LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055553.D
Acq On : 11 Nov 2022 00:24
Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055553.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.330	3	7	12	rBV	248255	373624	12.21%	2.264%
2	3.371	12	14	26	rVB2	34208	49677	1.62%	0.301%
3	5.322	339	346	356	rVB	159989	247192	8.08%	1.498%
4	5.798	419	427	440	rBV	1034582	1701097	55.60%	10.310%
5	7.402	692	700	711	rBV	1040030	1782025	58.24%	10.800%
6	8.265	840	847	854	rBV	170495	291375	9.52%	1.766%
7	9.441	1038	1047	1056	rBV	580952	1042293	34.07%	6.317%
8	10.845	1280	1286	1294	rBV	33490	55170	1.80%	0.334%
9	11.097	1321	1329	1337	rBV	222322	398949	13.04%	2.418%
10	13.512	1733	1740	1748	rVB	1284907	2066530	67.54%	12.524%
11	14.887	1966	1974	1981	rVB	360666	560646	18.32%	3.398%
12	16.362	2218	2225	2235	rBV	1259609	1914825	62.58%	11.605%
13	17.625	2433	2440	2448	rVB	493193	726429	23.74%	4.403%
14	17.737	2454	2459	2463	rVB3	29992	38928	1.27%	0.236%
15	18.483	2582	2586	2600	rBV2	52772	87736	2.87%	0.532%
16	19.746	2797	2801	2807	rBV3	35969	50101	1.64%	0.304%
17	20.210	2874	2880	2887	rBV	2294172	3059600	100.00%	18.543%
18	21.532	3100	3105	3113	rBV2	125181	191032	6.24%	1.158%
19	21.920	3165	3171	3182	rVB2	527098	879220	28.74%	5.329%
20	22.114	3201	3204	3208	rVB2	24070	31256	1.02%	0.189%
21	22.766	3311	3315	3323	rVB4	23322	47089	1.54%	0.285%
22	25.340	3743	3753	3769	rVB2	294477	905295	29.59%	5.487%

Sum of corrected areas: 16500089

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Instrument :
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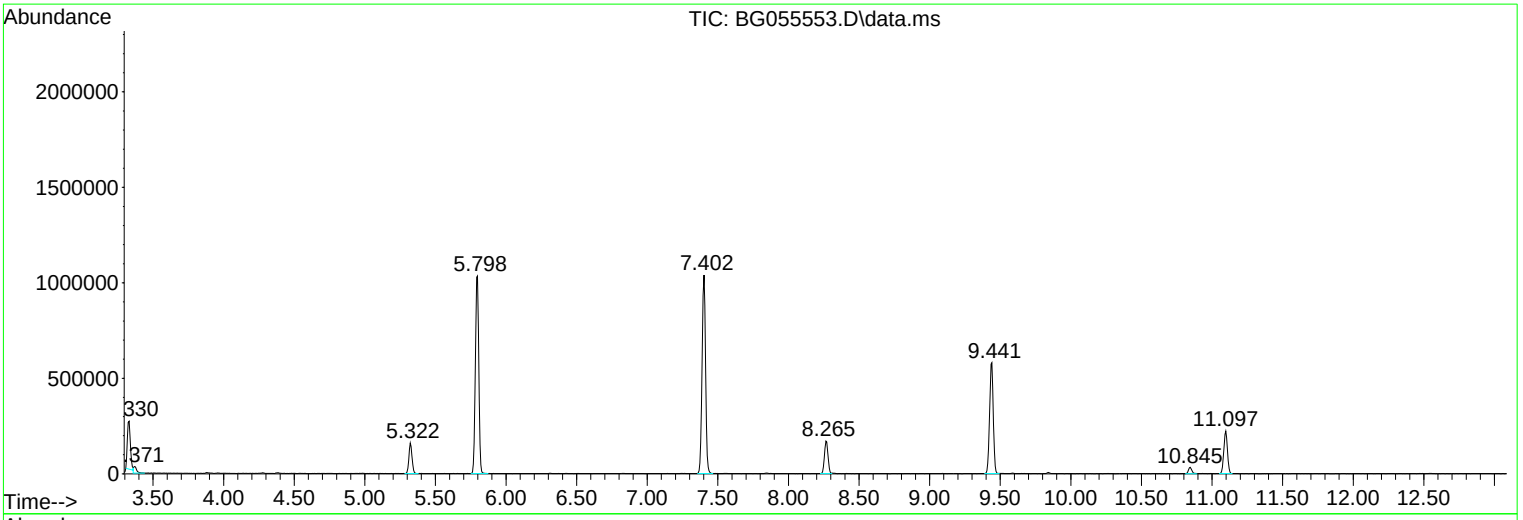
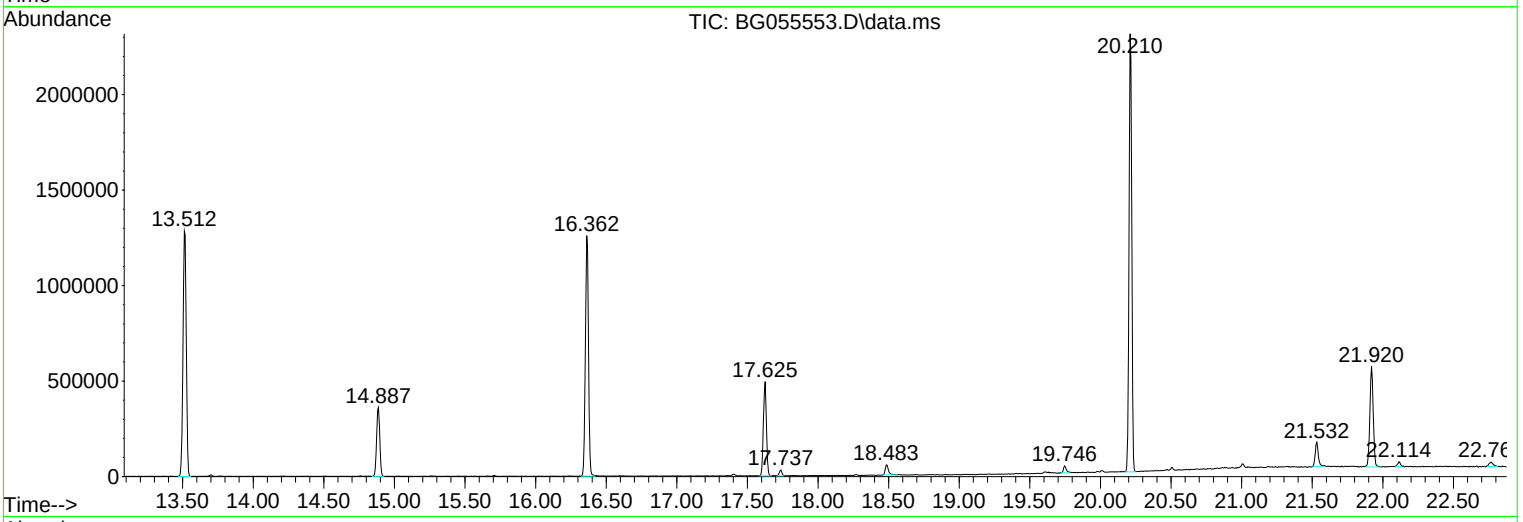
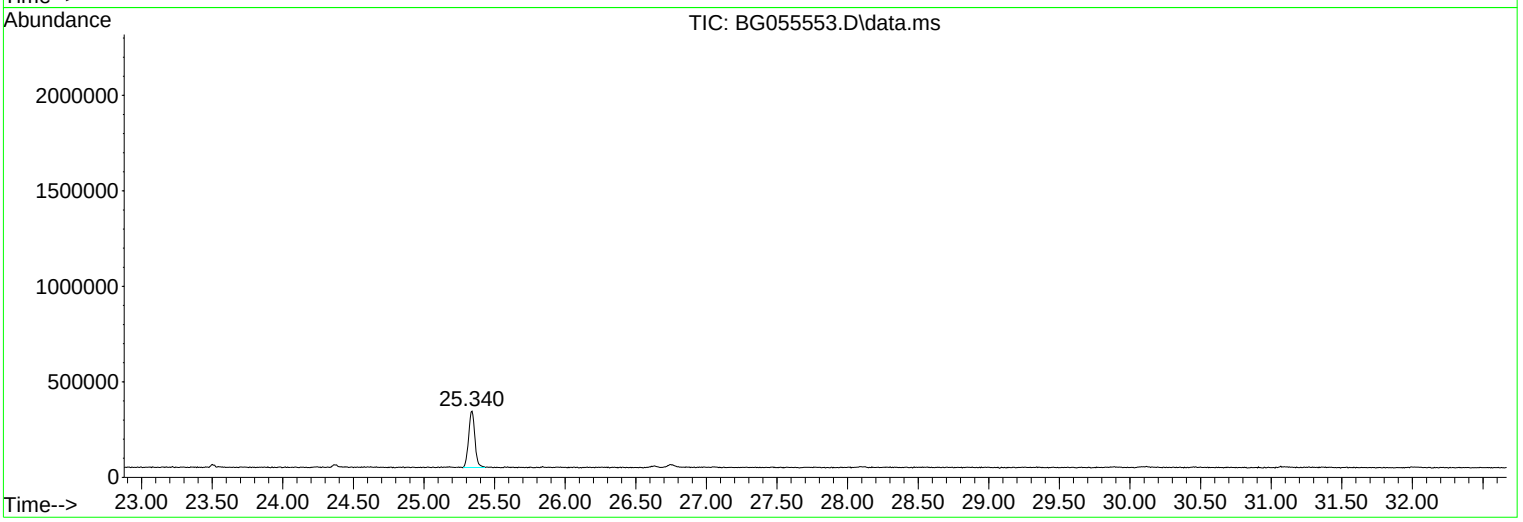
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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Acq On : 11 Nov 2022 00:24
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

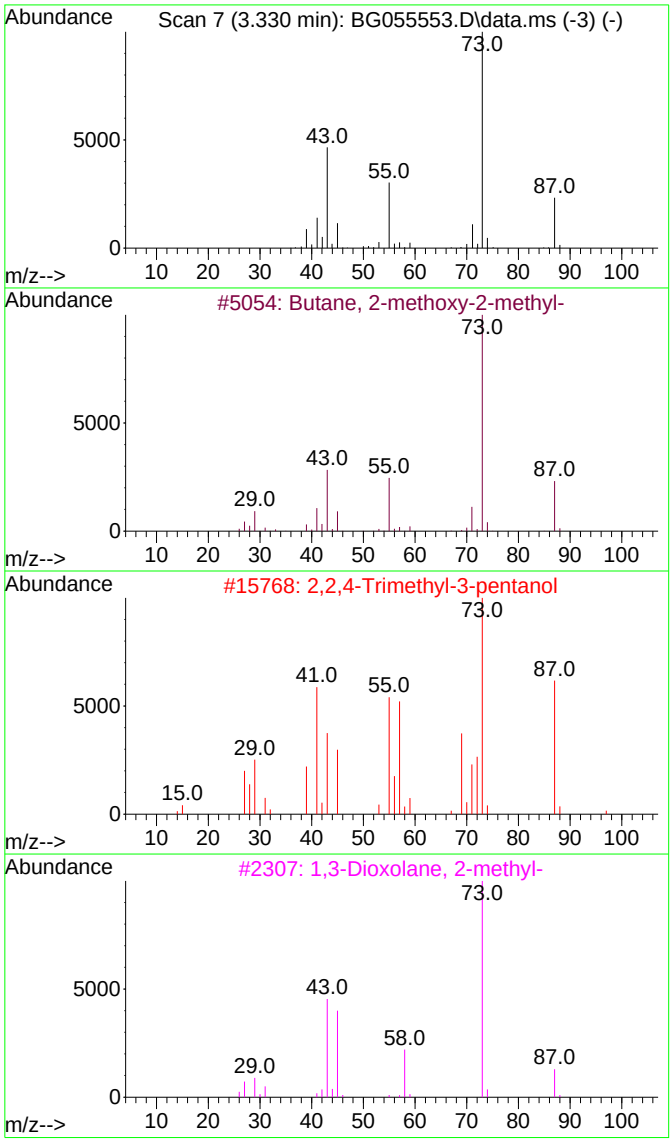
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

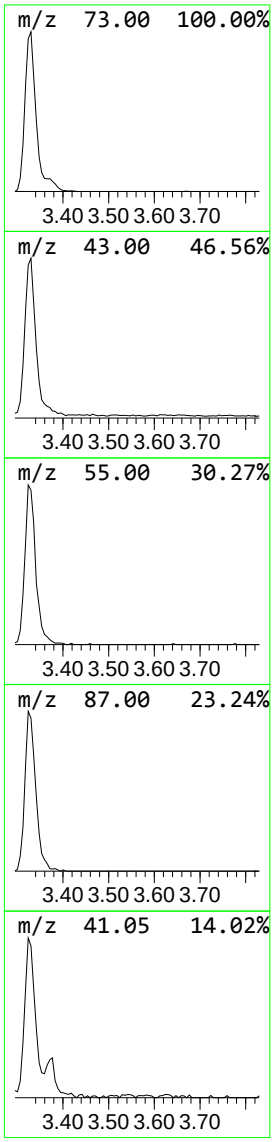
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.330	25.65 ng	373624	1,4-Dichlorobenzene-d4	8.265

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Data File : BG055553.D
Acq On : 11 Nov 2022 00:24
Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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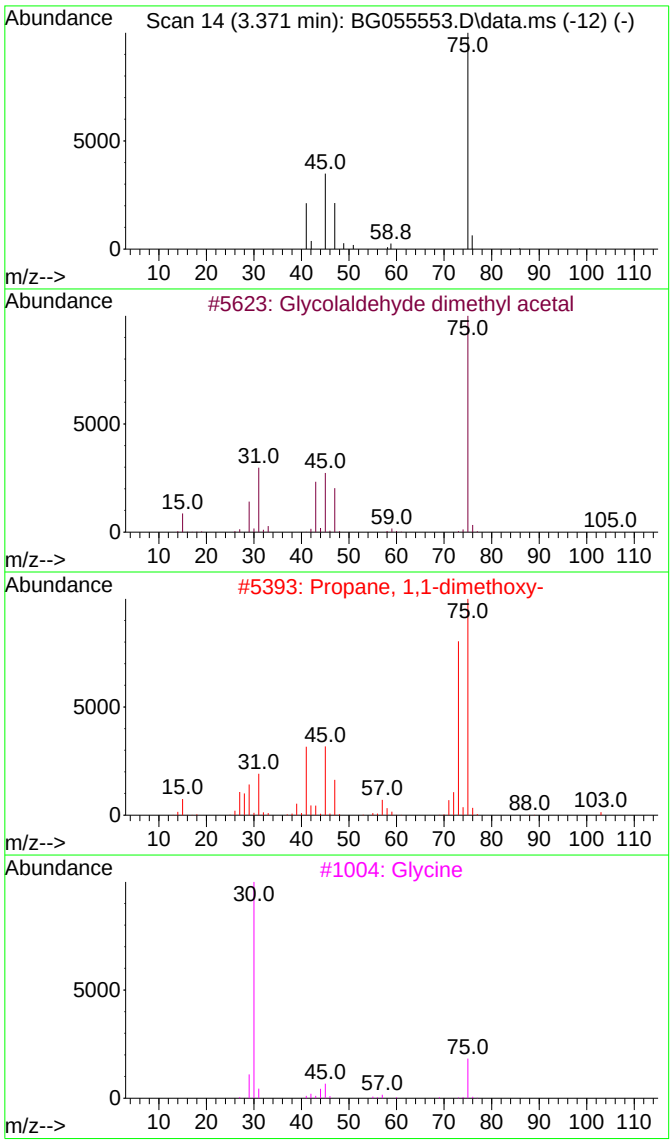
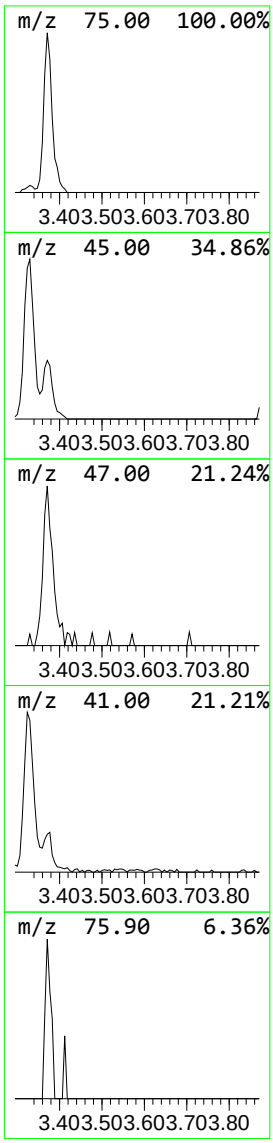
Peak Number 2 Glycolaldehyde dimethyl acetal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.371	3.41 ng	49677	1,4-Dichlorobenzene-d4	8.265

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	64
2	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
3	Glycine	75	C2H5NO2	000056-40-6	4
4	Ethanethioamide	75	C2H5NS	000062-55-5	4
5	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	4





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Sample : N5360-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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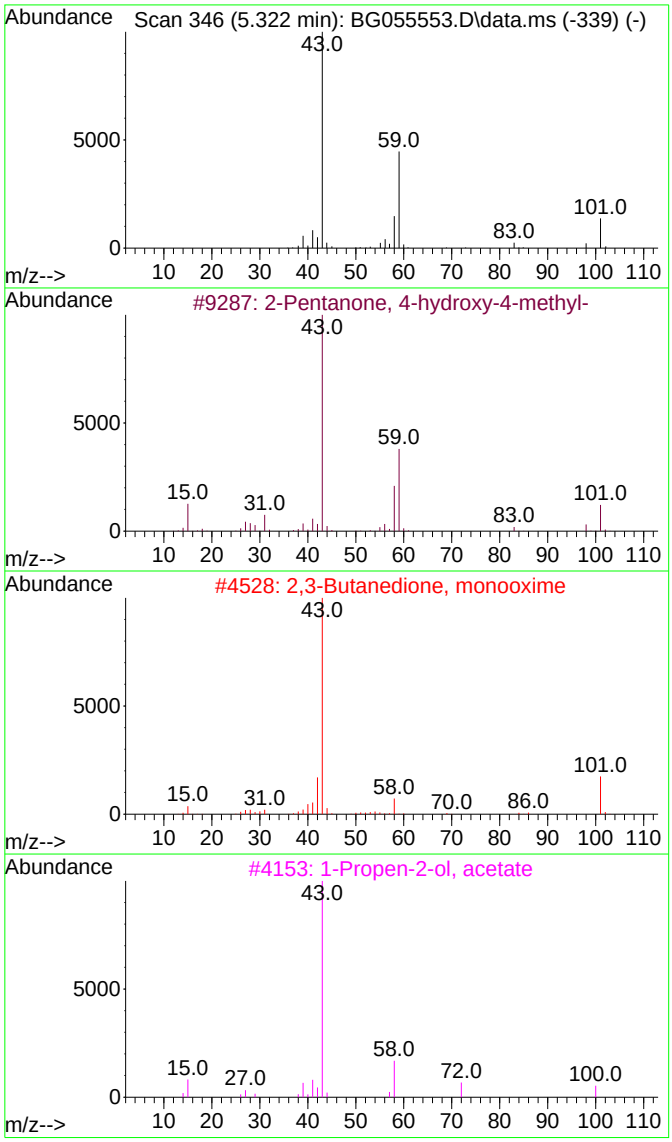
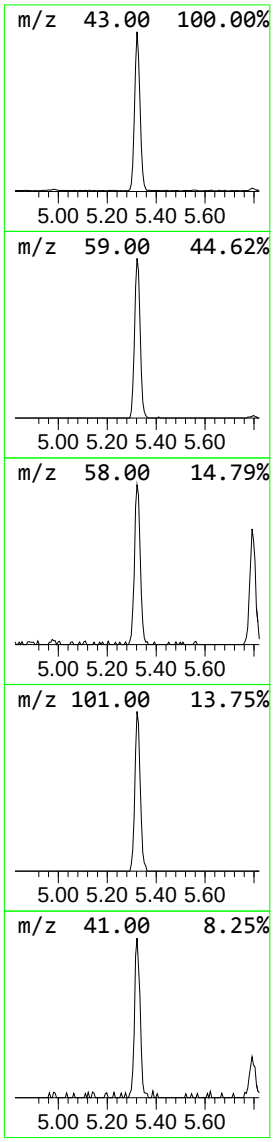
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.322	16.97 ng	247192	1,4-Dichlorobenzene-d4	8.265

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Sample : N5360-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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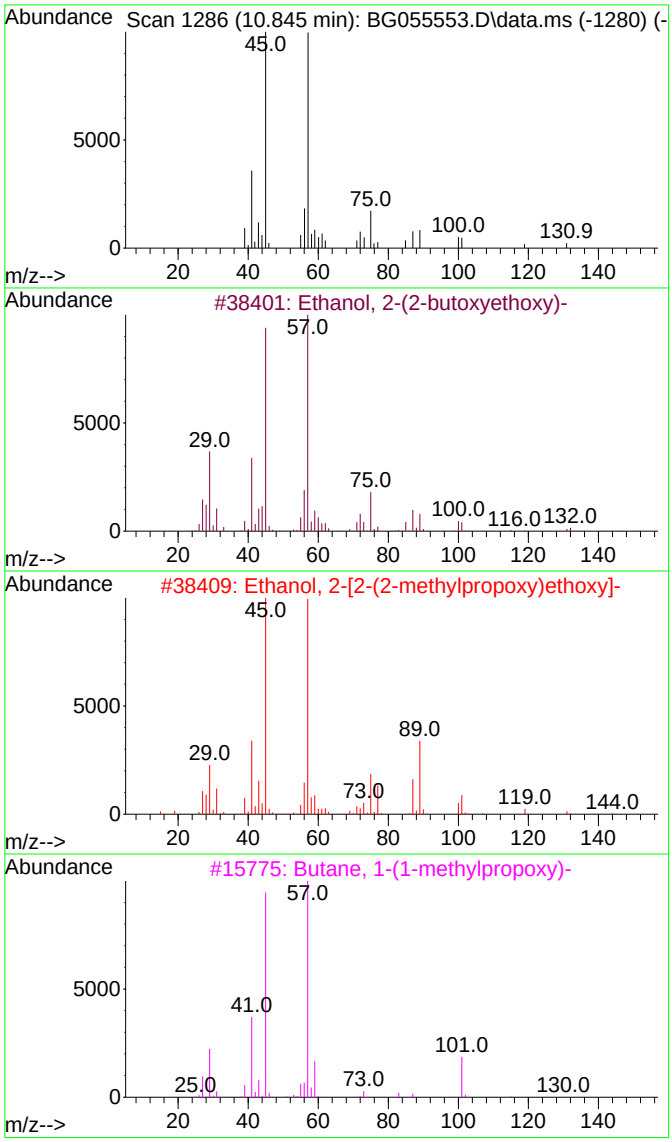
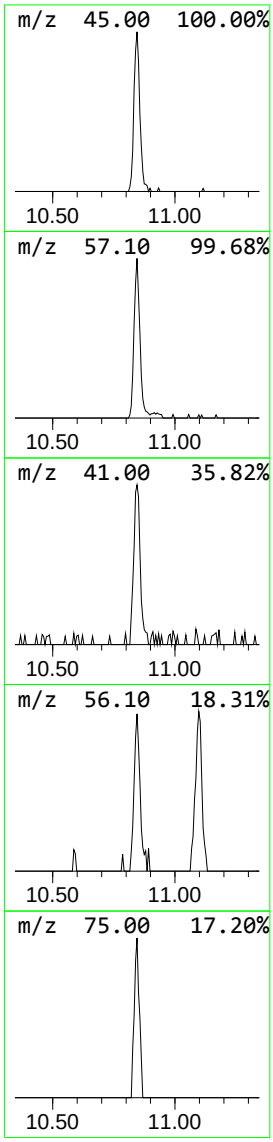
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	2.77 ng	55170	Naphthalene-d8	11.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
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Operator : CG/JU
Sample : N5360-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
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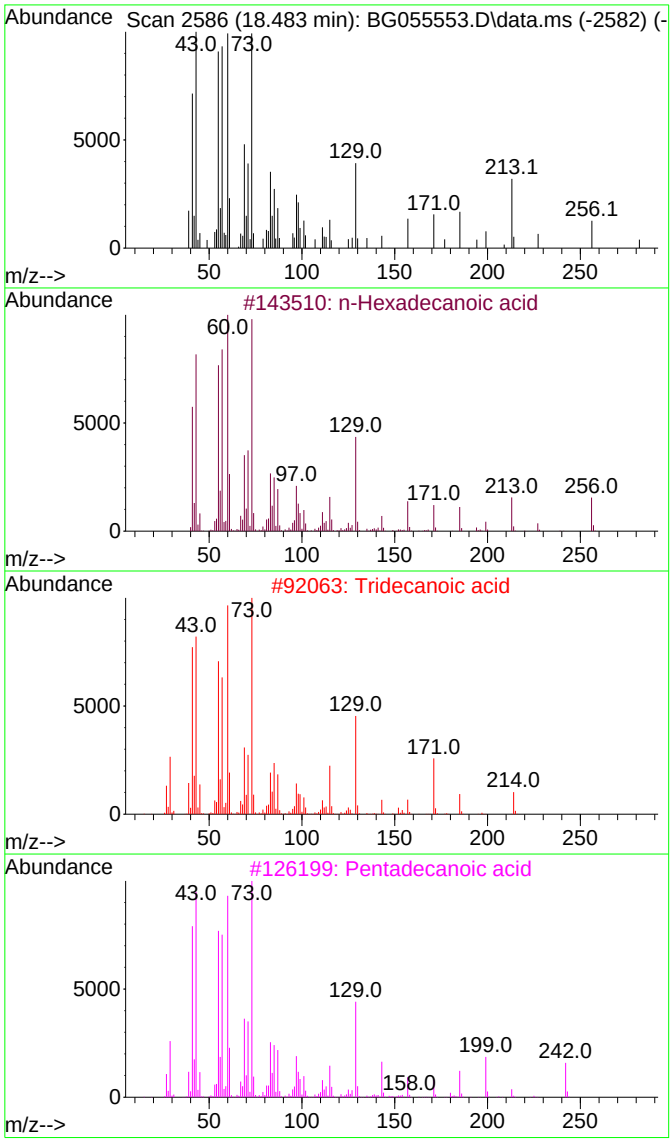
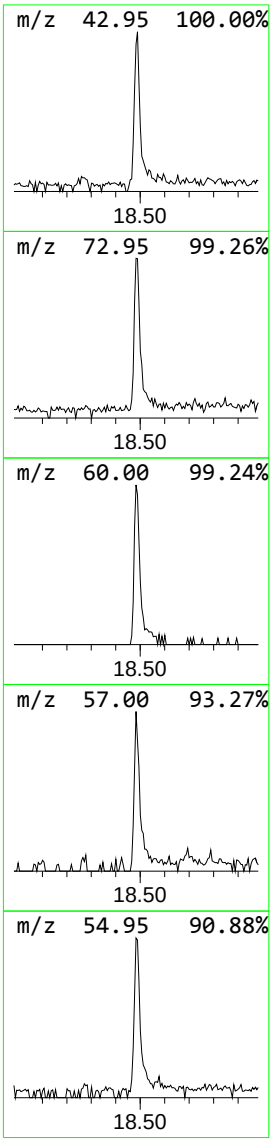
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.483	2.42 ng	87736	Phenanthrene-d10	17.625

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	18
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221113-COMP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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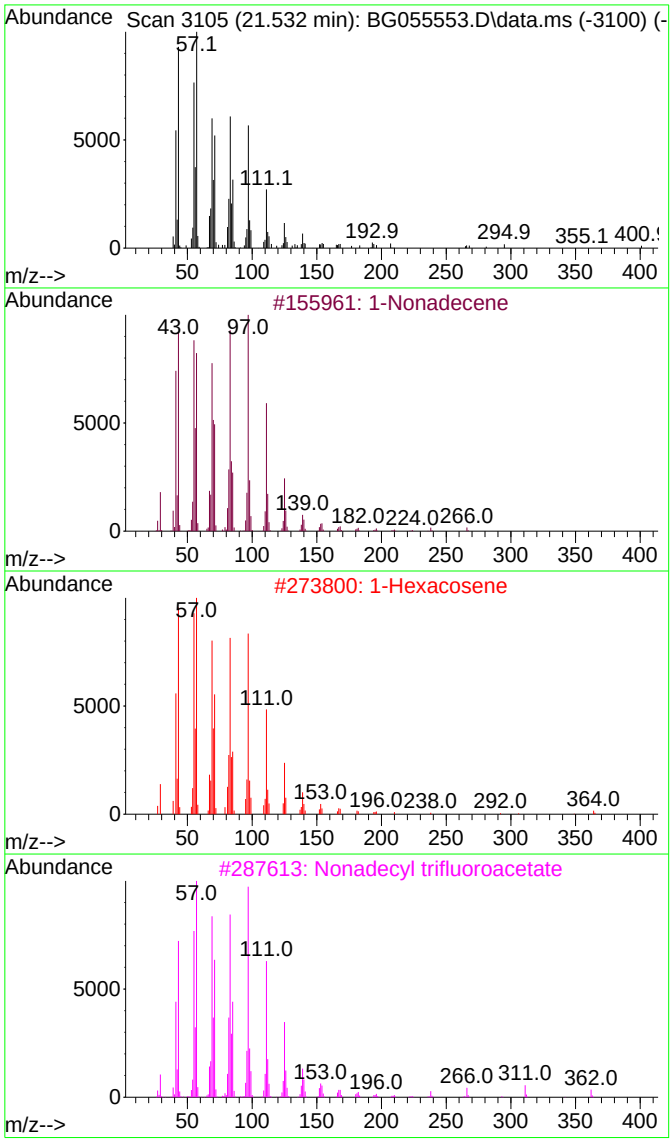
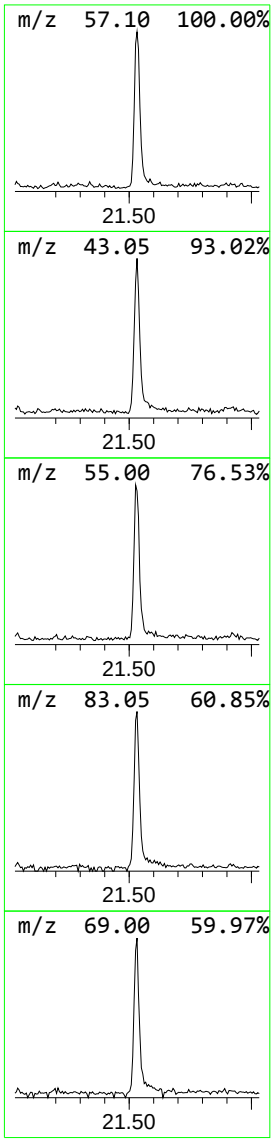
Peak Number 6 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.532	4.35 ng	191032	Chrysene-d12	21.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Cyclooctacosane	392	C28H56	000297-24-5	91





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-metho...	3.330	25.6	ng	373624	1	8.265	291375	20.0
Glycolaldehyde ...	3.371	3.4	ng	49677	1	8.265	291375	20.0
2-Pentanone, 4-...	5.322	17.0	ng	247192	1	8.265	291375	20.0
Ethanol, 2-(2-b...	10.845	2.8	ng	55170	2	11.097	398949	20.0
n-Hexadecanoic ...	18.483	2.4	ng	87736	4	17.625	726429	20.0
1-Nonadecene	21.532	4.3	ng	191032	5	21.920	879220	20.0