

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062421\
 Data File : BG049081.D
 Acq On : 24 Jun 2021 16:10
 Operator : CG/JU
 Sample : M2795-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B1GW

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: BG049081.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	28	rBV	128774	293168	10.59%	2.760%
2	3.231	29	33	44	rVB	64495	114366	4.13%	1.077%
3	5.658	437	446	455	rBV	275178	458047	16.55%	4.312%
4	7.256	710	718	725	rBV	165299	290476	10.49%	2.734%
5	8.102	856	862	869	rBV2	103333	181532	6.56%	1.709%
6	8.325	895	900	908	rVB2	37580	62791	2.27%	0.591%
7	9.271	1053	1061	1070	rBV	380901	689436	24.90%	6.490%
8	10.687	1295	1302	1308	rBV	33453	62123	2.24%	0.585%
9	10.928	1335	1343	1349	rBV	131909	250666	9.05%	2.360%
10	13.372	1751	1759	1766	rBV	923452	1418127	51.23%	13.349%
11	14.747	1986	1993	1999	rBV	208479	335236	12.11%	3.156%
12	16.233	2239	2246	2257	rBV	891438	1377220	49.75%	12.964%
13	17.497	2454	2461	2467	rBV	298133	441446	15.95%	4.155%
14	18.378	2605	2611	2620	rBV	242704	354694	12.81%	3.339%
15	19.641	2821	2826	2833	rBV	175892	252962	9.14%	2.381%
16	20.100	2898	2904	2910	rBV	2034691	2768399	100.00%	26.060%
17	21.416	3123	3128	3137	rVB3	55357	99233	3.58%	0.934%
18	21.780	3184	3190	3197	rVB	336147	570725	20.62%	5.372%
19	25.105	3745	3756	3768	rBV	197202	602600	21.77%	5.672%

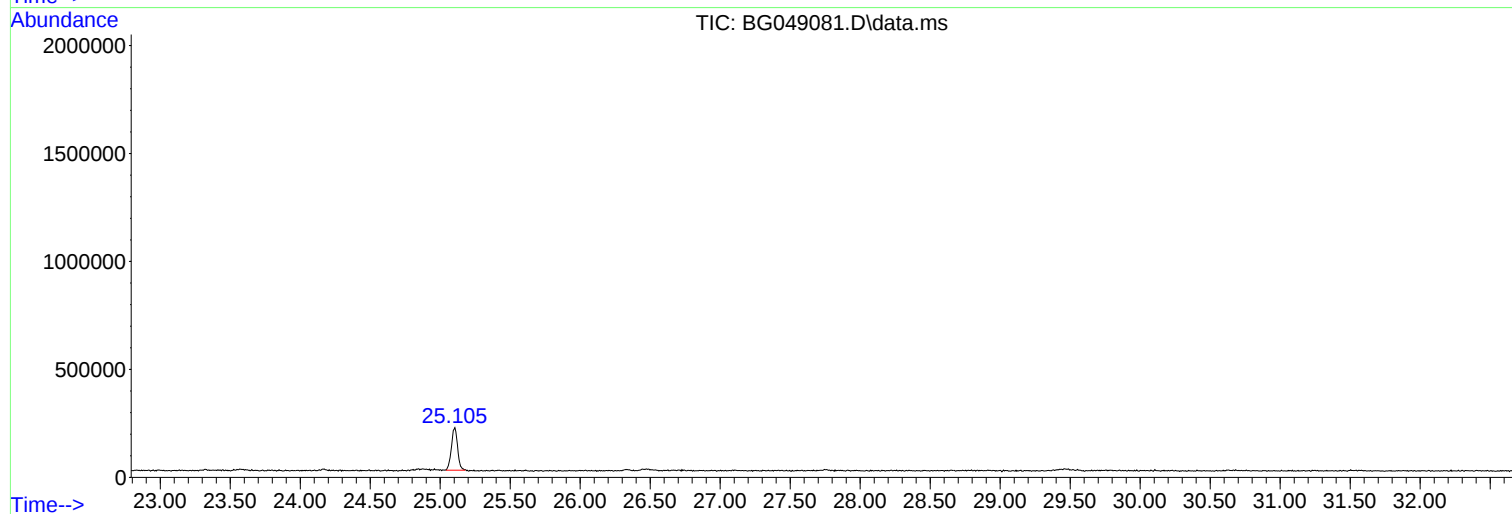
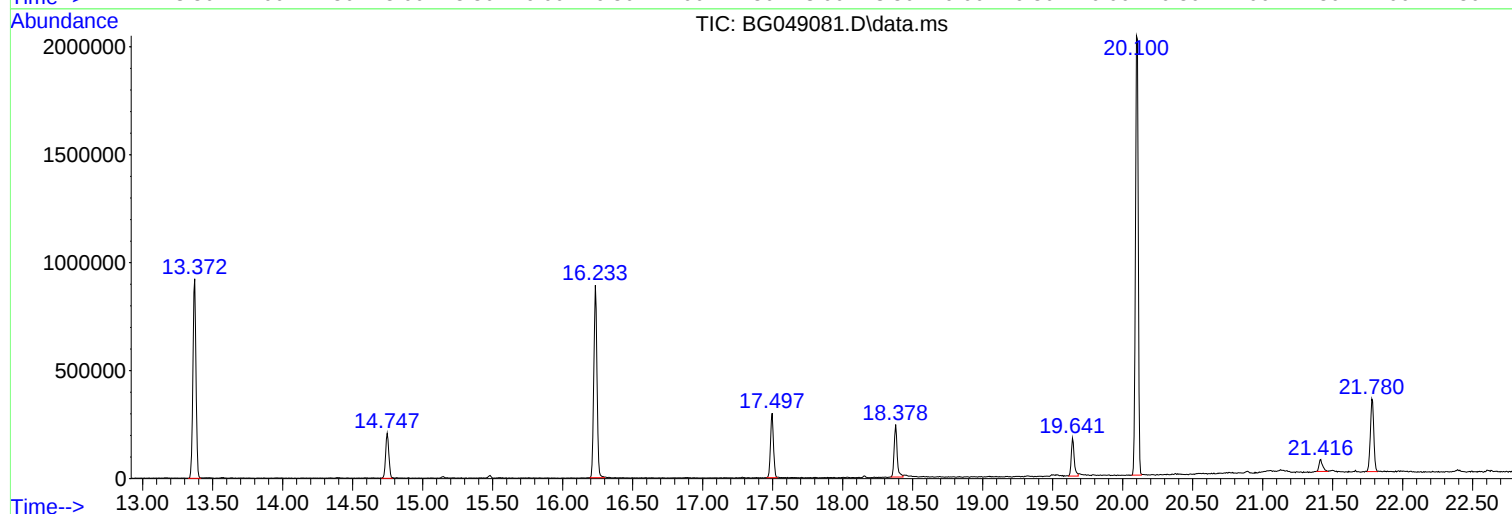
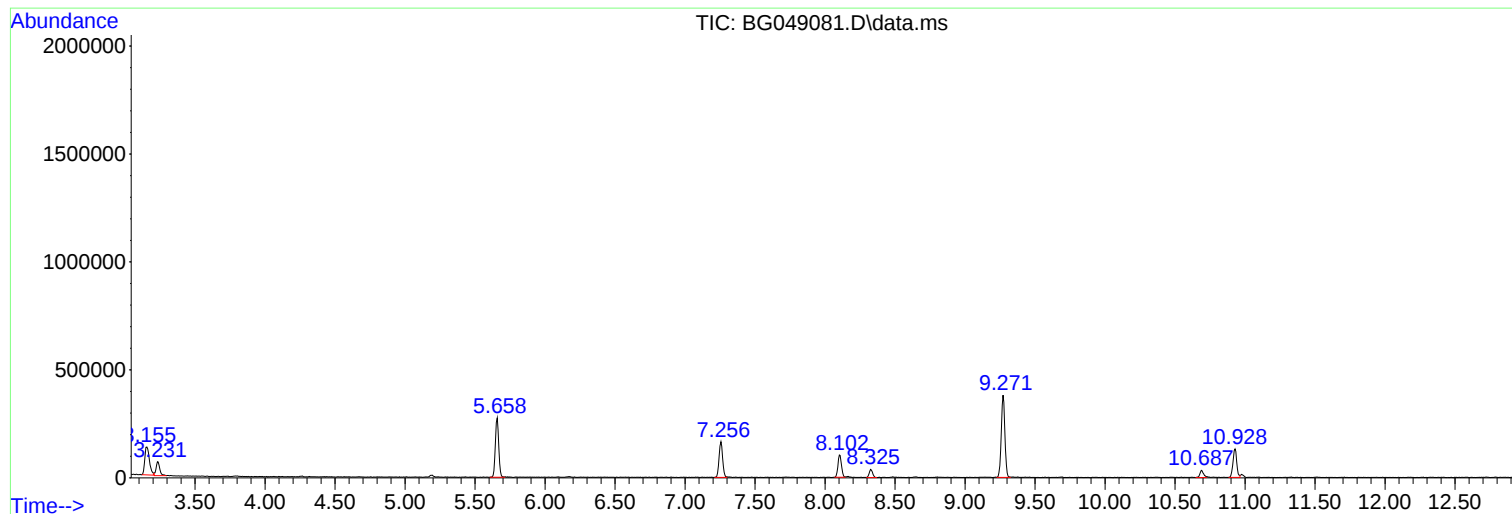
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
Sample : M2795-08
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Instrument :
BNA_G
ClientSampleId :
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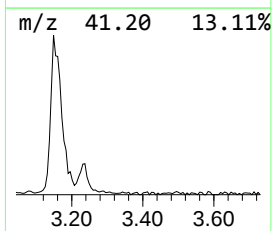
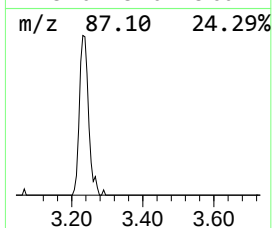
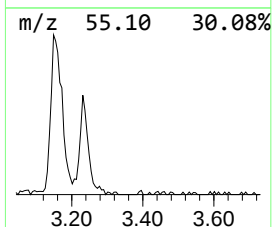
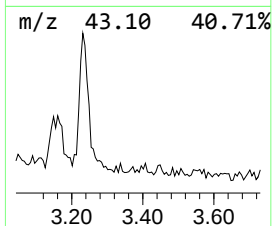
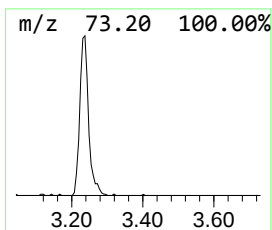
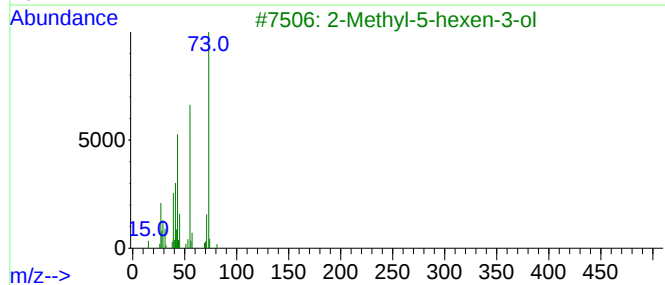
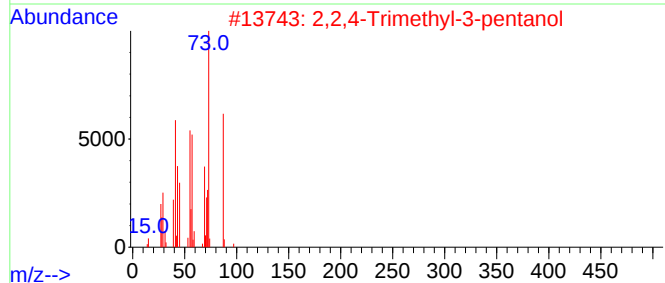
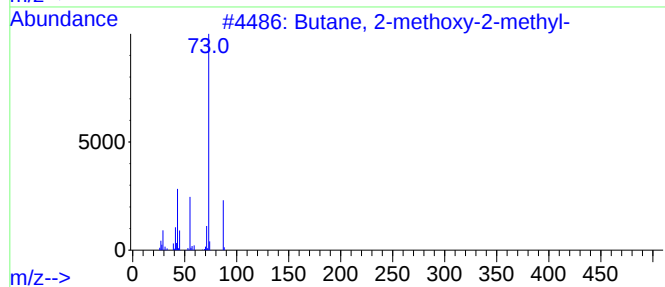
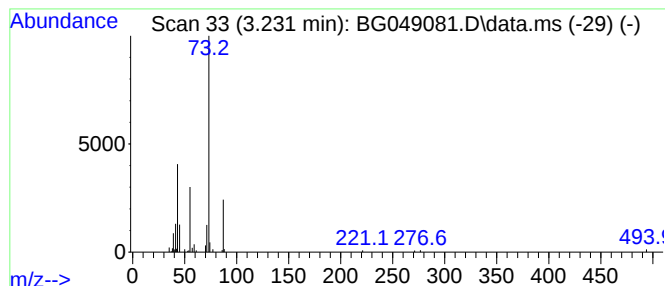
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.231	12.60 ng	114366	1,4-Dichlorobenzene-d4	8.108

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	45
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	9



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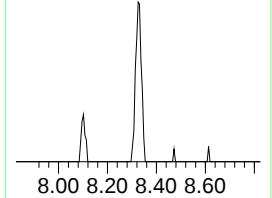
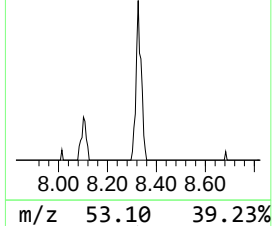
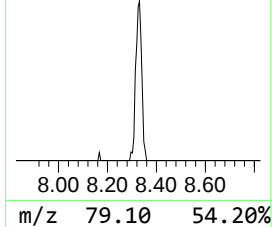
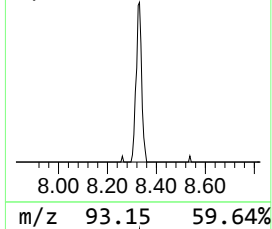
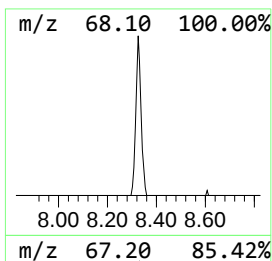
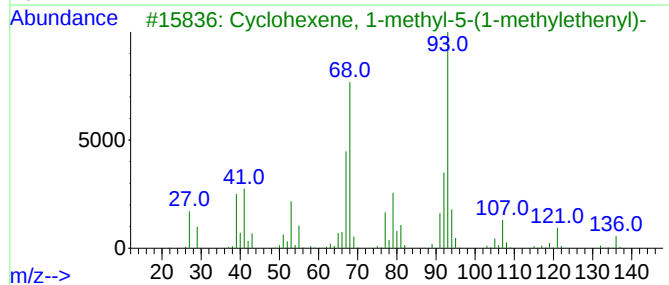
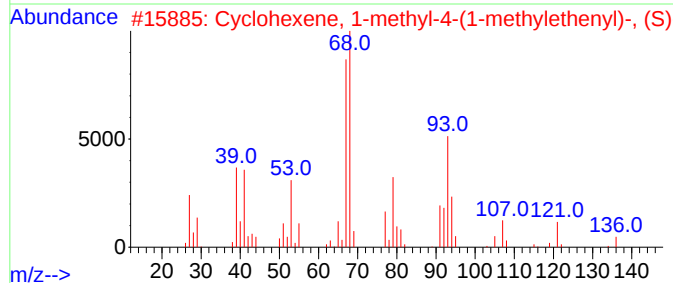
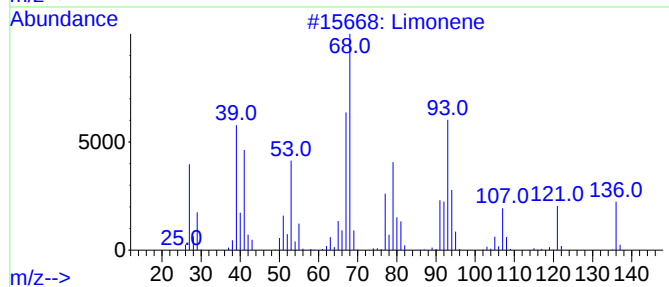
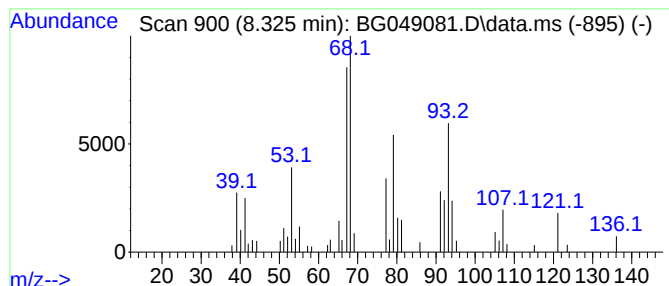
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.325	6.92 ng	62791	1,4-Dichlorobenzene-d4	8.108

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Limonene	136	C10H16	000138-86-3	91
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	90
3			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	81
4			D-Limonene	136	C10H16	005989-27-5	64
5			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	50



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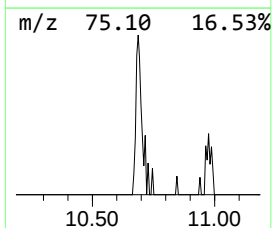
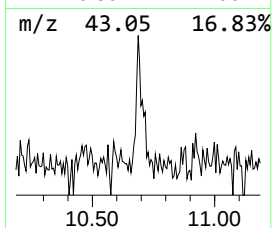
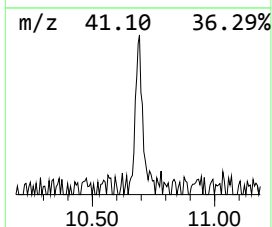
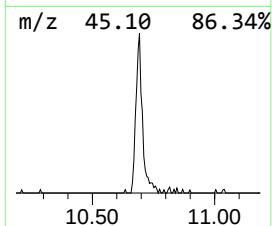
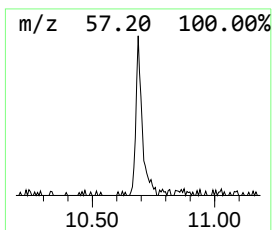
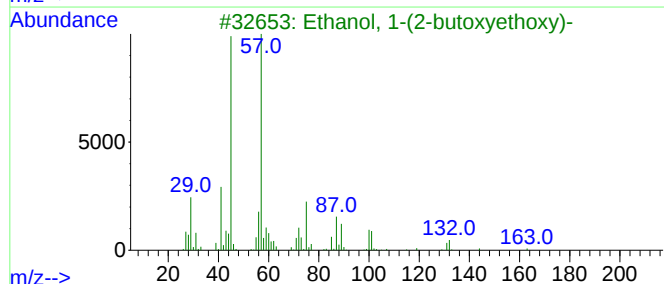
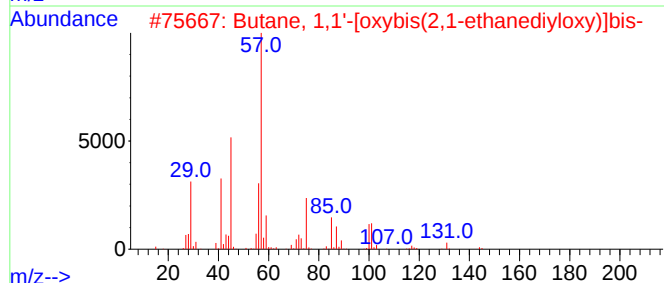
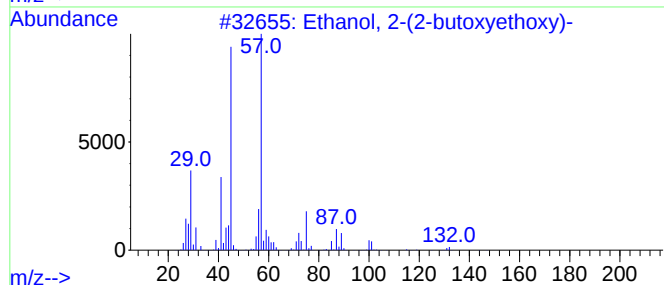
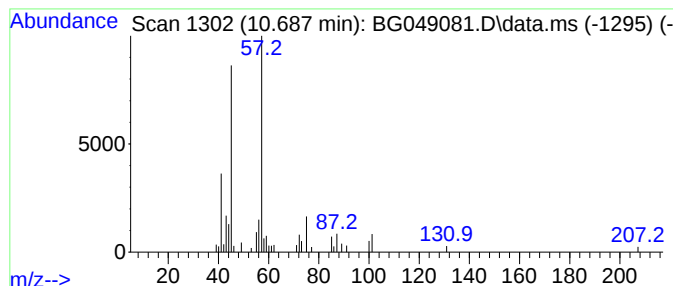
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.687	4.96 ng	62123	Naphthalene-d8	10.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	78
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
5			Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53



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Instrument :
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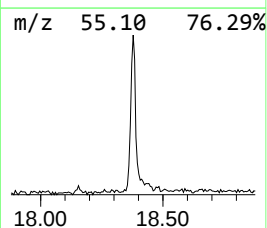
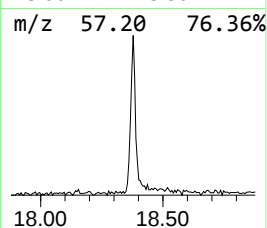
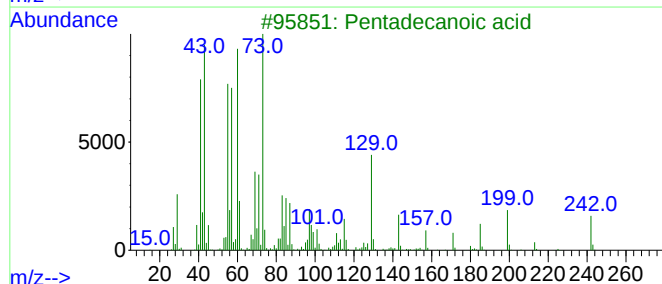
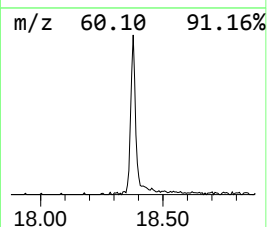
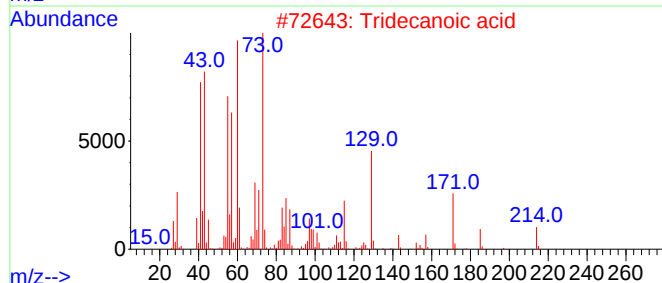
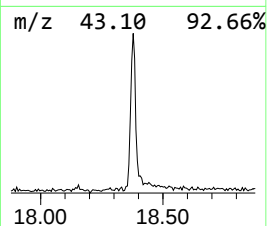
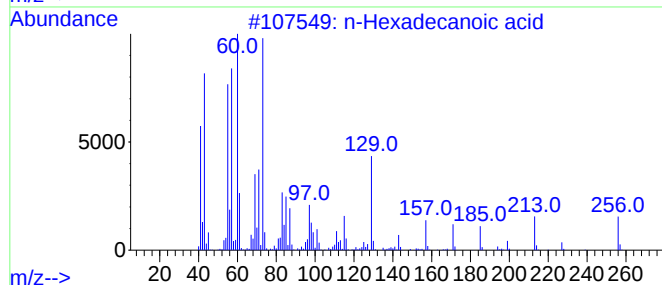
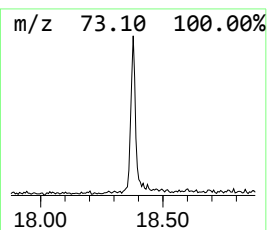
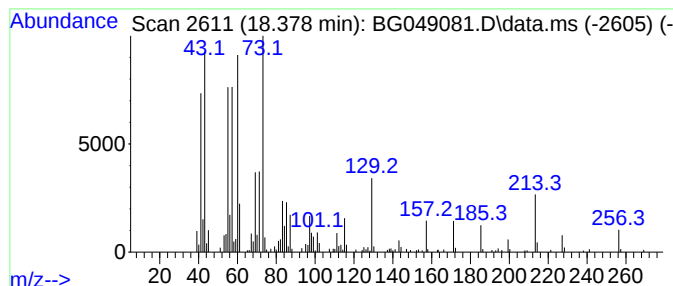
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.378	16.07 ng	354694	Phenanthrene-d10	17.497

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	59
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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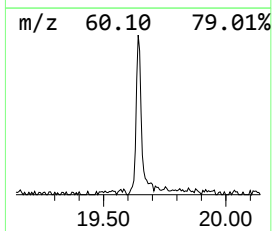
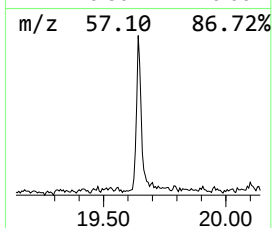
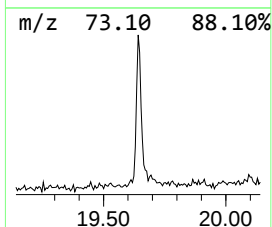
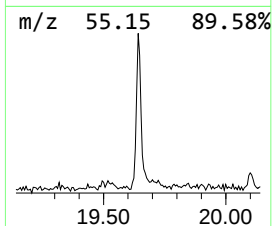
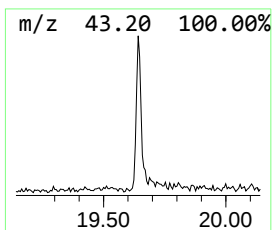
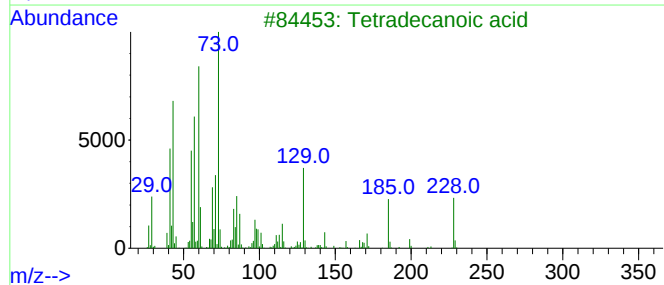
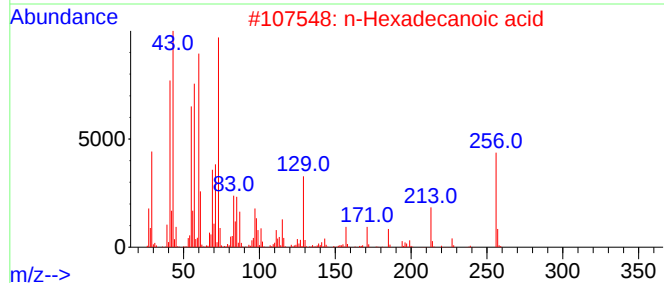
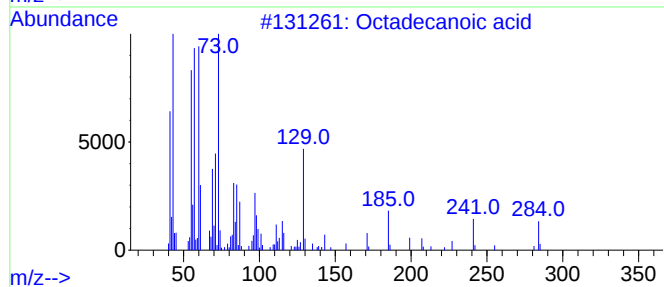
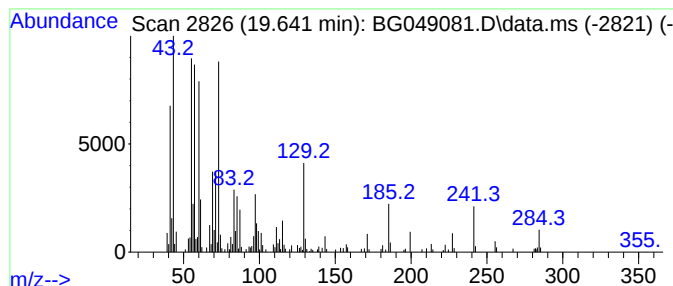
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.641	8.86 ng	252962	Chrysene-d12	21.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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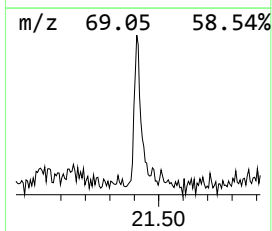
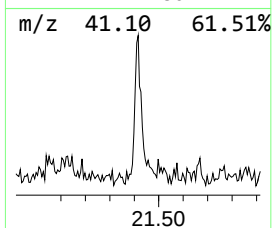
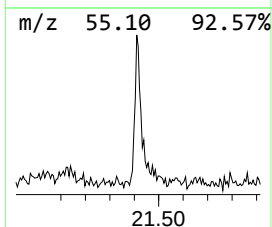
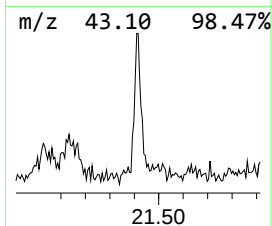
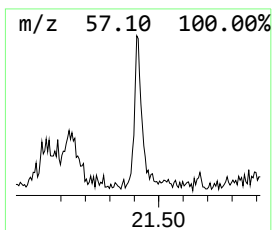
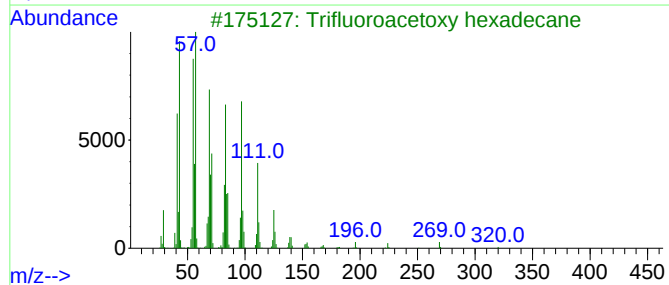
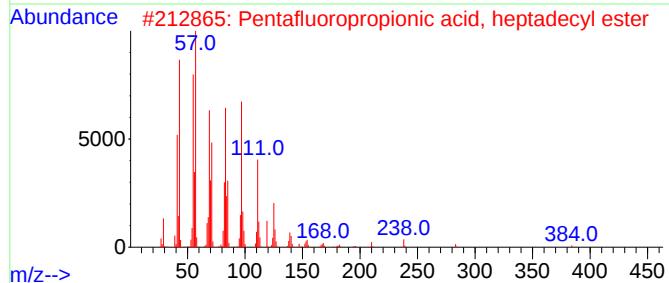
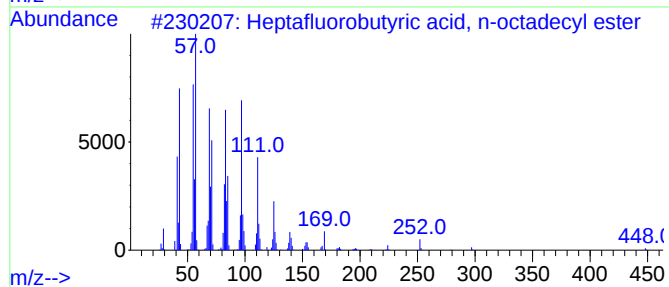
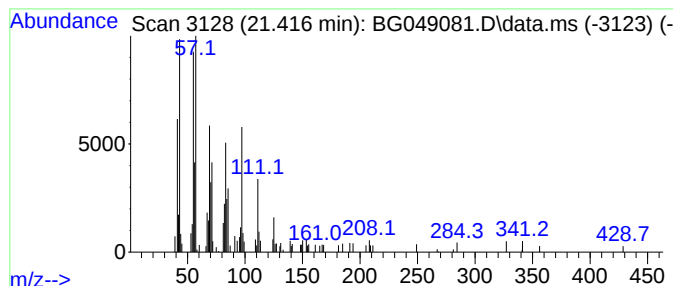
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	3.48 ng	99233	Chrysene-d12	21.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062421\
Data File : BG049081.D
Acq On : 24 Jun 2021 16:10
Operator : CG/JU
Sample : M2795-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B1GW

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.231	12.6	ng	114366	1	8.108	181532	20.0
Limonene	8.325	6.9	ng	62791	1	8.108	181532	20.0
Ethanol, 2-(2-b...	10.687	5.0	ng	62123	2	10.928	250666	20.0
n-Hexadecanoic ...	18.378	16.1	ng	354694	4	17.497	441446	20.0
Octadecanoic acid	19.641	8.9	ng	252962	5	21.780	570725	20.0
Heptafluorobuty...	21.416	3.5	ng	99233	5	21.780	570725	20.0