LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049061.D
Acq On : 23 Jun 2021 14:44
Operator : CG/JU
Sample : M2748-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-9A

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.155	14	20	29	rBV2	47152	93904	5.57%	1.320%
2	3.231	30	33	40	rVB2	11851	19339	1.15%	0.272%
3	4.583	258	263	270	rVB2	20965	36566	2.17%	0.514%
4	5.188	361	366	377	rVB	111002	176464	10.47%	2.481%
5	5.658	439	446	455	rBV	277403	464708	27.57%	6.533%
6	7.256	711	718	728	rBV	299605	534326	31.70%	7.512%
7	8.108	856	863	869	rVB	97751	164122	9.74%	2.307%
8	9.271	1052	1061	1070	rBV	195617	356206	21.14%	5.008%
9	10.693	1297	1303	1310	rBV2	23325	43991	2.61%	0.618%
10	10.928	1335	1343	1352	rBV	124189	230627	13.68%	3.242%
11	13.372	1751	1759	1766	rBV	498415	779030	46.22%	10.952%
12	14.747	1985	1993	2000	rBV	210457	337068	20.00%	4.738%
13	15.540	2123	2128	2133	rBV	39205	52034	3.09%	0.731%
14	16.234	2238	2246	2255	rBV	167921	284995	16.91%	4.006%
15	17.497	2455	2461	2471	rBV	315145	490148	29.08%	6.890%
16	18.161	2569	2574	2580	rVB2	18881	23702	1.41%	0.333%
17	18.378	2605	2611	2614	rBV3	18467	25594	1.52%	0.360%
18	20.106	2899	2905	2910	rBV	1289404	1685375	100.00%	23.693%
19	21.416	3124	3128	3140	rBV5	52468	106587	6.32%	1.498%
20	21.786	3185	3191	3198	rVB	349277	578622	34.33%	8.134%
21	25.106	3745	3756	3777	rVB2	193746	630025	37.38%	8.857%

Sum of corrected areas: 7113433

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Misc :
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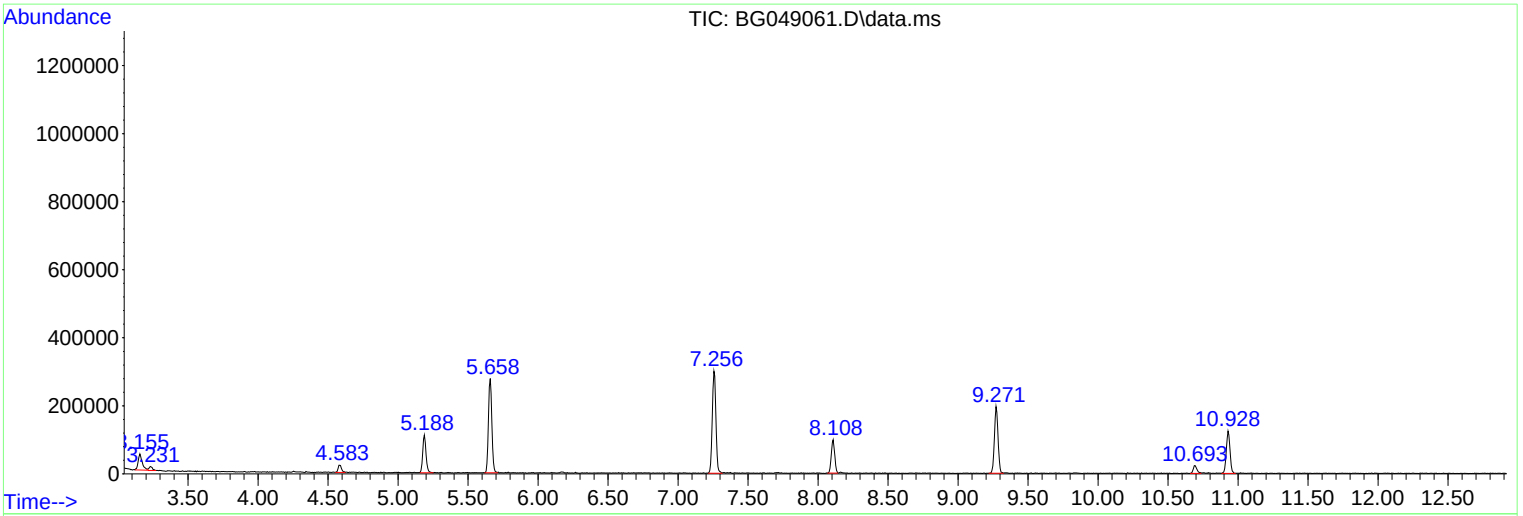
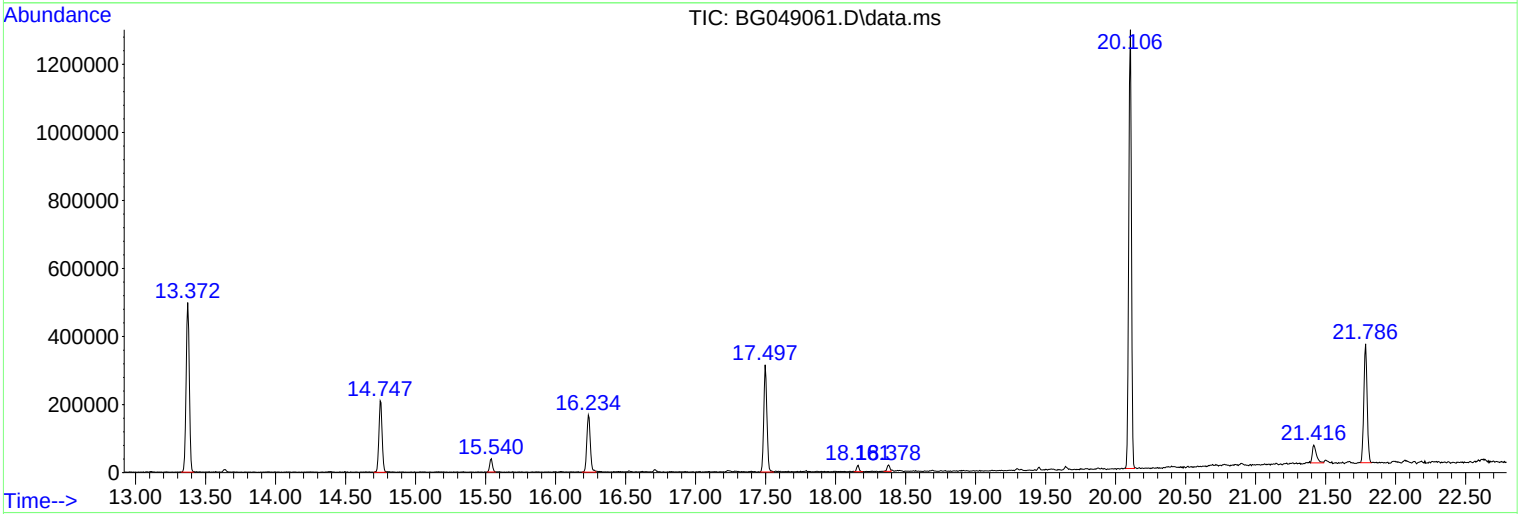
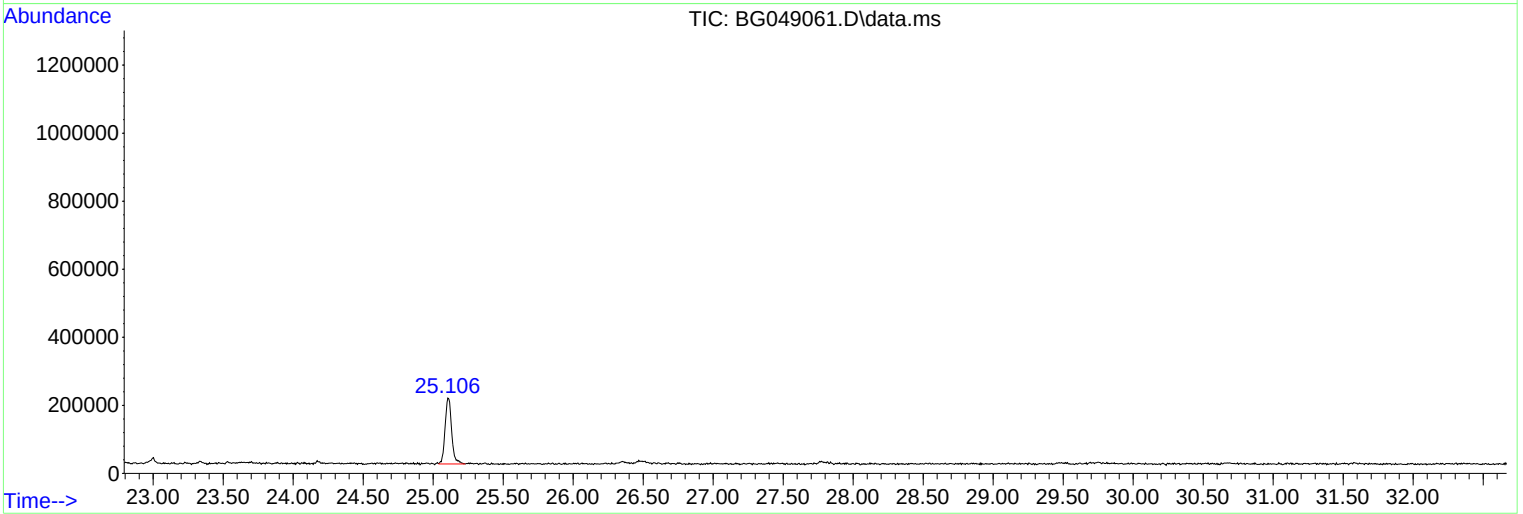
Instrument :
BNA_G
ClientSampleId :
SB-9A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

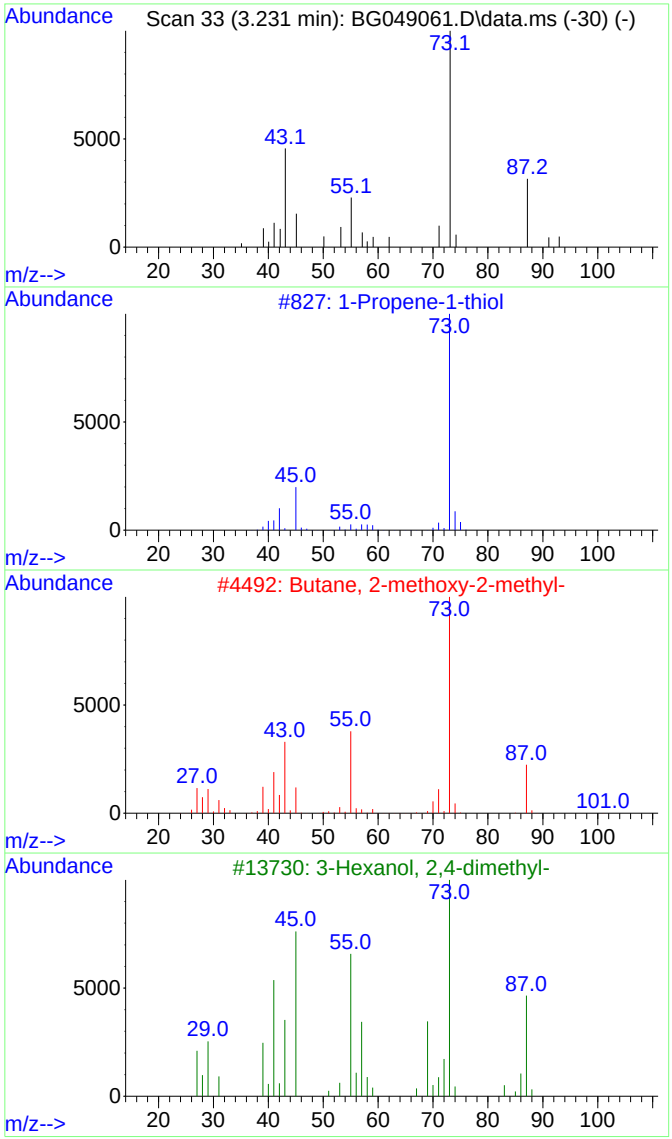
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

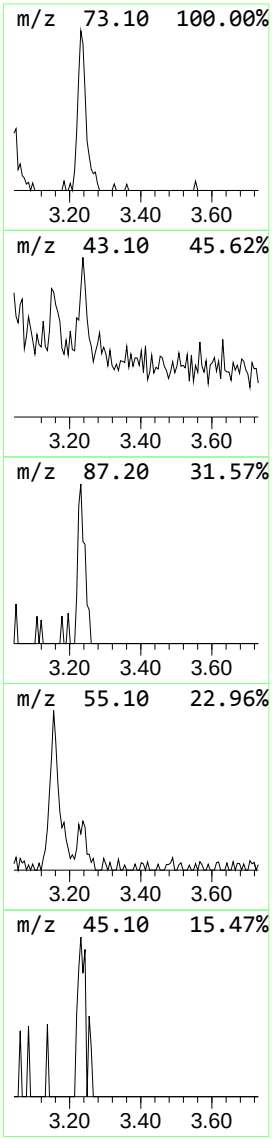
****

Peak Number 2 unknown3.231 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.231	2.36 ng	19339	1,4-Dichlorobenzene-d4	8.108

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9





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Data File : BG049061.D
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Operator : CG/JU
Sample : M2748-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-9A

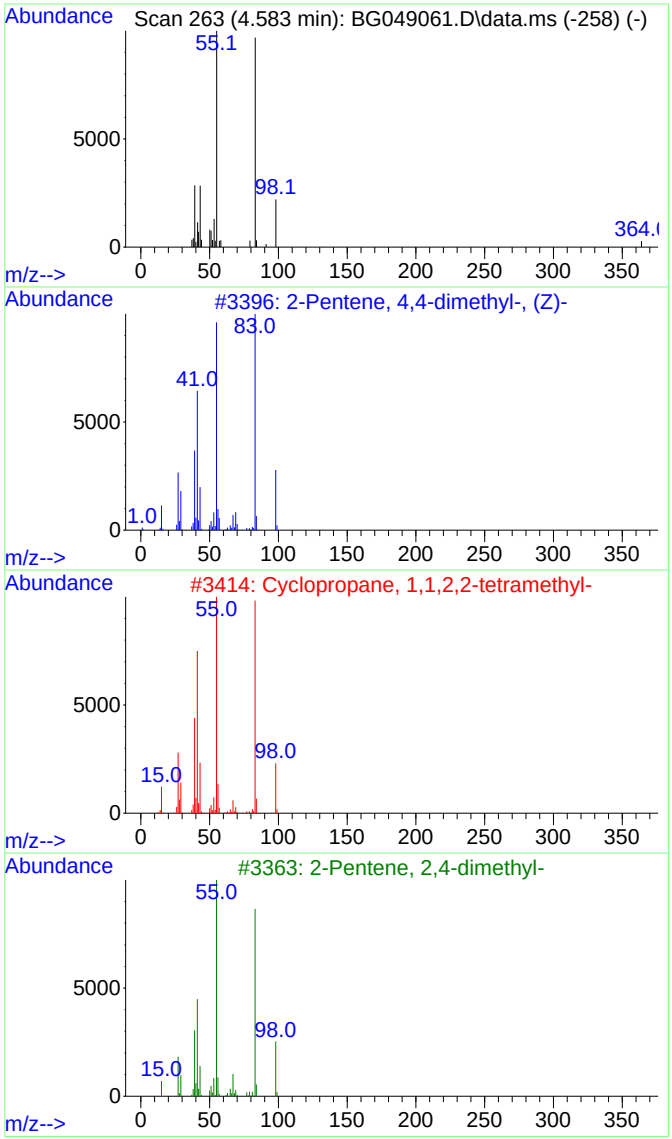
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

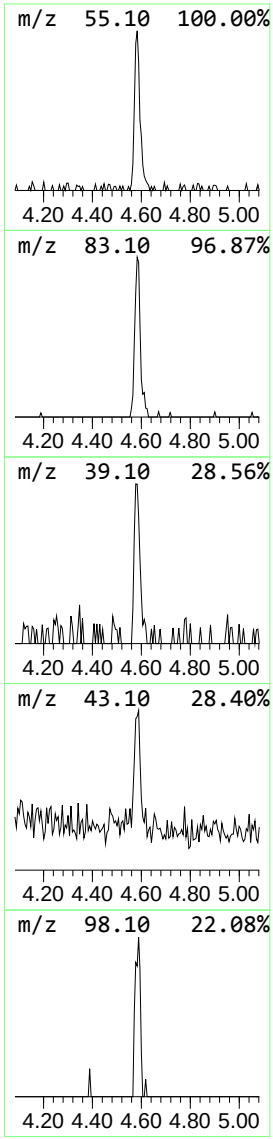
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentene, 4,4-dimethyl-, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.583	4.46 ng	36566	1,4-Dichlorobenzene-d4	8.108

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
2	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	72
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	64





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Acq On : 23 Jun 2021 14:44
Operator : CG/JU
Sample : M2748-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-9A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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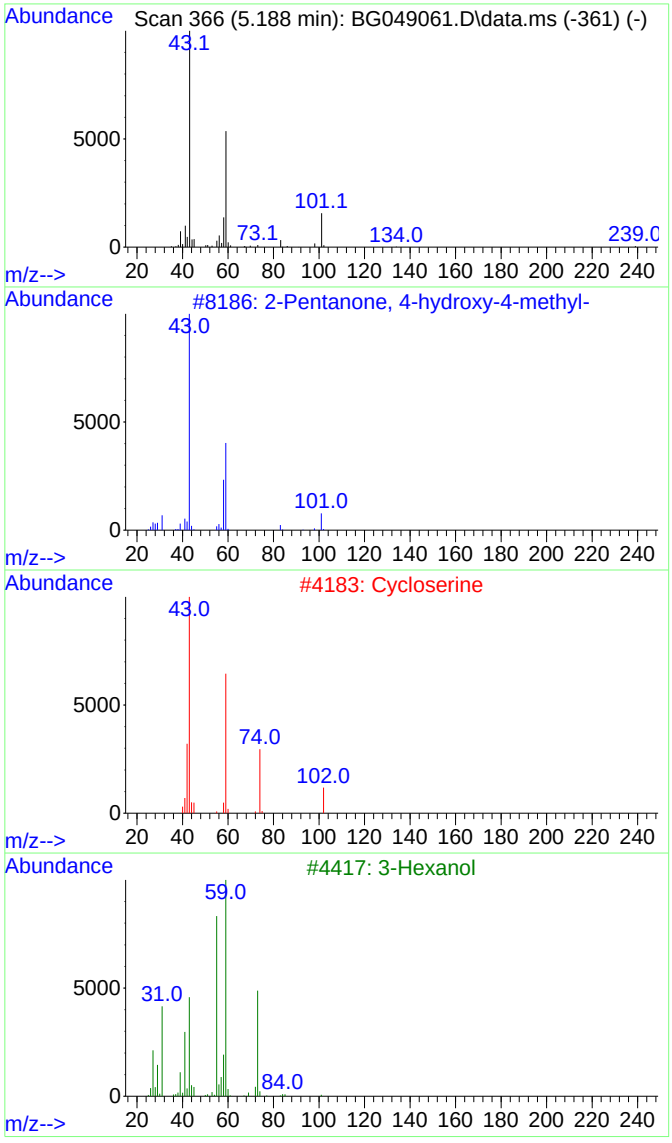
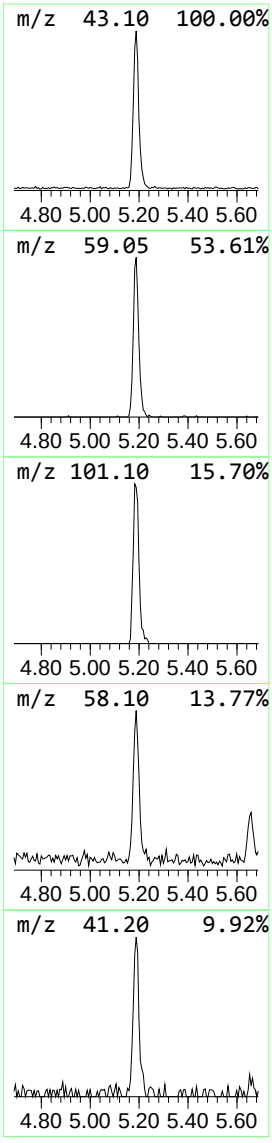
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.188	21.50 ng	176464	1,4-Dichlorobenzene-d4	8.108

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Cycloserine	102	C3H6N2O2	000068-41-7	45
3	3-Hexanol	102	C6H14O	000623-37-0	36
4	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	36
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33





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Operator : CG/JU
Sample : M2748-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-9A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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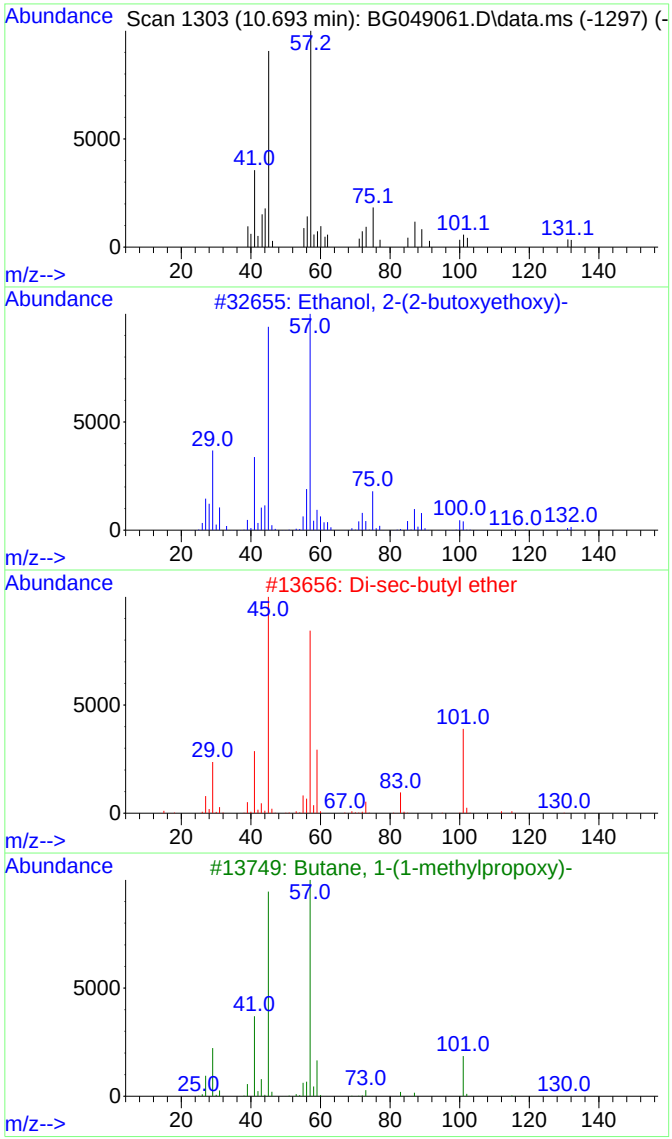
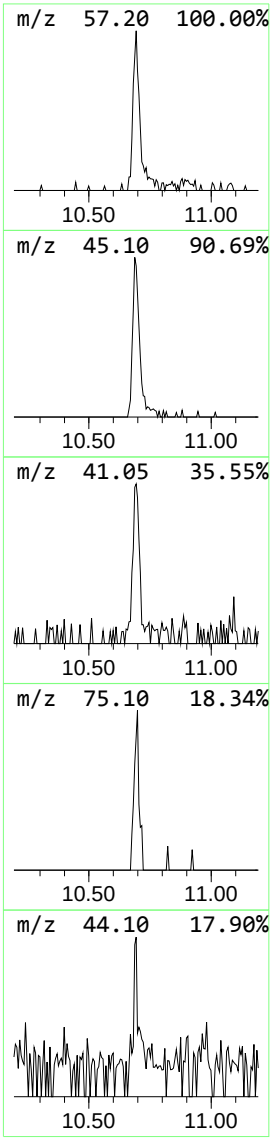
****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.693	3.81 ng	43991	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	42





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TIC Library : C:\Database\NIST11.L
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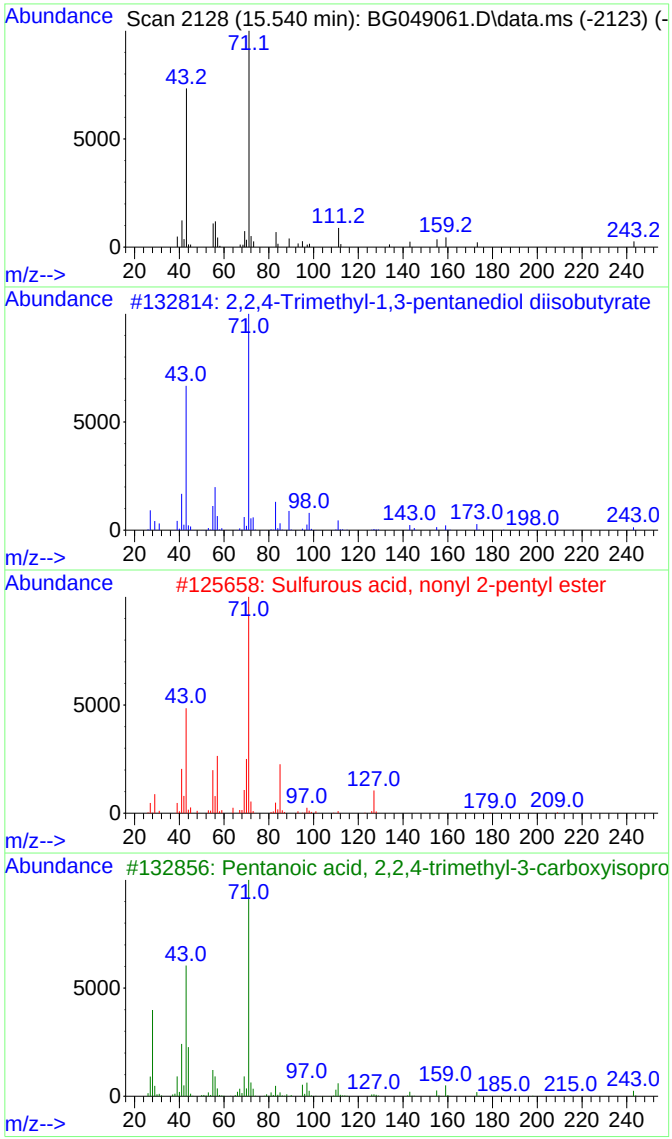
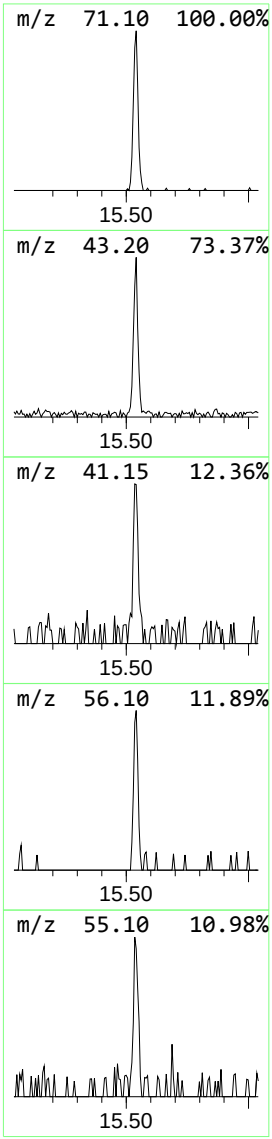
****
Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.540	3.09 ng	52034	Acenaphthene-d10	14.753

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1000309-15-8	50
3	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	50
4	3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	47
5	Disulfide, bis(1,1-dimethylpropyl)	206	C10H22S2	034965-30-5	45





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TIC Library : C:\Database\NIST11.L
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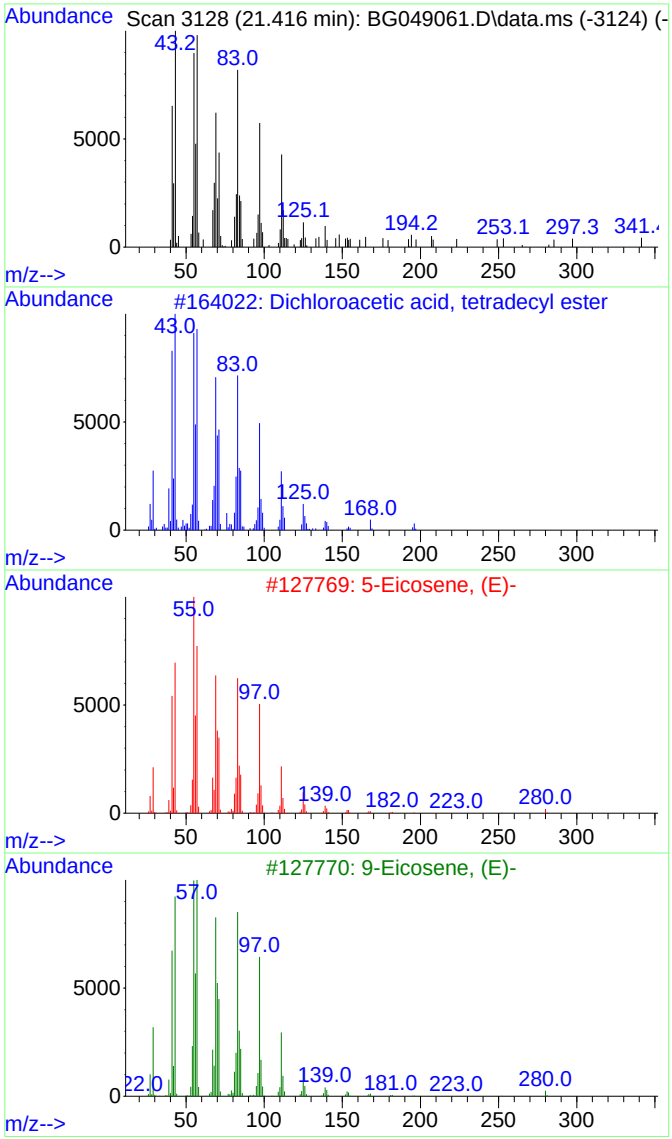
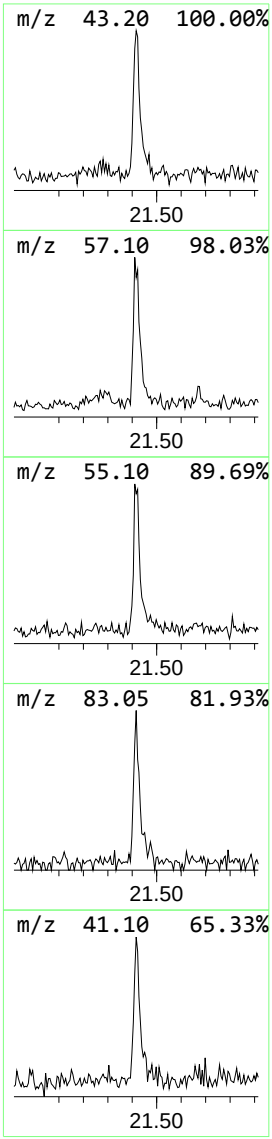
****
Peak Number 7 Dichloroacetic acid, tetrad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	3.68 ng	106587	Chrysene-d12	21.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	87
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	80
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	80
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	80
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80





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
unknown3.231	3.231	2.4	ng	19339	1	8.108	164122	20.0
2-Pentene, 4,4-...	4.583	4.5	ng	36566	1	8.108	164122	20.0
2-Pentanone, 4-...	5.188	21.5	ng	176464	1	8.108	164122	20.0
Ethanol, 2-(2-b...	10.693	3.8	ng	43991	2	10.928	230627	20.0
2,2,4-Trimethyl...	15.540	3.1	ng	52034	3	14.753	337068	20.0
Dichloroacetic ...	21.416	3.7	ng	106587	5	21.786	578622	20.0