LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070121\
Data File : BG049154.D
Acq On : 1 Jul 2021 15:18
Operator : CG/JU
Sample : M2901-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124035

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_G\METHODS\8270-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.129	10	15	25	rVV3	36449	93272	3.13%	0.653%
2	3.217	25	30	37	rVB3	19828	35360	1.18%	0.247%
3	5.174	357	363	370	rBV	21197	34433	1.15%	0.241%
4	5.644	436	443	456	rBV	744045	1287330	43.14%	9.008%
5	7.242	706	715	728	rBV	781326	1401341	46.96%	9.805%
6	8.088	851	859	866	rVB	135093	234263	7.85%	1.639%
7	9.257	1050	1058	1069	rBV	496464	907381	30.41%	6.349%
8	10.321	1232	1239	1247	rVB3	34715	61964	2.08%	0.434%
9	10.668	1292	1298	1314	rBV	213395	375439	12.58%	2.627%
10	10.908	1331	1339	1348	rBV	177432	318482	10.67%	2.228%
11	13.353	1747	1755	1763	rBV	1227611	1941426	65.06%	13.584%
12	14.733	1981	1990	1998	rVB	291389	455253	15.26%	3.185%
13	16.220	2237	2243	2252	rBV	1185453	1822036	61.05%	12.749%
14	17.483	2450	2458	2463	rBV	357198	576779	19.33%	4.036%
15	17.524	2463	2465	2473	rVB3	22598	34157	1.14%	0.239%
16	18.141	2563	2570	2576	rBV	25954	36863	1.24%	0.258%
17	18.359	2601	2607	2613	rBV3	34674	59155	1.98%	0.414%
18	19.534	2800	2807	2812	rBV	42190	65426	2.19%	0.458%
19	19.892	2864	2868	2873	rVB	34094	46475	1.56%	0.325%
20	20.092	2895	2902	2907	rBV	2208880	2984283	100.00%	20.881%
21	21.396	3119	3124	3131	rBV3	73955	157037	5.26%	1.099%
22	21.766	3180	3187	3193	rBV2	382102	652467	21.86%	4.565%
23	23.500	3478	3482	3488	rVB6	14910	34084	1.14%	0.238%
24	25.080	3739	3751	3763	rBV2	227247	676825	22.68%	4.736%

Sum of corrected areas: 14291531

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Instrument :
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ClientSampleId :
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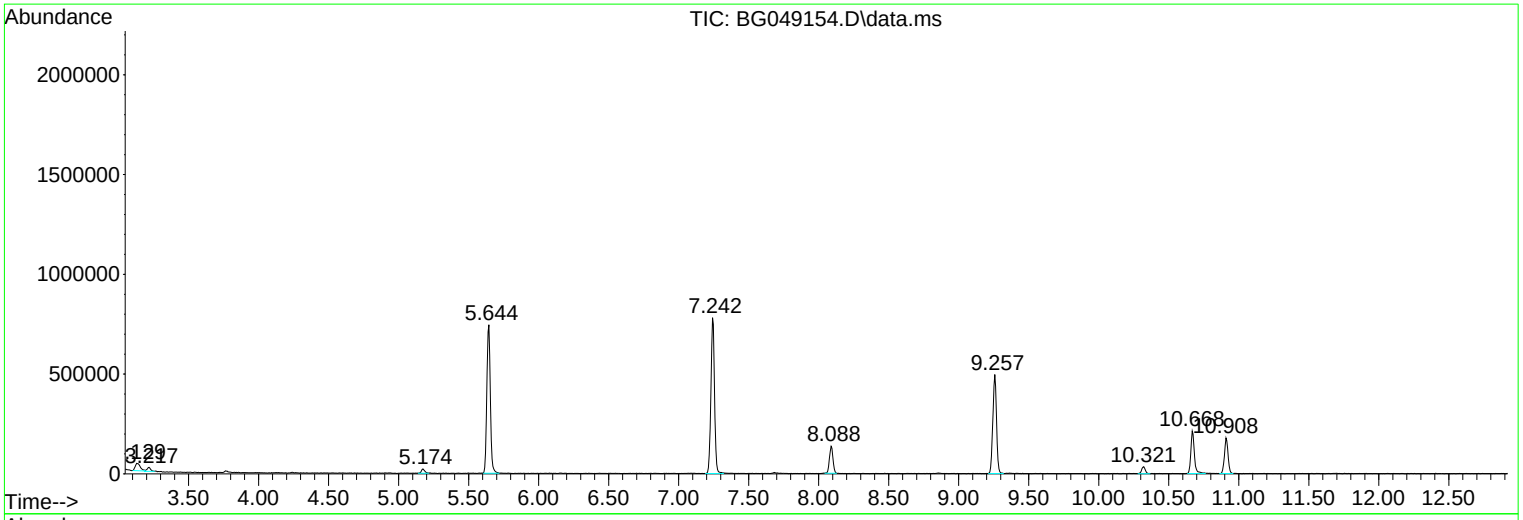
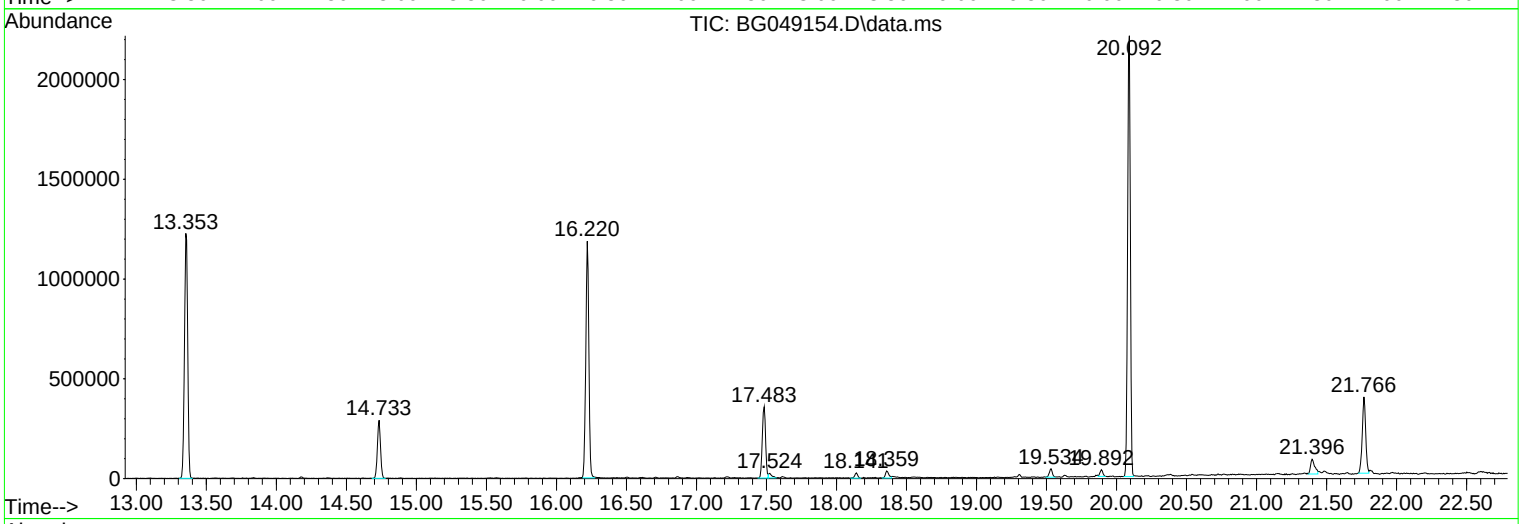
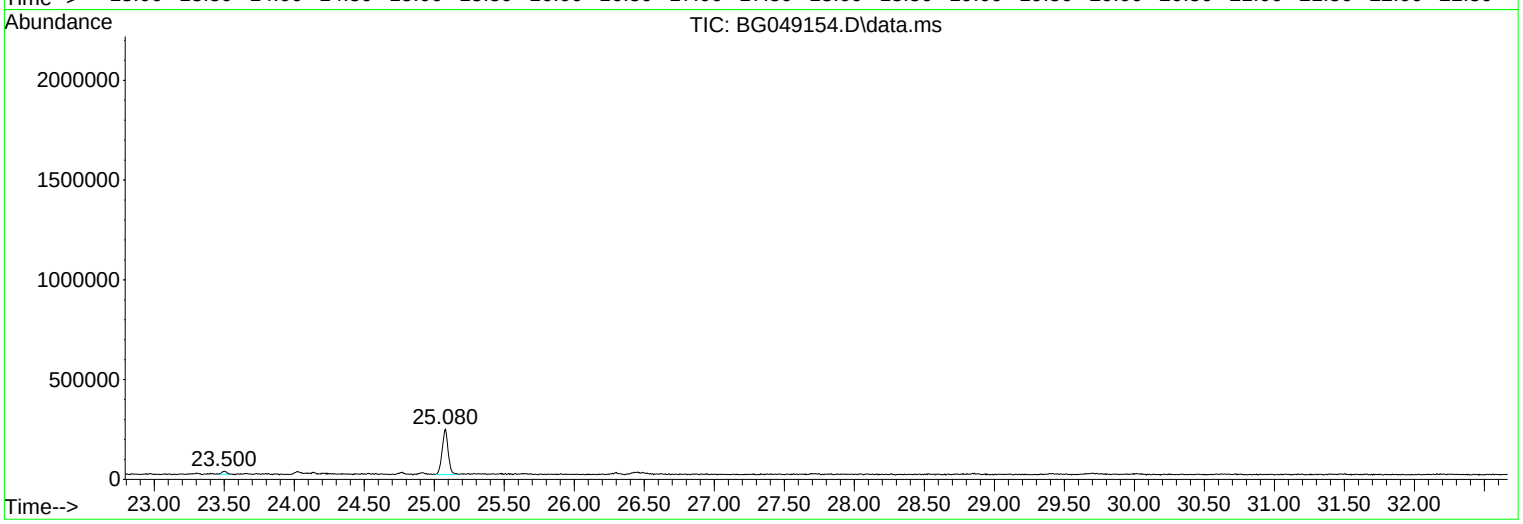
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BG049154.D
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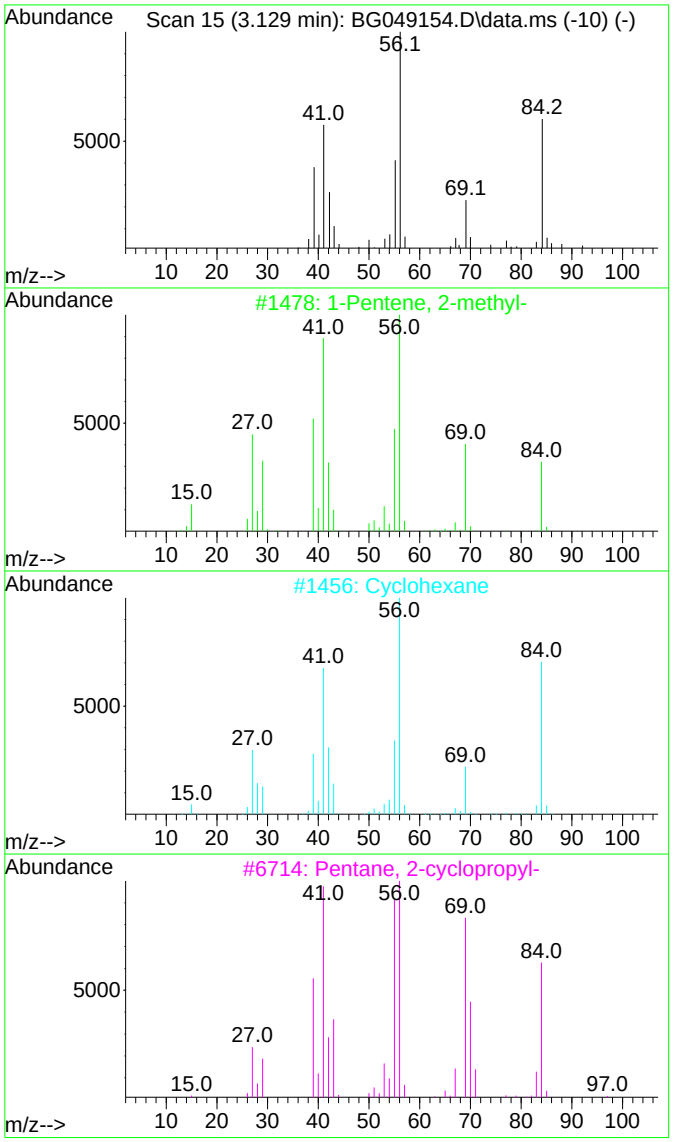
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

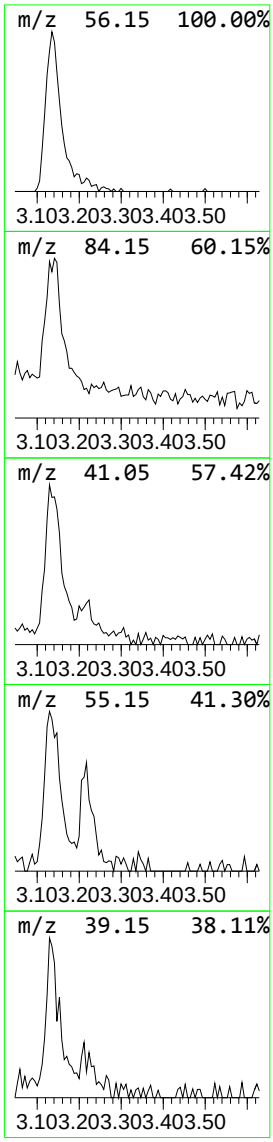
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.129	7.96 ng	93272	1,4-Dichlorobenzene-d4	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
2	Cyclohexane	84	C6H12	000110-82-7	76
3	Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	64
4	2,2-Dimethylglutaric anhydride	142	C7H10O3	002938-48-9	43
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	40





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Sample : M2901-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

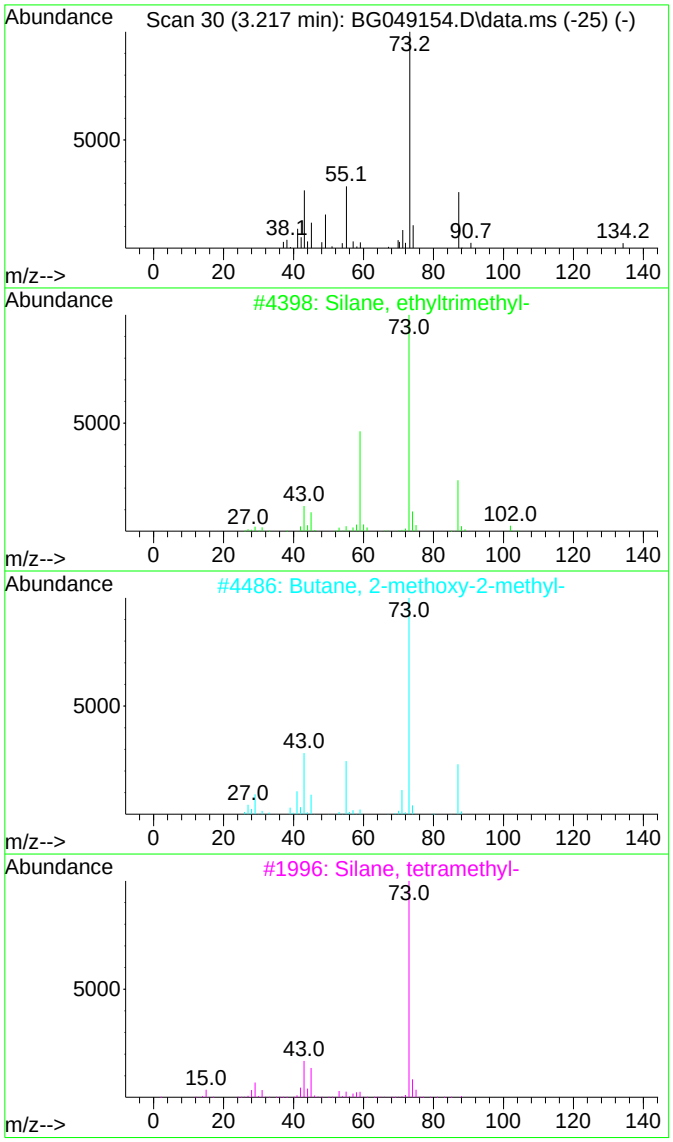
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

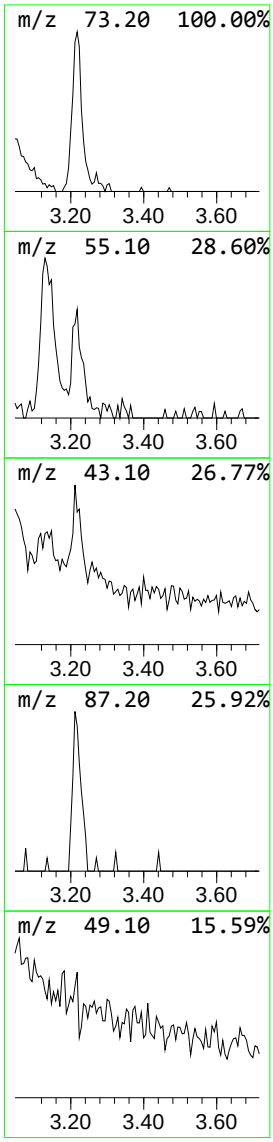
****

Peak Number 2 unknown3.217 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.217	3.02 ng	35360	1,4-Dichlorobenzene-d4	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070121\
Data File : BG049154.D
Acq On : 1 Jul 2021 15:18
Operator : CG/JU
Sample : M2901-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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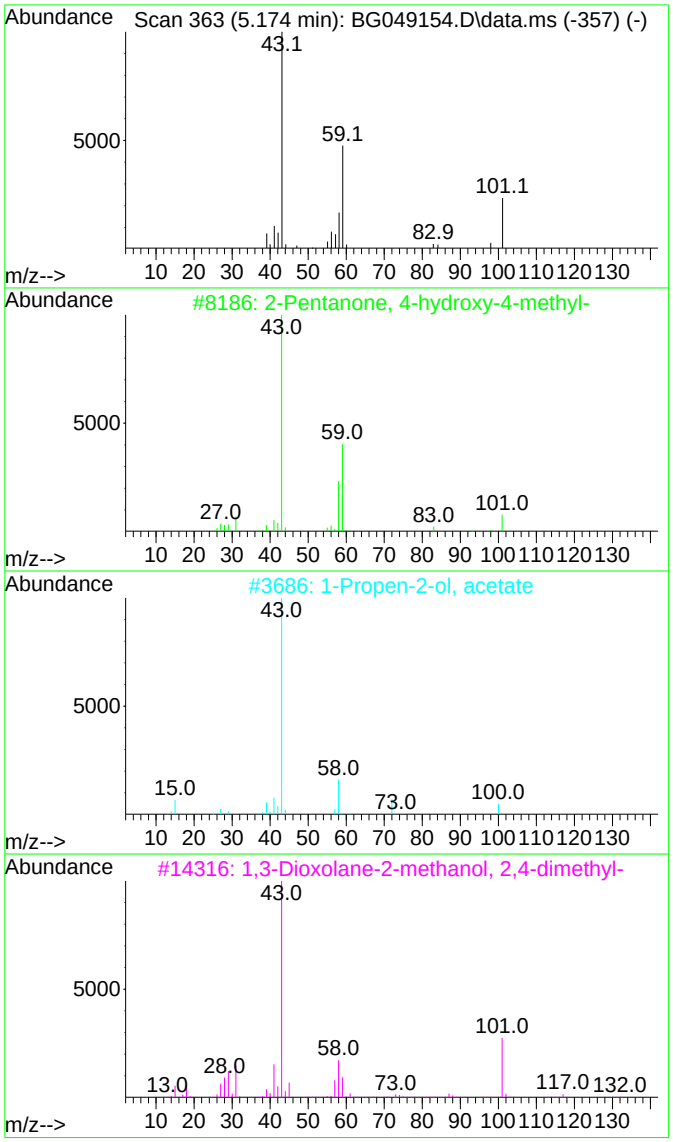
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

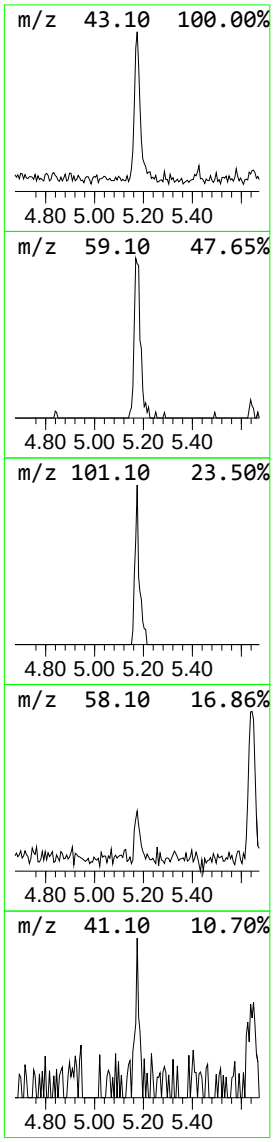
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.174	2.94 ng	34433	1,4-Dichlorobenzene-d4	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9
4	2-Nonanone	142	C9H18O	000821-55-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Sample : M2901-01
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Instrument :
BNA_G
ClientSampleId :
124035

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

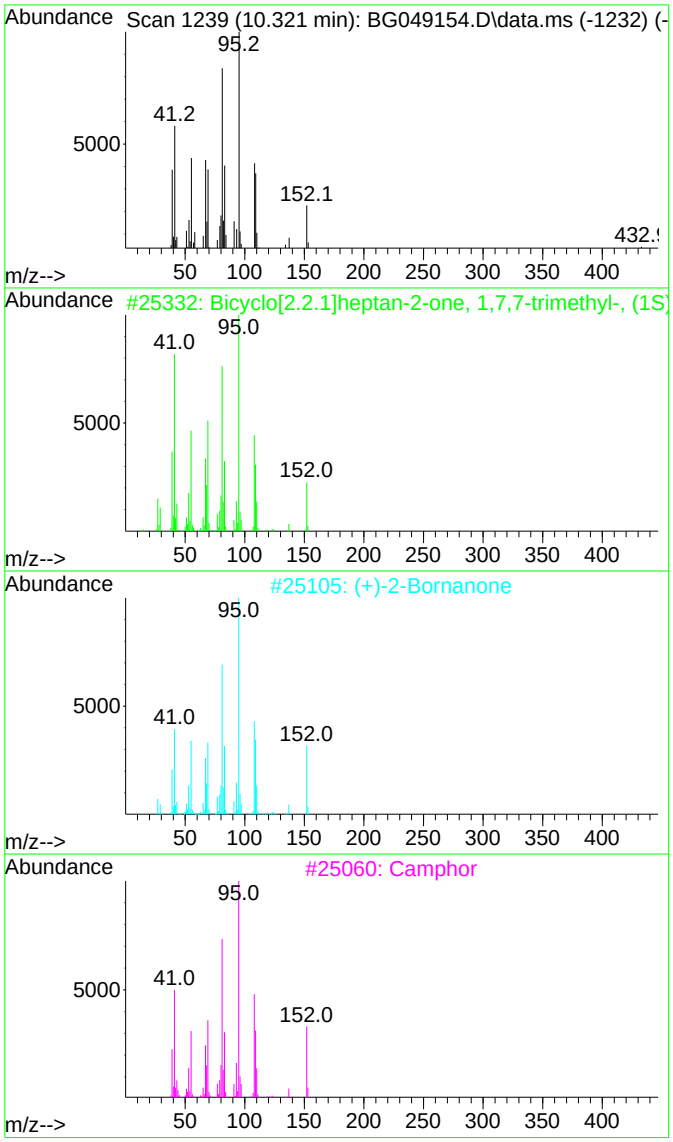
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

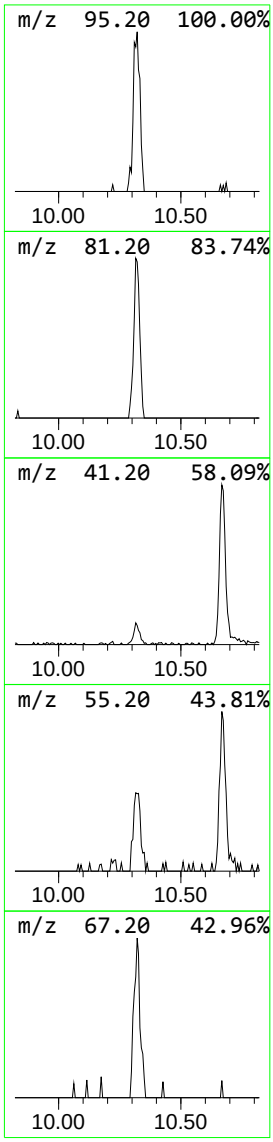
****

Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.321	3.89 ng	61964	Naphthalene-d8	10.908

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	93
3	Camphor	152	C10H16O	000076-22-2	91
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	43
5	Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	38





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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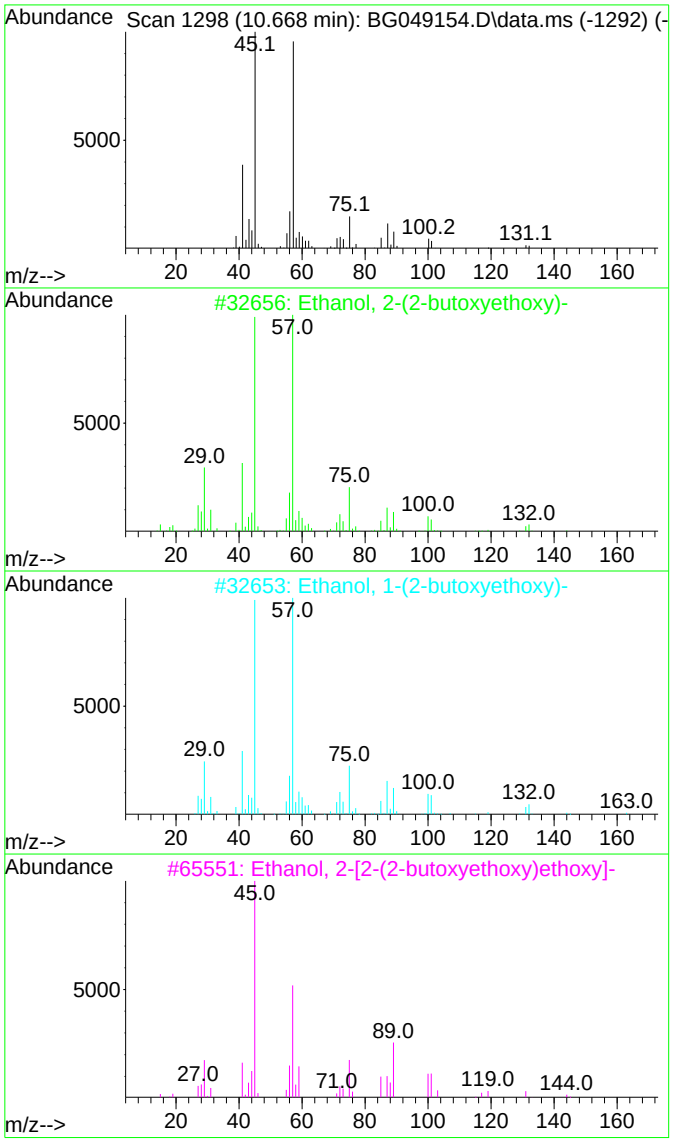
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

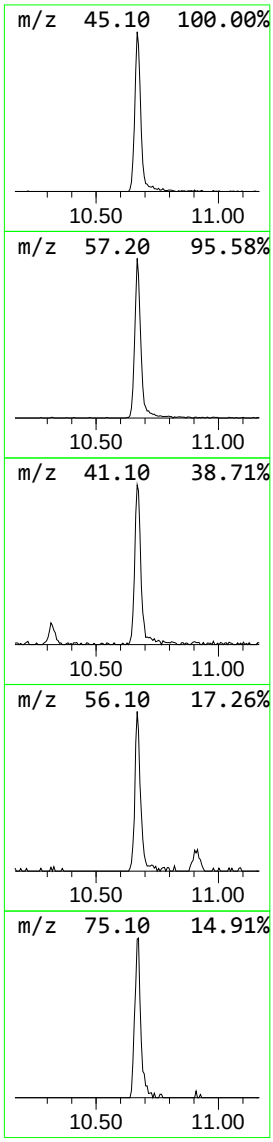
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.668	23.58 ng	375439	Naphthalene-d8	10.908

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	47
5	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	47





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BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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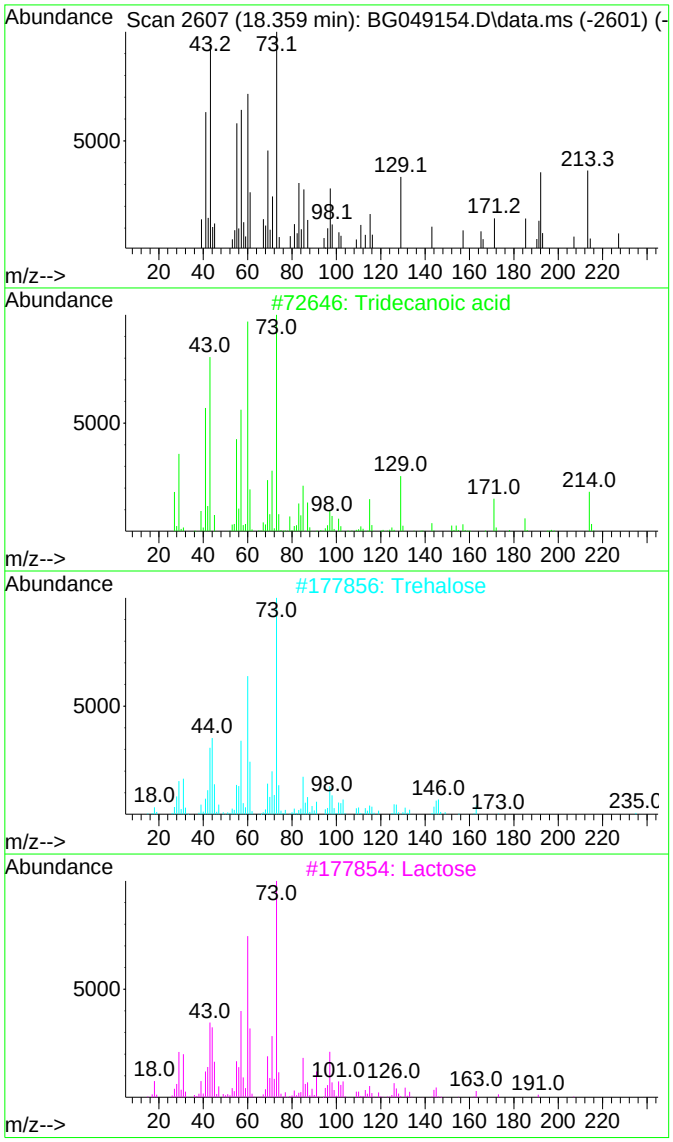
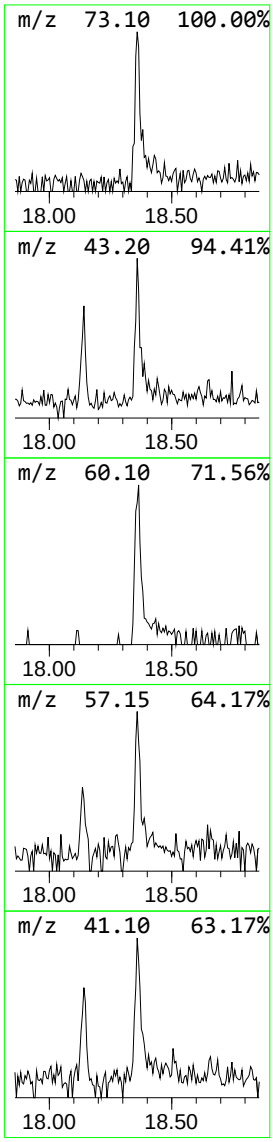
****

Peak Number 6 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.358	2.05 ng	59155	Phenanthrene-d10	17.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	Trehalose	342	C12H22O11	000099-20-7	43
3	Lactose	342	C12H22O11	000063-42-3	38
4	n-Decanoic acid	172	C10H20O2	000334-48-5	35
5	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	27





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Operator : CG/JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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BNA_G
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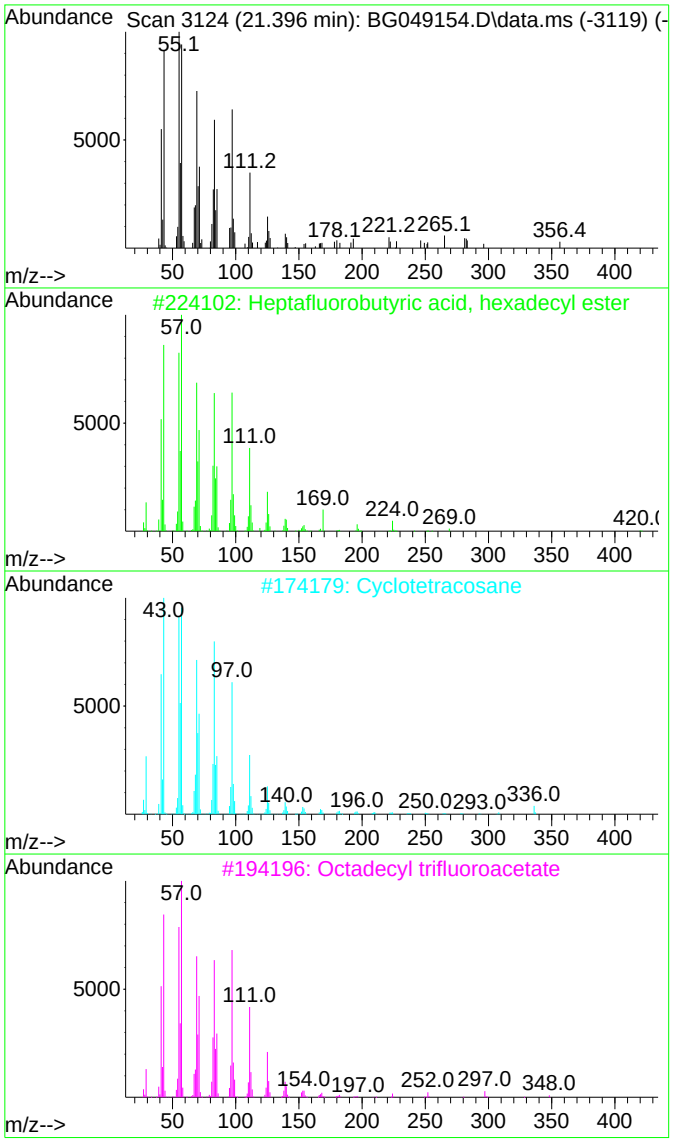
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

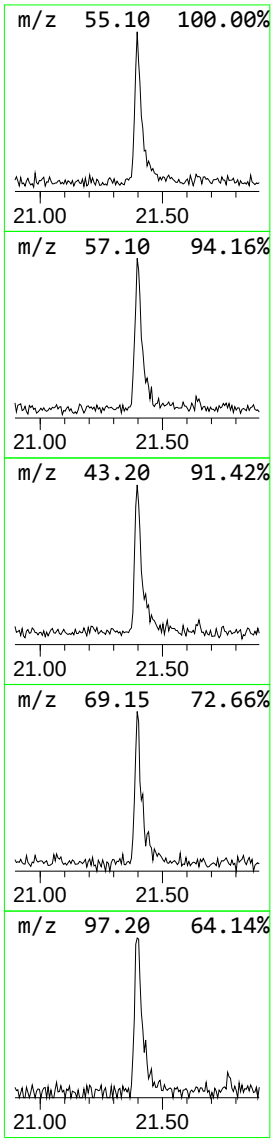
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptafluorobutyric acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.396	4.81 ng	157037	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
2	Cyclotetracosane	336	C24H48	000297-03-0	90
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4	E-7-Octadecene	252	C18H36	1000130-92-0	87
5	17-Pentatriacontene	491	C35H70	006971-40-0	87





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
1-Pentene, 2-me...	3.129	8.0	ng	93272	1	8.088	234263	20.0
unknown3.217	3.217	3.0	ng	35360	1	8.088	234263	20.0
2-Pentanone, 4-...	5.174	2.9	ng	34433	1	8.088	234263	20.0
Bicyclo[2.2.1]h...	10.321	3.9	ng	61964	2	10.908	318482	20.0
Ethanol, 2-(2-b...	10.668	23.6	ng	375439	2	10.908	318482	20.0
Tridecanoic acid	18.358	2.0	ng	59155	4	17.483	576779	20.0
Heptafluorobuty...	21.396	4.8	ng	157037	5	21.766	652467	20.0