LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036194.D
Acq On : 10 Aug 2022 16:16
Operator : CG/JU
Sample : N3972-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-2R

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: BM036194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.981	147	152	160	rVB	311989	399286	3.17%	0.660%
2	4.281	194	203	217	rBV	808928	1098489	8.72%	1.816%
3	4.928	307	313	322	rBV3	257527	427609	3.39%	0.707%
4	5.322	374	380	384	rBV	102322	155320	1.23%	0.257%
5	5.416	390	396	400	rBV	2839731	3993352	31.68%	6.602%
6	5.452	400	402	412	rVB	235686	424391	3.37%	0.702%
7	5.828	459	466	471	rBV	210971	311839	2.47%	0.516%
8	6.475	571	576	584	rBV	200816	289139	2.29%	0.478%
9	7.034	664	671	685	rBV	1828296	2871081	22.78%	4.747%
10	7.834	799	807	813	rBV	923903	1450777	11.51%	2.398%
11	7.899	813	818	823	rBV	224851	363983	2.89%	0.602%
12	9.004	998	1006	1013	rBV	2586609	4097265	32.51%	6.774%
13	9.569	1097	1102	1109	rVB	86844	143050	1.13%	0.236%
14	10.634	1276	1283	1289	rBV	1204143	2012899	15.97%	3.328%
15	10.687	1289	1292	1299	rVB	86283	144674	1.15%	0.239%
16	11.598	1441	1447	1459	rVB	142726	298177	2.37%	0.493%
17	13.104	1695	1703	1710	rBV	5999953	8789339	69.73%	14.531%
18	13.333	1736	1742	1750	rBV	1107365	1572935	12.48%	2.600%
19	14.475	1928	1936	1944	rBV	1717763	2508854	19.90%	4.148%
20	15.969	2178	2190	2206	rBV	4559718	6732147	53.41%	11.130%
21	17.216	2396	2402	2409	rBV	1988622	2760998	21.91%	4.565%
22	18.116	2550	2555	2565	rBV	157995	284871	2.26%	0.471%
23	19.392	2769	2772	2784	rBV4	61250	130565	1.04%	0.216%
24	19.845	2843	2849	2854	rBV	10346875	12604211	100.00%	20.838%
25	21.398	3108	3113	3119	rBV	2577981	3238783	25.70%	5.354%
26	23.745	3506	3512	3523	rVB2	1711809	3383117	26.84%	5.593%

Sum of corrected areas: 60487151

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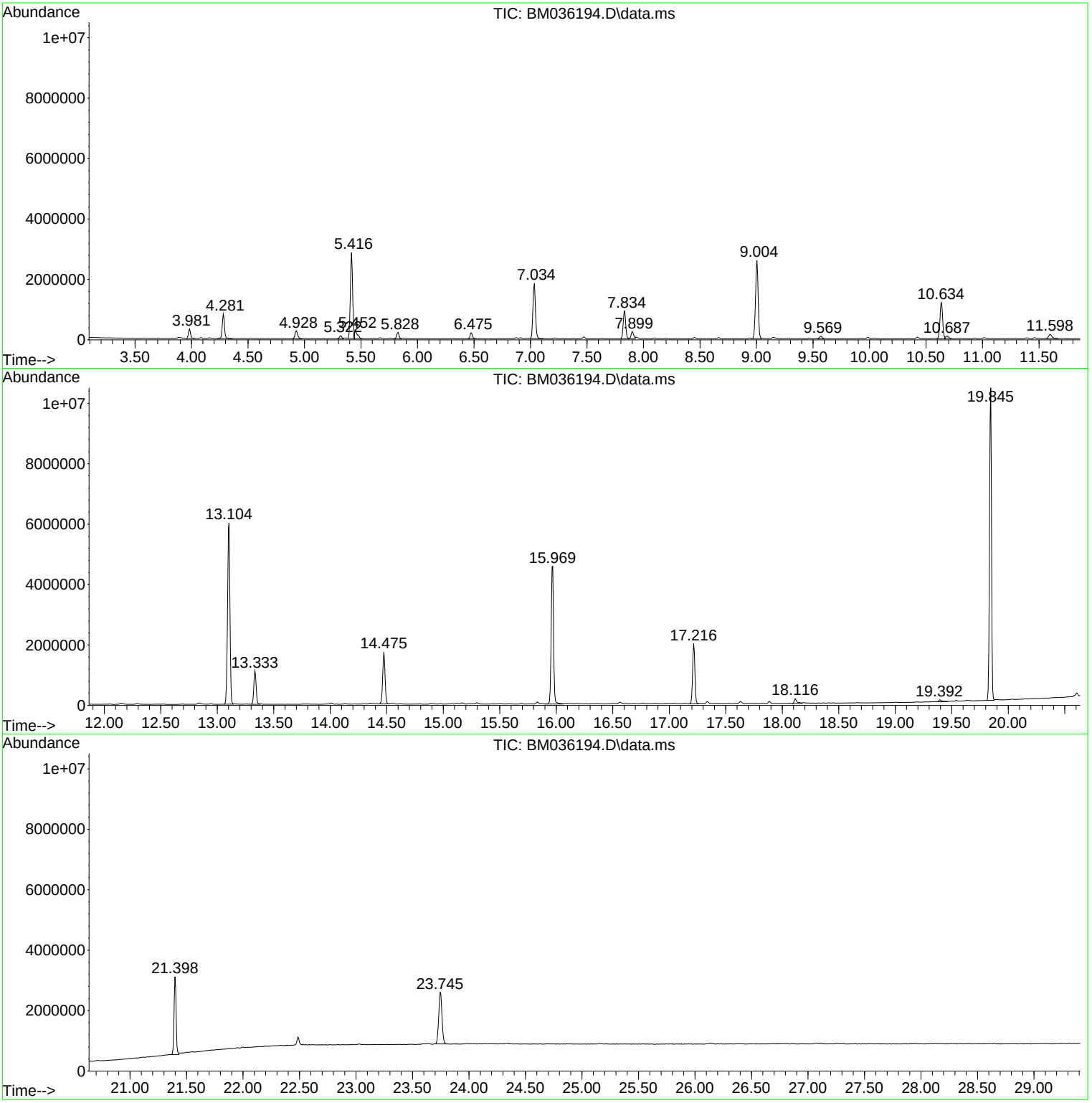
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM036194.D
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Operator : CG/JU
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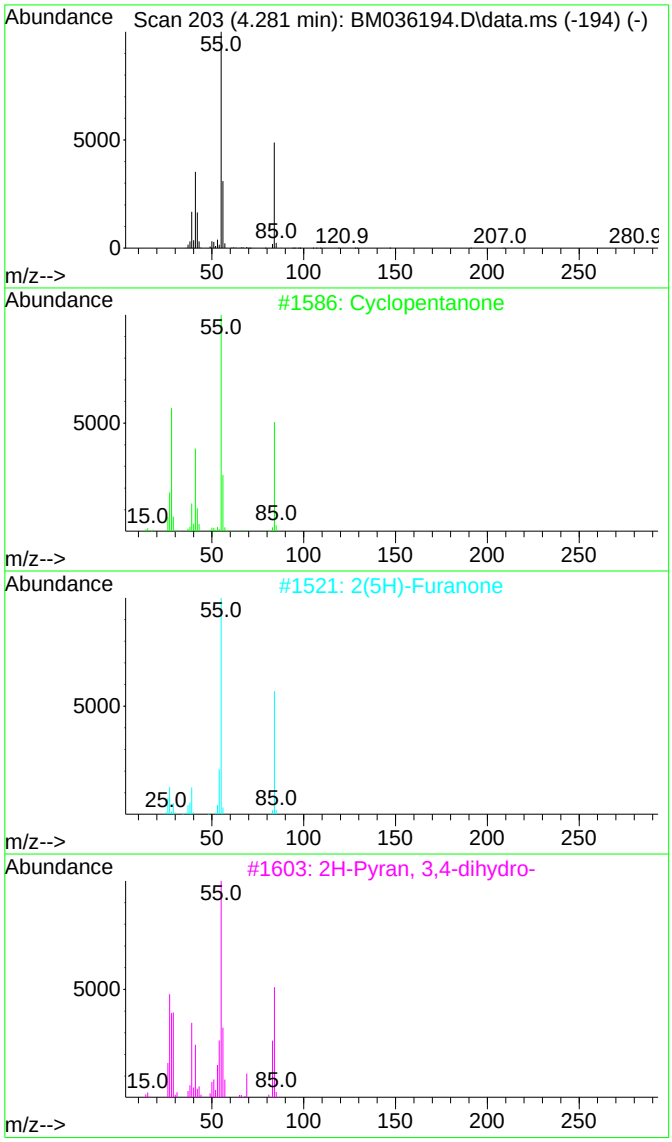
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

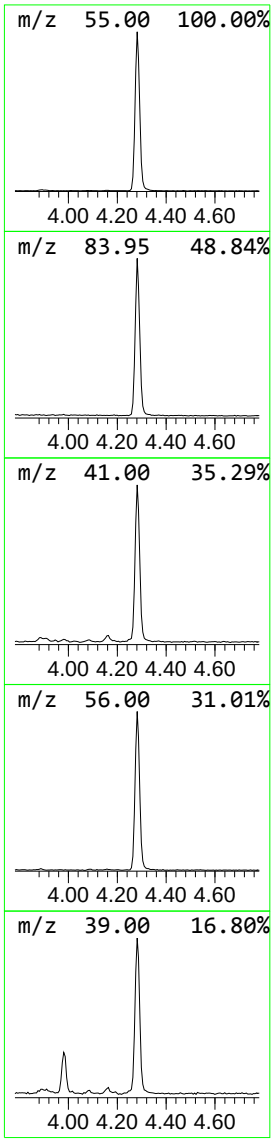
****

Peak Number 2 Cyclopentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	15.14 ng	1098490	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2(5H)-Furanone	84	C4H4O2	000497-23-4	52
3	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
4	3-Hexene	84	C6H12	000592-47-2	45
5	Aminoacetonitrile	56	C2H4N2	000540-61-4	9





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Operator : CG/JU
Sample : N3972-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-2R

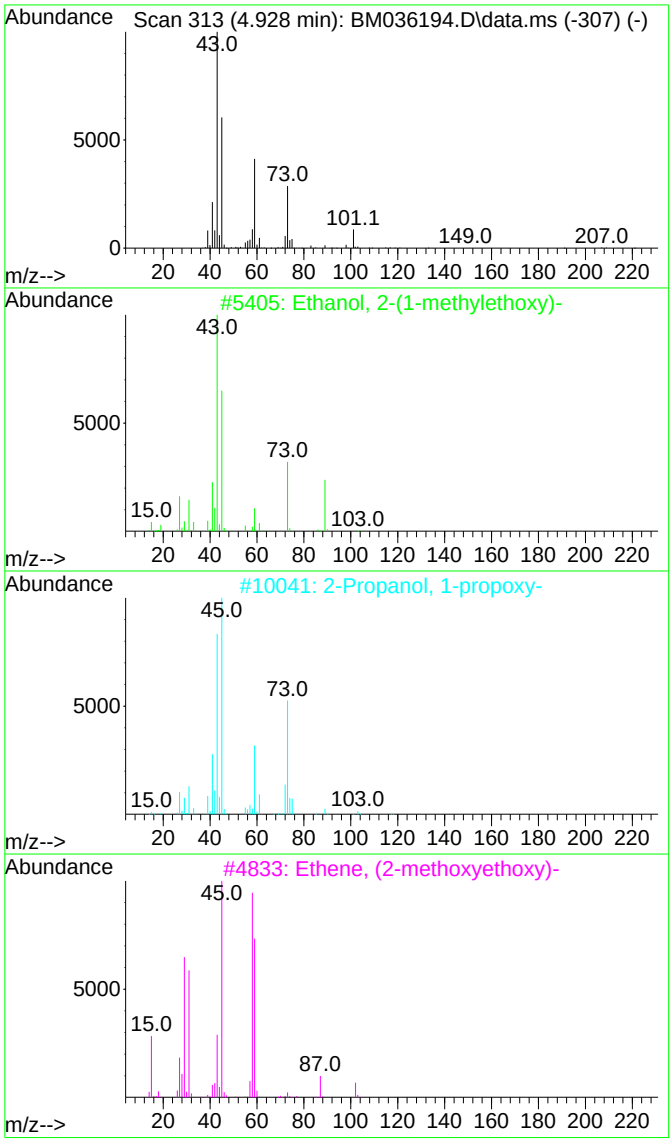
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

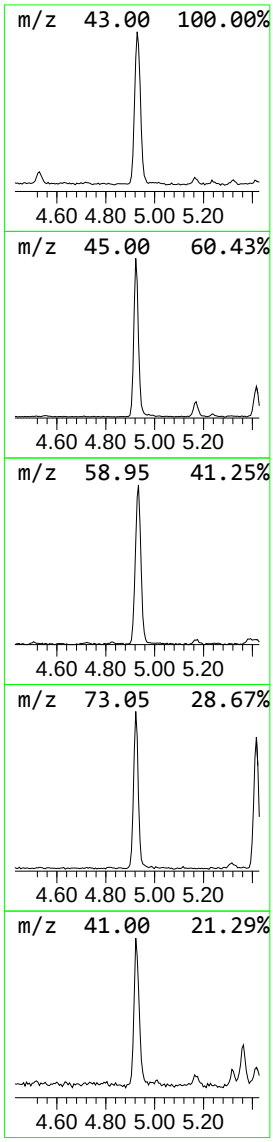
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(1-methylethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	5.89 ng	427609	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	53
2	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	43
3	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	38
4	Diacetamide	101	C4H7NO2	000625-77-4	38
5	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036194.D
Acq On : 10 Aug 2022 16:16
Operator : CG/JU
Sample : N3972-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COP-2R

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

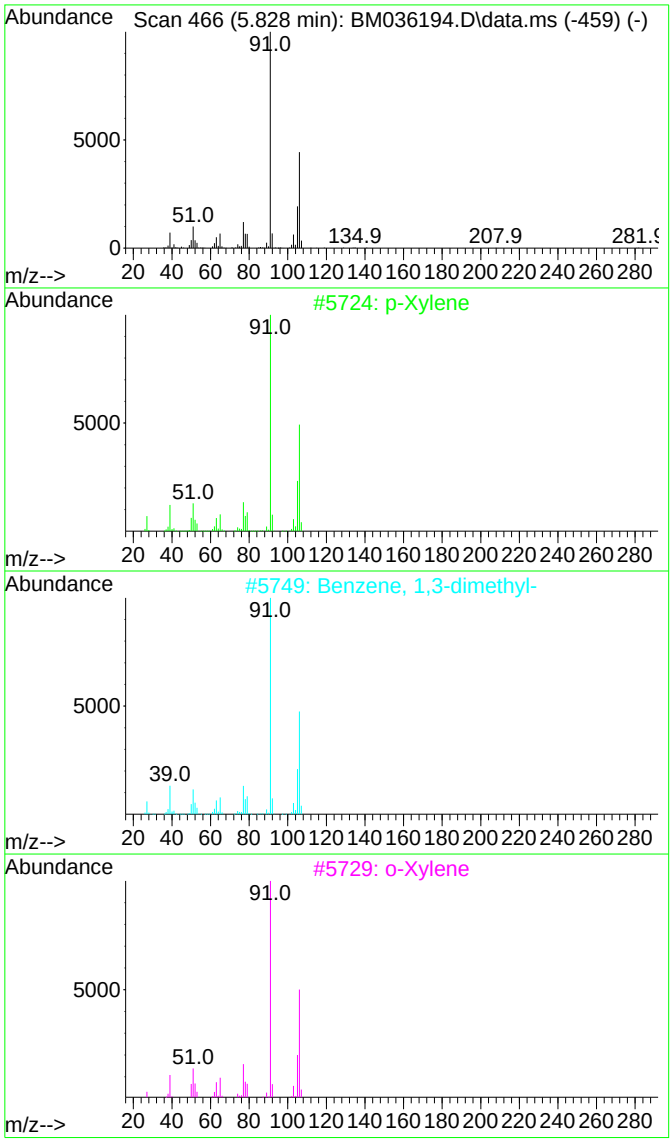
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

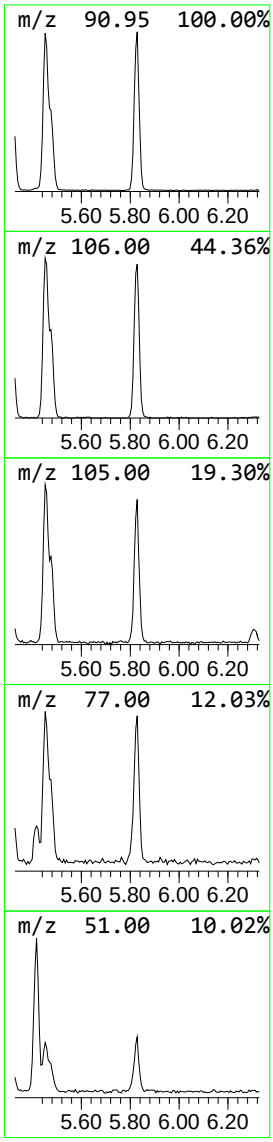
****

Peak Number 5 p-Xylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	4.30 ng	311839	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	97
2	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
3	o-Xylene	106	C8H10	000095-47-6	97
4	Ethylbenzene	106	C8H10	000100-41-4	87
5	Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	86





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Sample : N3972-07
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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

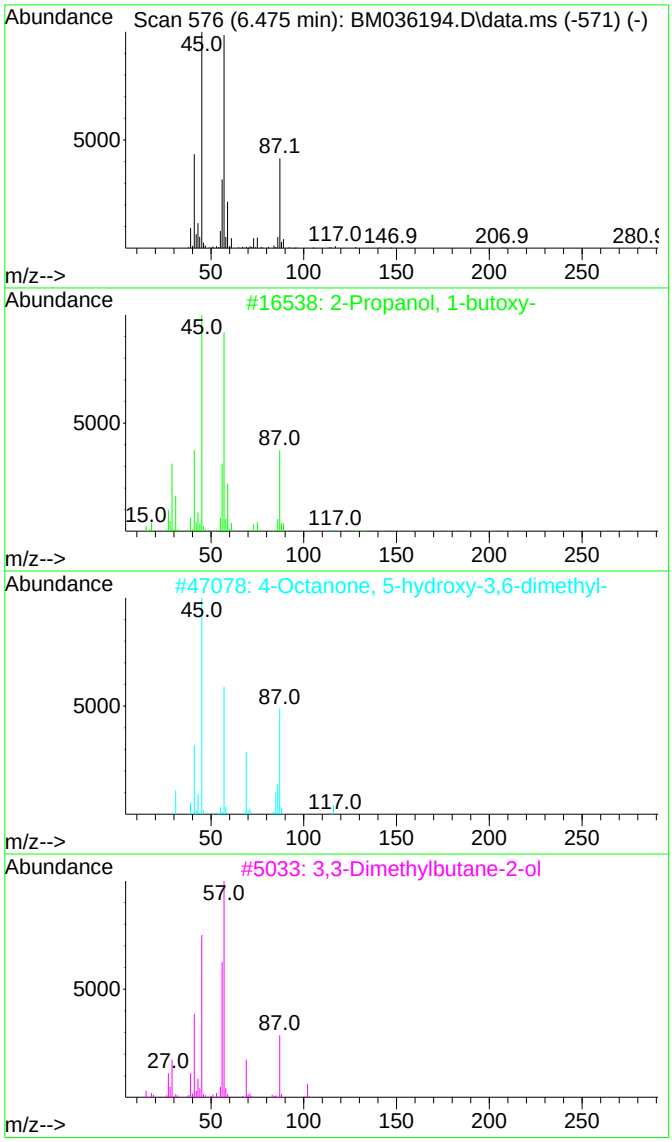
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

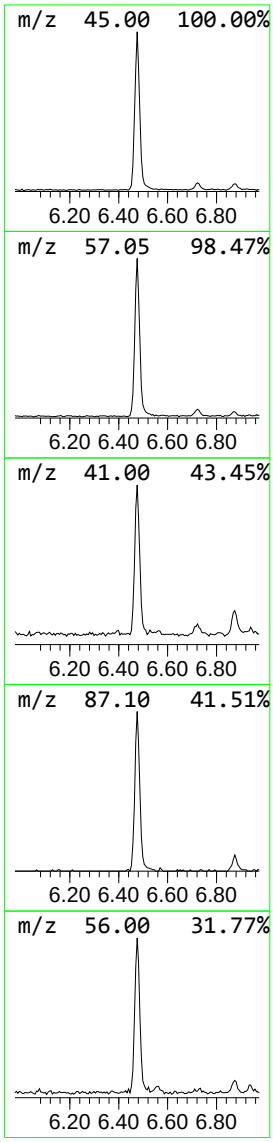
****

Peak Number 6 2-Propanol, 1-butoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	3.99 ng	289139	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	4-Octanone, 5-hydroxy-3,6-dimethyl-	172	C10H20O2	062759-47-1	53
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
5	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	50





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

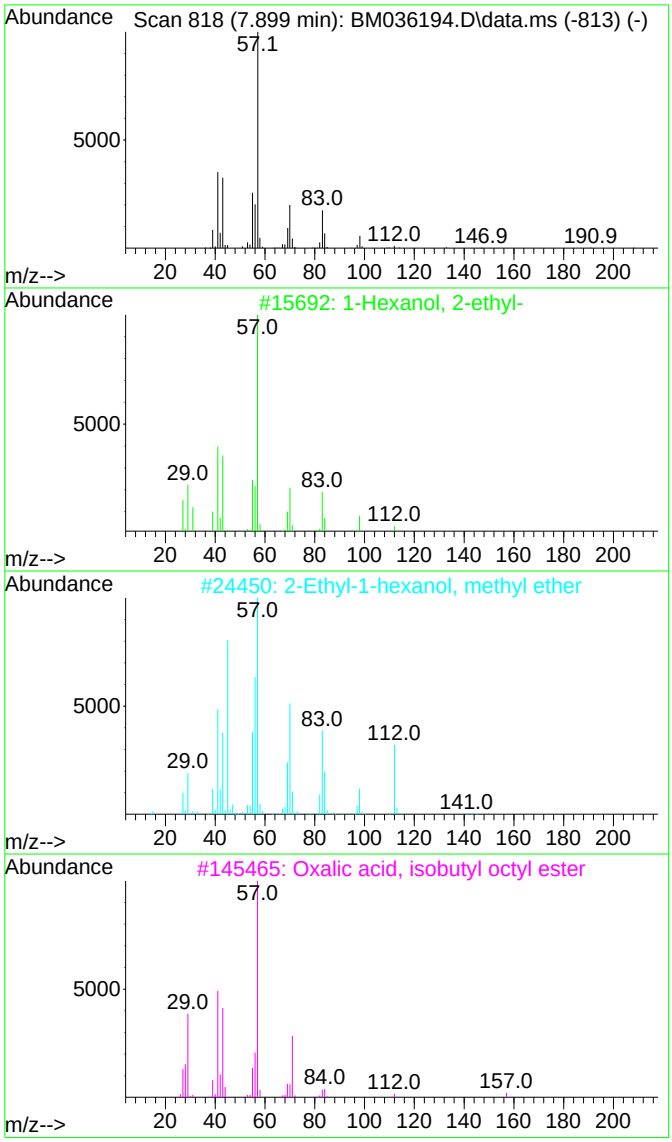
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

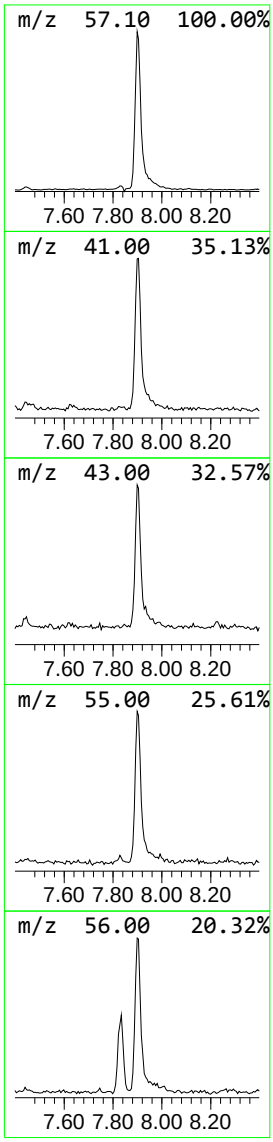
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.899	5.02 ng	363983	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
3	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47





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ClientSampleId :
COP-2R

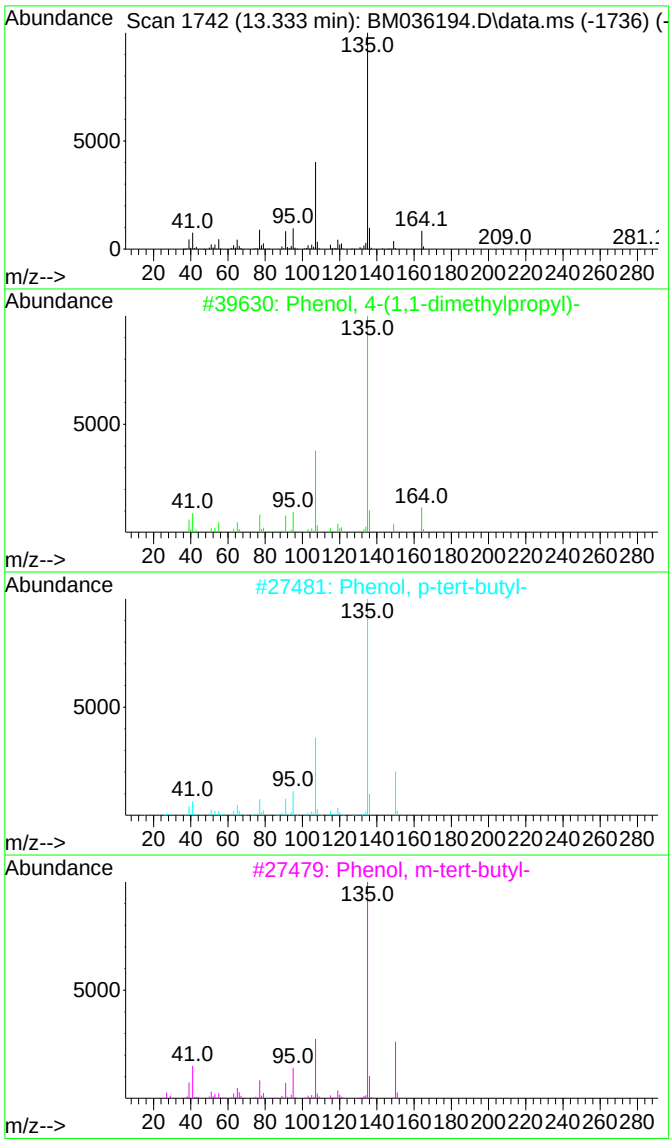
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

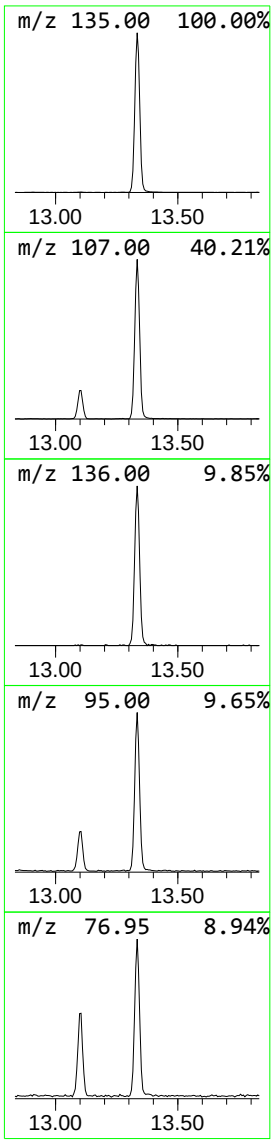
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.334	12.54 ng	1572940	Acenaphthene-d10	14.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





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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

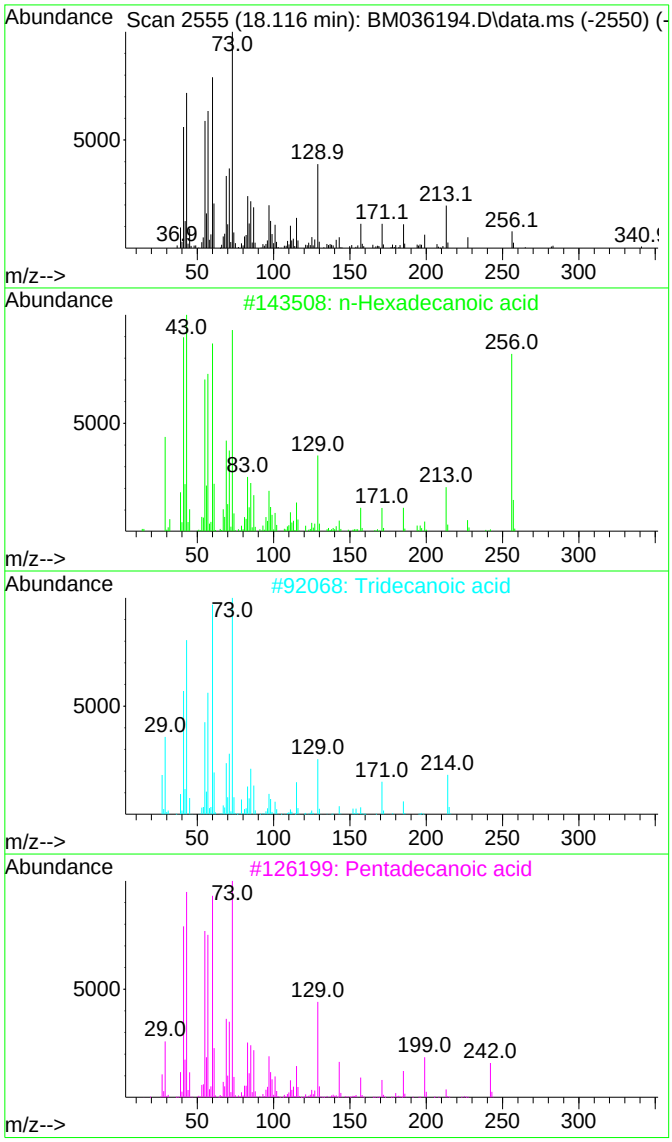
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

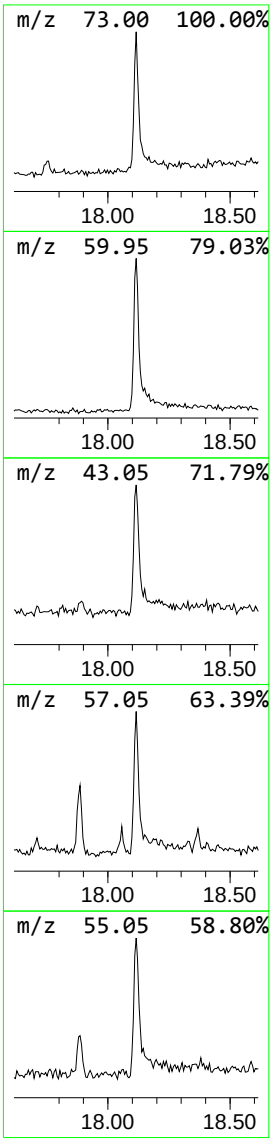
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	2.06 ng	284871	Phenanthrene-d10	17.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Tentatively Identified Compound (LSC) summary

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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	15.1	ng	1098490	1	7.834	1450780	20.0
Ethanol, 2-(1-m...	4.928	5.9	ng	427609	1	7.834	1450780	20.0
p-Xylene	5.828	4.3	ng	311839	1	7.834	1450780	20.0
2-Propanol, 1-b...	6.475	4.0	ng	289139	1	7.834	1450780	20.0
1-Hexanol, 2-et...	7.899	5.0	ng	363983	1	7.834	1450780	20.0
Phenol, 4-(1,1-...	13.334	12.5	ng	1572940	3	14.475	2508850	20.0
n-Hexadecanoic ...	18.116	2.1	ng	284871	4	17.216	2761000	20.0