LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
Data File : BM036216.D
Acq On : 11 Aug 2022 19:22
Operator : CG/JU
Sample : N3971-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-26R

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: BM036216.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.275	197	202	213	rVB	710720	1027448	5.67%	1.466%
2	4.916	305	311	319	rBV2	231264	377435	2.08%	0.539%
3	5.404	388	394	407	rVB	2260734	3315542	18.29%	4.731%
4	6.469	567	575	585	rBV	259903	395183	2.18%	0.564%
5	7.022	662	669	682	rBV	1365100	2225996	12.28%	3.176%
6	7.822	798	805	812	rBV	740544	1190854	6.57%	1.699%
7	7.892	812	817	832	rVV	259515	438095	2.42%	0.625%
8	8.998	998	1005	1014	rBV	2665040	4322874	23.85%	6.168%
9	9.981	1166	1172	1181	rVB	110254	190877	1.05%	0.272%
10	10.628	1275	1282	1290	rBV	1046808	1732139	9.56%	2.471%
11	11.457	1417	1423	1434	rBV2	119129	205977	1.14%	0.294%
12	11.598	1441	1447	1463	rVB	161970	379881	2.10%	0.542%
13	13.098	1694	1702	1716	rBV	7037637	10408317	57.42%	14.851%
14	13.327	1734	1741	1755	rVB	2077733	2986350	16.47%	4.261%
15	14.469	1927	1935	1943	rBV	1723498	2435870	13.44%	3.476%
16	15.963	2182	2189	2205	rBV	6100165	8944475	49.34%	12.762%
17	17.210	2395	2401	2409	rBV	2220898	3021563	16.67%	4.311%
18	17.880	2510	2515	2521	rVB	217288	271551	1.50%	0.387%
19	19.839	2842	2848	2853	rBV	15105020	18127684	100.00%	25.865%
20	20.603	2974	2978	2981	rBV	298414	353741	1.95%	0.505%
21	21.392	3107	3112	3119	rBV	3119205	3820949	21.08%	5.452%
22	23.739	3504	3511	3521	rVB2	1978897	3911960	21.58%	5.582%

Sum of corrected areas: 70084761

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
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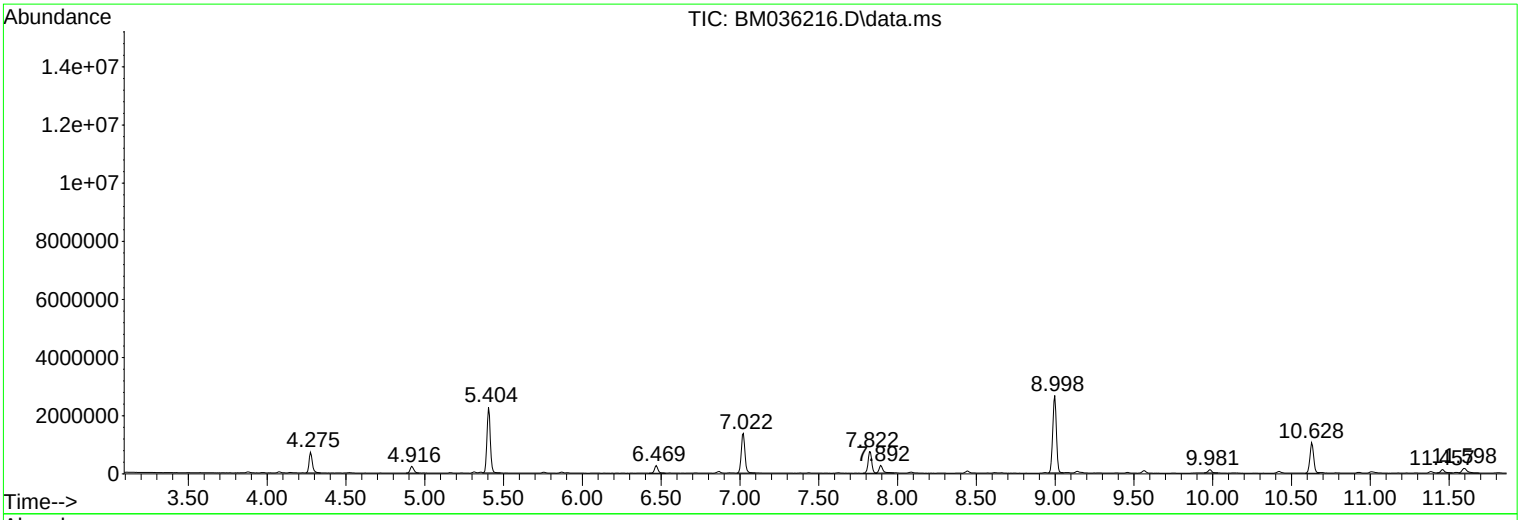
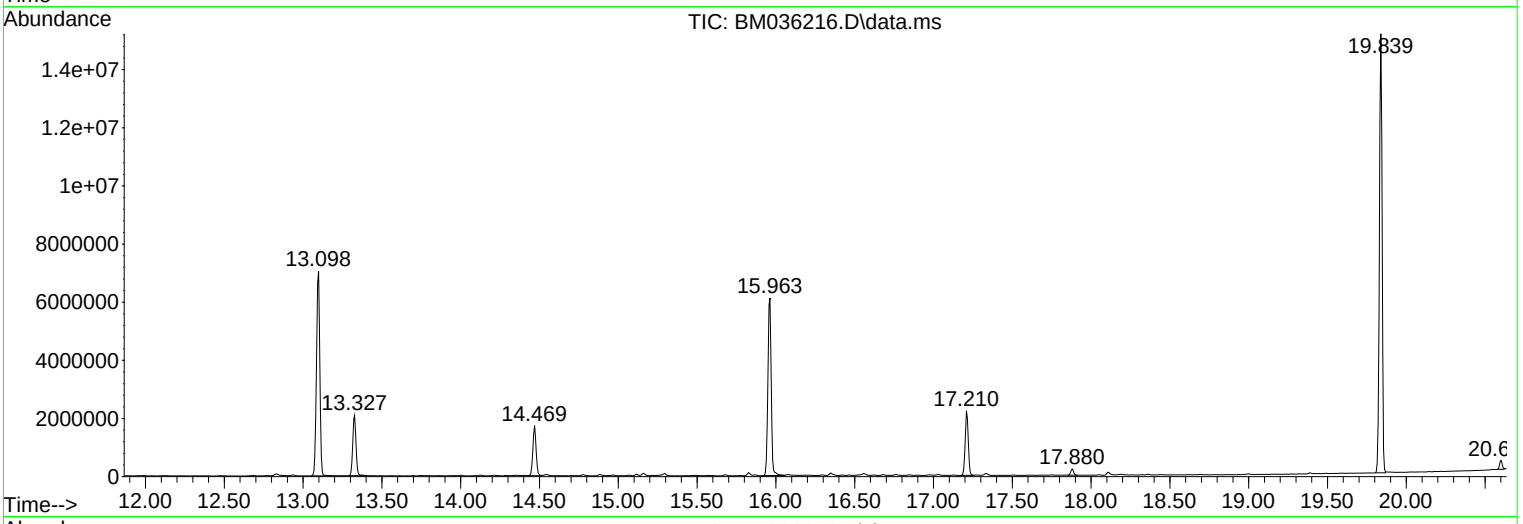
Misc :
ALS Vial : 12 Sample Multiplier: 1

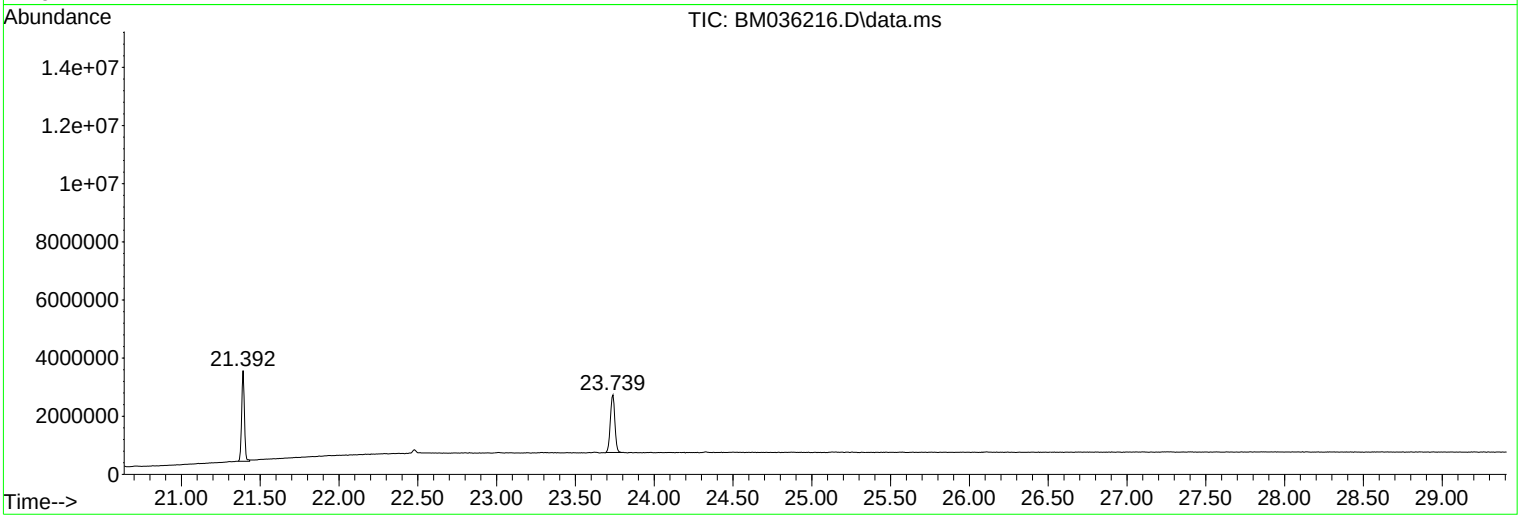
Instrument :
BNA_M
ClientSampleId :
MW-26R

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 : BM036216.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

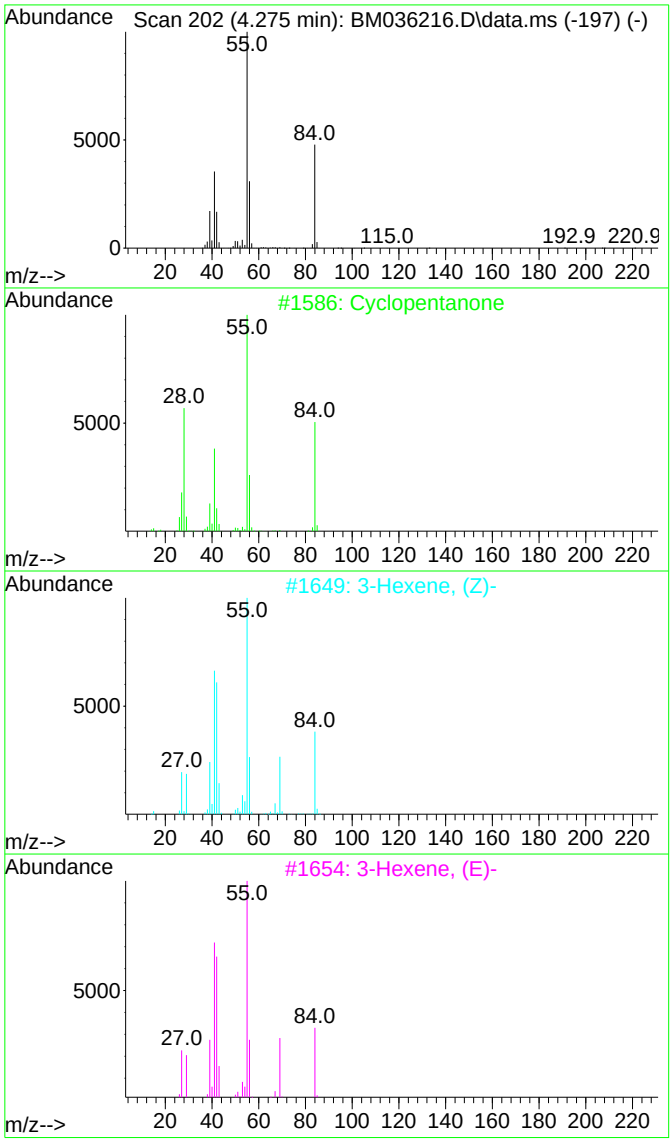
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

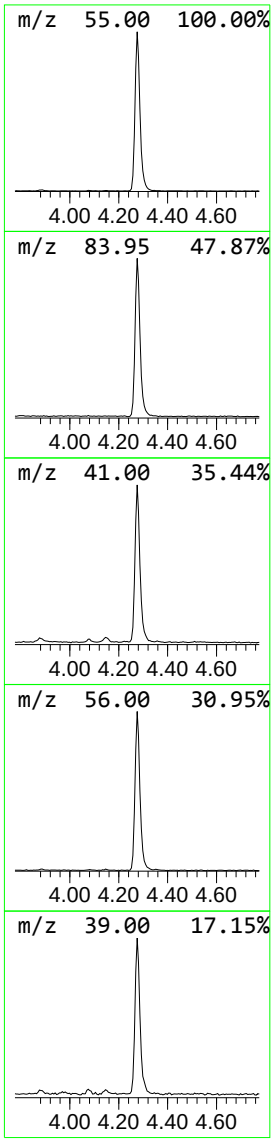
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.275	17.26 ng	1027450	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	3-Hexene, (Z)-	84	C6H12	007642-09-3	59
3	3-Hexene, (E)-	84	C6H12	013269-52-8	45
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
5	2(5H)-Furanone	84	C4H4O2	000497-23-4	40





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Instrument :
BNA_M
ClientSampleId :
MW-26R

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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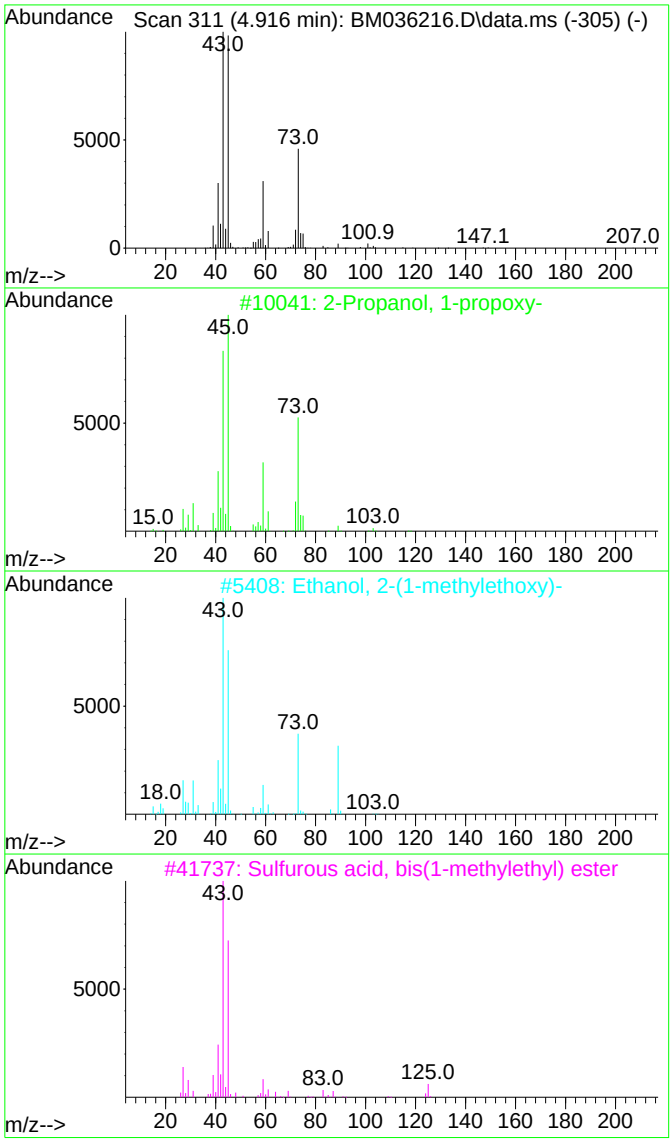
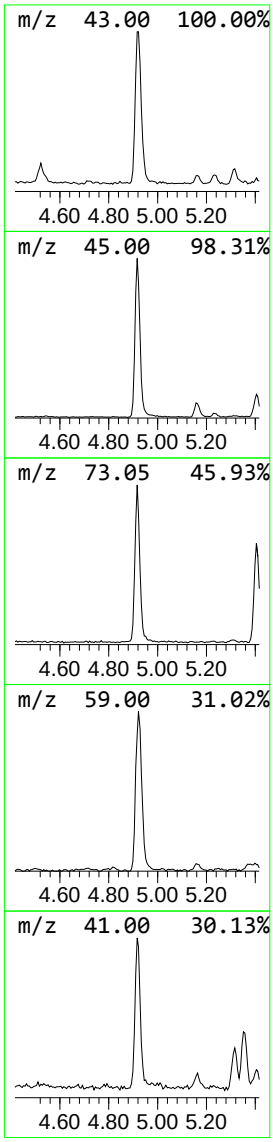
Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	6.34 ng	377435	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	Sulfurous acid, bis(1-methylethy...	166	C6H14O3S	004773-13-1	50
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
5	Monomethyl oxalate	104	C3H4O4	000600-23-7	50





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Acq On : 11 Aug 2022 19:22
Operator : CG/JU
Sample : N3971-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-26R

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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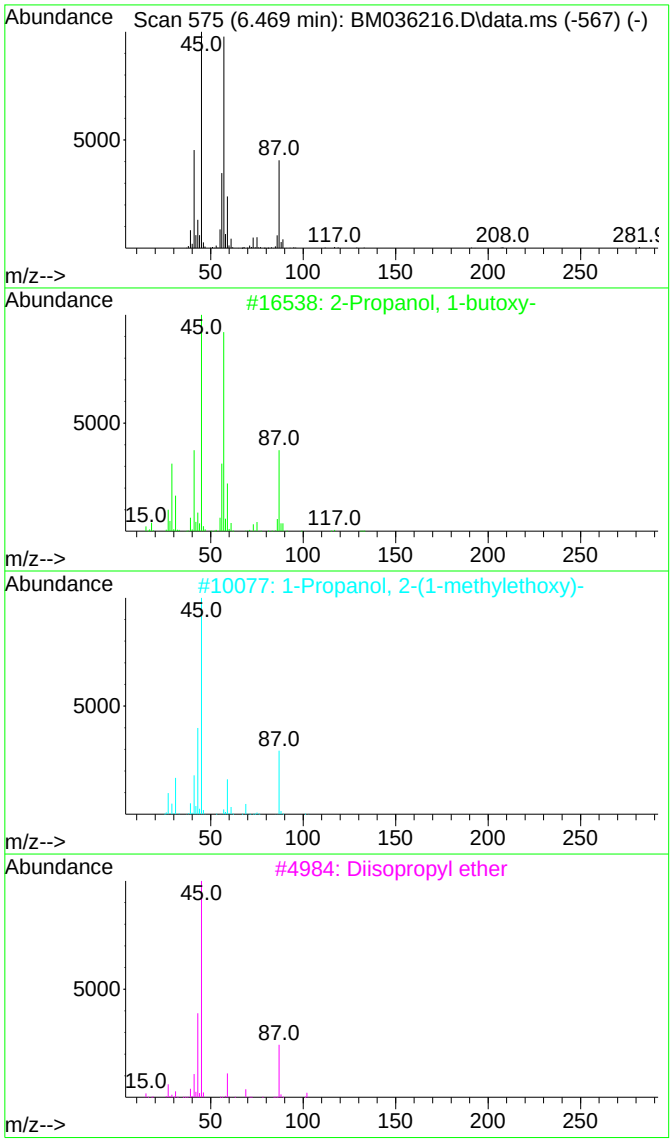
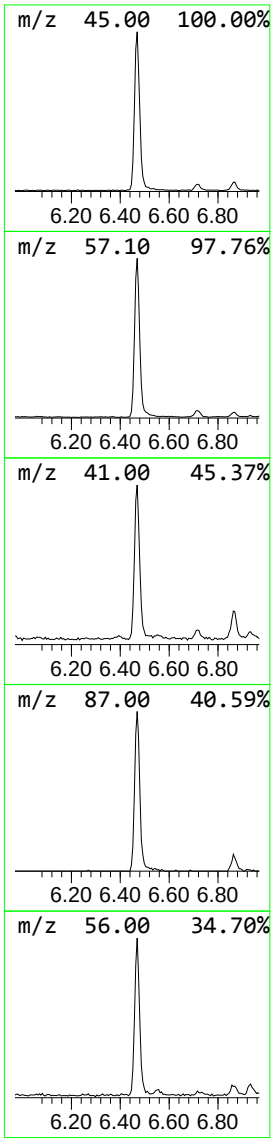
Peak Number 3 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.469	6.64 ng	395183	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	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3	Diisopropyl ether	102	C6H14O	000108-20-3	42
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
5	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	40





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Sample : N3971-18
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ALS Vial : 12 Sample Multiplier: 1

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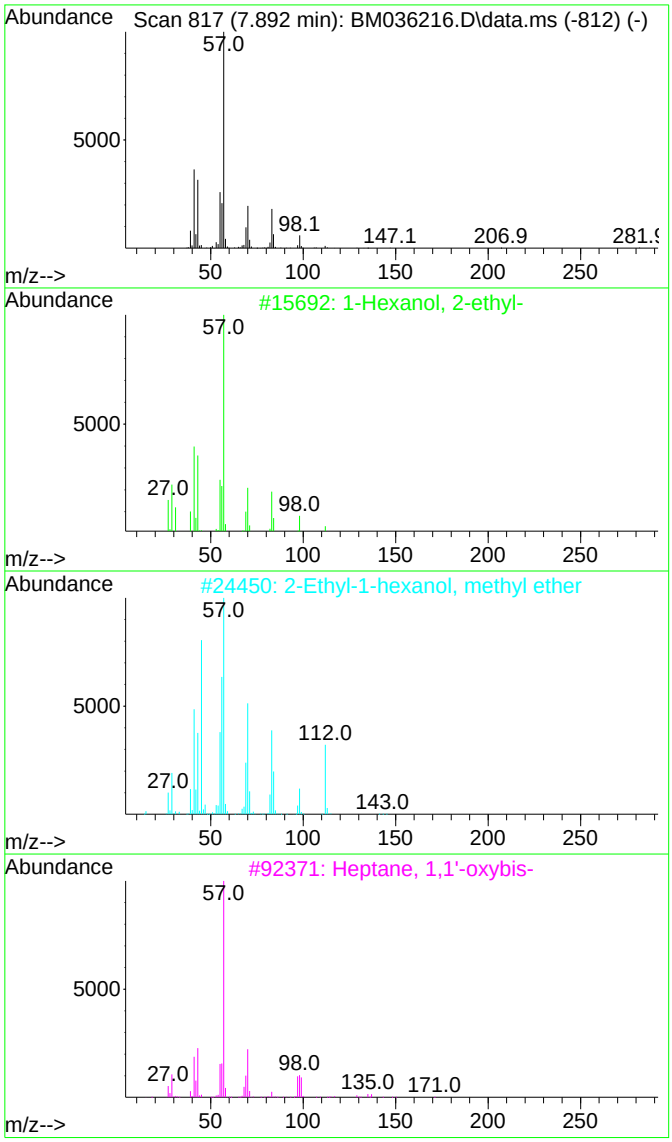
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

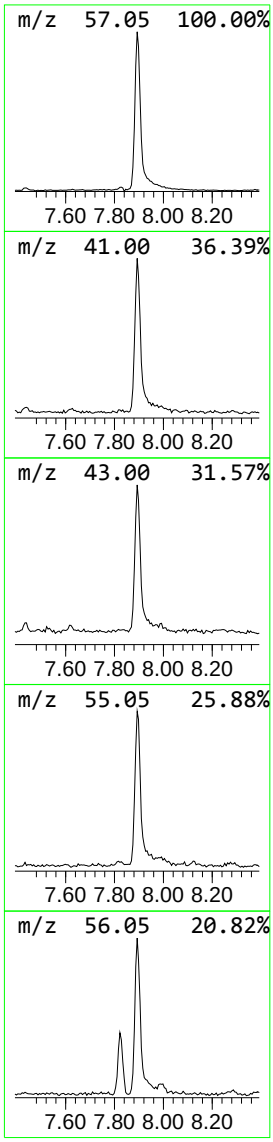
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	7.36 ng	438095	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	90
2	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42





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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

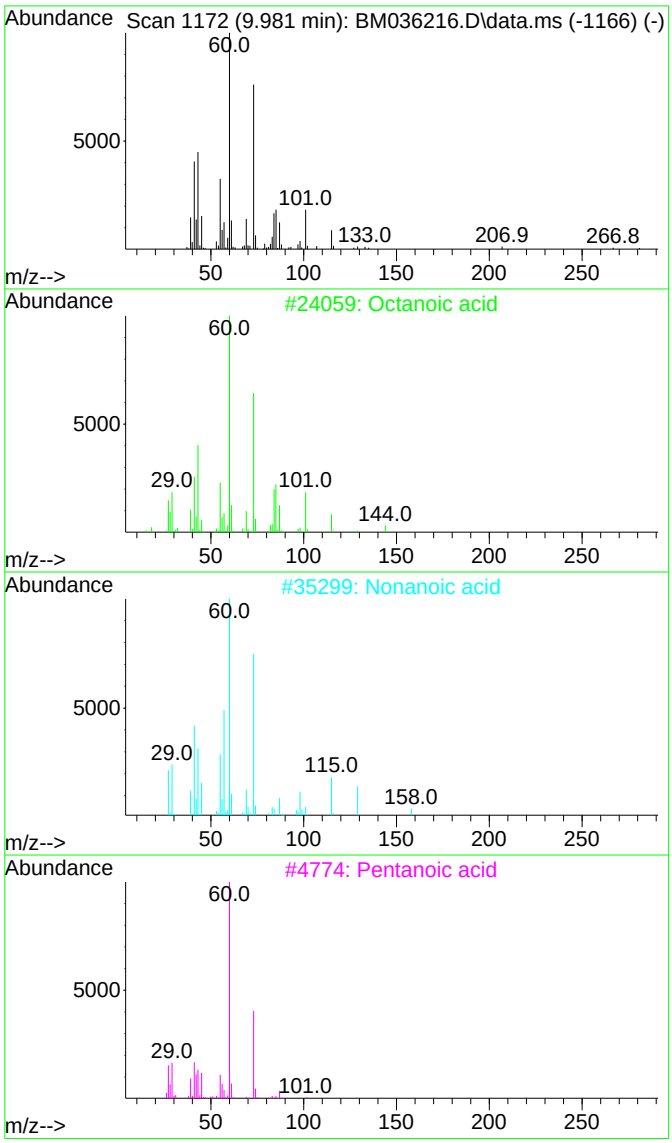
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

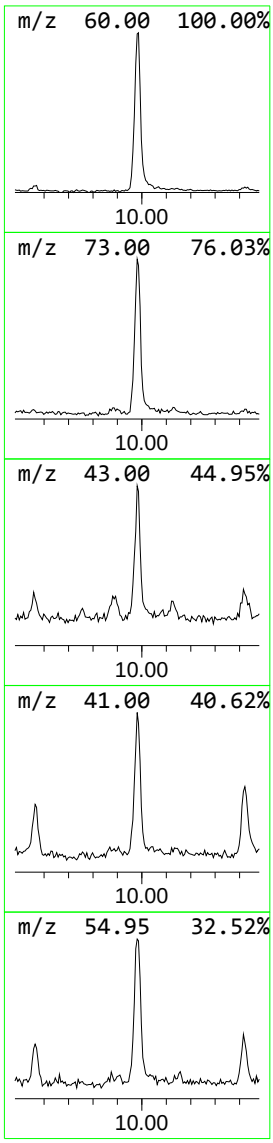
****

Peak Number 5 Octanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.981	2.20 ng	190877	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	Nonanoic acid	158	C9H18O2	000112-05-0	64
3	Pentanoic acid	102	C5H10O2	000109-52-4	58
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
5	Hexanoic acid	116	C6H12O2	000142-62-1	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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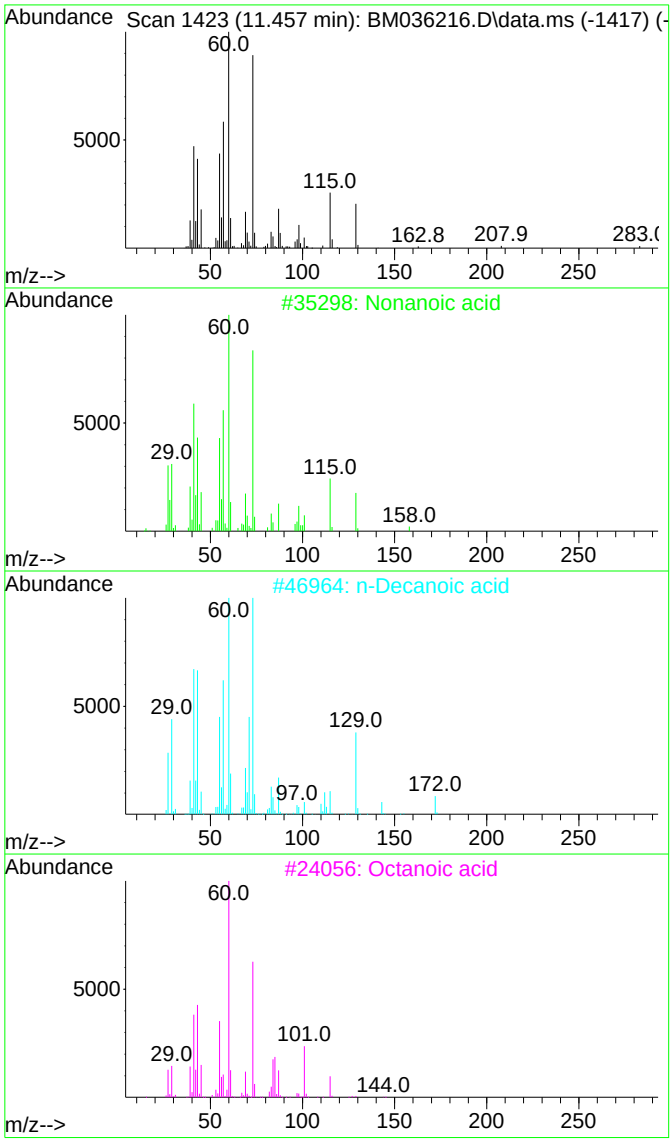
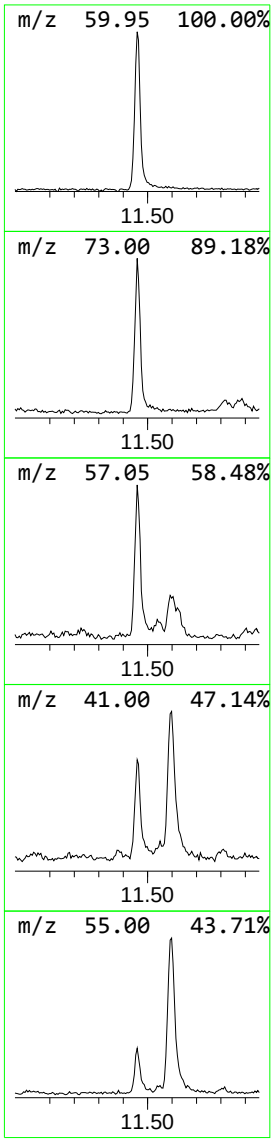
****

Peak Number 6 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	2.38 ng	205977	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	86
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Octanoic acid	144	C8H16O2	000124-07-2	53
4	Hexanoic acid	116	C6H12O2	000142-62-1	47
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43





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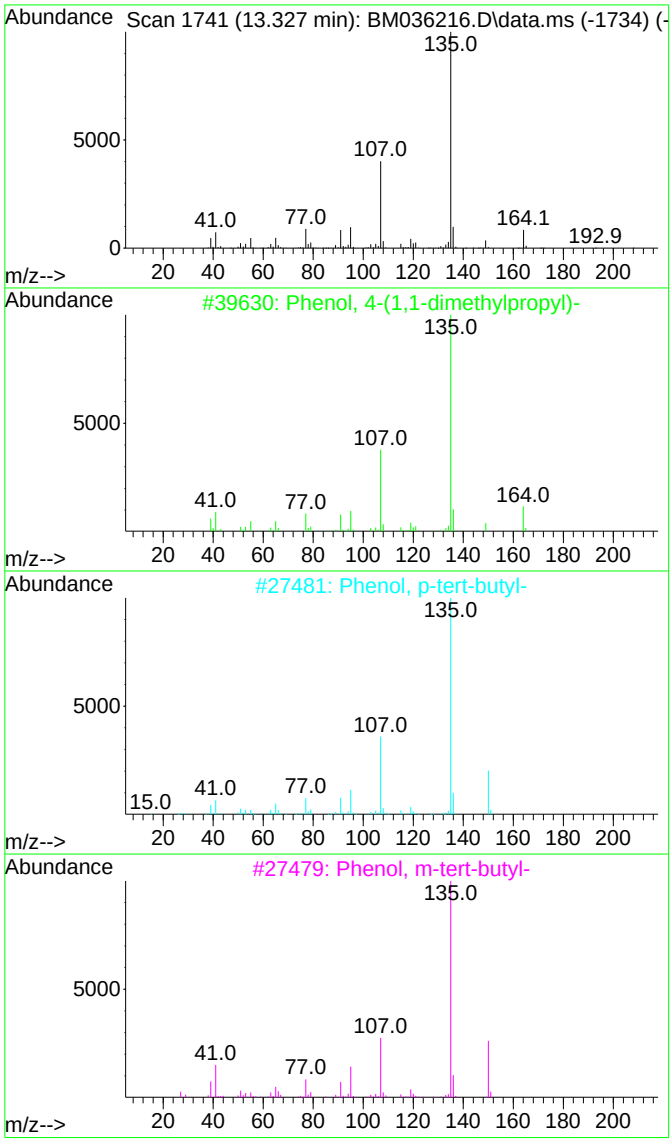
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

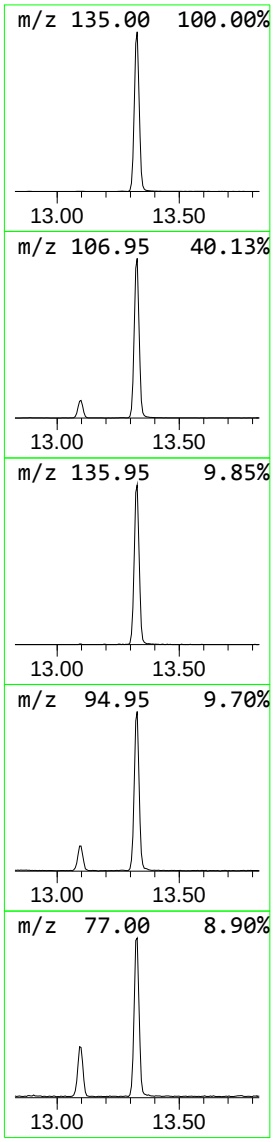
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	24.52 ng	2986350	Acenaphthene-d10	14.469

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	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	64
5	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentanone	4.275	17.3	ng	1027450	1	7.828	1190850	20.0
2-Propanol, 1-p...	4.916	6.3	ng	377435	1	7.828	1190850	20.0
2-Propanol, 1-b...	6.469	6.6	ng	395183	1	7.828	1190850	20.0
1-Hexanol, 2-et...	7.892	7.4	ng	438095	1	7.828	1190850	20.0
Octanoic acid	9.981	2.2	ng	190877	2	10.628	1732140	20.0
Nonanoic acid	11.457	2.4	ng	205977	2	10.628	1732140	20.0
Phenol, 4-(1,1-...	13.327	24.5	ng	2986350	3	14.469	2435870	20.0