LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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: BM036195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.887	131	136	144	rBV2	73422	125558	1.07%	0.159%
2	3.981	147	152	164	rVB	658137	857235	7.34%	1.087%
3	4.281	194	203	215	rVB	936492	1300331	11.13%	1.649%
4	4.928	307	313	320	rBV2	515250	828057	7.09%	1.050%
5	5.322	374	380	384	rBV	223303	319499	2.74%	0.405%
6	5.416	390	396	400	rBV	2682924	3755990	32.16%	4.763%
7	5.451	400	402	413	rVB	424798	754139	6.46%	0.956%
8	5.828	459	466	472	rVB	391636	579330	4.96%	0.735%
9	6.475	567	576	587	rBV	453189	659032	5.64%	0.836%
10	7.034	664	671	684	rBV	1685319	2685857	23.00%	3.406%
11	7.475	741	746	752	rVB	94078	152091	1.30%	0.193%
12	7.834	797	807	813	rBV	1775117	2810746	24.06%	3.564%
13	7.898	813	818	823	rBV	233199	373054	3.19%	0.473%
14	8.086	845	850	861	rBV	68176	144911	1.24%	0.184%
15	8.663	944	948	956	rVB	81960	133031	1.14%	0.169%
16	9.004	999	1006	1014	rBV	2473626	3980737	34.08%	5.048%
17	9.163	1025	1033	1044	rVB3	107361	267309	2.29%	0.339%
18	9.569	1091	1102	1109	rVB	164476	297060	2.54%	0.377%
19	10.422	1241	1247	1255	rBV2	139142	269732	2.31%	0.342%
20	10.633	1276	1283	1289	rBV	2345957	3902275	33.41%	4.948%
21	10.686	1289	1292	1300	rVB	146946	248357	2.13%	0.315%
22	11.016	1341	1348	1356	rBV	105303	233802	2.00%	0.296%
23	11.392	1406	1412	1419	rBV	70256	143541	1.23%	0.182%
24	11.598	1440	1447	1458	rVB	505287	963375	8.25%	1.222%
25	12.839	1653	1658	1666	rBV	133654	239501	2.05%	0.304%
26	13.104	1694	1703	1715	rBV	5890122	8940419	76.54%	11.336%
27	13.333	1736	1742	1753	rBV	2024881	2831122	24.24%	3.590%
28	14.474	1928	1936	1944	rBV	3321214	4772067	40.86%	6.051%
29	15.298	2072	2076	2082	rVB	100718	143064	1.22%	0.181%
30	15.833	2163	2167	2171	rBV	119500	164005	1.40%	0.208%
31	15.962	2183	2189	2199	rBV	4141496	5933402	50.80%	7.523%
32	16.562	2287	2291	2298	rVB2	90589	143459	1.23%	0.182%
33	17.215	2396	2402	2411	rBV	3717394	5152792	44.12%	6.534%
34	17.339	2417	2423	2431	rVB4	105939	174535	1.49%	0.221%
35	17.498	2445	2450	2459	rVB3	97508	154177	1.32%	0.195%
36	17.627	2462	2472	2478	rBV	140141	238974	2.05%	0.303%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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

37	17.886	2512	2516	2523	rVB2	121819	156522	1.34%	0.198%
38	18.115	2551	2555	2563	rBV4	89548	155867	1.33%	0.198%
39	19.844	2843	2849	2854	rBV	9706366	11680010	100.00%	14.810%
40	21.397	3108	3113	3119	rBV	4684388	5722273	48.99%	7.256%
41	22.485	3295	3298	3304	rVB	295484	374342	3.20%	0.475%
42	23.750	3506	3513	3525	rVB2	3076015	6103741	52.26%	7.739%

Sum of corrected areas: 78865321

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
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Acq On : 10 Aug 2022 16:54
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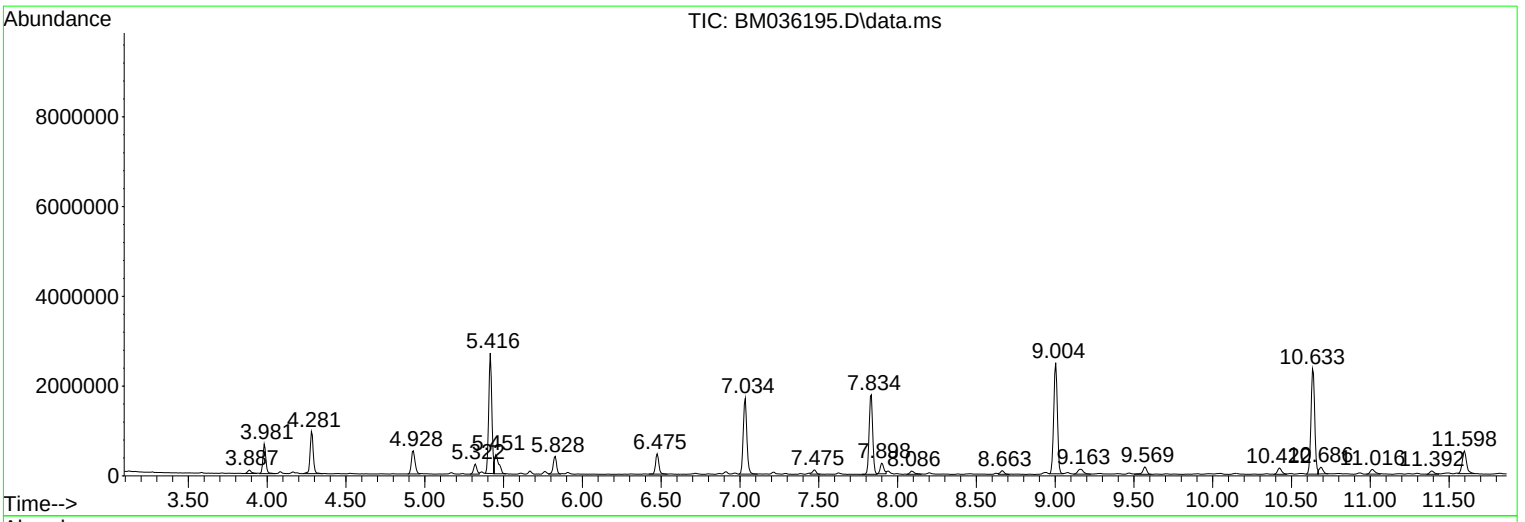
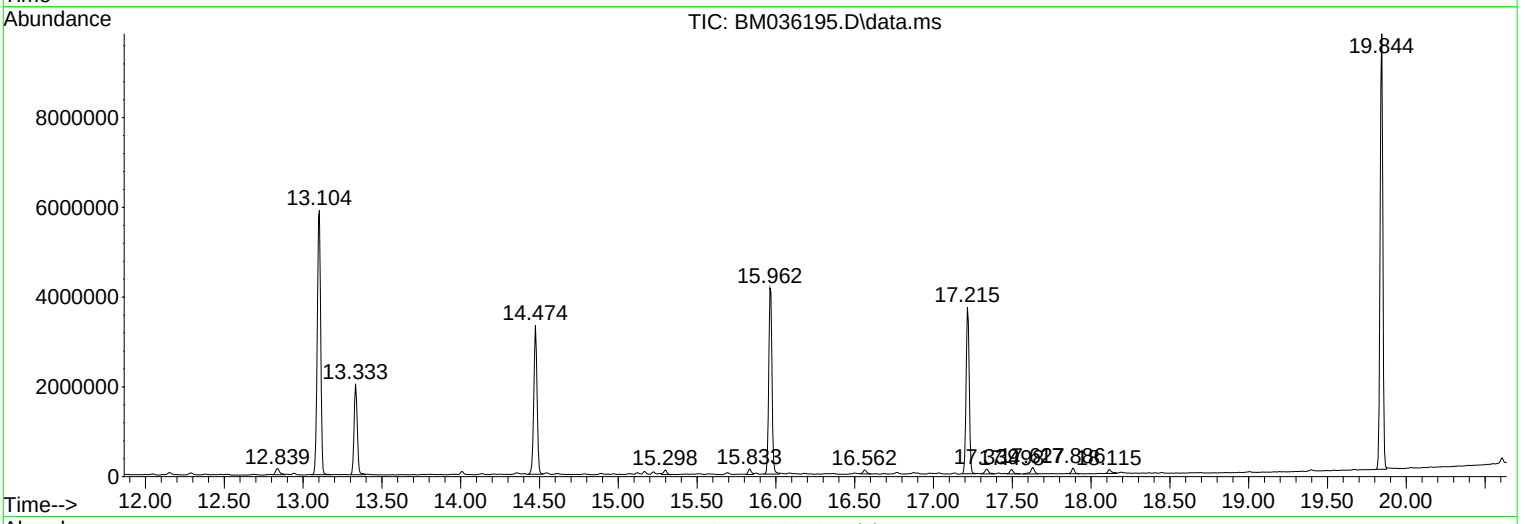
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

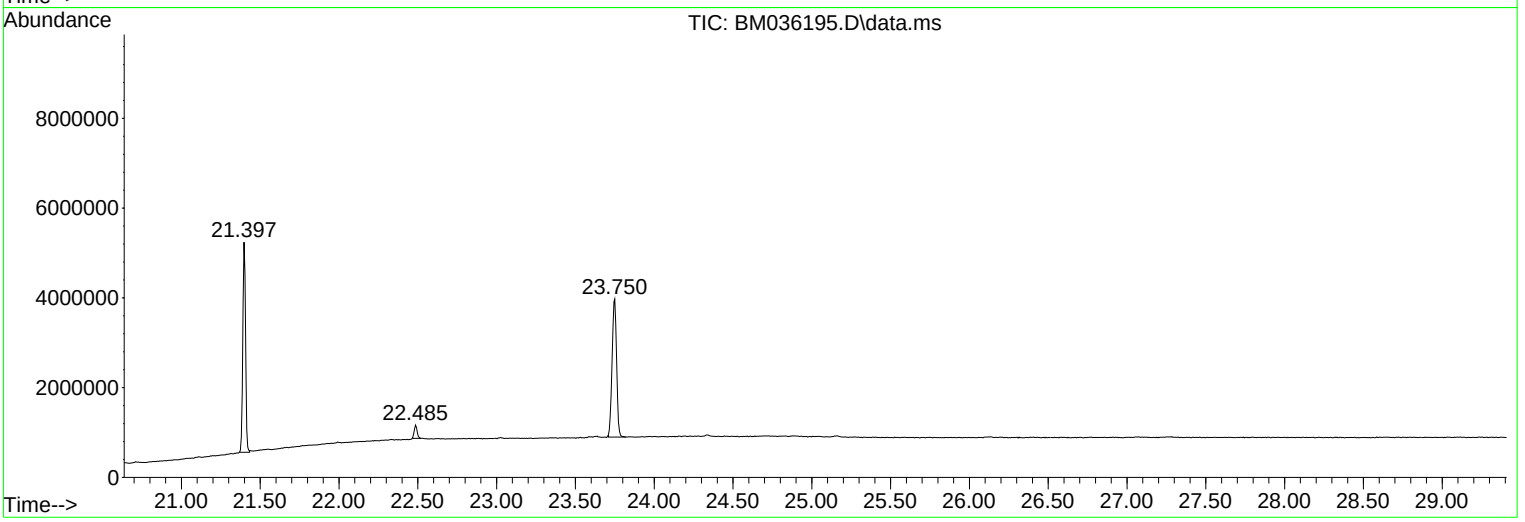
Instrument :
BNA_M
ClientSampleId :
COP-1R

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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

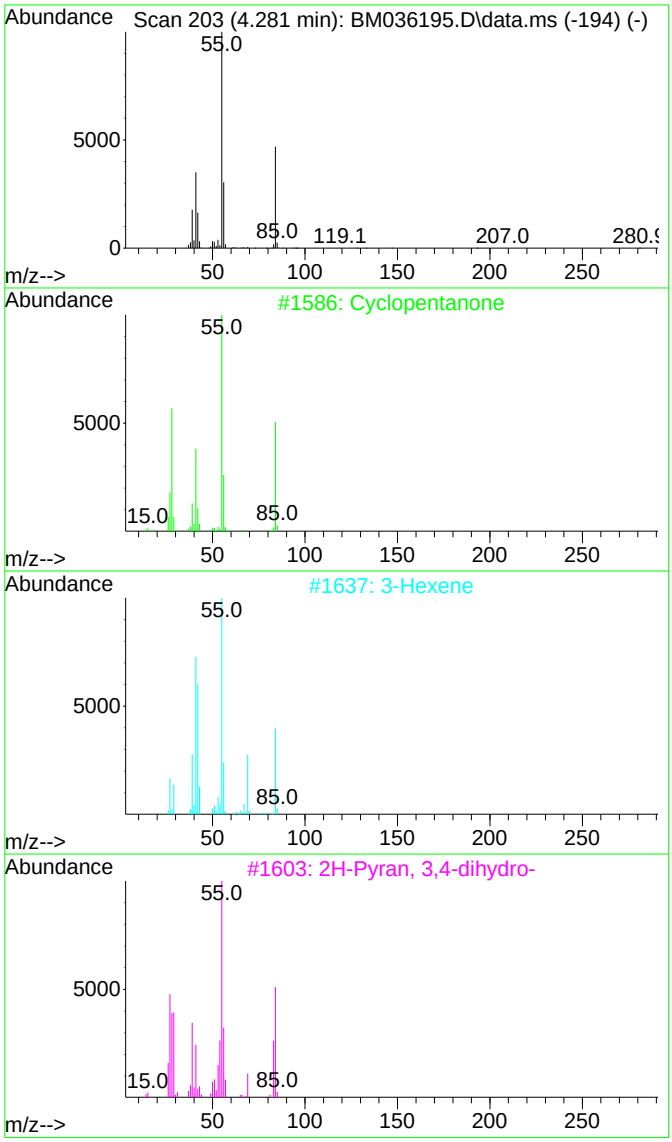
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

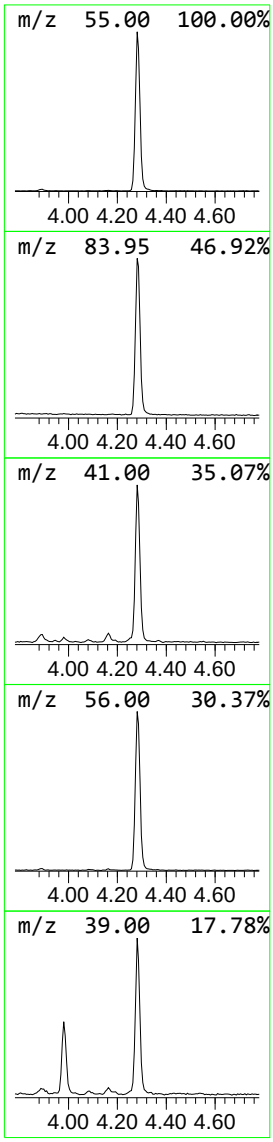
****

Peak Number 2 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	9.25 ng	1300330	1,4-Dichlorobenzene-d4	7.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	3-Hexene	84	C6H12	000592-47-2	45
3	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	42
5	2(3H)-Furanone	84	C4H4O2	020825-71-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

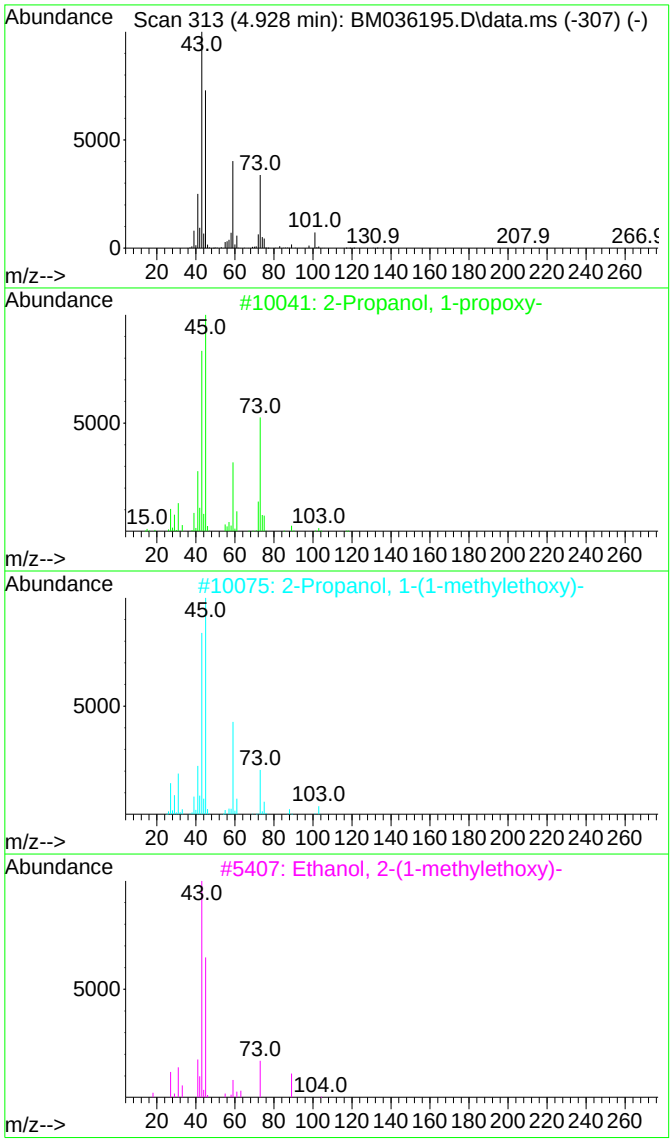
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

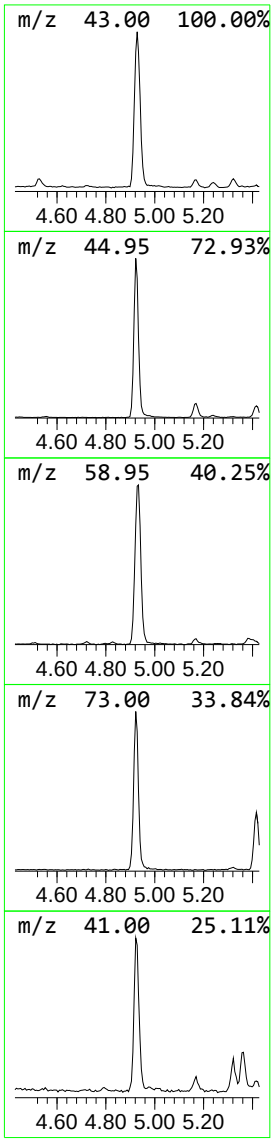
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-propoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	5.89 ng	828057	1,4-Dichlorobenzene-d4	7.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	59
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	53
3	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	53
4	Diethyl carbitol	162	C8H18O3	000112-36-7	40
5	Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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

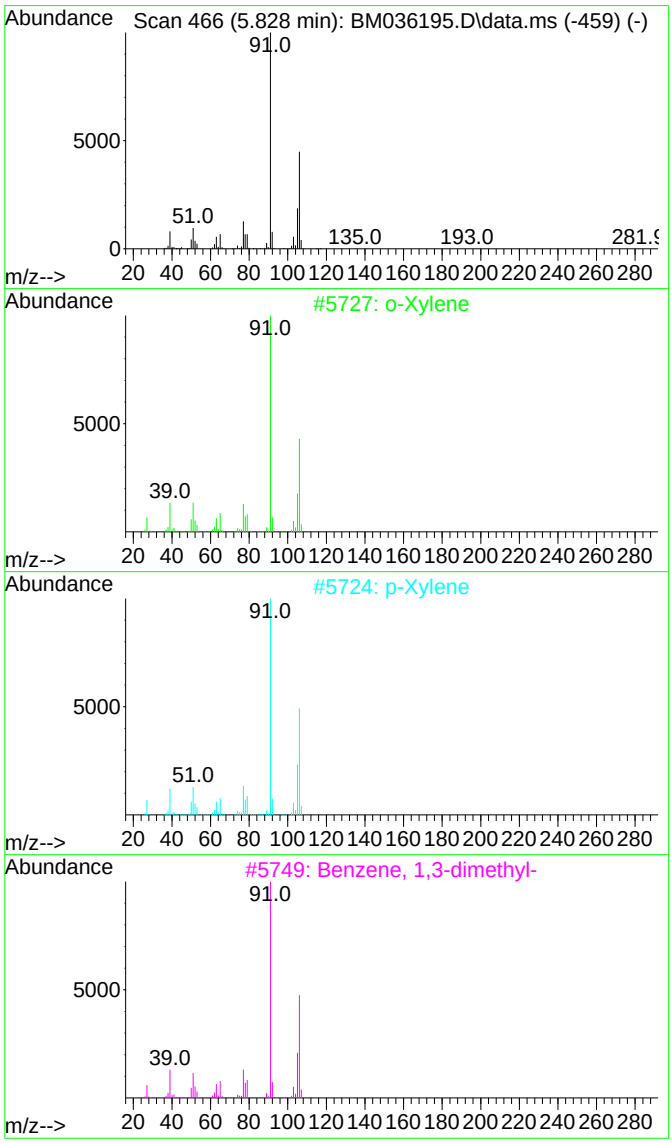
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

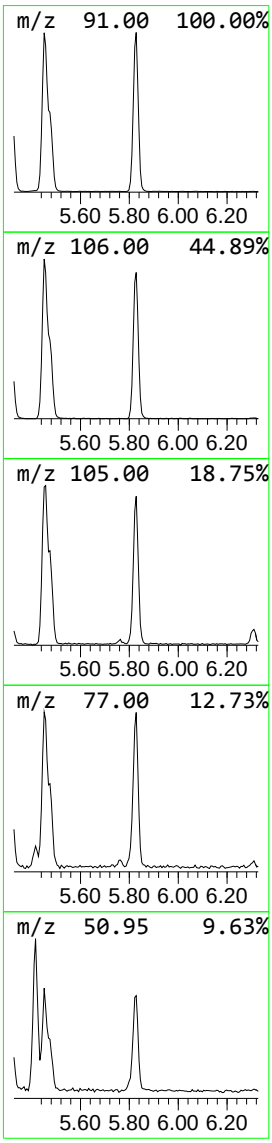
****

Peak Number 5 o-Xylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	4.12 ng	579330	1,4-Dichlorobenzene-d4	7.833

Hit# of 4	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Xylene	106	C8H10	000095-47-6	97
2	p-Xylene	106	C8H10	000106-42-3	97
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
4	Ethylbenzene	106	C8H10	000100-41-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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

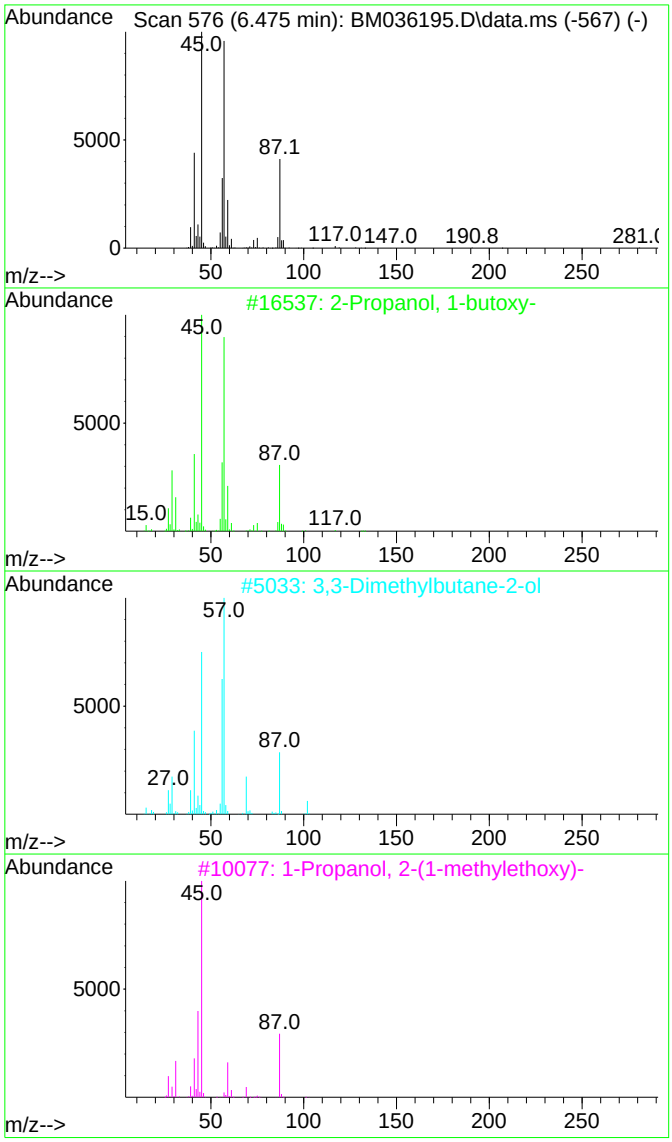
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

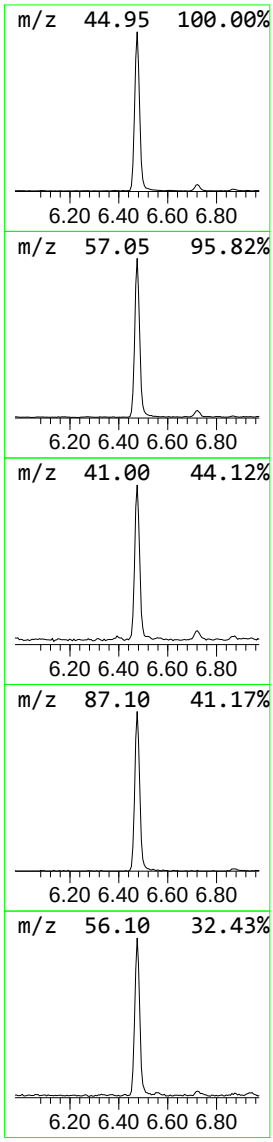
****

Peak Number 6 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	4.69 ng	659032	1,4-Dichlorobenzene-d4	7.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
4	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	50
5	Diisopropyl ether	102	C6H14O	000108-20-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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

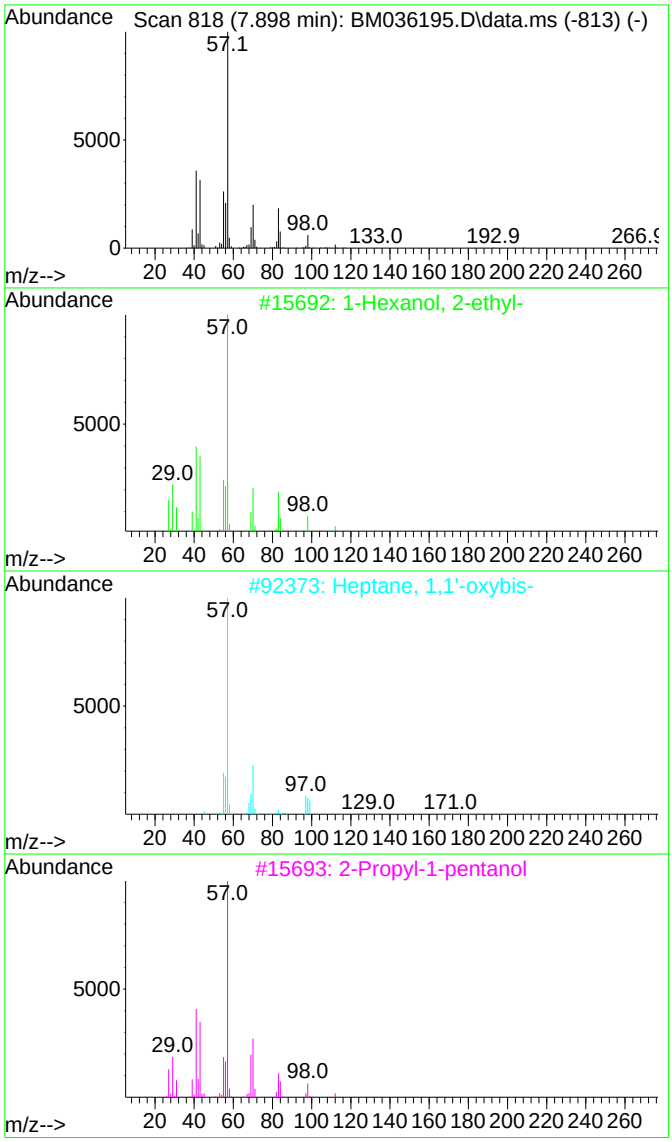
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

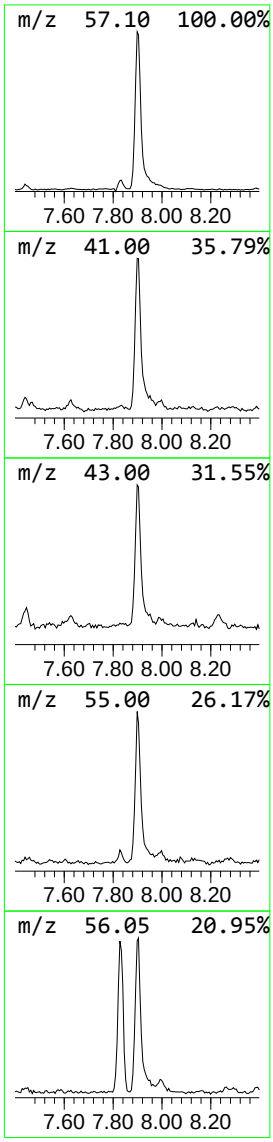
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	2.65 ng	373054	1,4-Dichlorobenzene-d4	7.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50
5	Decyl heptyl ether	256	C17H36O	1000406-39-1	50





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Data File : BM036195.D
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Operator : CG/JU
Sample : N3971-24
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

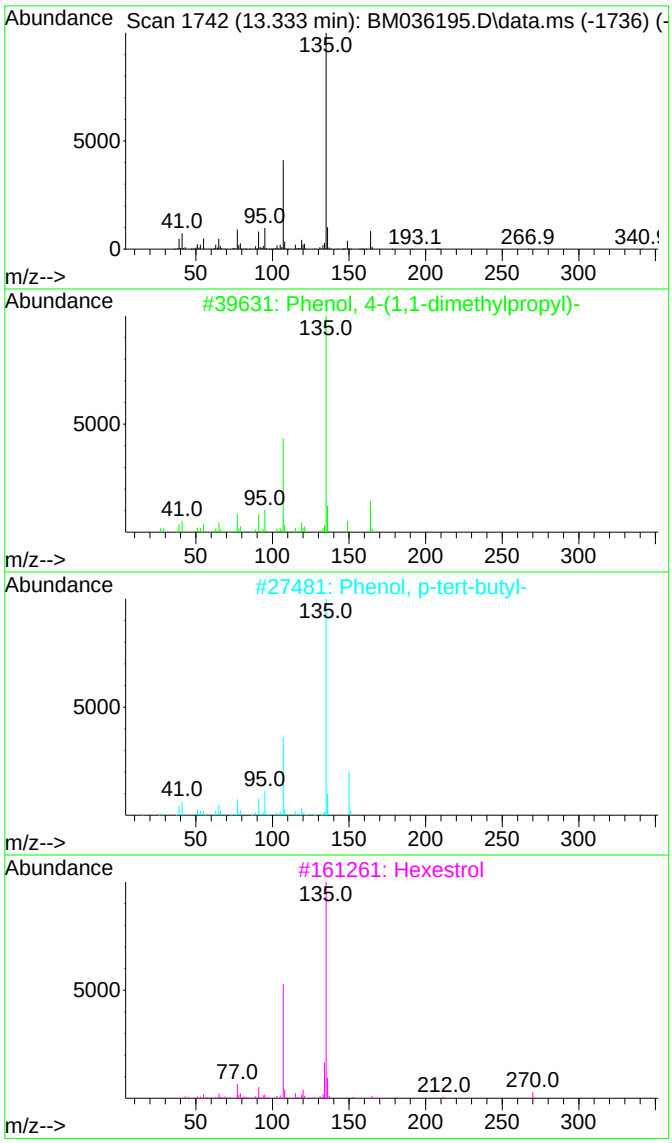
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

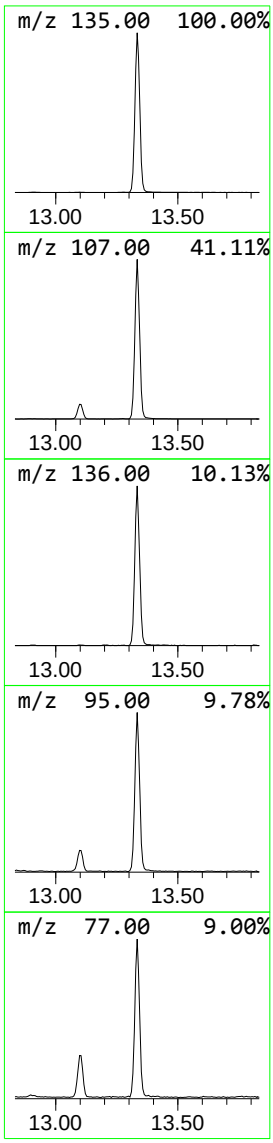
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	11.87 ng	2831120	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	Hexestrol	270	C18H22O2	000084-16-2	72
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	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 : BM036195.D
Acq On : 10 Aug 2022 16:54
Operator : CG/JU
Sample : N3971-24
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-1R

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
Cyclopentanone	4.281	9.3	ng	1300330	1	7.833	2810750	20.0
2-Propanol, 1-p...	4.928	5.9	ng	828057	1	7.833	2810750	20.0
o-Xylene	5.828	4.1	ng	579330	1	7.833	2810750	20.0
2-Propanol, 1-b...	6.475	4.7	ng	659032	1	7.833	2810750	20.0
1-Hexanol, 2-et...	7.898	2.6	ng	373054	1	7.833	2810750	20.0
Phenol, 4-(1,1-...	13.333	11.9	ng	2831120	3	14.474	4772070	20.0