

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
 Data File : BG048950.D
 Acq On : 14 Jun 2021 15:25
 Operator : CG/JU
 Sample : M2687-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 17-B6(100-104)

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: BG048950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	16	21	35	rVB	173237	305707	19.09%	2.990%
2	3.288	38	42	51	rVB2	72895	108443	6.77%	1.061%
3	3.787	122	127	132	rBV4	17139	28075	1.75%	0.275%
4	4.275	202	210	215	rVB6	9616	17305	1.08%	0.169%
5	5.203	363	368	376	rBV	50259	83861	5.24%	0.820%
6	5.662	440	446	455	rBV	523868	852796	53.26%	8.341%
7	5.738	455	459	468	rVB3	19494	46551	2.91%	0.455%
8	6.114	519	523	528	rBV3	10855	16761	1.05%	0.164%
9	7.260	708	718	727	rBV	546040	955570	59.68%	9.346%
10	8.117	856	864	871	rBV	130288	228121	14.25%	2.231%
11	9.287	1055	1063	1072	rVB	318667	579880	36.22%	5.672%
12	10.703	1298	1304	1317	rBV2	106967	178164	11.13%	1.743%
13	10.944	1335	1345	1352	rBV	171347	315281	19.69%	3.084%
14	13.388	1754	1761	1768	rBV	672254	1065425	66.54%	10.420%
15	13.588	1789	1795	1799	rBV3	10535	16835	1.05%	0.165%
16	14.763	1988	1995	2004	rVB	277103	443348	27.69%	4.336%
17	16.161	2227	2233	2237	rBV	50515	68735	4.29%	0.672%
18	16.243	2241	2247	2255	rBV	637695	1029006	64.27%	10.064%
19	17.512	2456	2463	2470	rBV	366727	576685	36.02%	5.640%
20	17.630	2478	2483	2490	rVB3	32670	49279	3.08%	0.482%
21	18.170	2570	2575	2580	rBV7	26214	39004	2.44%	0.381%
22	18.394	2608	2613	2623	rBV3	44975	80265	5.01%	0.785%
23	19.322	2768	2771	2774	rBV5	11543	16878	1.05%	0.165%
24	19.663	2825	2829	2833	rBV5	23691	35895	2.24%	0.351%
25	19.898	2865	2869	2872	rVB3	16588	18070	1.13%	0.177%
26	20.115	2900	2906	2917	rVB	1176438	1601145	100.00%	15.660%
27	20.797	3017	3022	3027	rBV6	16643	29611	1.85%	0.290%
28	20.879	3032	3036	3039	rVB3	23956	33591	2.10%	0.329%
29	21.437	3127	3131	3140	rBV2	66367	122665	7.66%	1.200%
30	21.690	3171	3174	3179	rVB	43812	61366	3.83%	0.600%
31	21.801	3187	3193	3200	rVB2	356866	587303	36.68%	5.744%
32	23.035	3398	3403	3410	rVB7	33173	59776	3.73%	0.585%
33	25.145	3752	3762	3772	rVB2	192604	573019	35.79%	5.604%

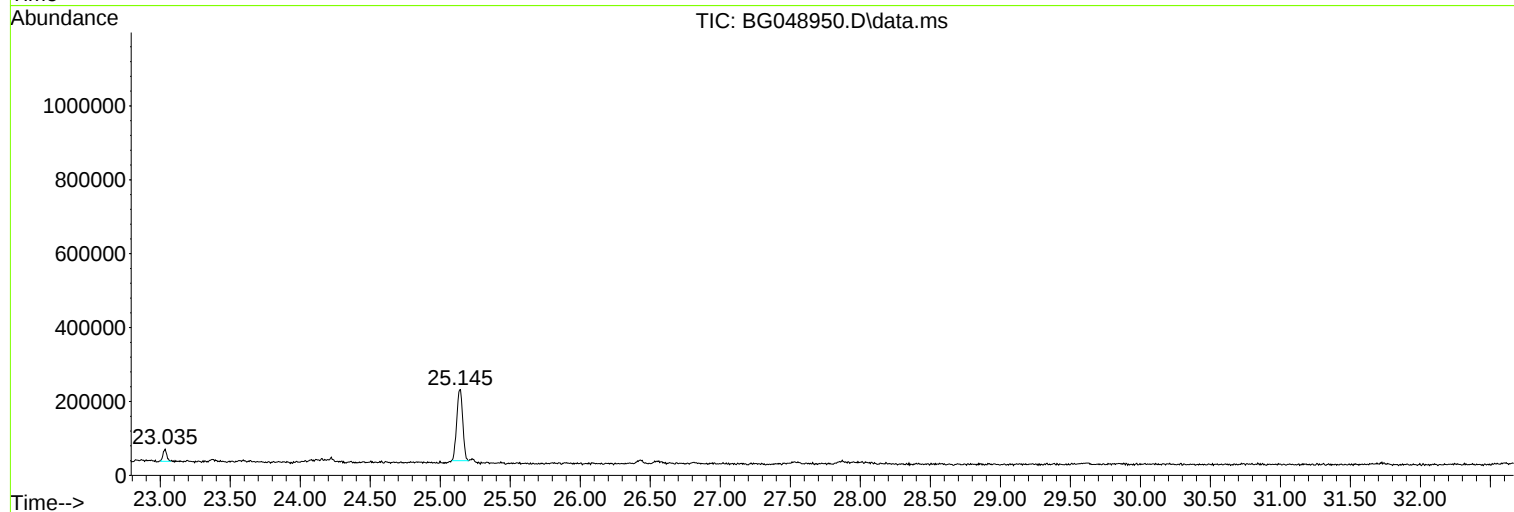
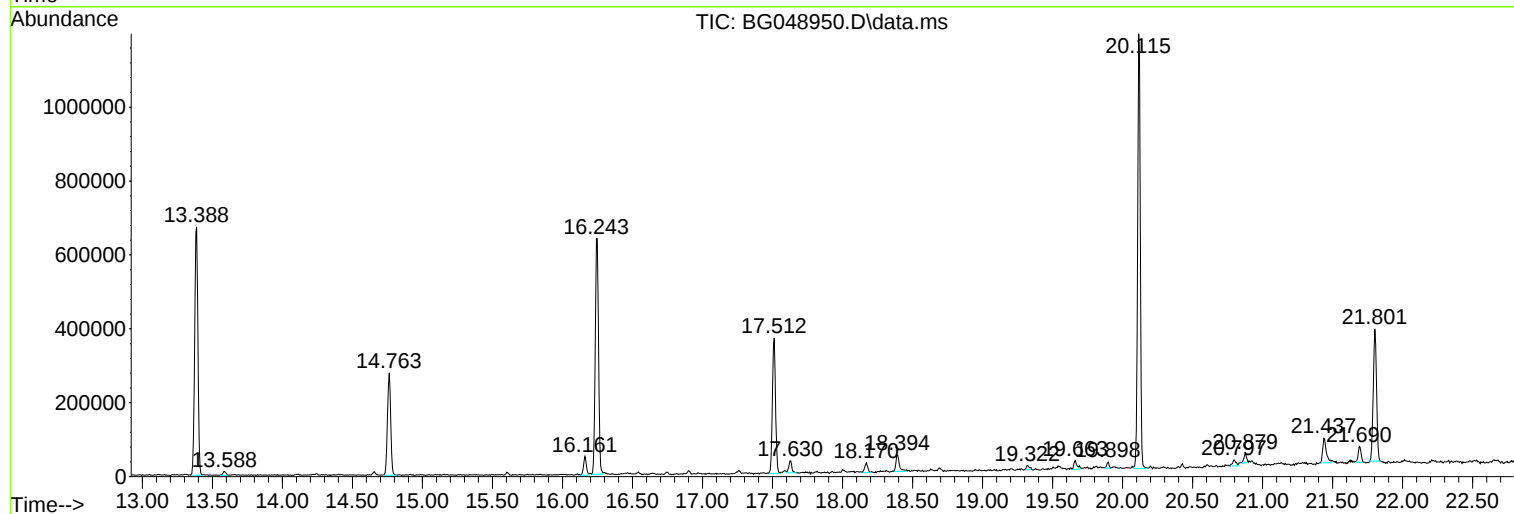
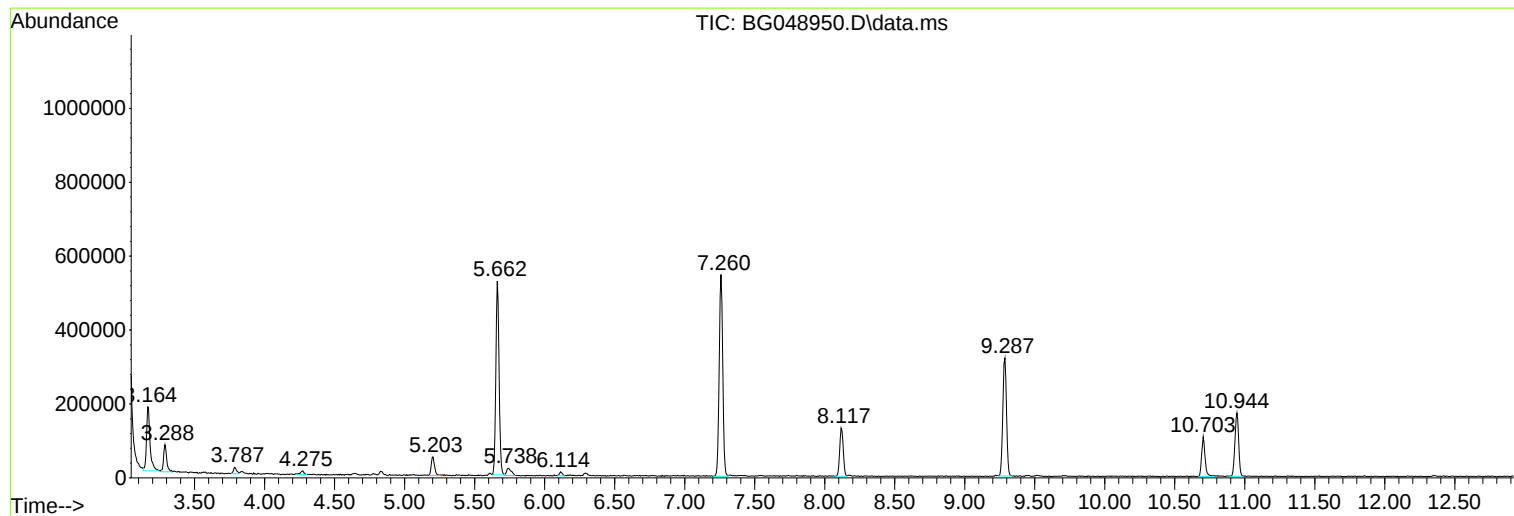
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Instrument :
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ClientSampleId :
17-B6(100-104)

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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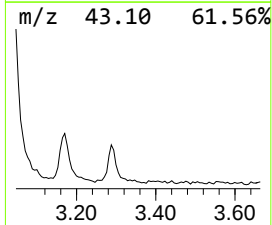
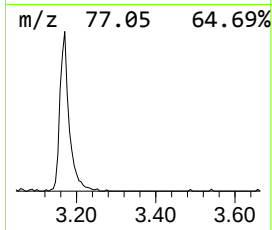
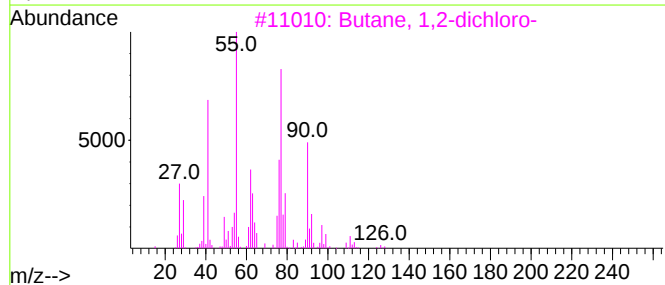
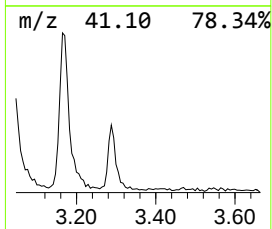
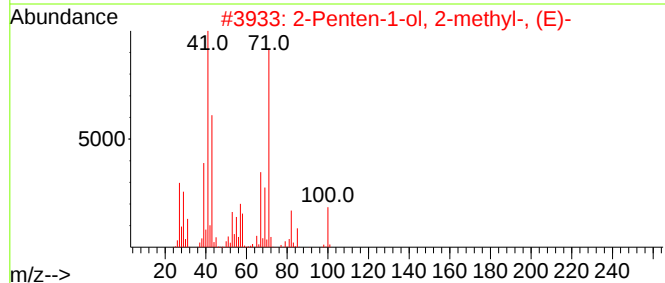
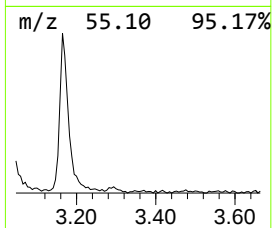
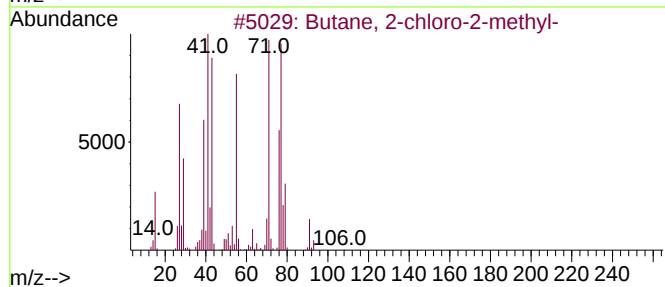
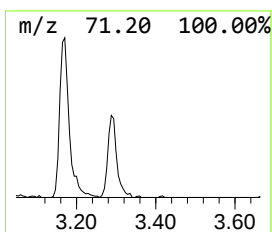
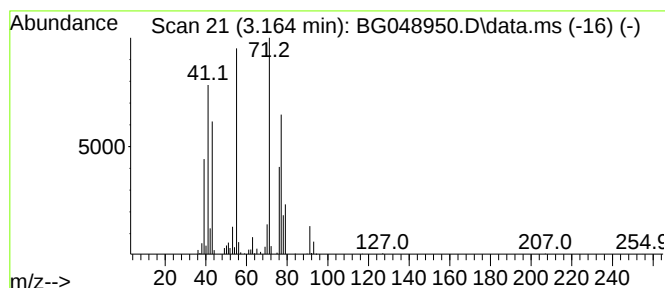
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	26.80 ng	305707	1,4-Dichlorobenzene-d4	8.117

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	72
2			2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	25
3			Butane, 1,2-dichloro-	126	C4H8Cl2	000616-21-7	25
4			Allyl chloride	76	C3H5Cl	000107-05-1	22
5			Tetrahydrofurfuryl acrylate	156	C8H12O3	002399-48-6	22



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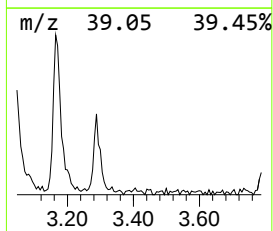
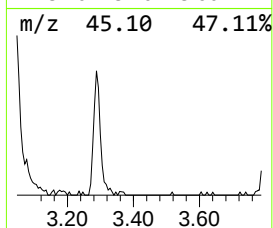
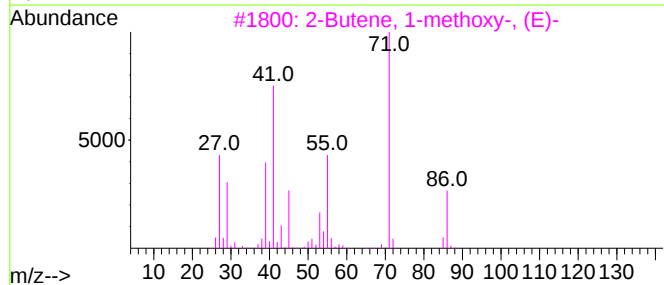
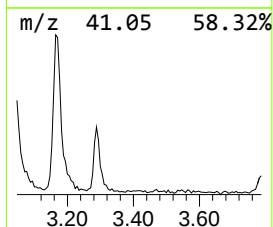
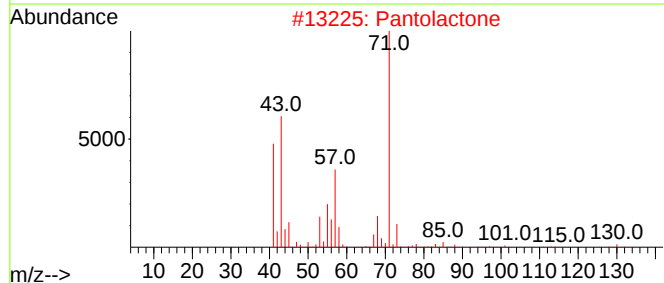
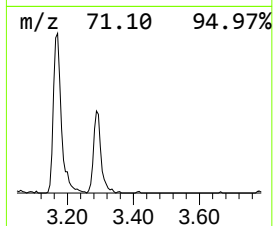
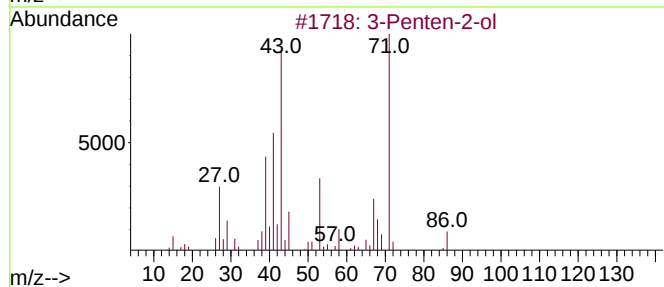
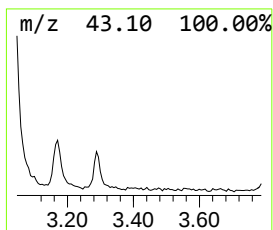
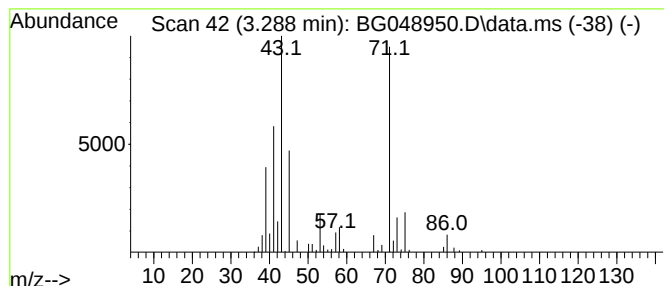
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.288	9.51 ng	108443	1,4-Dichlorobenzene-d4	8.117

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-ol	86	C5H10O	001569-50-2	62
2		Pantolactone	130	C6H10O3	000599-04-2	50
3		2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	40
4		1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	40
5		1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	37



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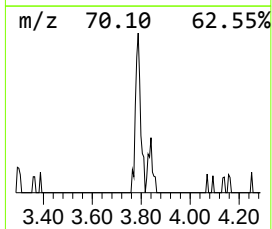
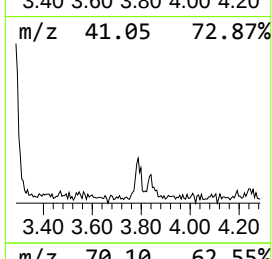
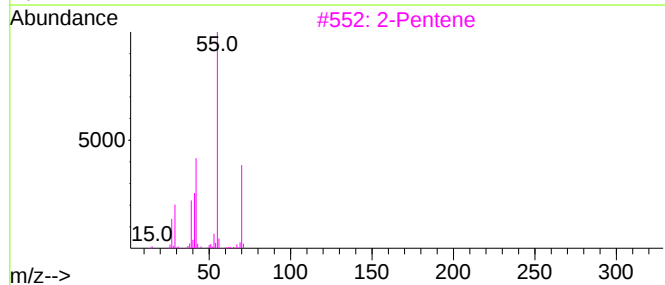
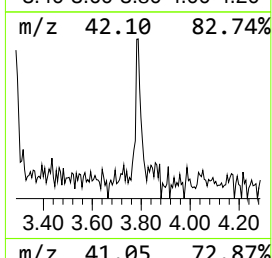
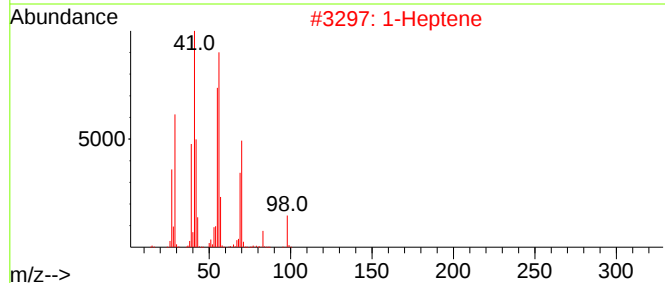
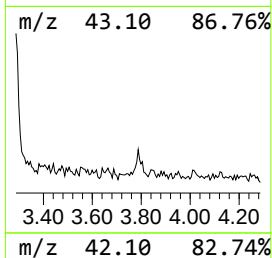
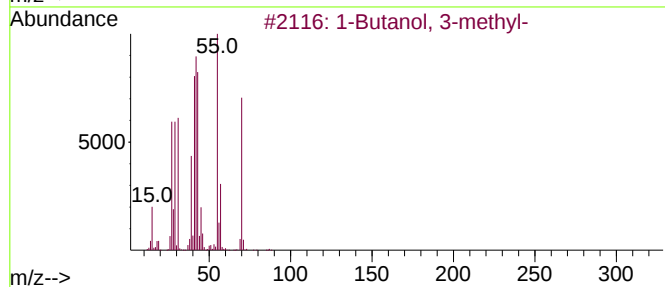
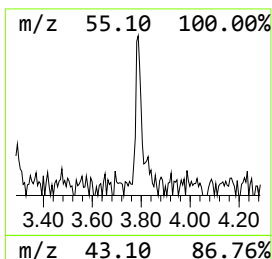
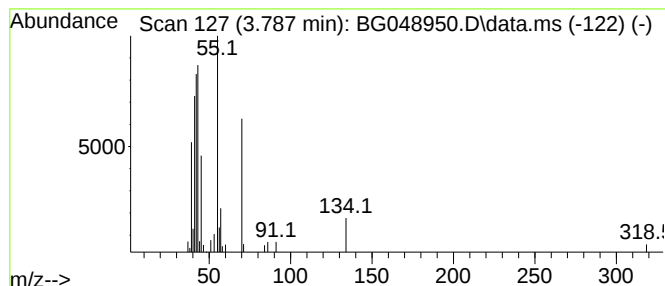
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Butanol, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.787	2.46 ng	28075	1,4-Dichlorobenzene-d4	8.117

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	59
2		1-Heptene	98	C7H14	000592-76-7	53
3		2-Pentene	70	C5H10	000109-68-2	53
4		2-Pentene, (Z)-	70	C5H10	000627-20-3	53
5		2-Pentene, (E)-	70	C5H10	000646-04-8	50



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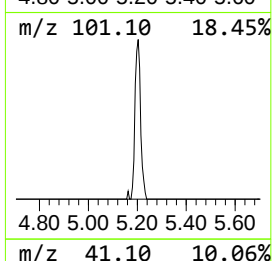
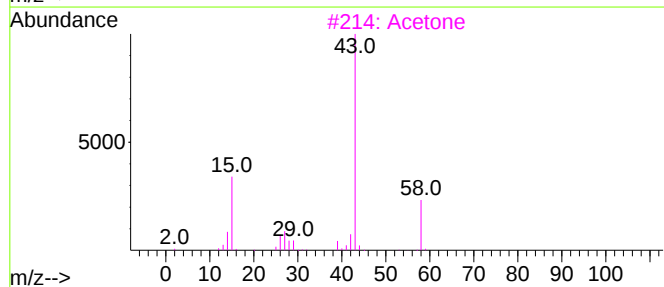
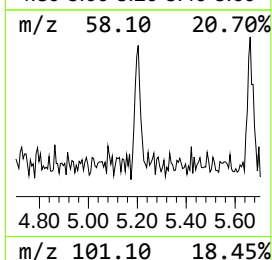
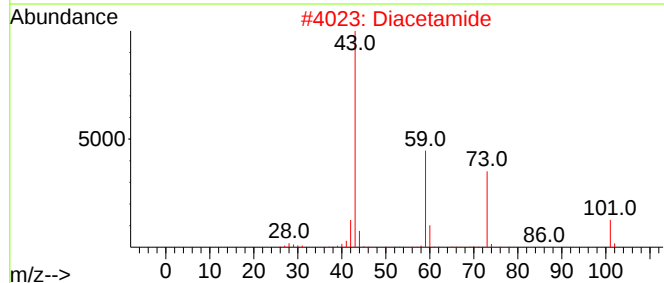
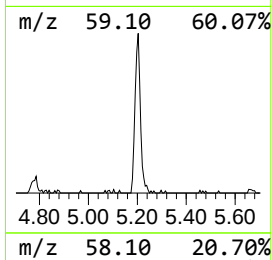
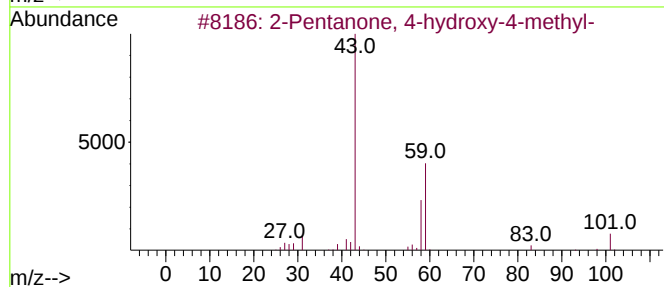
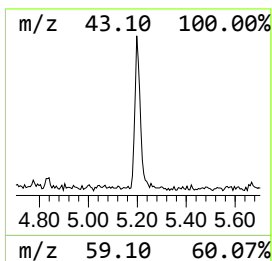
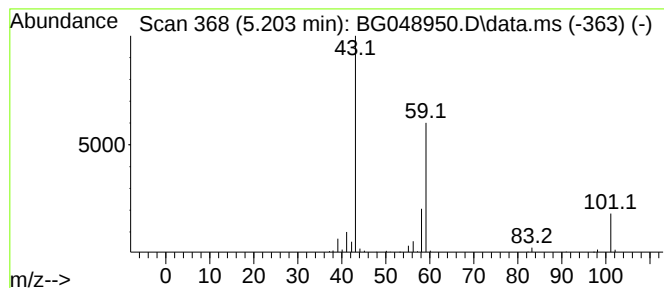
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.203	7.35 ng	83861	1,4-Dichlorobenzene-d4	8.117

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45	
2	Diacetamide	101	C4H7NO2	000625-77-4	33	
3	Acetone	58	C3H6O	000067-64-1	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9	



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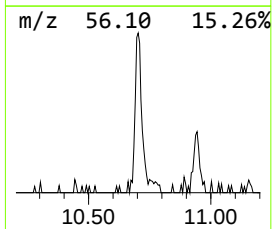
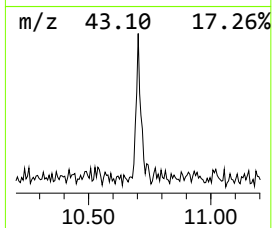
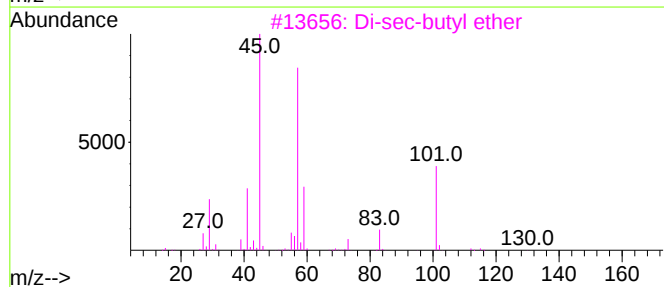
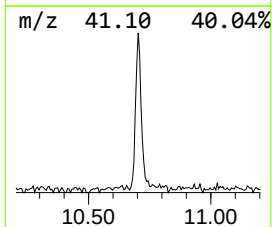
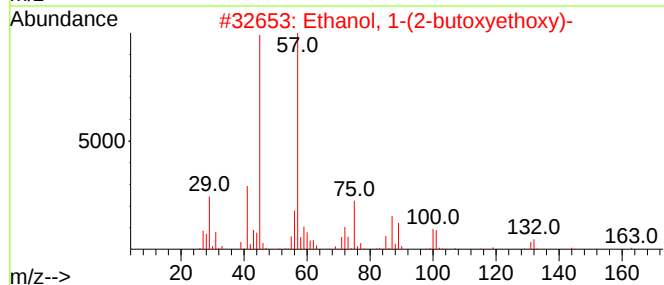
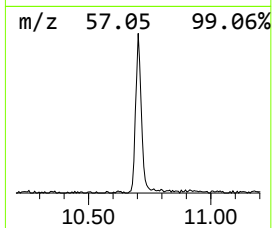
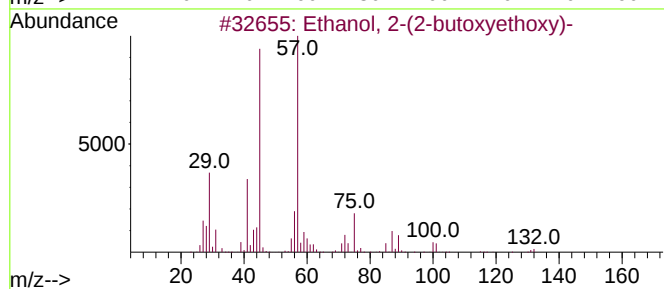
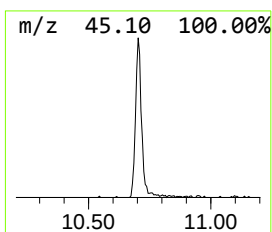
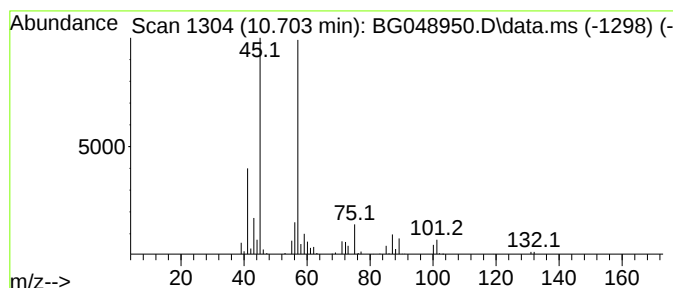
Instrument :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.703	11.30 ng	178164	Naphthalene-d8	10.944	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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17-B6(100-104)

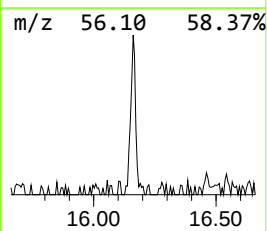
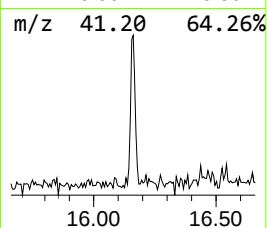
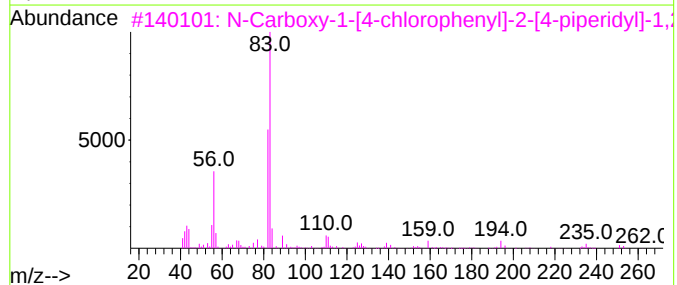
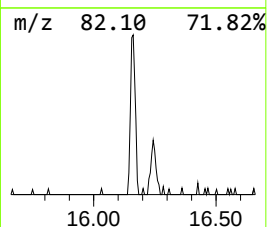
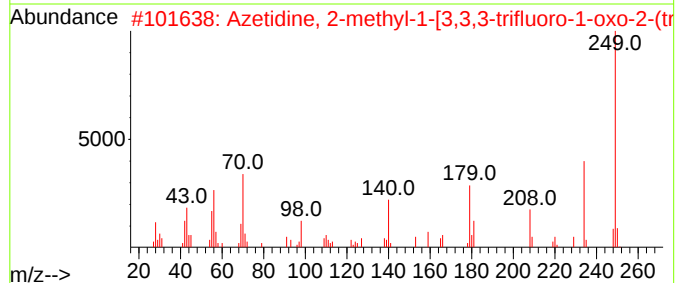
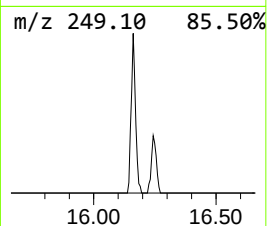
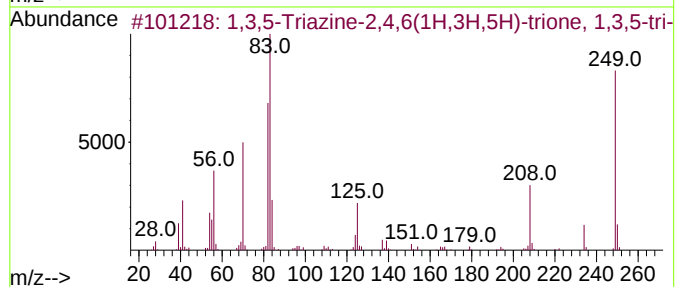
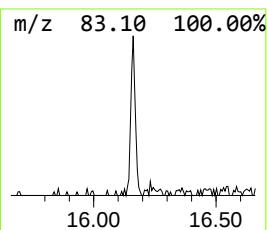
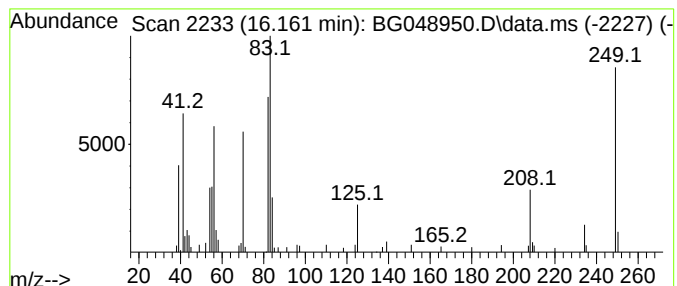
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.161	2.38 ng	68735	Phenanthrene-d10	17.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	95		
2	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	25		
3	N-Carboxy-1-[4-chlorophenyl]-2-[...	295	C15H18ClNO3	058158-38-6	25		
4	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	17		
5	n-Pentadecylcyclohexane	294	C21H42	006006-95-7	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048950.D
Acq On : 14 Jun 2021 15:25
Operator : CG/JU
Sample : M2687-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(100-104)

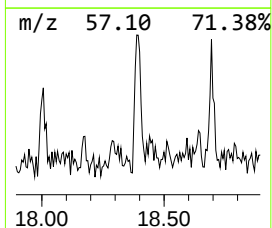
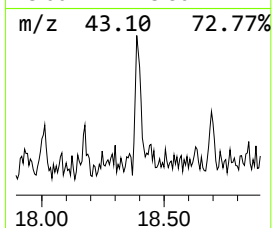
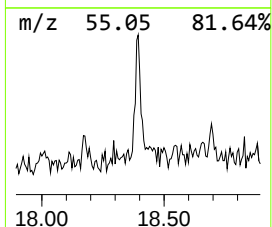
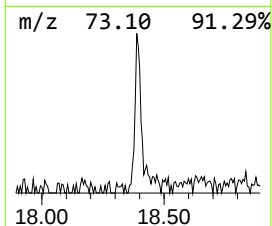
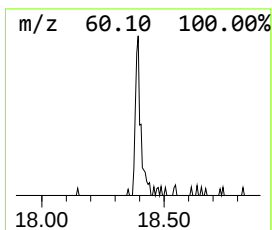
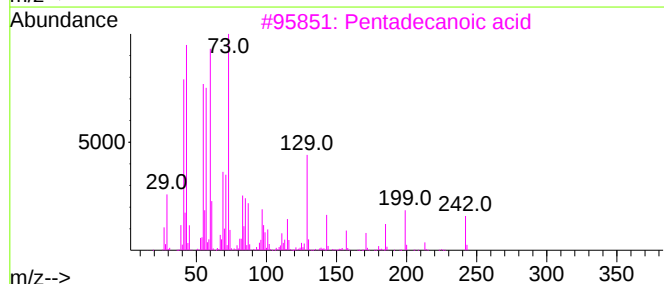
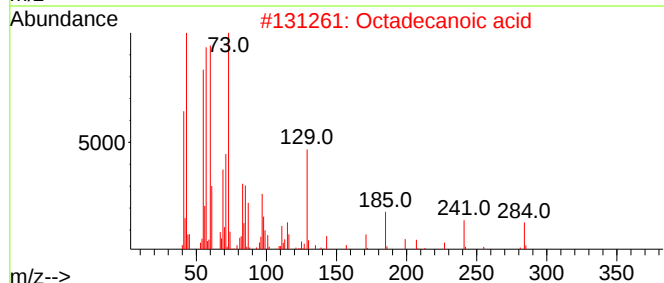
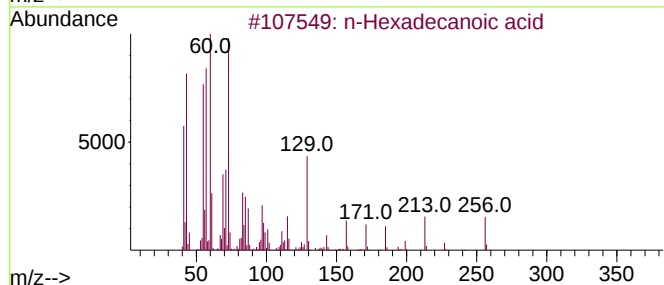
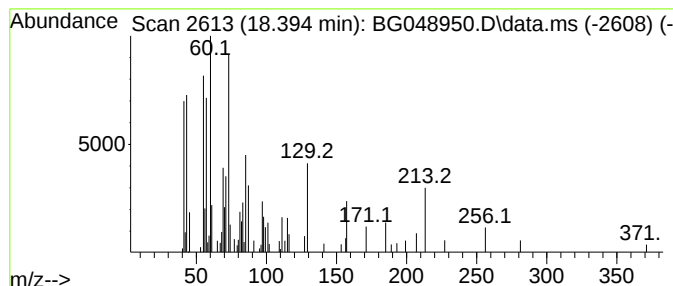
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.394	2.78 ng	80265	Phenanthrene-d10	17.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048950.D
Acq On : 14 Jun 2021 15:25
Operator : CG/JU
Sample : M2687-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

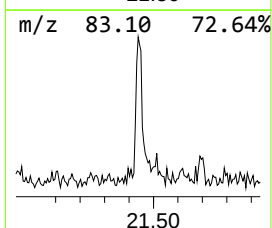
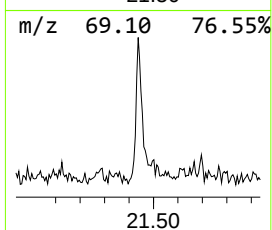
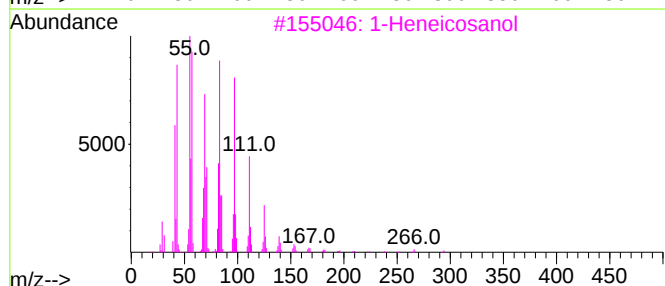
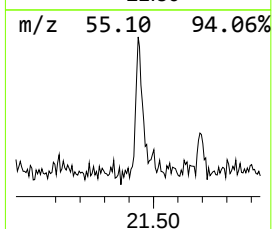
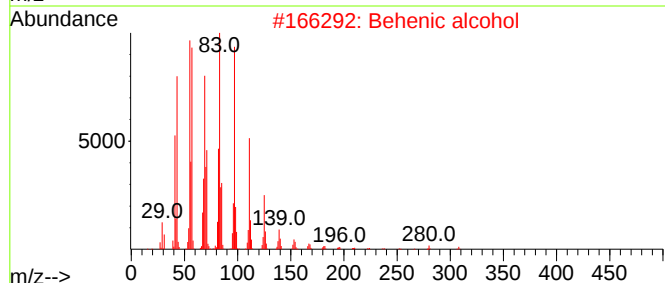
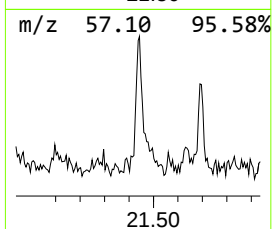
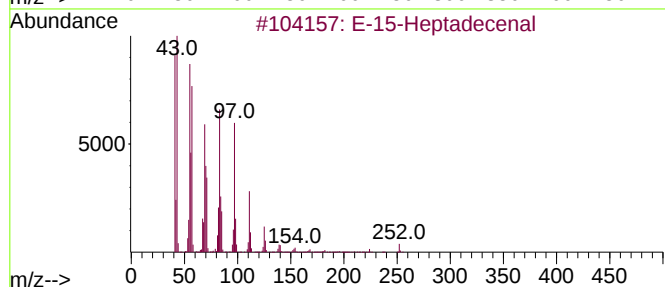
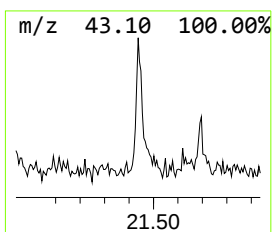
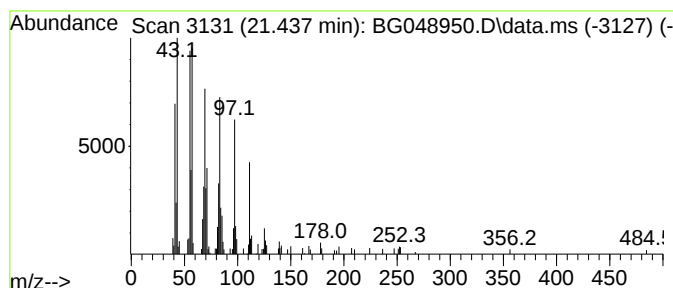
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ClientSampleId :
17-B6(100-104)

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 9 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.437	4.18 ng	122665	Chrysene-d12	21.801	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	1-Heneicosanol	312	C21H44O	015594-90-8	90
4	1-Octadecene	252	C18H36	000112-88-9	89
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048950.D
Acq On : 14 Jun 2021 15:25
Operator : CG/JU
Sample : M2687-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

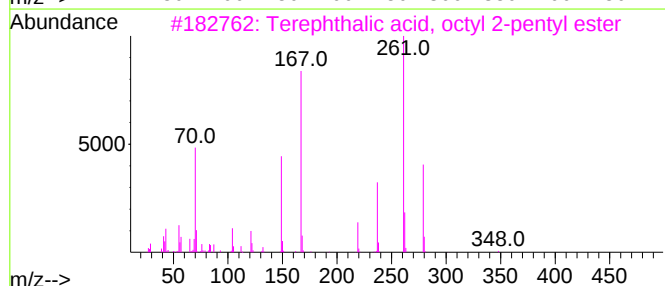
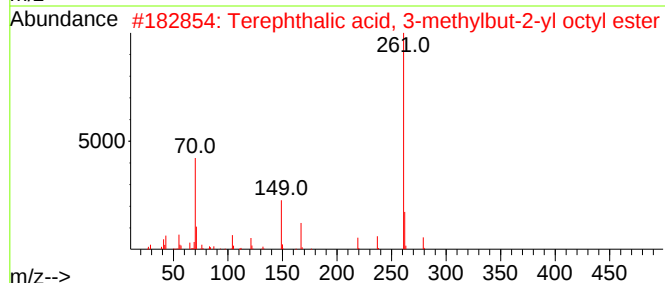
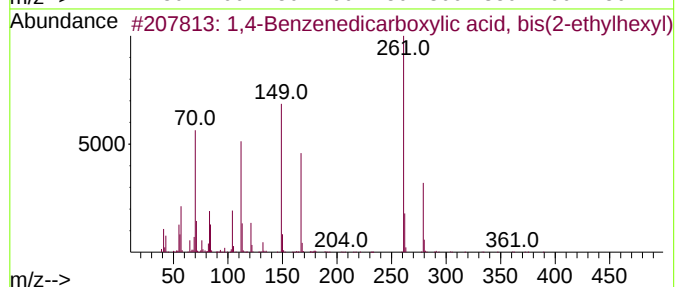
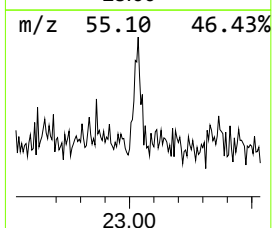
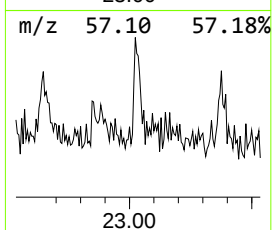
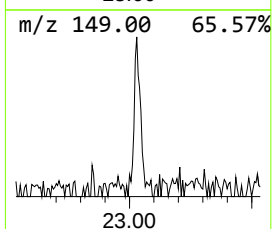
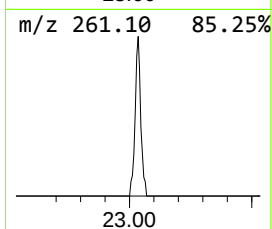
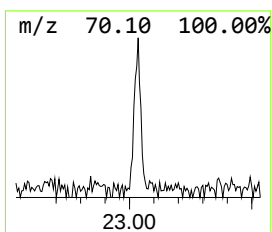
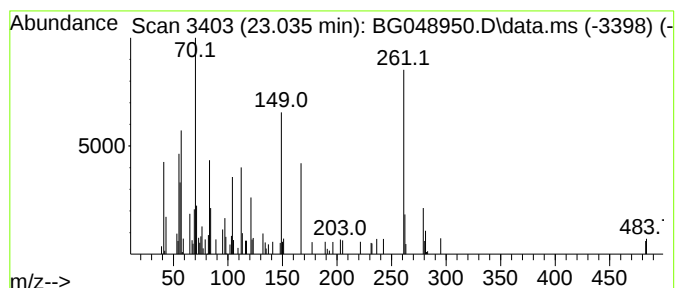
Instrument :
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ClientSampleId :
17-B6(100-104)

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 10 1,4-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.035	2.04 ng	59776	Chrysene-d12	21.801	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	59
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
3	Terephthalic acid, octyl 2-penty...	348	C21H32O4	1000323-55-2	47
4	Isophthalic acid, hept-3-yl octy...	376	C23H36O4	1000356-51-7	35
5	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048950.D
Acq On : 14 Jun 2021 15:25
Operator : CG/JU
Sample : M2687-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(100-104)

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-chlor...	3.164	26.8	ng	305707	1	8.117	228121	20.0
3-Penten-2-ol	3.288	9.5	ng	108443	1	8.117	228121	20.0
1-Butanol, 3-me...	3.787	2.5	ng	28075	1	8.117	228121	20.0
2-Pentanone, 4-...	5.203	7.3	ng	83861	1	8.117	228121	20.0
Ethanol, 2-(2-b...	10.703	11.3	ng	178164	2	10.944	315281	20.0
1,3,5-Triazine-...	16.161	2.4	ng	68735	4	17.512	576685	20.0
n-Hexadecanoic ...	18.394	2.8	ng	80265	4	17.512	576685	20.0
E-15-Heptadecenal	21.437	4.2	ng	122665	5	21.801	587303	20.0
1,4-Benzenedica...	23.035	2.0	ng	59776	5	21.801	587303	20.0