

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
 Data File : BG049060.D
 Acq On : 23 Jun 2021 14:03
 Operator : CG/JU
 Sample : M2748-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-5A

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: BG049060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	14	19	29	rBV2	52757	105795	6.87%	1.266%
2	4.580	256	262	270	rBV	99274	159003	10.32%	1.903%
3	5.191	359	366	375	rBV	827494	1311774	85.14%	15.703%
4	5.661	440	446	454	rBV	60541	102817	6.67%	1.231%
5	7.259	711	718	727	rBV	209053	366650	23.80%	4.389%
6	8.111	852	863	868	rBV	88248	159176	10.33%	1.905%
7	8.158	868	871	881	rVB2	10348	19203	1.25%	0.230%
8	9.274	1052	1061	1069	rBV2	182737	337805	21.93%	4.044%
9	10.931	1336	1343	1350	rVB	118411	218189	14.16%	2.612%
10	13.375	1752	1759	1769	rBV	457249	738845	47.95%	8.845%
11	14.750	1987	1993	1999	rBV	203739	319796	20.76%	3.828%
12	15.538	2121	2127	2133	rBV	60990	91476	5.94%	1.095%
13	16.002	2197	2206	2207	rBV2	12544	28169	1.83%	0.337%
14	16.325	2256	2261	2262	rBV	13082	15575	1.01%	0.186%
15	16.378	2262	2270	2273	rVV3	20629	55497	3.60%	0.664%
16	16.707	2309	2326	2327	rBV	121217	306363	19.88%	3.667%
17	17.071	2381	2388	2392	rBV6	7524	20850	1.35%	0.250%
18	17.500	2454	2461	2471	rVB	279085	449300	29.16%	5.379%
19	18.381	2605	2611	2622	rBV5	32959	87592	5.69%	1.049%
20	19.644	2822	2826	2828	rBV3	30218	39981	2.59%	0.479%
21	20.103	2898	2904	2910	rBV	1168820	1540710	100.00%	18.444%
22	20.620	2986	2992	2998	rVB4	27493	56391	3.66%	0.675%
23	21.372	3115	3120	3124	rBV3	24892	48548	3.15%	0.581%
24	21.425	3124	3129	3136	rVV3	52452	129273	8.39%	1.548%
25	21.501	3137	3142	3148	rVB2	61185	106704	6.93%	1.277%
26	21.666	3167	3170	3175	rVB3	15457	21727	1.41%	0.260%
27	21.789	3184	3191	3199	rVB	313828	553907	35.95%	6.631%
28	22.459	3300	3305	3309	rBV7	14684	28488	1.85%	0.341%
29	22.529	3313	3317	3323	rVV5	27391	47187	3.06%	0.565%
30	22.706	3345	3347	3352	rVB6	12867	16972	1.10%	0.203%
31	22.999	3388	3397	3405	rBV5	43720	103895	6.74%	1.244%
32	23.240	3433	3438	3445	rVB5	18537	38121	2.47%	0.456%
33	23.340	3450	3455	3462	rVB6	23491	49091	3.19%	0.588%
34	25.115	3747	3757	3776	rVB3	194140	638653	41.45%	7.645%
35	28.058	4250	4258	4259	rBV8	17479	40041	2.60%	0.479%

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ClientSampleId :
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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

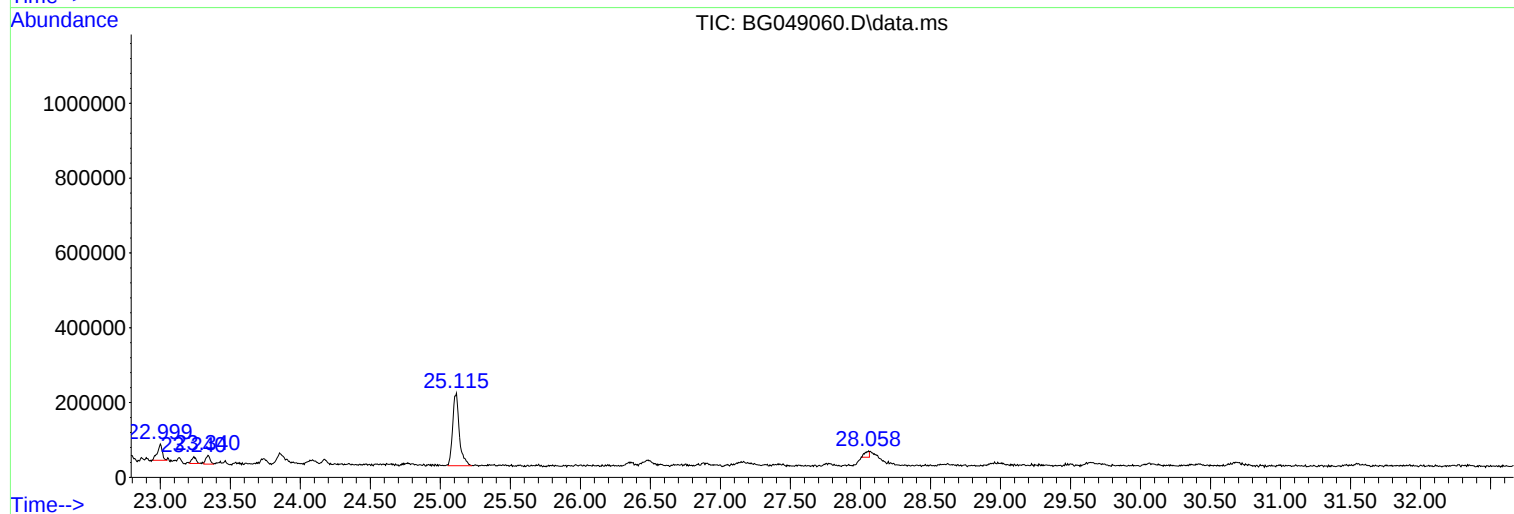
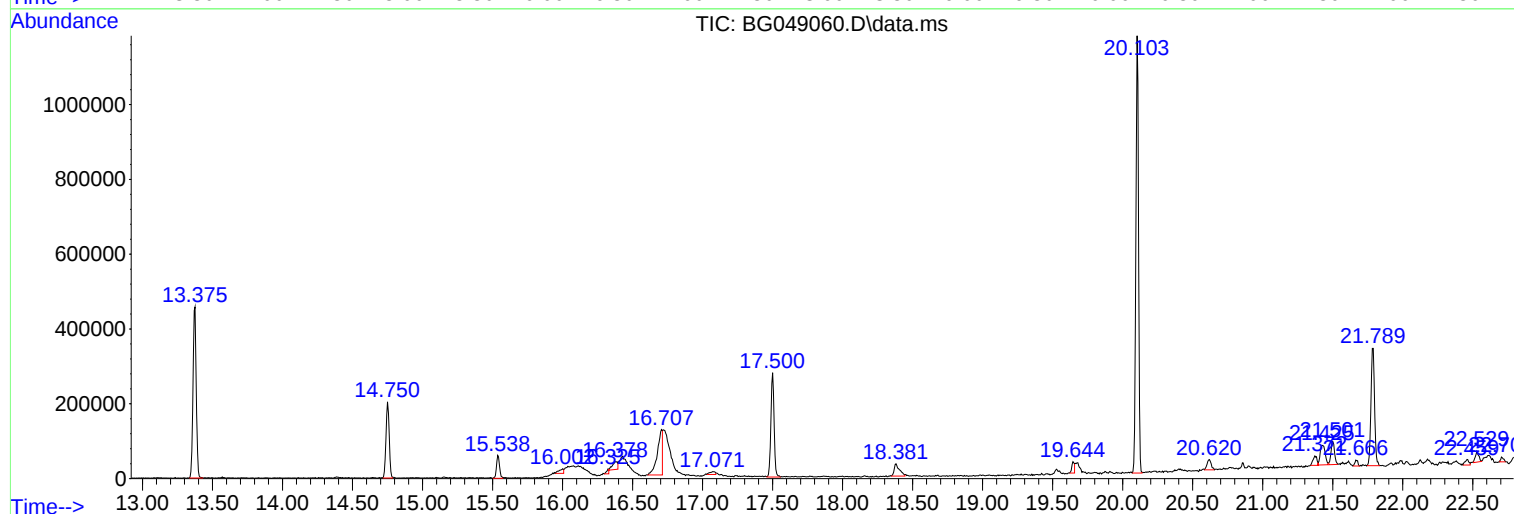
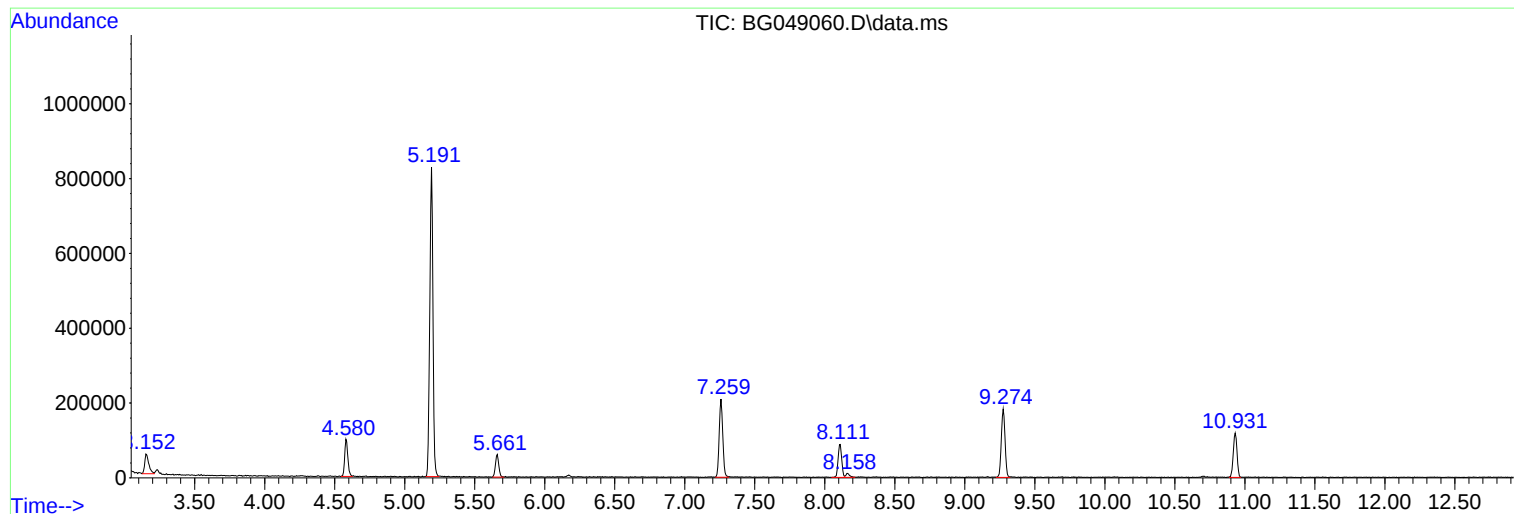
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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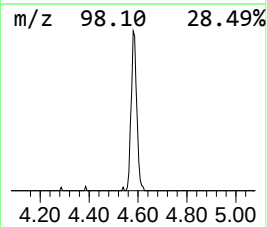
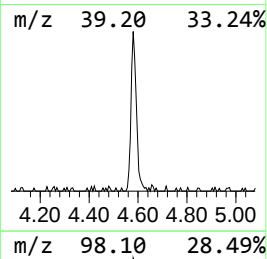
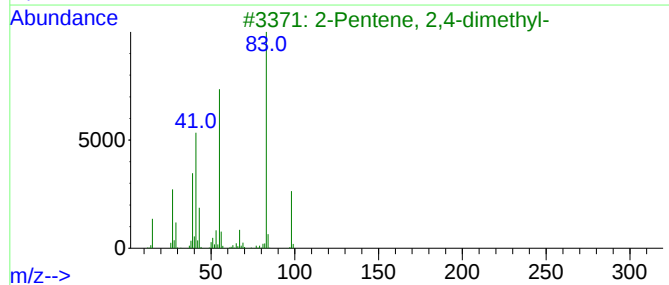
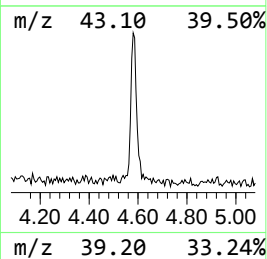
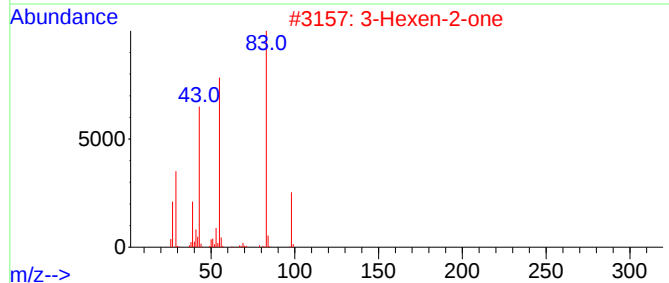
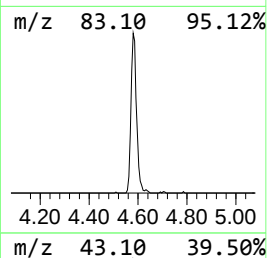
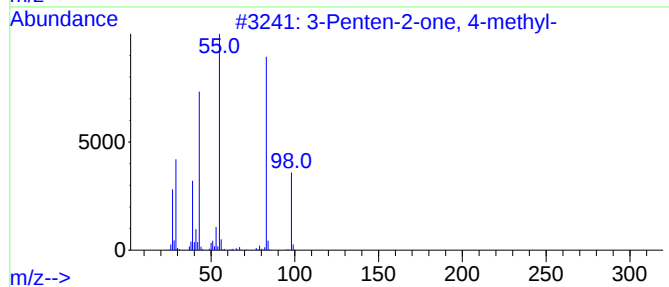
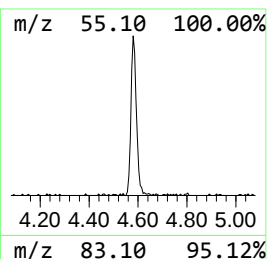
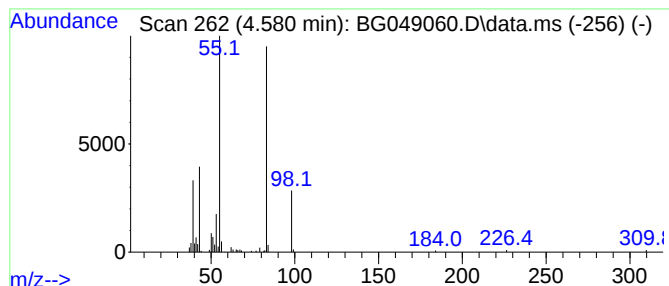
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.580	19.98 ng	159003	1,4-Dichlorobenzene-d4	8.111

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			3-Hexen-2-one	98	C6H10O	000763-93-9	78
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64



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Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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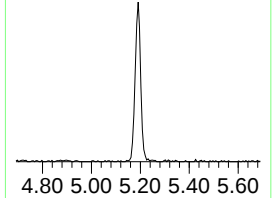
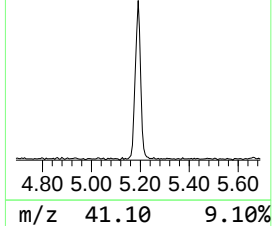
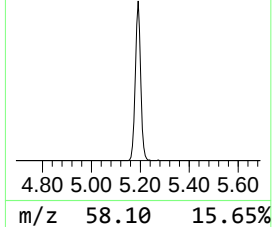
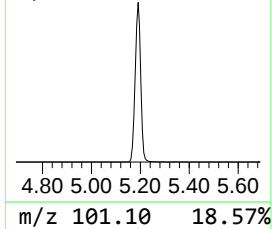
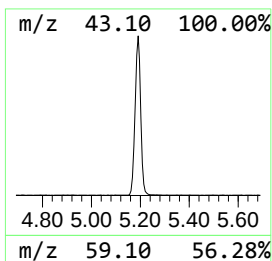
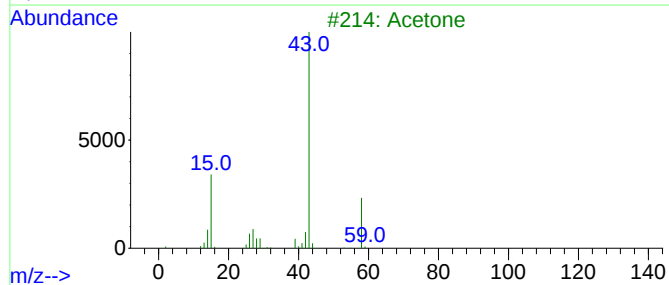
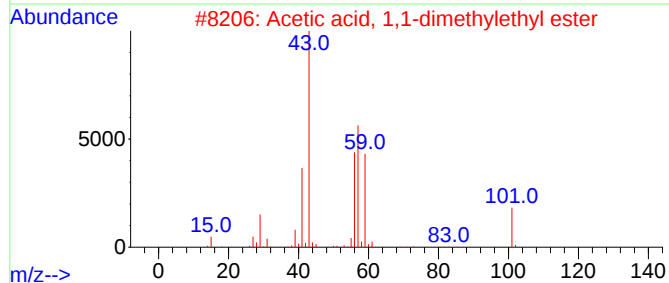
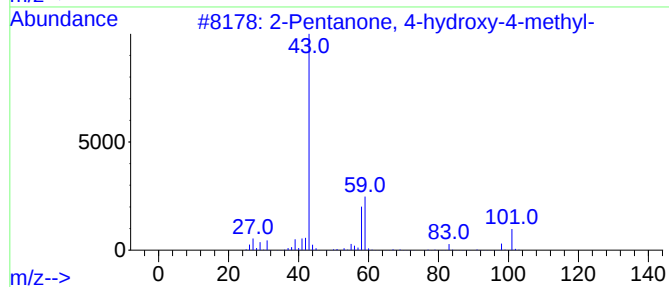
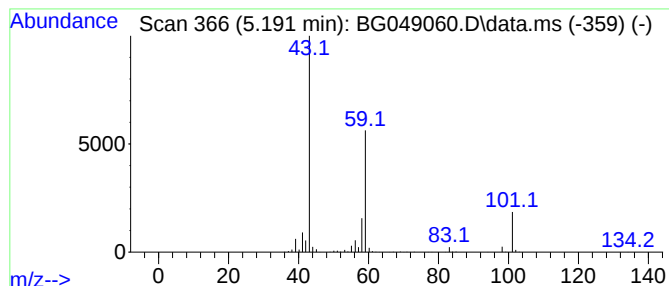
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	164.82 ng	1311770	1,4-Dichlorobenzene-d4	8.111

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetone	58	C3H6O	000067-64-1	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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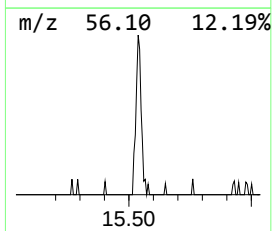
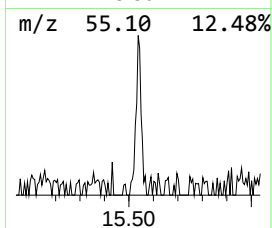
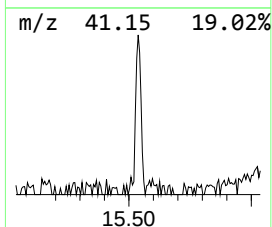
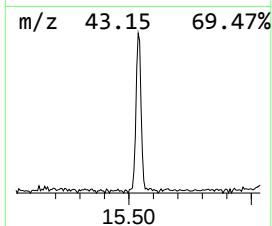
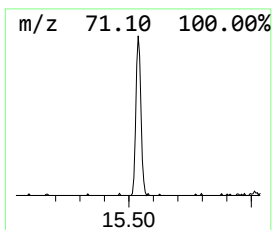
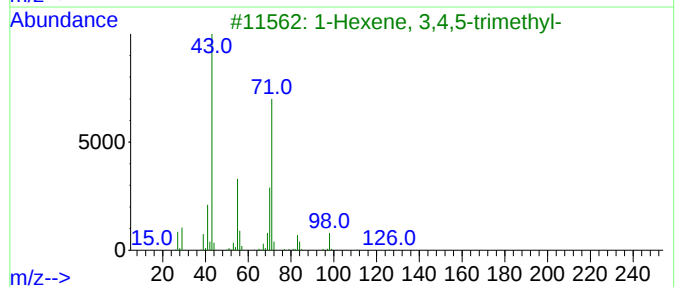
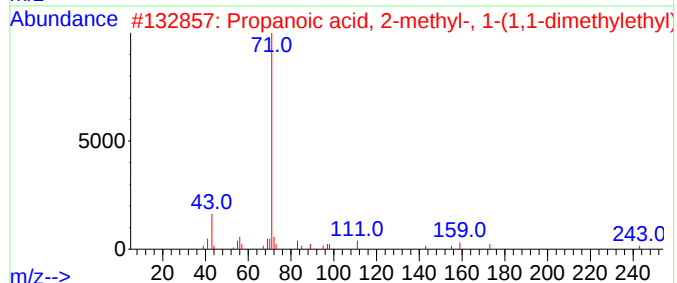
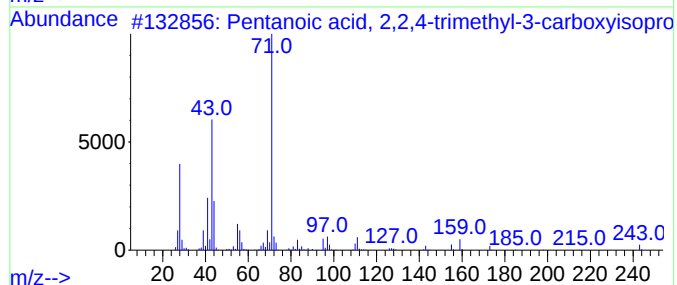
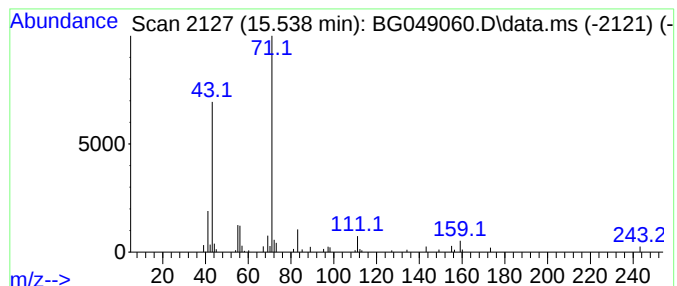
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentanoic acid, 2,2,4-trime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	5.72 ng	91476	Acenaphthene-d10	14.750

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	78
2			Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	72
3			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	64
4			Propanoic acid, 2-methyl-, 2-(hy...	216	C12H24O3	074367-32-1	56
5			Sulfurous acid, dodecyl 2-pentyl...	320	C17H36O3S	1000309-16-1	56



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ClientSampled :
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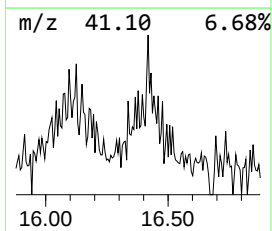
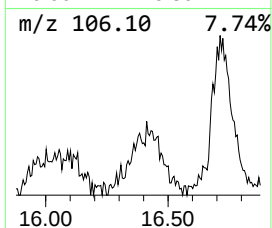
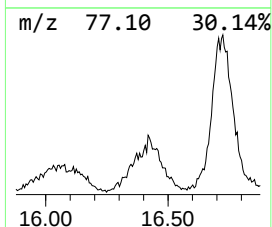
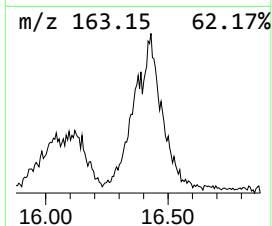
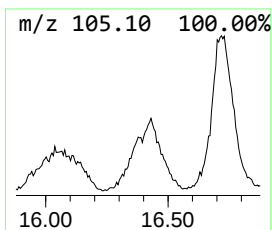
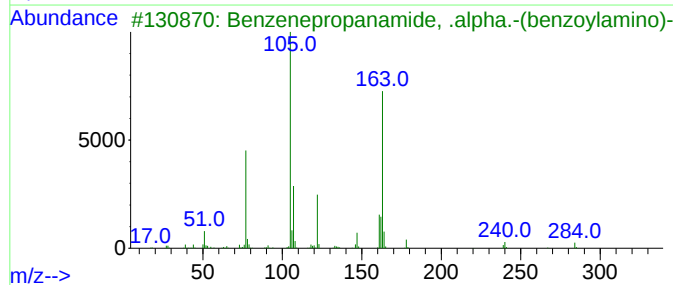
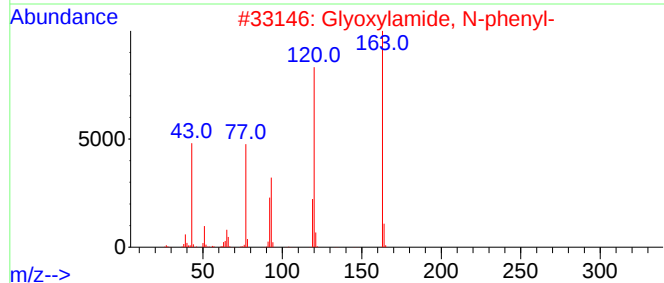
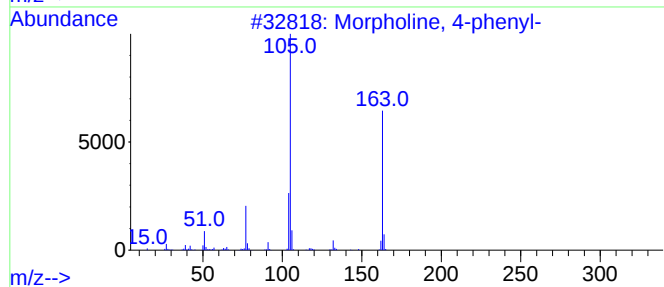
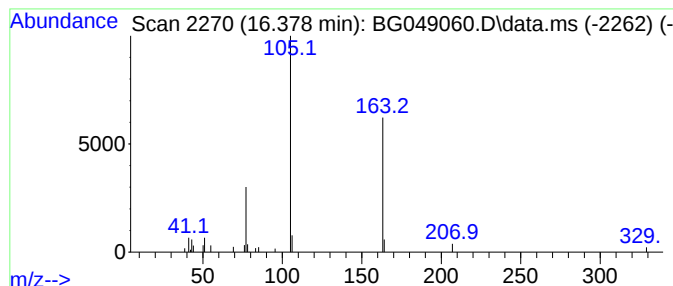
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Peak Number 5 Morpholine, 4-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.378	2.47 ng	55497	Phenanthrene-d10	17.500

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
3			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	39
4			Ethyl 2-benzamido-3,3,3-trifluor...	459	C19H20F3N3O5S	339352-43-1	35
5			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	35



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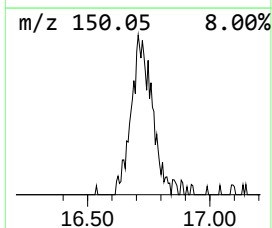
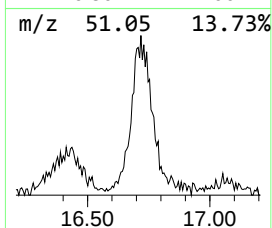
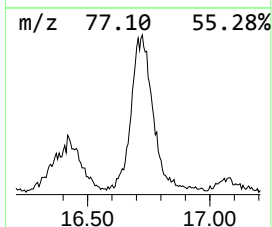
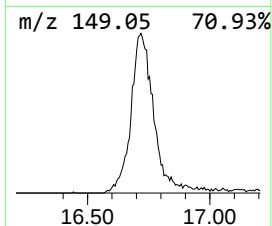
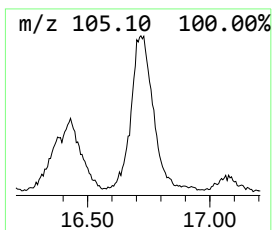
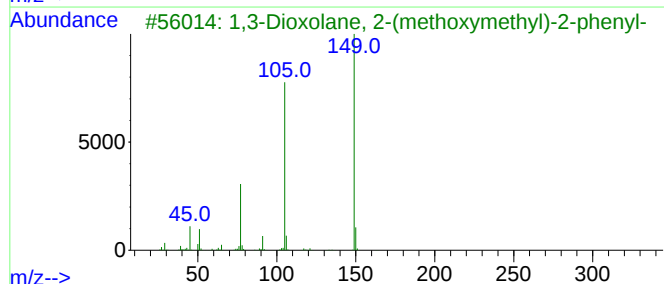
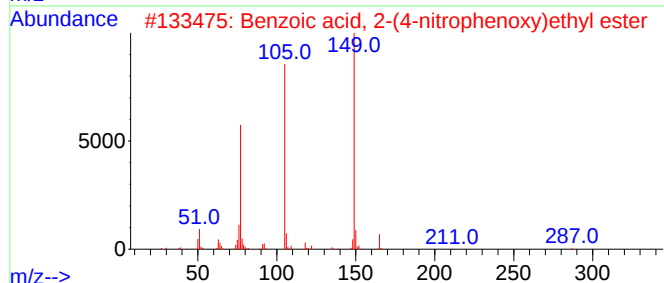
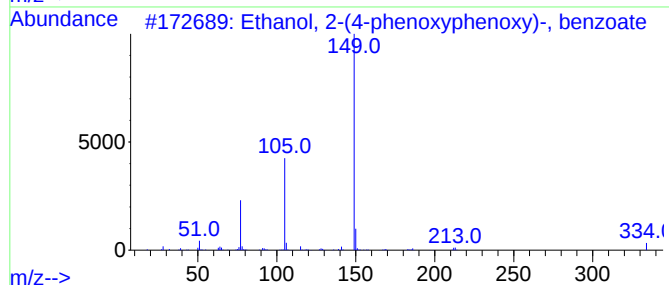
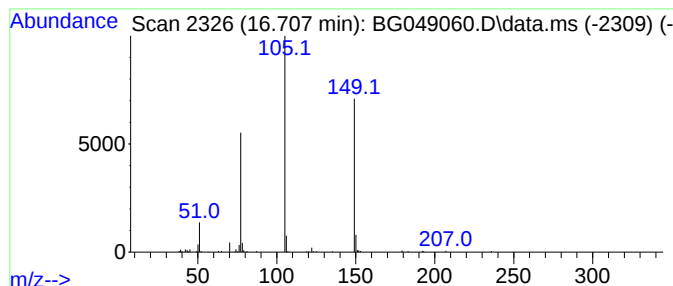
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Ethanol, 2-(4-phenoxypheno... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.707	13.64 ng	306363	Phenanthrene-d10	17.500

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	83
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	59
5			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049060.D
Acq On : 23 Jun 2021 14:03
Operator : CG/JU
Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

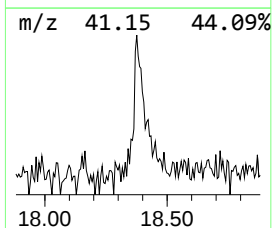
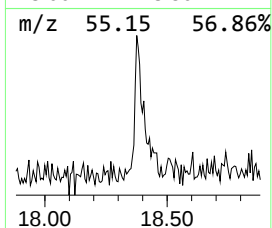
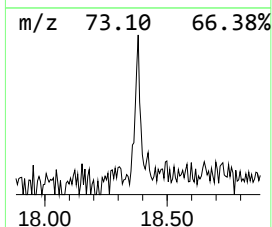
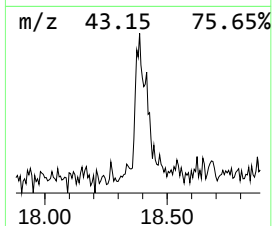
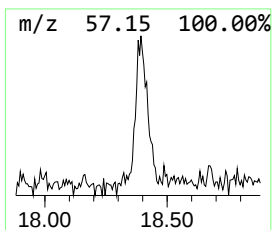
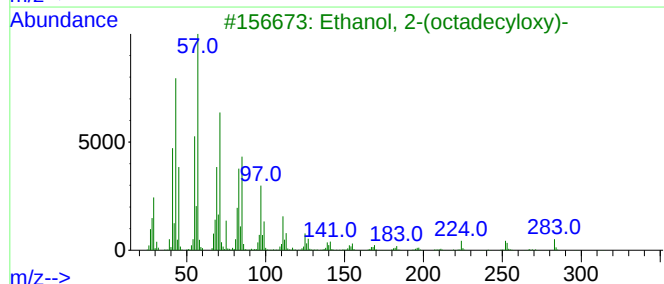
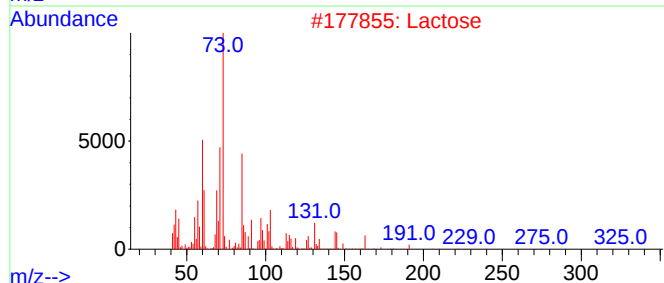
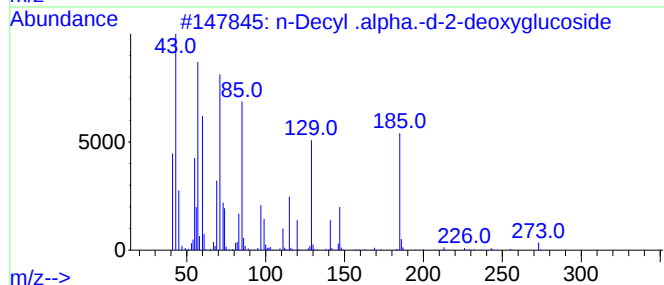
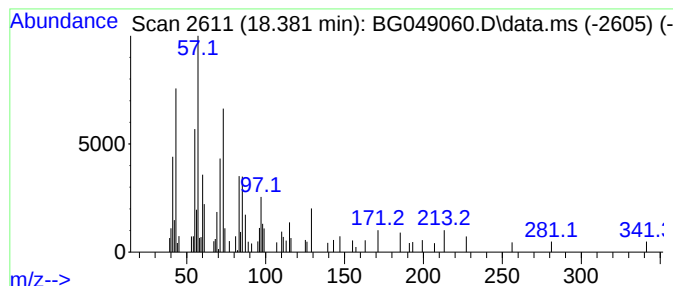
Instrument :
BNA_G
ClientSampleId :
SB-5A

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 n-Decyl .alpha.-d-2-deoxygl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.381	3.90 ng	87592	Phenanthrene-d10		17.500	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Decyl .alpha.-d-2-deoxyglucoside		304	C16H32O5	1000211-42-8	53
2	Lactose		342	C12H22O11	000063-42-3	50
3	Ethanol, 2-(octadecyloxy)-		314	C20H42O2	002136-72-3	38
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	35
5	Sulfurous acid, pentadecyl 2-pro...		334	C18H38O3S	1000309-12-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049060.D
Acq On : 23 Jun 2021 14:03
Operator : CG/JU
Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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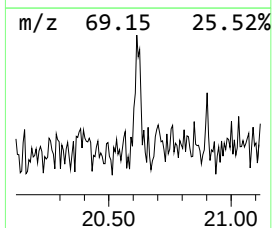
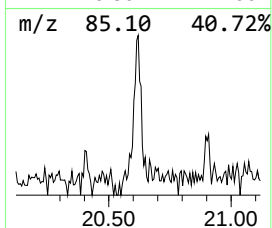
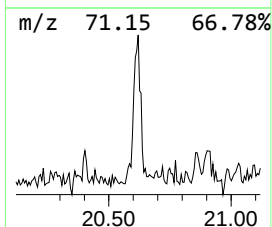
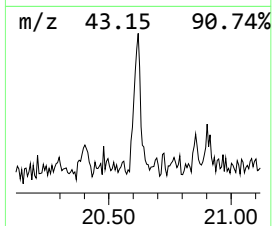
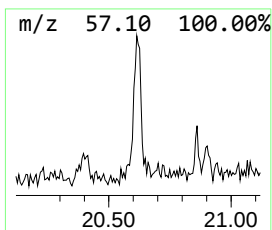
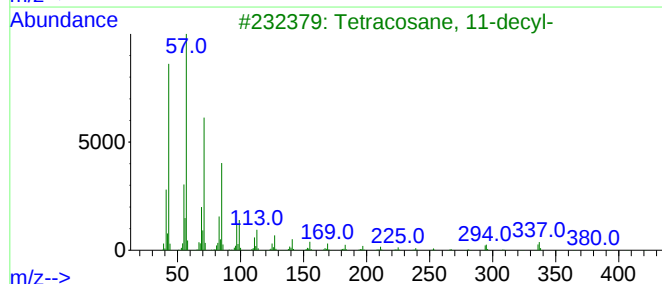
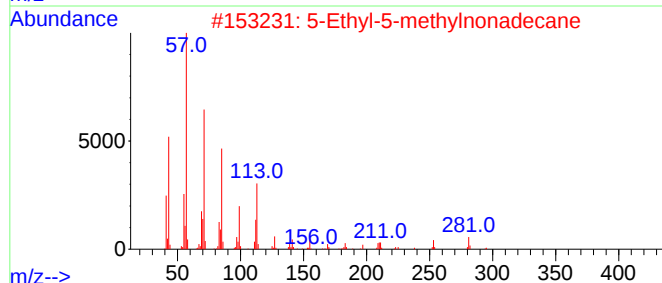
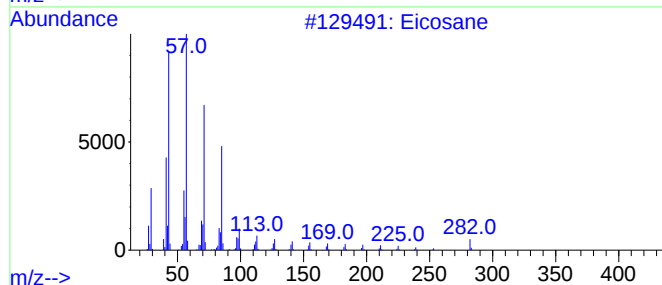
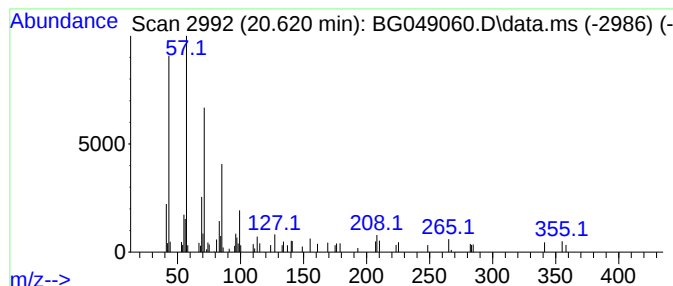
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.620	2.04 ng	56391	Chrysene-d12	21.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	83
2			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	64
4			Tridecane, 6-propyl-	226	C16H34	055045-10-8	64
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049060.D
Acq On : 23 Jun 2021 14:03
Operator : CG/JU
Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5A

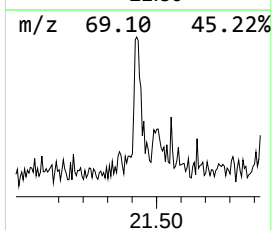
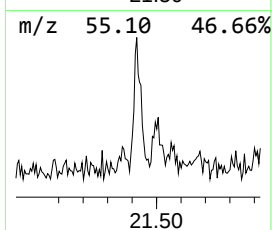
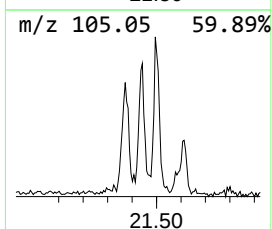
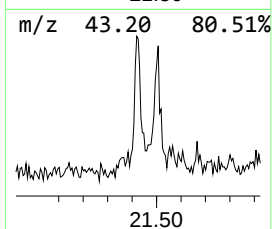
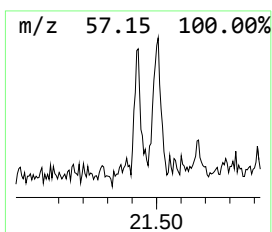
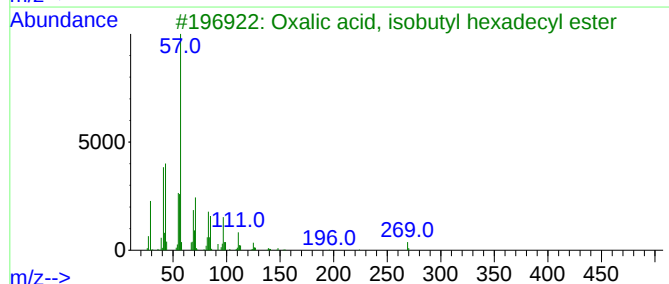
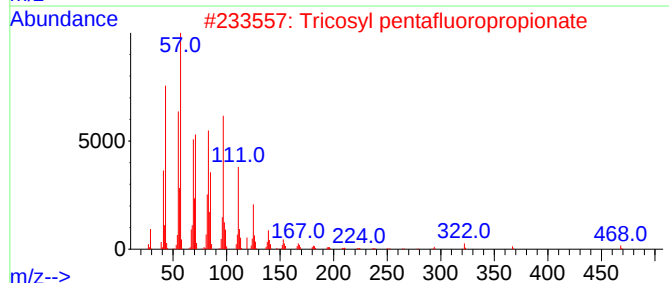
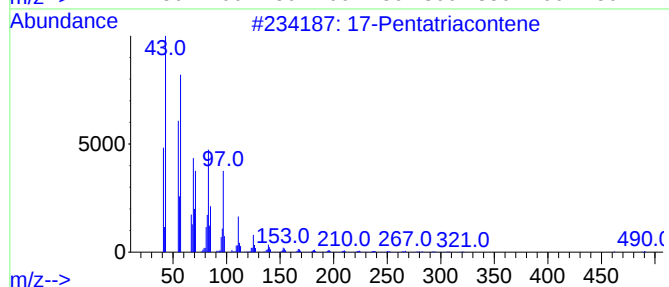
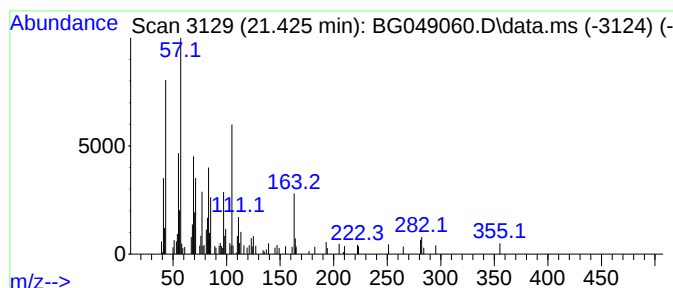
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.425	4.67 ng	129273	Chrysene-d12	21.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	50
2			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	49
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	49
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	43
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049060.D
Acq On : 23 Jun 2021 14:03
Operator : CG/JU
Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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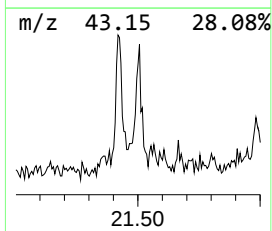
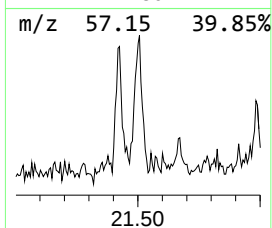
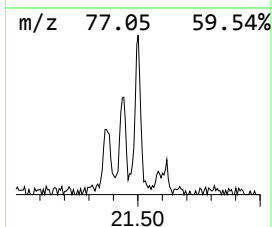
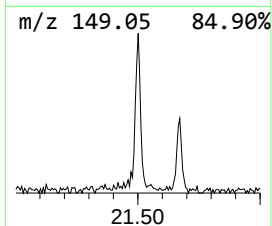
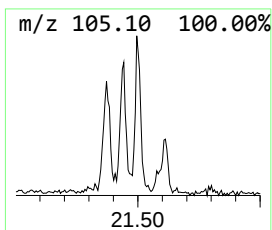
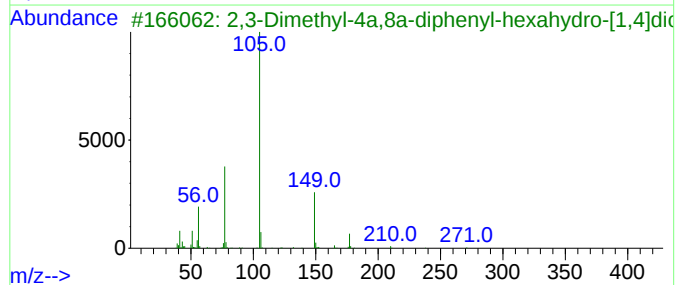
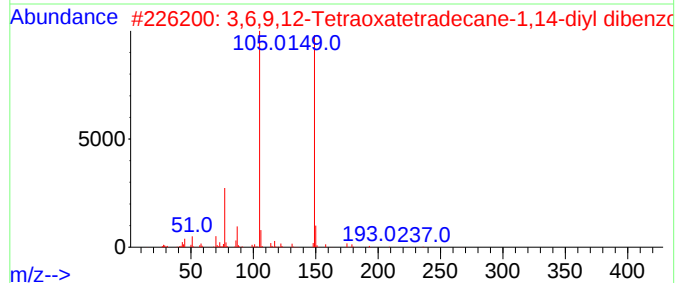
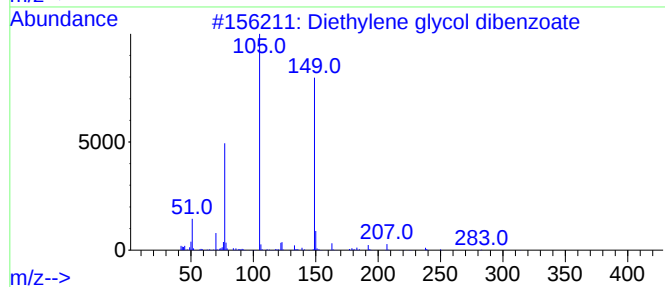
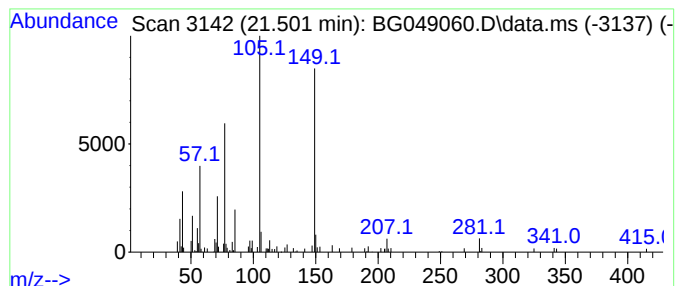
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.501	3.85 ng	106704	Chrysene-d12	21.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
2			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	50
3			2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	50
4			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	50
5			Phthalic acid, isohexyl tetradec...	446	C28H46O4	1000309-05-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
Data File : BG049060.D
Acq On : 23 Jun 2021 14:03
Operator : CG/JU
Sample : M2748-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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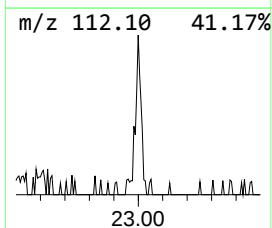
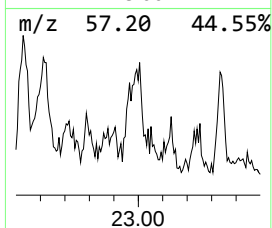
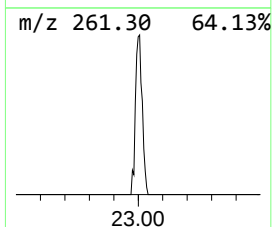
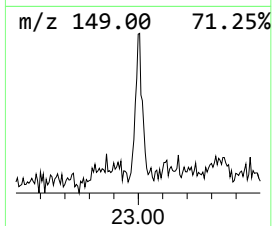
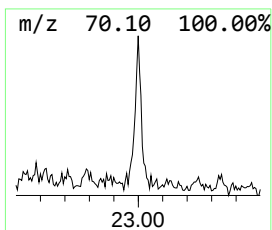
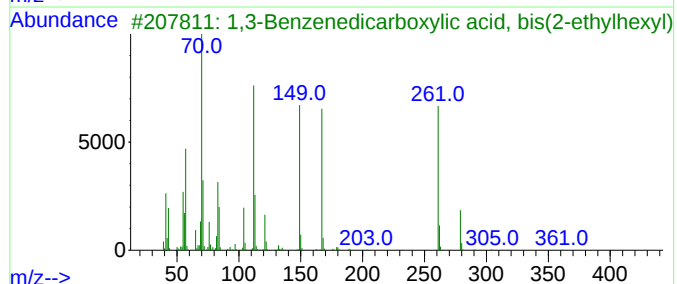
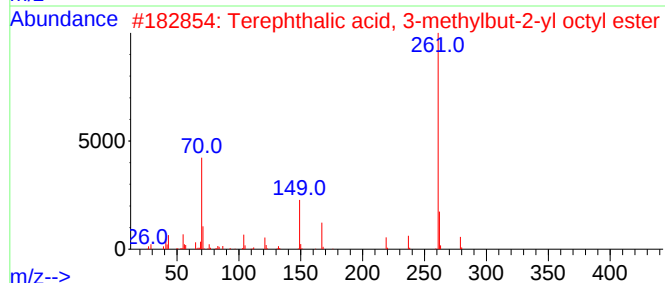
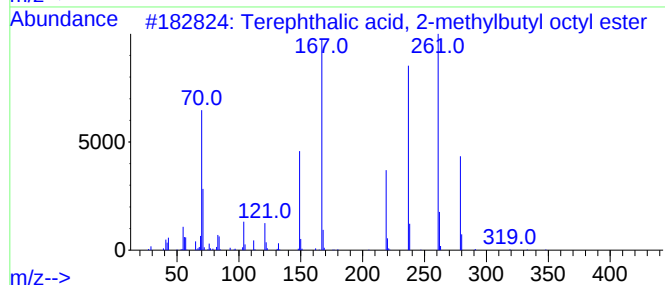
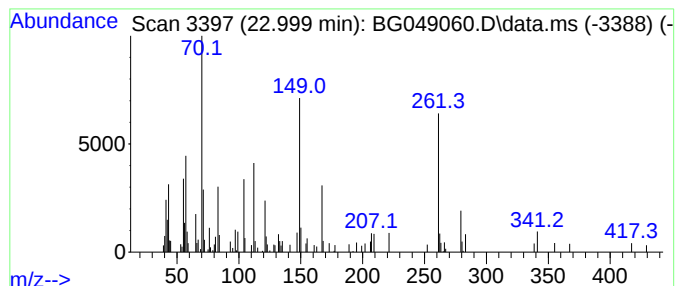
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.999 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.999	3.75 ng	103895	Chrysene-d12	21.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 2-methylbutyl...	348	C21H32O4	1000323-90-4	43
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	40
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	40
4			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
5			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
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Operator : CG/JU
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.191	164.8	ng	1311770	1	8.111	159176	20.0
Pentanoic acid,...	15.538	5.7	ng	91476	3	14.750	319796	20.0
Morpholine, 4-p...	16.378	2.5	ng	55497	4	17.500	449300	20.0
Ethanol, 2-(4-p...	16.707	13.6	ng	306363	4	17.500	449300	20.0
n-Decyl .alpha....	18.381	3.9	ng	87592	4	17.500	449300	20.0
Eicosane	20.620	2.0	ng	56391	5	21.789	553907	20.0
17-Pentatriacon...	21.425	4.7	ng	129273	5	21.789	553907	20.0
Diethylene glyc...	21.501	3.9	ng	106704	5	21.789	553907	20.0
unknown22.999	22.999	3.8	ng	103895	5	21.789	553907	20.0