

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
 Data File : BG048987.D
 Acq On : 15 Jun 2021 21:26
 Operator : CG/JU
 Sample : M2672-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 17-B6(48-52)

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: BG048987.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	15	20	36	rVB	142439	250458	10.83%	2.131%
2	3.282	36	41	48	rVB	57801	84529	3.65%	0.719%
3	5.667	439	447	454	rBV	569452	956202	41.34%	8.135%
4	5.737	454	459	466	rVB2	16483	38835	1.68%	0.330%
5	7.265	710	719	734	rBV	571183	1036602	44.82%	8.819%
6	8.111	856	863	870	rBV	115909	199870	8.64%	1.700%
7	9.280	1054	1062	1069	rBV	365568	643893	27.84%	5.478%
8	10.702	1298	1304	1313	rVB3	15607	27855	1.20%	0.237%
9	10.937	1337	1344	1350	rBV	147303	266470	11.52%	2.267%
10	13.381	1753	1760	1768	rBV	855454	1330995	57.54%	11.324%
11	14.756	1986	1994	2002	rVB	245491	398710	17.24%	3.392%
12	16.155	2227	2232	2238	rBV2	45648	60010	2.59%	0.511%
13	16.243	2240	2247	2256	rBV	856827	1298301	56.13%	11.045%
14	17.506	2455	2462	2468	rBV	358773	559653	24.20%	4.761%
15	17.624	2475	2482	2486	rBV4	46960	69431	3.00%	0.591%
16	18.158	2568	2573	2578	rBV3	40195	58223	2.52%	0.495%
17	18.387	2606	2612	2619	rBV2	115215	169289	7.32%	1.440%
18	19.310	2765	2769	2775	rBV5	14873	28373	1.23%	0.241%
19	19.656	2822	2828	2837	rBV	146612	208507	9.01%	1.774%
20	20.115	2900	2906	2916	rVB	1690933	2312986	100.00%	19.678%
21	20.785	3014	3020	3029	rBV9	16985	43728	1.89%	0.372%
22	20.867	3031	3034	3037	rVV4	27368	30264	1.31%	0.257%
23	20.920	3039	3043	3046	rVB2	23934	31688	1.37%	0.270%
24	21.431	3125	3130	3137	rBV3	59786	98706	4.27%	0.840%
25	21.684	3169	3173	3179	rVB2	47682	66939	2.89%	0.569%
26	21.795	3186	3192	3199	rVB	374905	632870	27.36%	5.384%
27	22.001	3224	3227	3232	rBV2	24904	32802	1.42%	0.279%
28	22.635	3331	3335	3341	rVB3	25219	40911	1.77%	0.348%
29	23.023	3396	3401	3407	rVB5	30130	58643	2.54%	0.499%
30	23.335	3448	3454	3455	rBV6	15141	26207	1.13%	0.223%
31	24.204	3596	3602	3609	rBV8	17188	40435	1.75%	0.344%
32	25.132	3749	3760	3771	rBV2	212905	651828	28.18%	5.545%

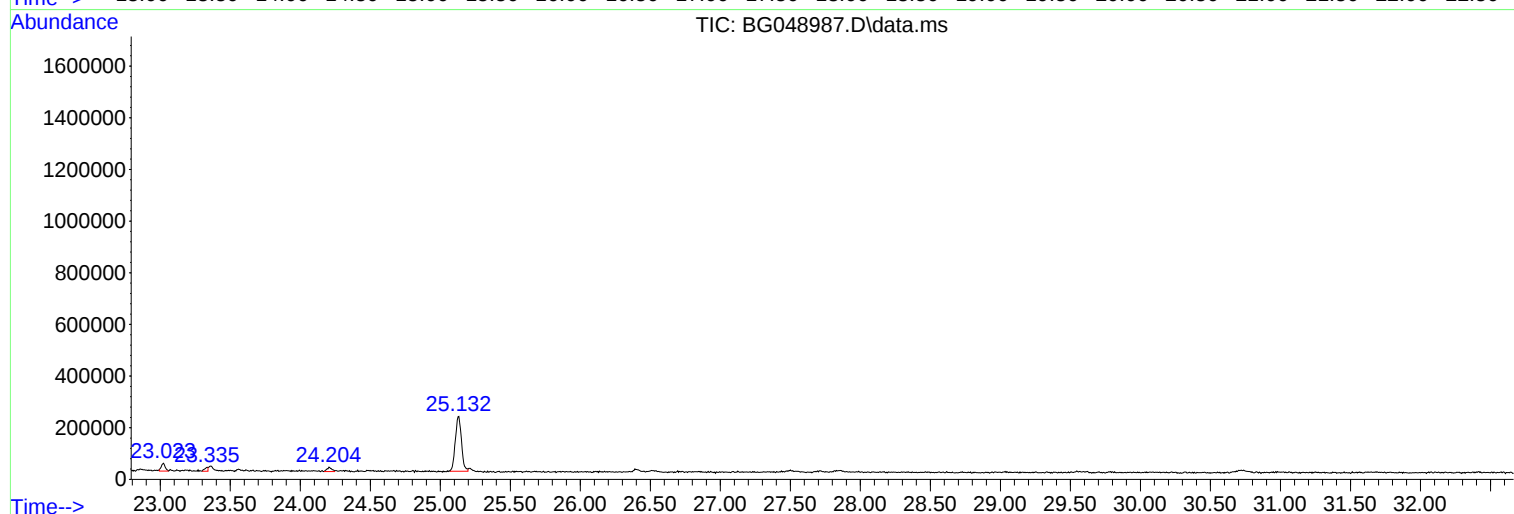
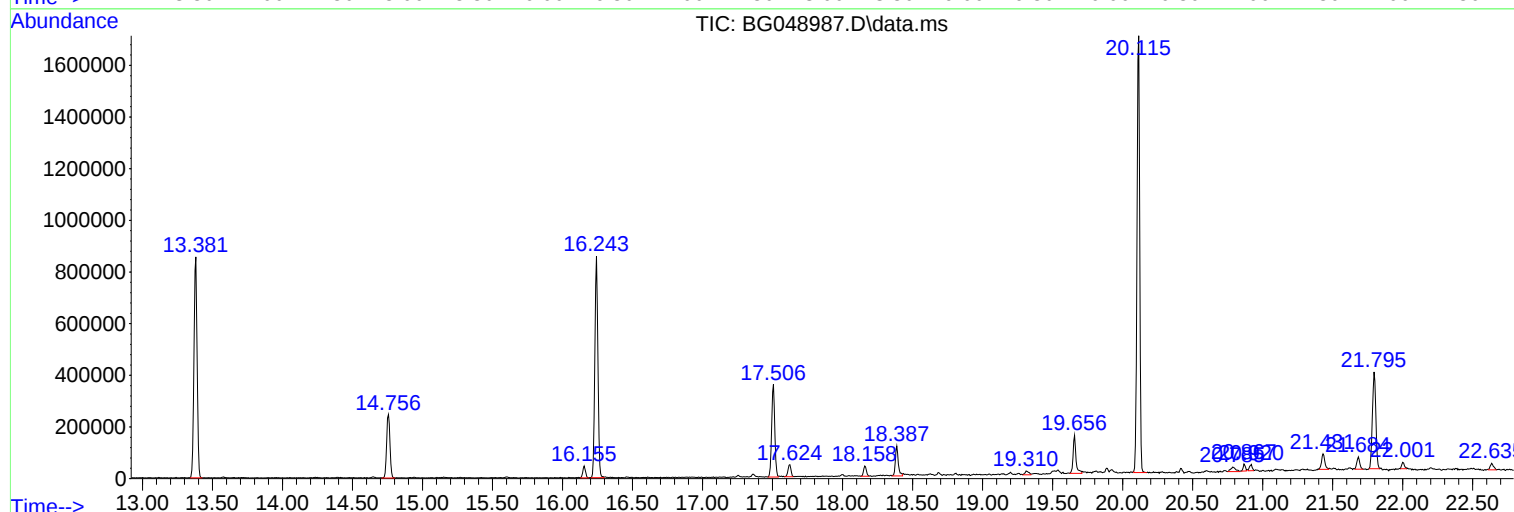
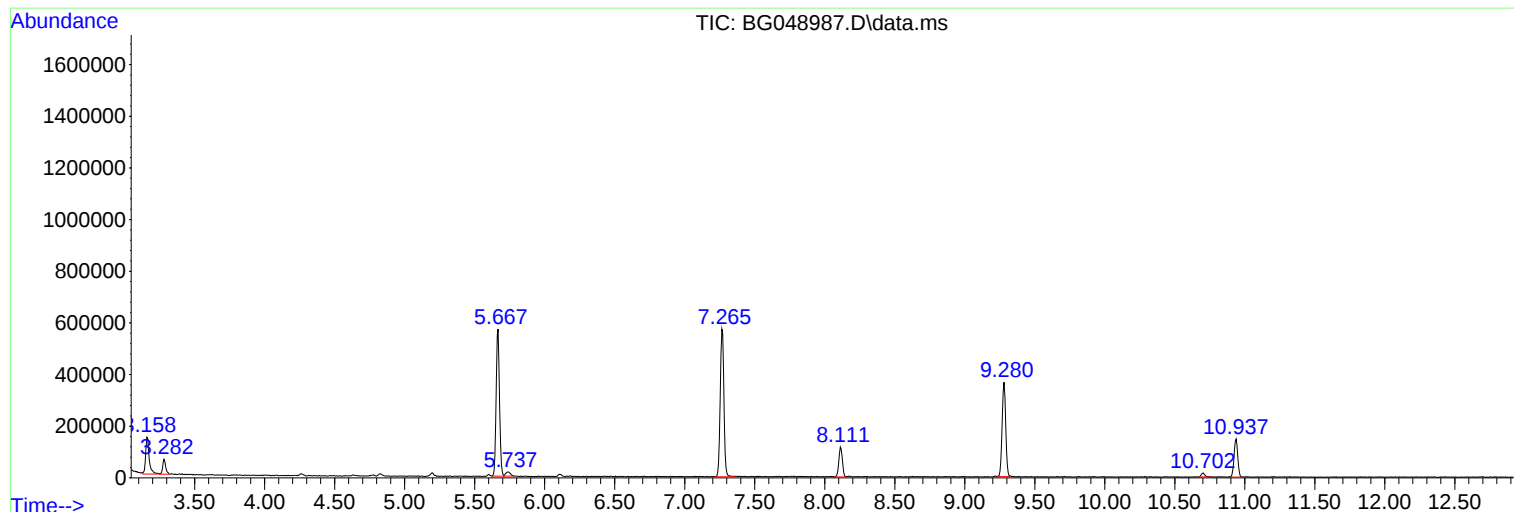
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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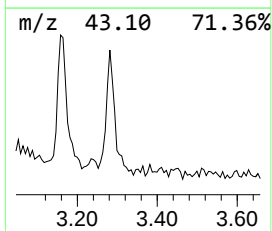
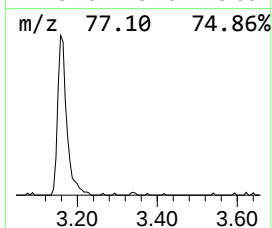
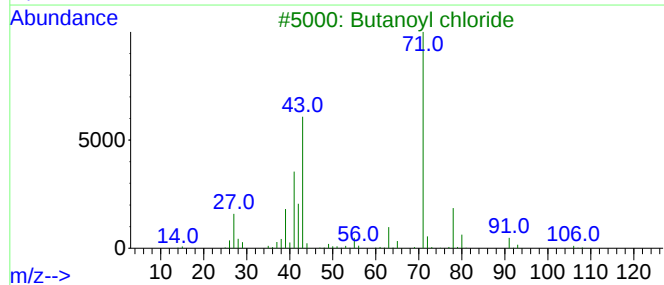
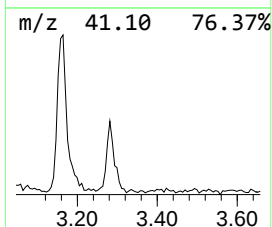
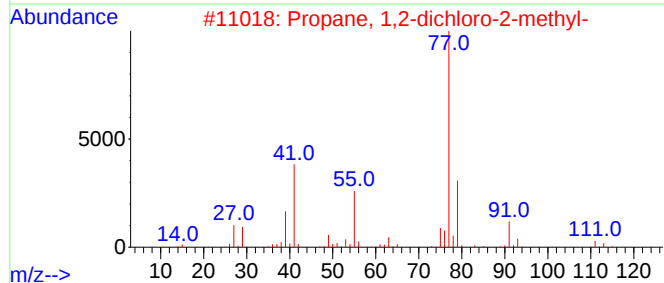
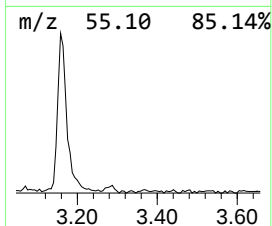
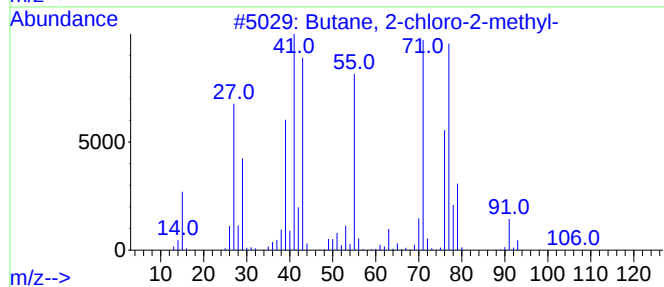
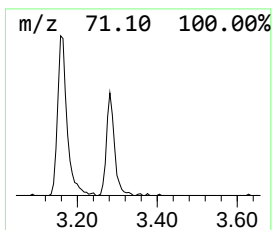
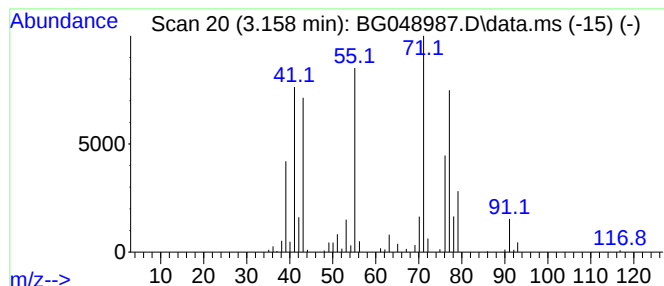
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.158	25.06 ng	250458	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	90
2			Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	27
3			Butanoyl chloride	106	C4H7ClO	000141-75-3	22
4			2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	16
5			Allyl chloride	76	C3H5Cl	000107-05-1	14



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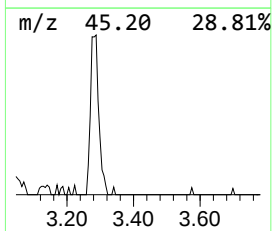
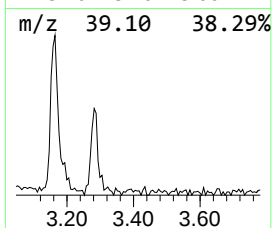
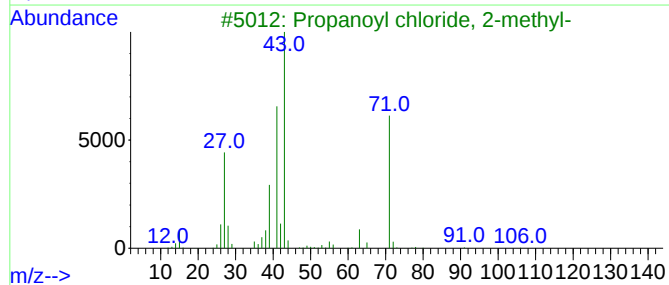
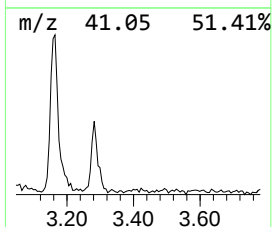
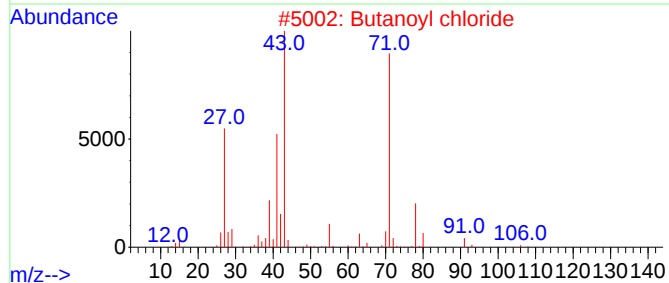
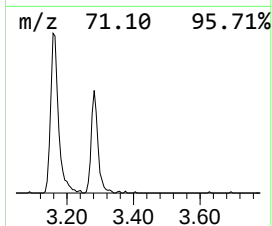
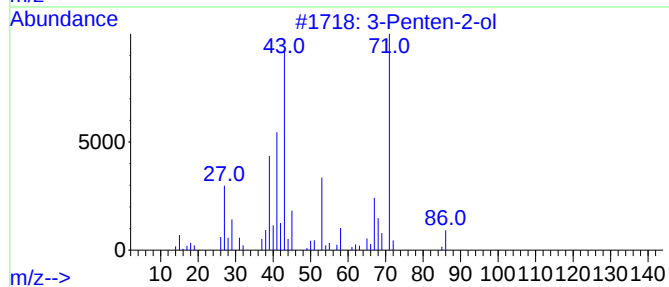
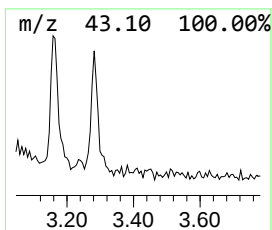
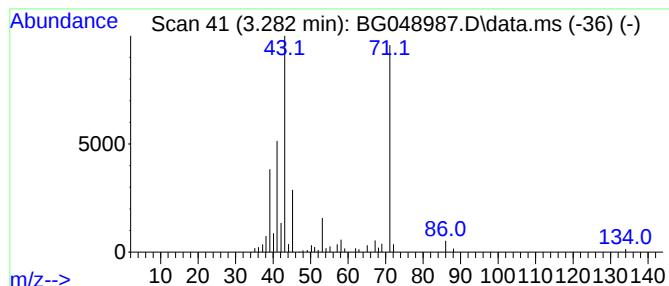
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.282	8.46 ng	84529	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	56
2			Butanoyl chloride	106	C4H7ClO	000141-75-3	47
3			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	43
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	40
5			Acetic acid, (1,2-dimethyl-1-pro...	128	C7H12O2	003814-41-3	38



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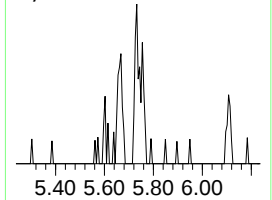
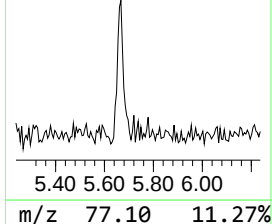
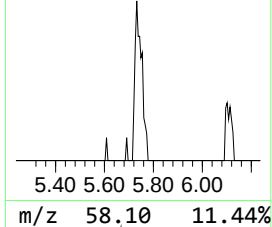
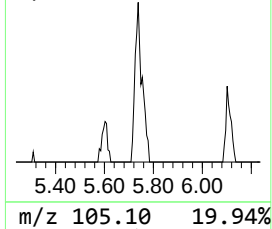
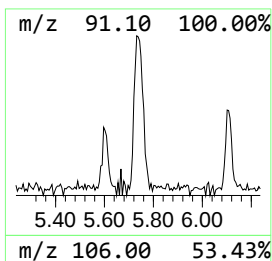
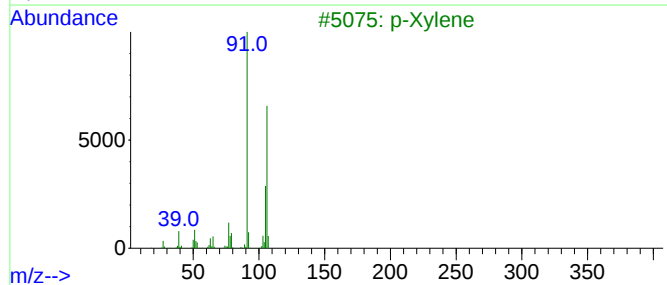
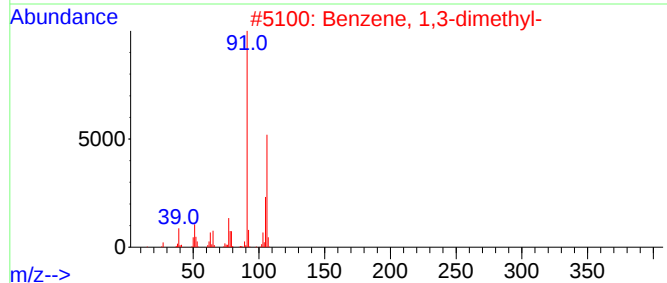
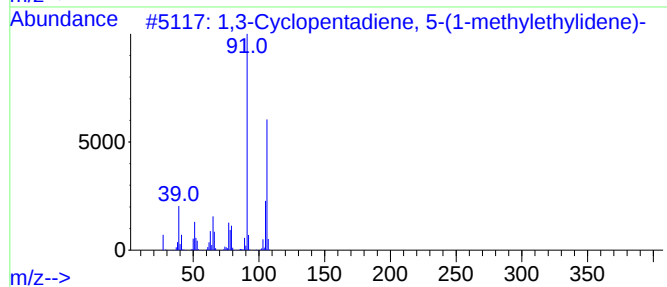
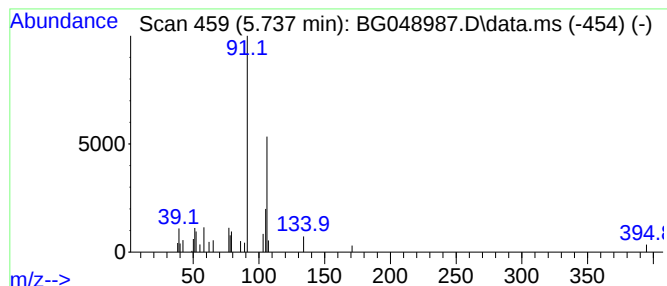
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 1,3-Cyclopentadiene, 5-(1-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.737	3.89 ng	38835	1,4-Dichlorobenzene-d4	8.117

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87
2		Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
3		p-Xylene	106	C8H10	000106-42-3	83
4		o-Xylene	106	C8H10	000095-47-6	83
5		1,3-Cyclopentadiene, 5-(1-methyl...	148	C11H16	061039-45-0	72



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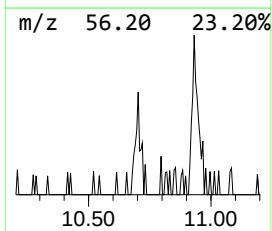
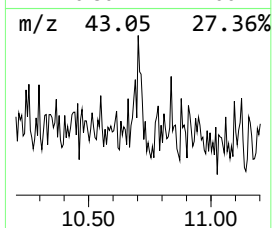
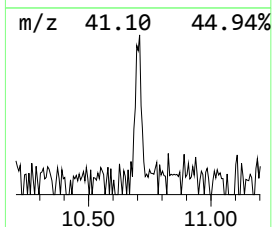
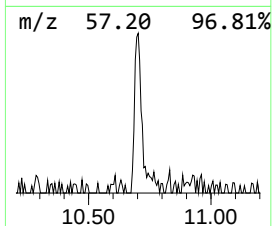
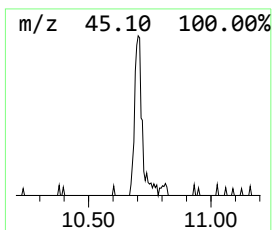
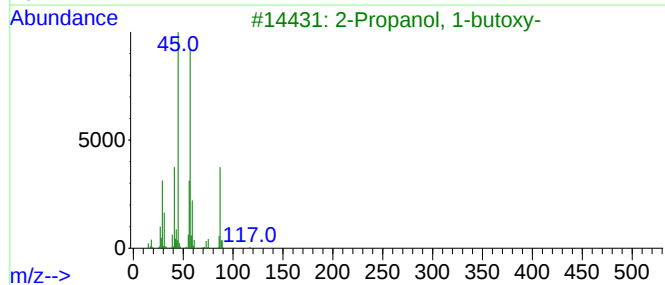
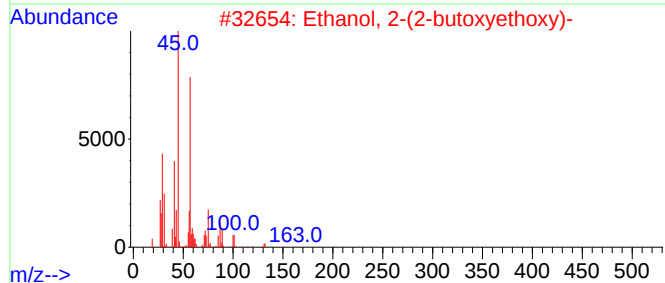
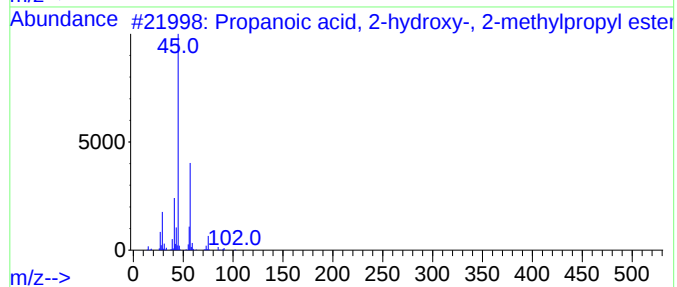
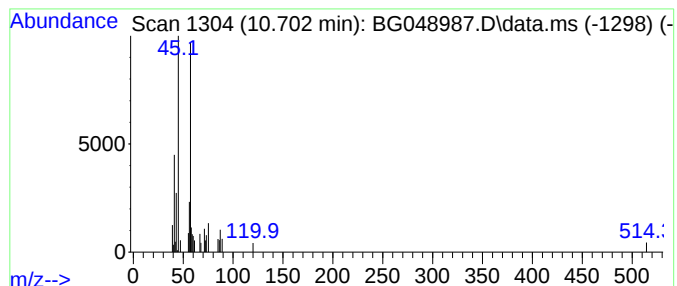
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Peak Number 4 Propanoic acid, 2-hydroxy-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.702	2.09 ng	27855	Naphthalene-d8	10.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	50
3			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	50
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	38
5			E-1-Methoxy-3-hexene	114	C7H14O	121441-40-5	38



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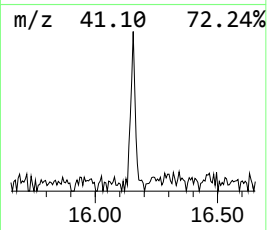
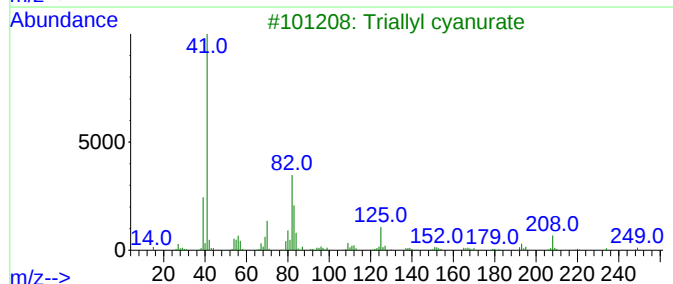
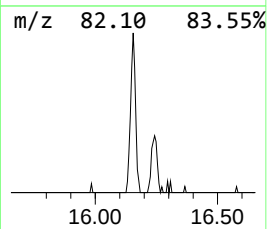
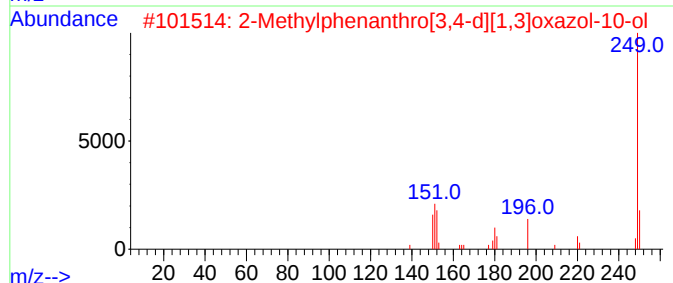
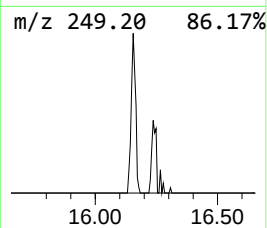
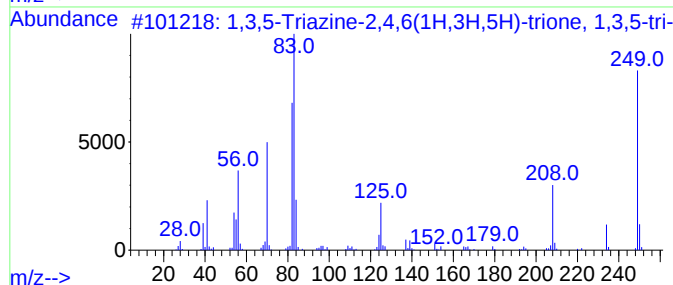
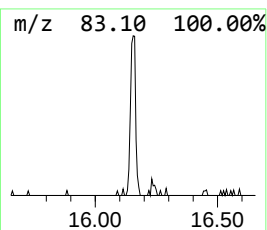
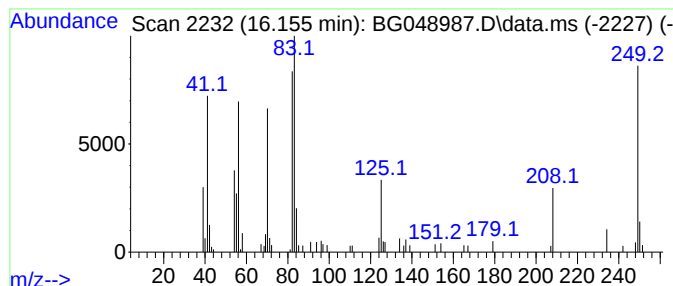
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Peak Number 5 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.155	2.14 ng	60010	Phenanthrene-d10	17.506

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	94		
2	2-Methylphenanthro[3,4-d][1,3]ox...	249	C16H11NO2	098033-24-0	45		
3	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	35		
4	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	25		
5	8,8-Dimethylspiro(4.6)undecane-6...	208	C13H20O2	068181-81-7	25		



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17-B6(48-52)

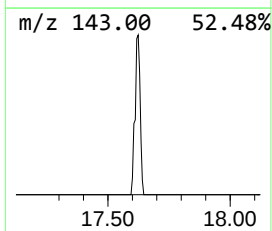
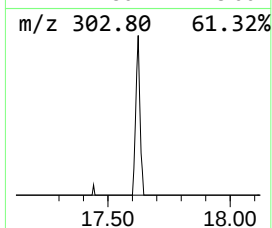
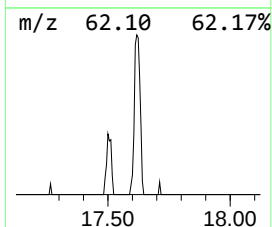
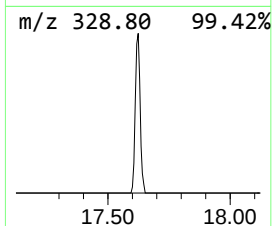
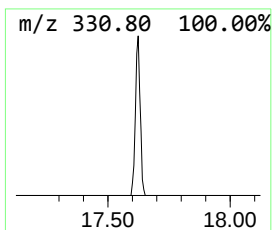
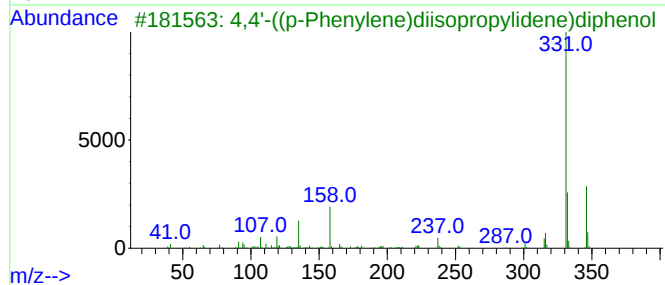
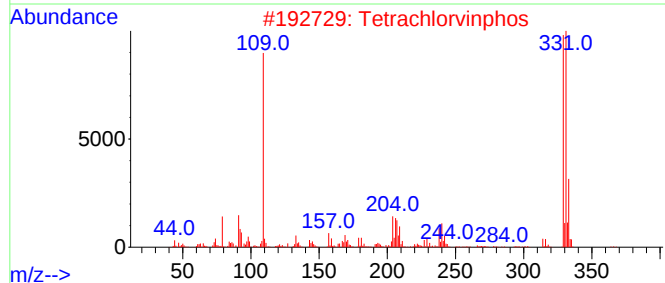
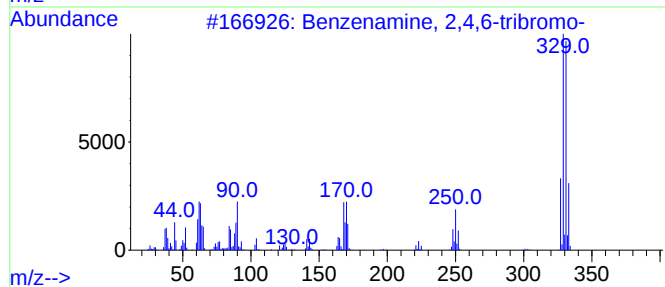
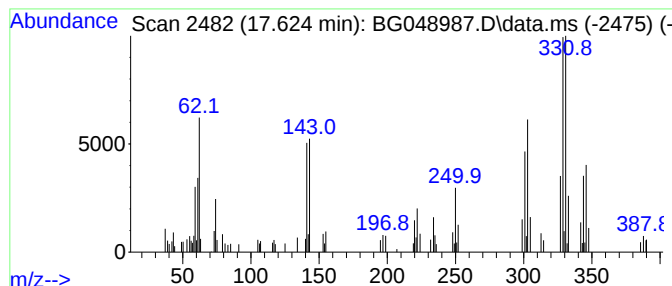
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.624 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.624	2.48 ng	69431	Phenanthrene-d10	17.506

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	46
2			Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	10
3			4,4'-(p-Phenylene)diisopropylid...	346	C24H26O2	002167-51-3	9
4			Morphinan-6-one, 3,4-dimethoxy-5...	329	C20H27NO3	085618-83-3	9
5			Acetophenone, 2,4-bis(trifluoroa...	344	C12H6F6O5	1000365-29-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048987.D
Acq On : 15 Jun 2021 21:26
Operator : CG/JU
Sample : M2672-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
17-B6(48-52)

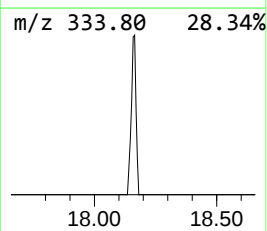
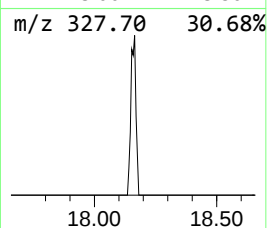
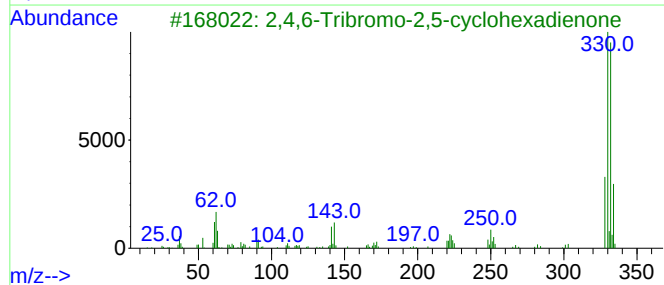
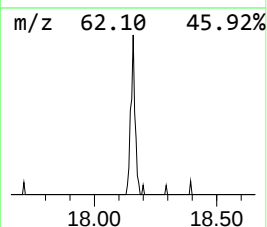
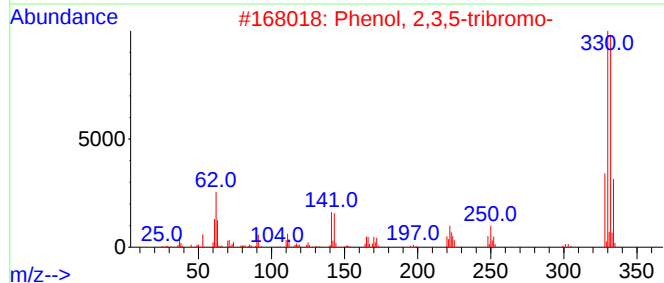
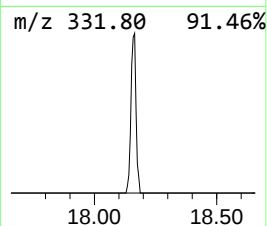
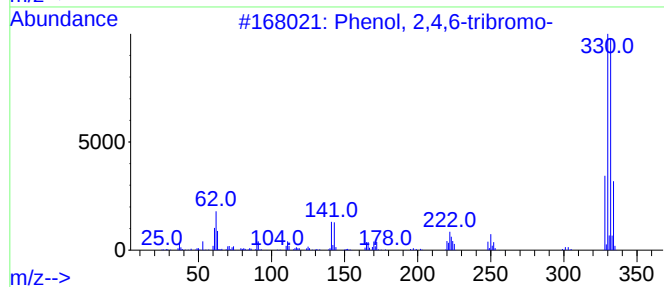
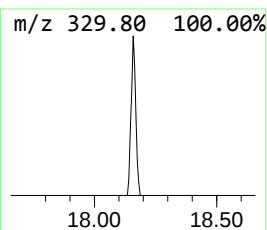
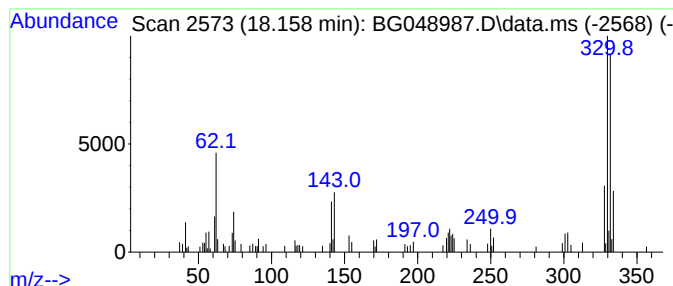
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 2,3,5-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.158	2.08 ng	58223	Phenanthrene-d10	17.506

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	98
2			Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	98
3			2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	96
4			Propane, 1-(2,4,6-tribromophenox...	526	C9H7Br5O	035109-60-5	64
5			Naphtho[2,1-b]thiophene-4-carbox...	330	C14H6ClF3O2S	052300-59-1	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048987.D
Acq On : 15 Jun 2021 21:26
Operator : CG/JU
Sample : M2672-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(48-52)

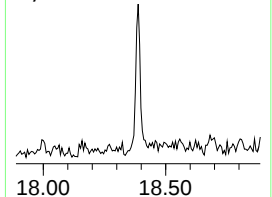
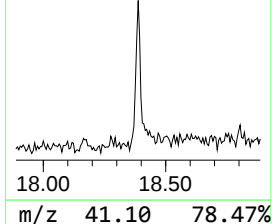
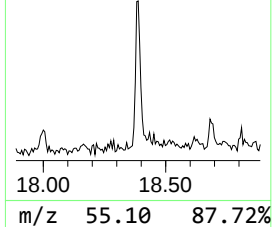
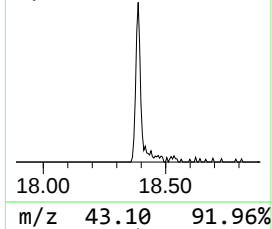
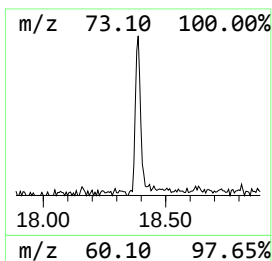
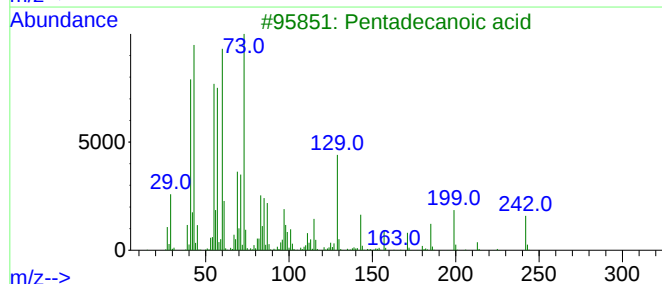
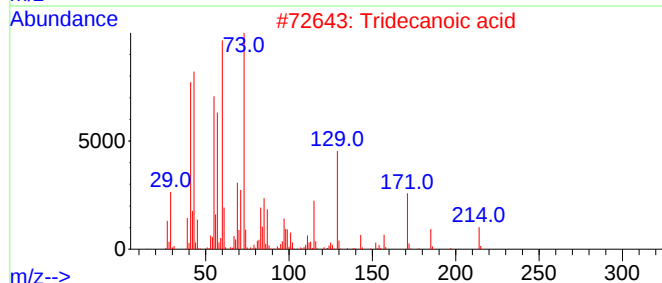
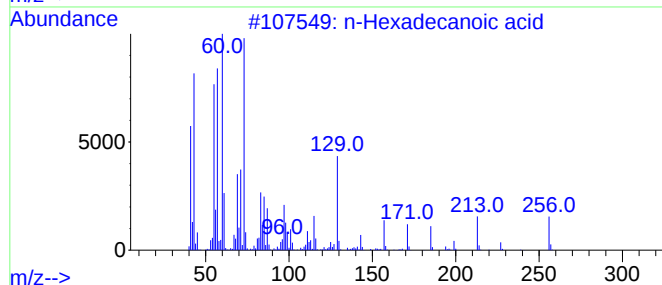
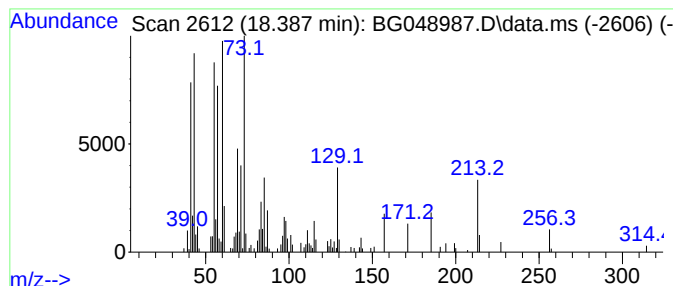
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.387	6.05 ng	169289	Phenanthrene-d10	17.506

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048987.D
Acq On : 15 Jun 2021 21:26
Operator : CG/JU
Sample : M2672-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(48-52)

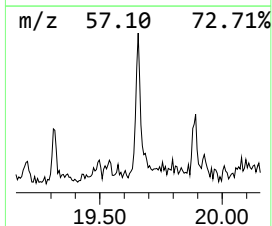
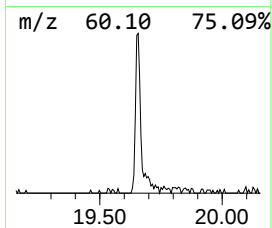
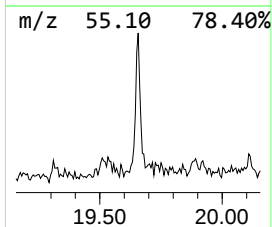
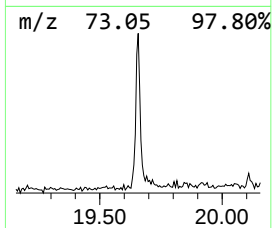
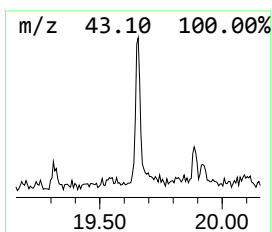
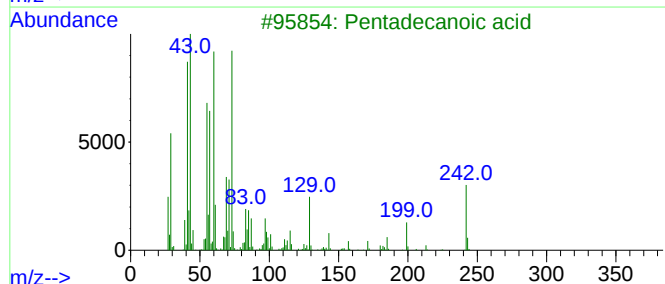
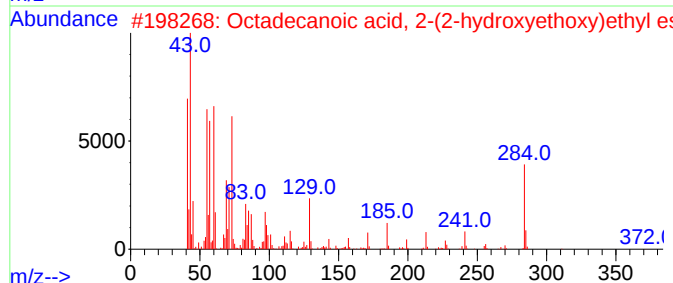
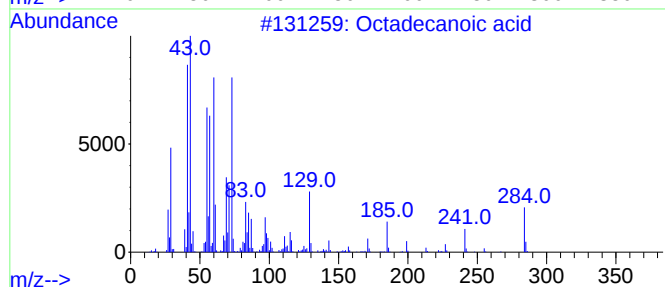
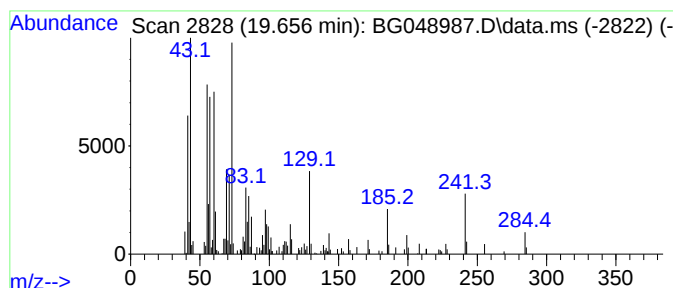
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.657	6.59 ng	208507	Chrysene-d12	21.795

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048987.D
Acq On : 15 Jun 2021 21:26
Operator : CG/JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
17-B6(48-52)

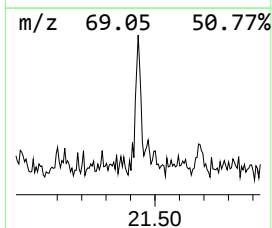
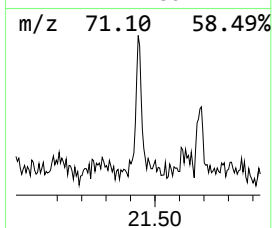
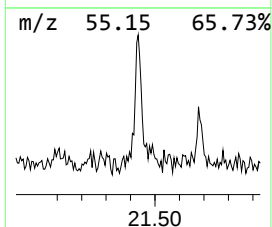
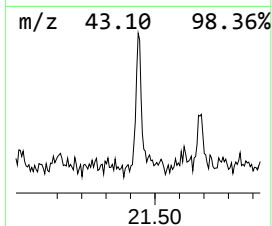
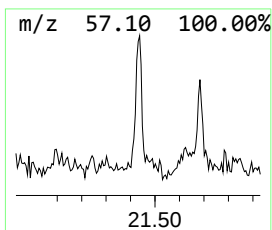
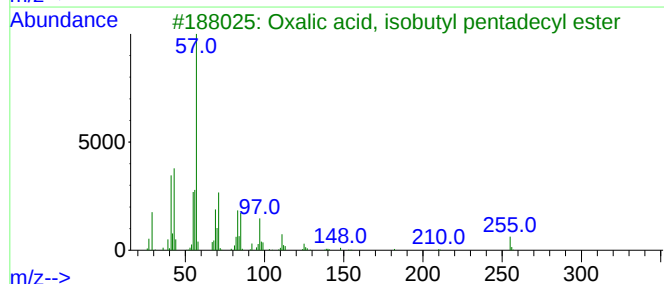
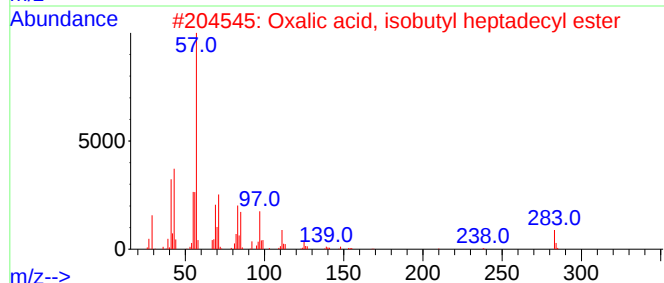
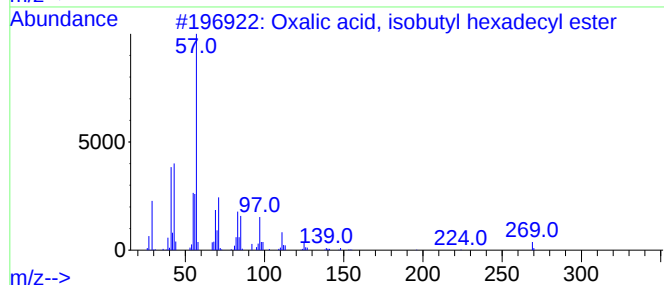
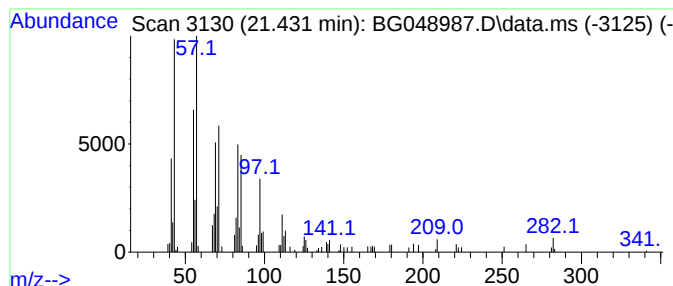
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, isobutyl hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.431	3.12 ng	98706	Chrysene-d12	21.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87		
2	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87		
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87		
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87		
5	Oxalic acid, cyclobutyl hexadecyl...	368	C22H40O4	1000309-70-6	86		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048987.D
Acq On : 15 Jun 2021 21:26
Operator : CG/JU
Sample : M2672-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
17-B6(48-52)

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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...	3.158	25.1	ng	250458	1	8.117	199870	20.0
3-Penten-2-ol	3.282	8.5	ng	84529	1	8.117	199870	20.0
1,3-Cyclopentad...	5.737	3.9	ng	38835	1	8.117	199870	20.0
Propanoic acid,...	10.702	2.1	ng	27855	2	10.937	266470	20.0
1,3,5-Triazine-...	16.155	2.1	ng	60010	4	17.506	559653	20.0
unknown17.624	17.624	2.5	ng	69431	4	17.506	559653	20.0
Phenol, 2,3,5-t...	18.158	2.1	ng	58223	4	17.506	559653	20.0
n-Hexadecanoic ...	18.387	6.0	ng	169289	4	17.506	559653	20.0
Octadecanoic acid	19.657	6.6	ng	208507	5	21.795	632870	20.0
Oxalic acid, is...	21.431	3.1	ng	98706	5	21.795	632870	20.0