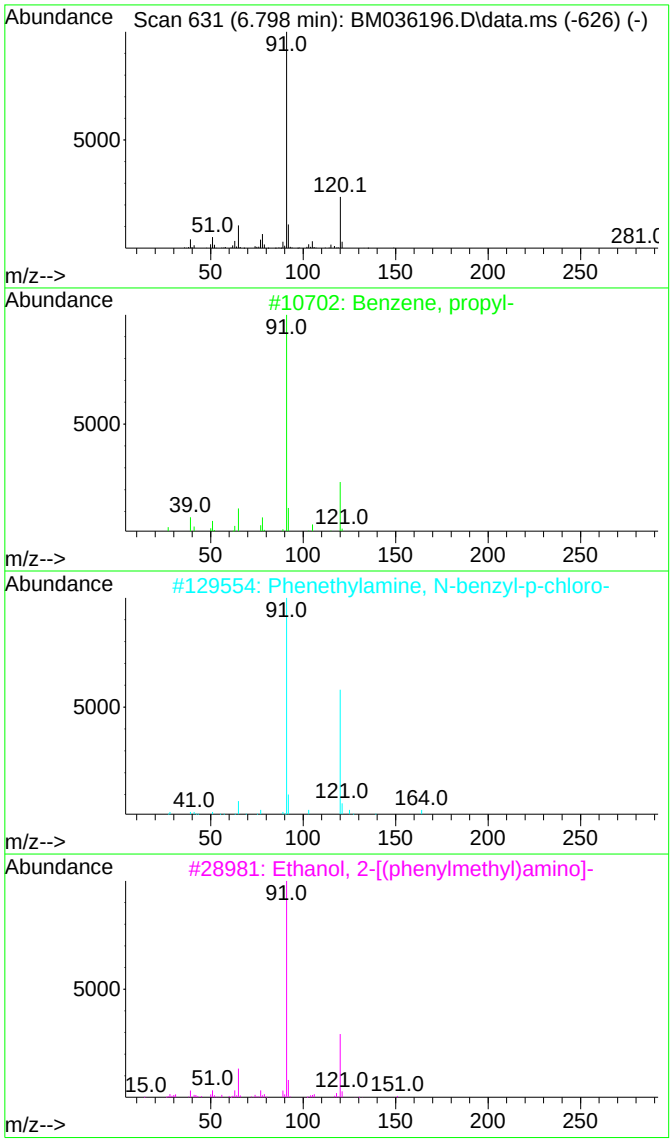
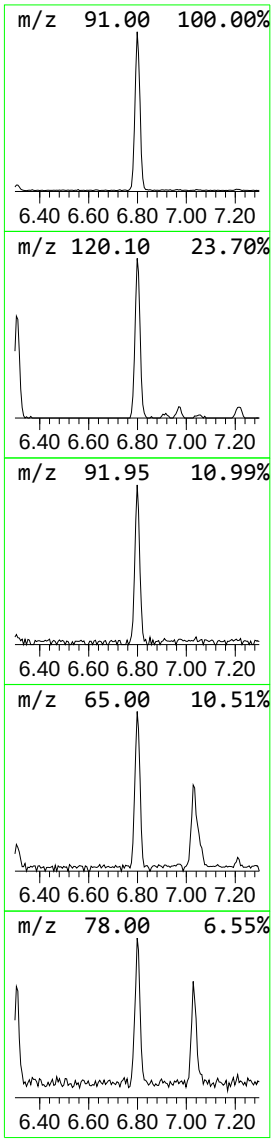
Peak Number 6 Benzene, propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.798	3.02 ng	225275	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	94
2	Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	78
3	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	78
4	1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	72
5	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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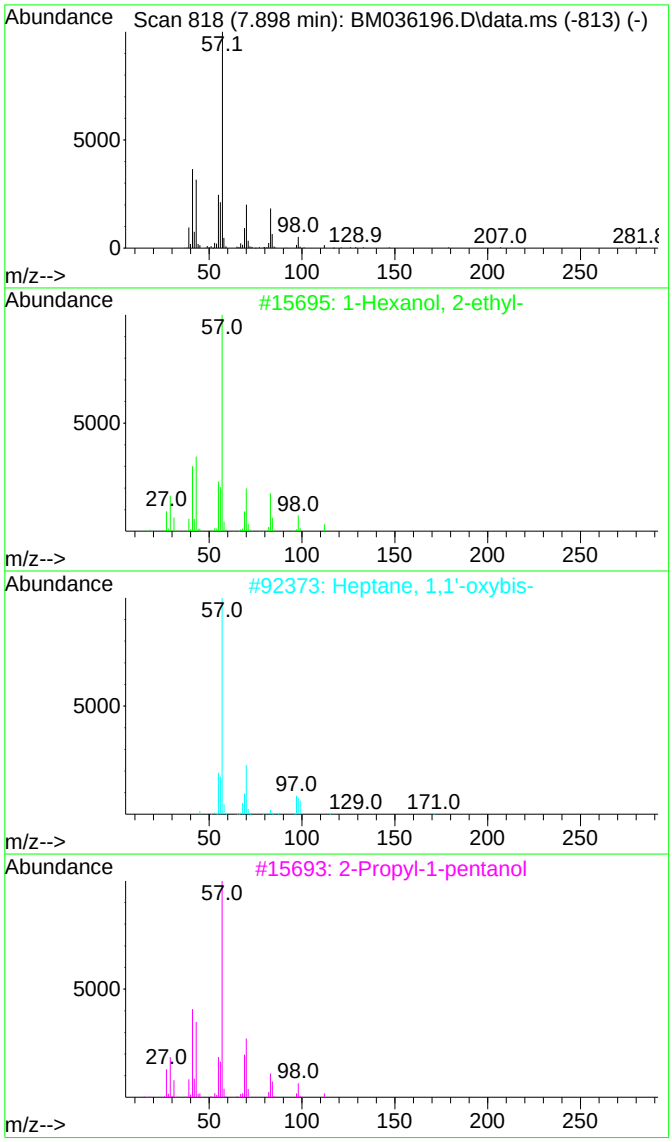
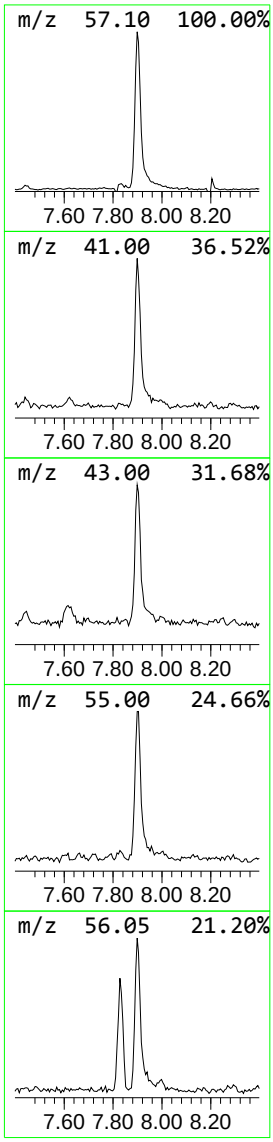
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	4.10 ng	306239	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	47
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45





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TIC Library : C:\Database\NIST20.L
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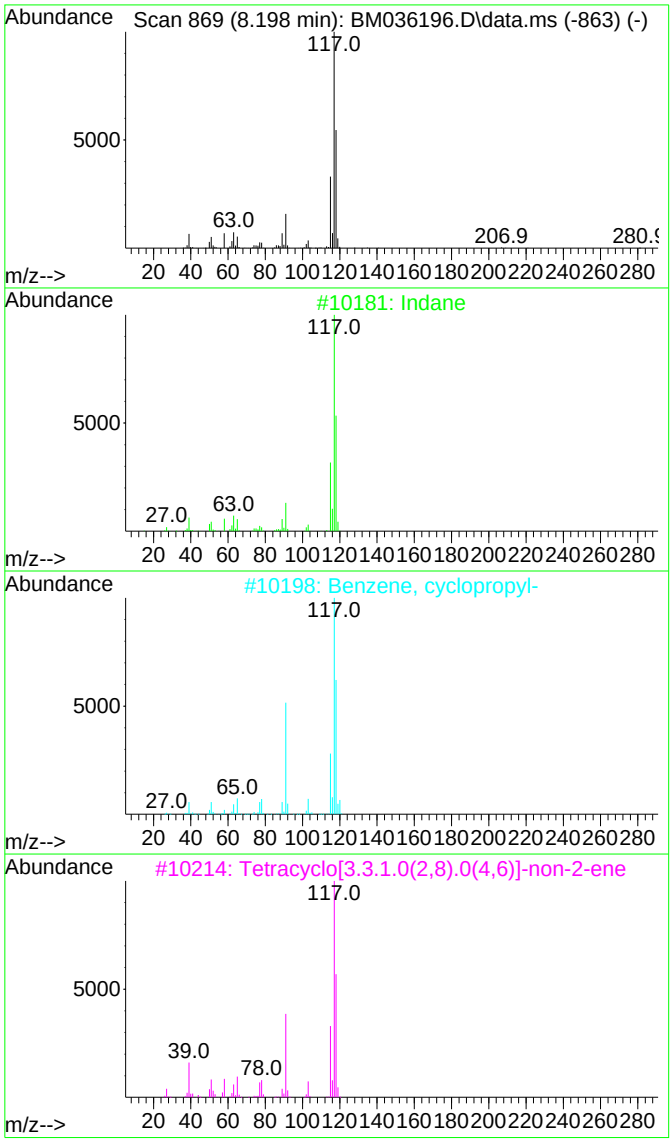
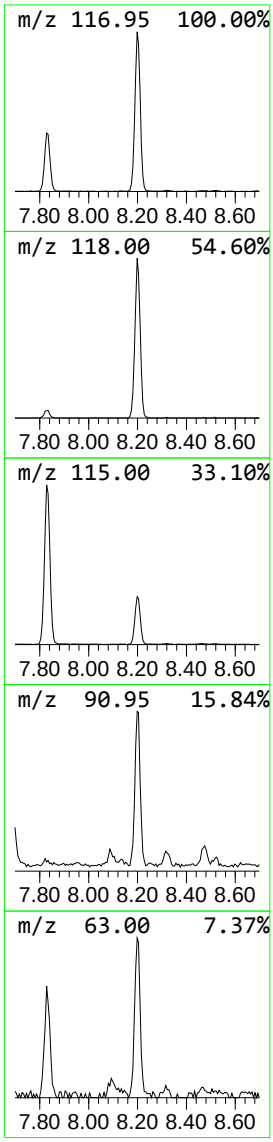
Peak Number 8 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.198	5.17 ng	386340	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4	Benzene, 1-(chloromethyl)-4-ethe...	152	C9H9Cl	001592-20-7	59
5	Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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TIC Library : C:\Database\NIST20.L
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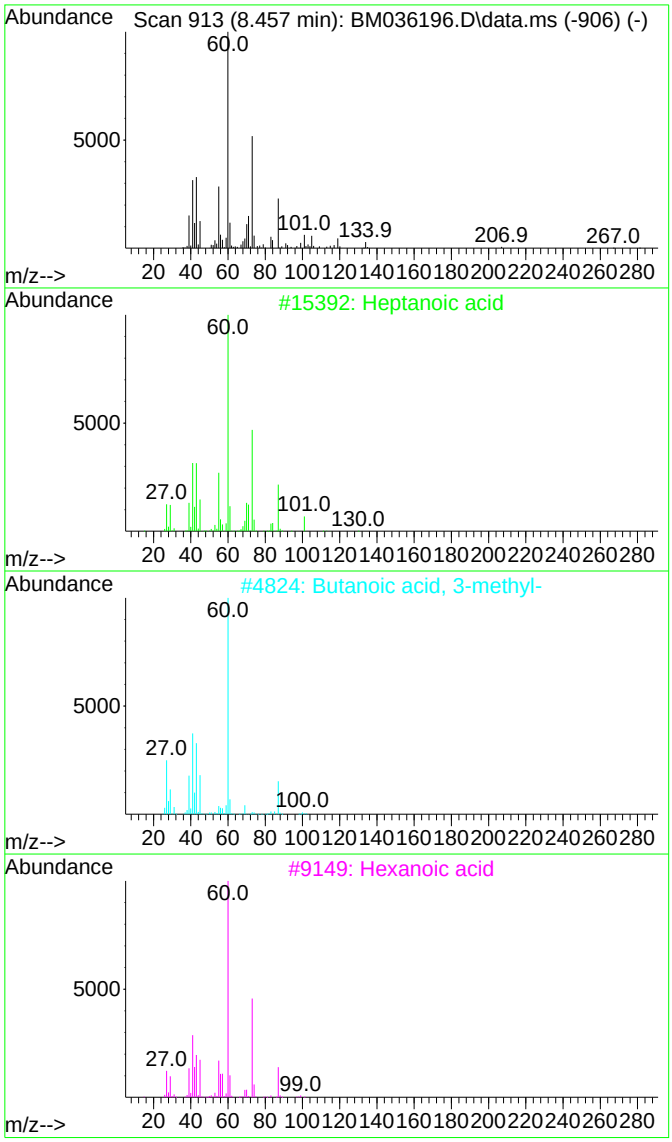
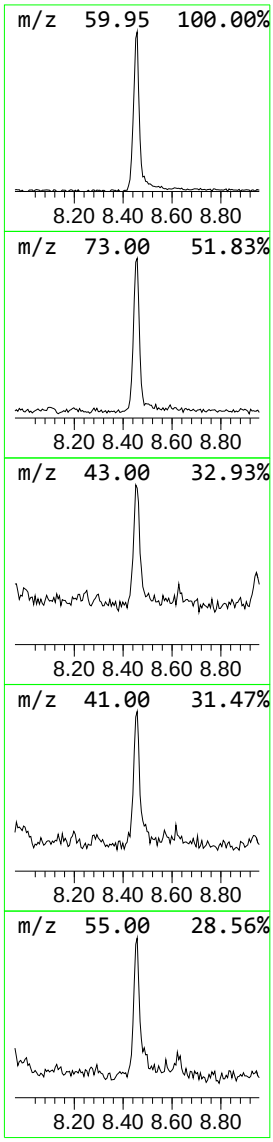
Peak Number 9 Heptanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.47 ng	184193	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	90
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036196.D
Acq On : 10 Aug 2022 17:31
Operator : CG/JU
Sample : N3972-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-9

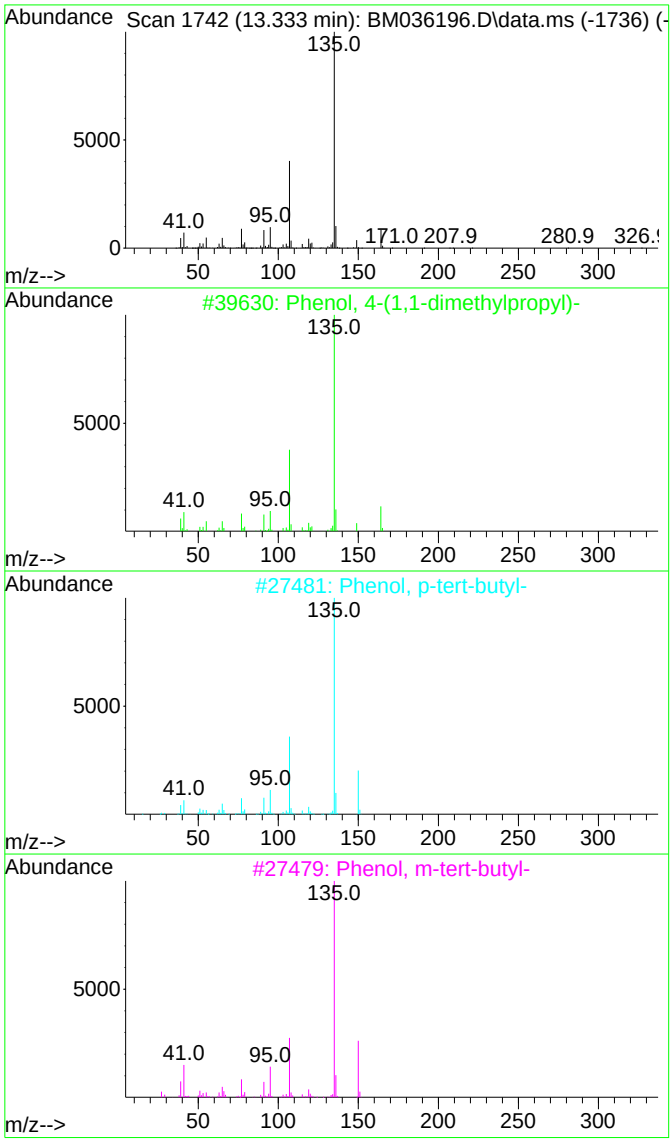
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

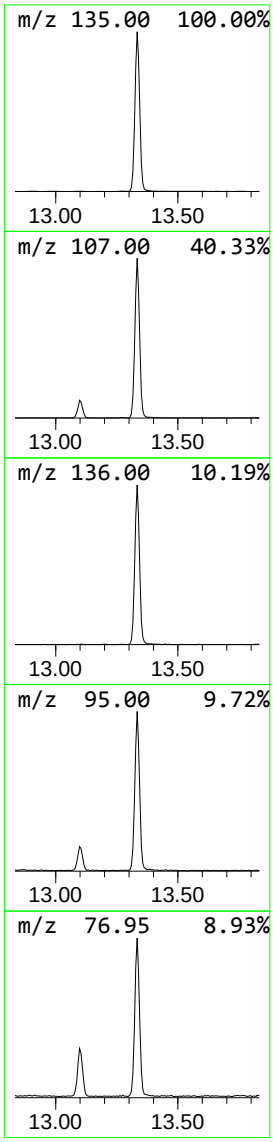
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	21.47 ng	2661960	Acenaphthene-d10	14.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
4	Hexestrol	270	C18H22O2	000084-16-2	72
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036196.D
Acq On : 10 Aug 2022 17:31
Operator : CG/JU
Sample : N3972-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Di-sec-Butyl ether	4.234	3.3	ng	244364	1	7.828	1493580	20.0
Cyclopentanone	4.281	28.6	ng	2133640	1	7.828	1493580	20.0
2-Propanol, 1-p...	4.922	8.2	ng	608880	1	7.828	1493580	20.0
Benzene, (1-met...	6.304	2.2	ng	162995	1	7.828	1493580	20.0
2-Propanol, 1-b...	6.475	8.1	ng	601291	1	7.828	1493580	20.0
Benzene, propyl-	6.798	3.0	ng	225275	1	7.828	1493580	20.0
1-Hexanol, 2-et...	7.898	4.1	ng	306239	1	7.828	1493580	20.0
Indane	8.198	5.2	ng	386340	1	7.828	1493580	20.0
Heptanoic acid	8.457	2.5	ng	184193	1	7.828	1493580	20.0
Phenol, 4-(1,1-...	13.333	21.5	ng	2661960	3	14.474	2479380	20.0