

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
 Data File : BG056349.D
 Acq On : 19 Jan 2023 16:20
 Operator : CG/JU
 Sample : 01209-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TWP-03

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	23	rVB	416063	533237	17.09%	3.660%
2	5.344	344	350	356	rBV	47645	72929	2.34%	0.501%
3	5.826	425	432	442	rVB	273055	435142	13.95%	2.987%
4	7.442	701	707	718	rVB	161585	283365	9.08%	1.945%
5	8.305	846	854	862	rBV	124832	205557	6.59%	1.411%
6	9.480	1046	1054	1062	rBV	349464	610626	19.57%	4.191%
7	11.137	1328	1336	1344	rBV	157354	280018	8.97%	1.922%
8	12.882	1630	1633	1644	rVB3	18970	37829	1.21%	0.260%
9	13.546	1738	1746	1754	rVB	1284264	1926951	61.76%	13.227%
10	14.222	1854	1861	1868	rBV	281468	407620	13.06%	2.798%
11	14.557	1911	1918	1927	rVB3	11522	31222	1.00%	0.214%
12	14.657	1927	1935	1940	rBV	242147	357402	11.46%	2.453%
13	14.921	1972	1980	1986	rBV	291158	457834	14.67%	3.143%
14	16.255	2199	2207	2211	rBV	124538	212347	6.81%	1.458%
15	16.331	2211	2220	2224	rVV5	99977	346395	11.10%	2.378%
16	16.396	2225	2231	2250	rVB	1003515	1873806	60.06%	12.862%
17	17.653	2439	2445	2452	rBV	401881	614736	19.70%	4.220%
18	18.499	2584	2589	2599	rVB	196500	272888	8.75%	1.873%
19	19.757	2795	2803	2815	rVB	281179	462612	14.83%	3.175%
20	20.233	2878	2884	2889	rVB	2335278	3119983	100.00%	21.416%
21	20.485	2923	2927	2931	rBV3	25296	47166	1.51%	0.324%
22	21.161	3039	3042	3049	rVB4	34231	55118	1.77%	0.378%
23	21.525	3100	3104	3110	rVB2	101060	143679	4.61%	0.986%
24	21.948	3169	3176	3184	rVB2	453347	794441	25.46%	5.453%
25	22.741	3308	3311	3317	rBV4	30032	44362	1.42%	0.305%
26	23.476	3429	3436	3444	rBV6	38773	97507	3.13%	0.669%
27	25.385	3751	3761	3772	rVB2	245200	761725	24.41%	5.229%
28	29.586	4468	4476	4478	rBV9	38973	82112	2.63%	0.564%

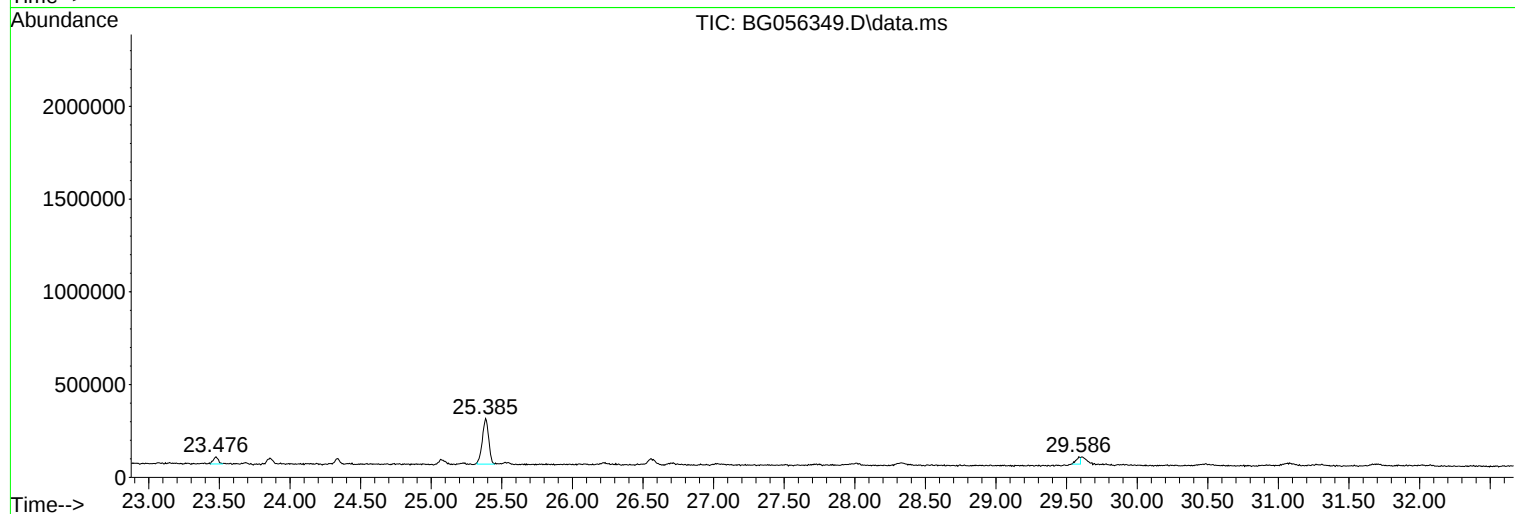
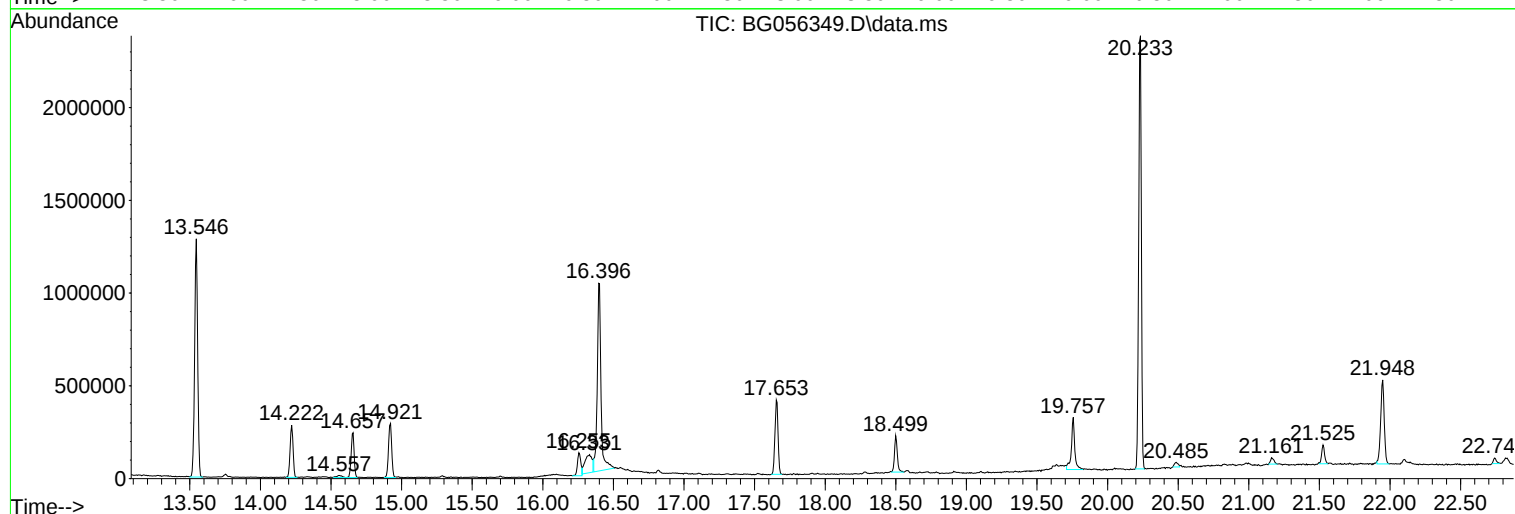
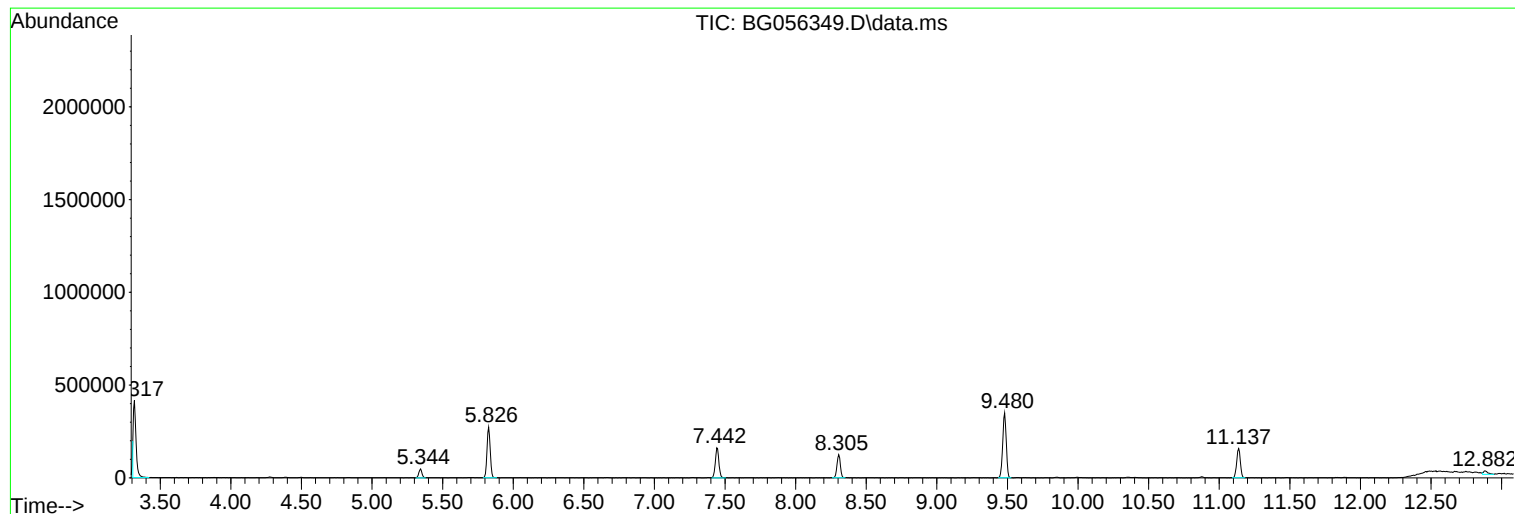
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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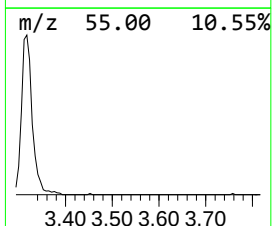
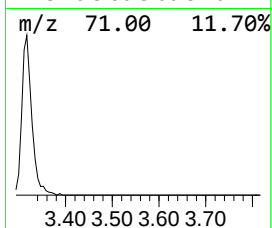
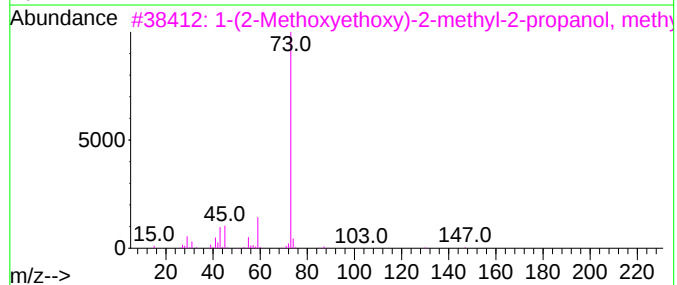
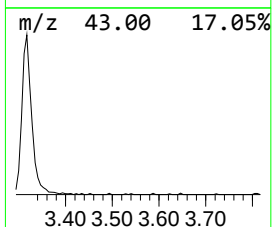
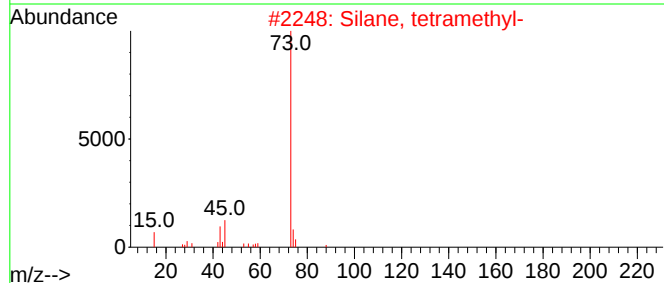
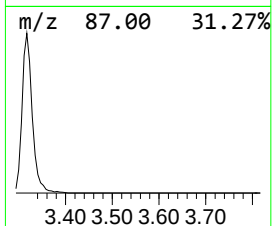
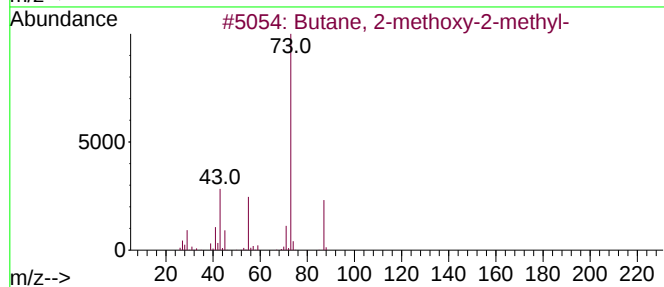
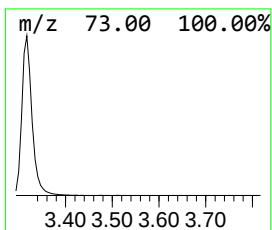
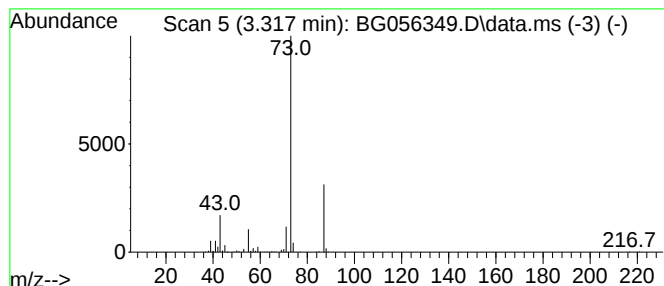
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.317	51.88 ng	533237	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
3			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	7



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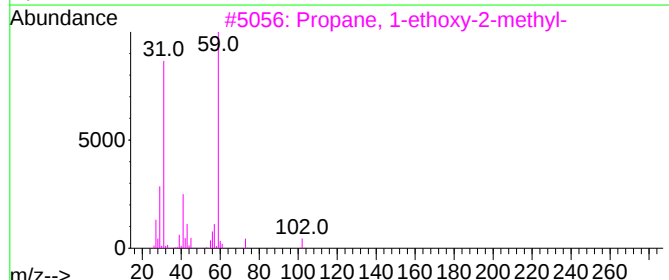
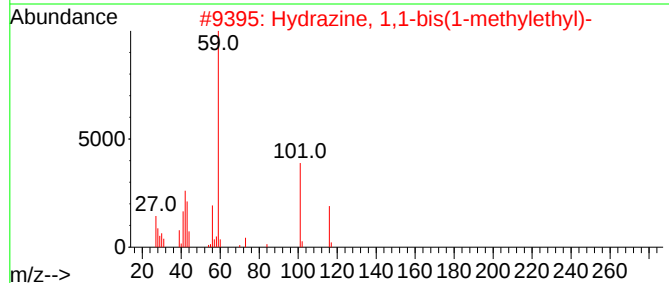
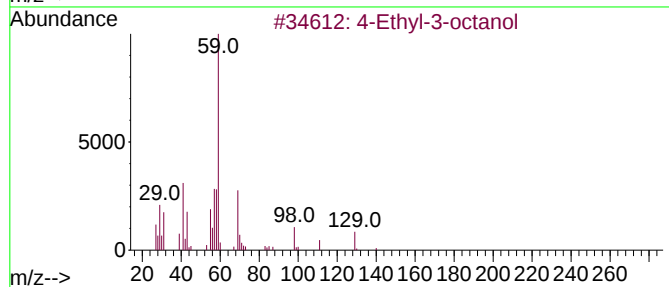
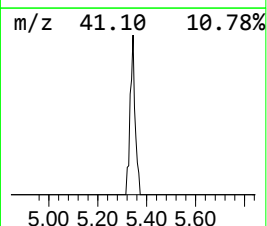
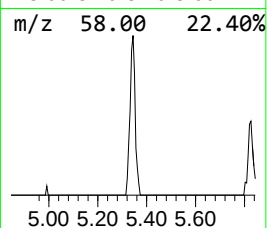
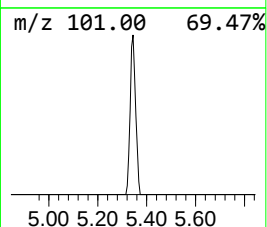
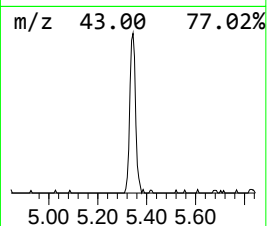
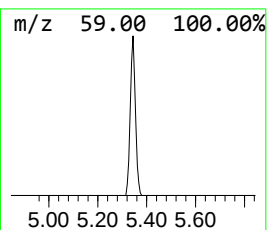
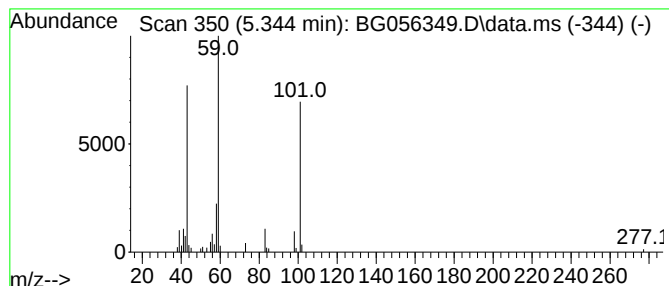
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.344 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	7.10 ng	72929	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethyl-3-octanol	158	C10H22O	019781-26-1	43
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
4			Butanoic acid, 4-(2,4,5-trichloro...	296	C11H11Cl3O3	025333-21-5	33
5			2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	32



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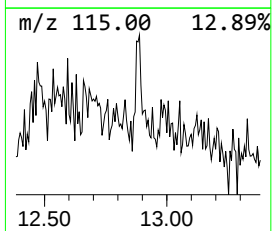
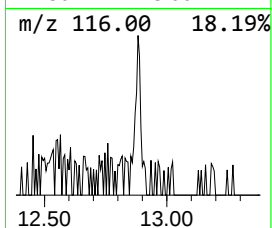
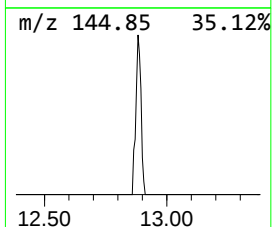
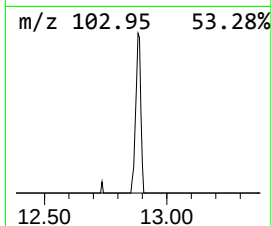
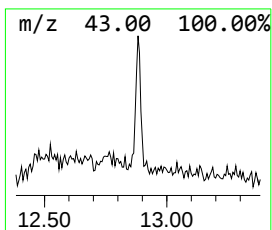
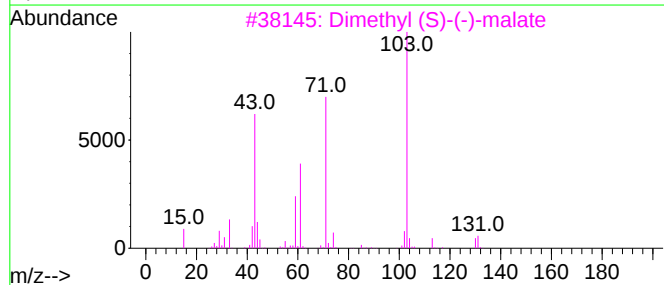
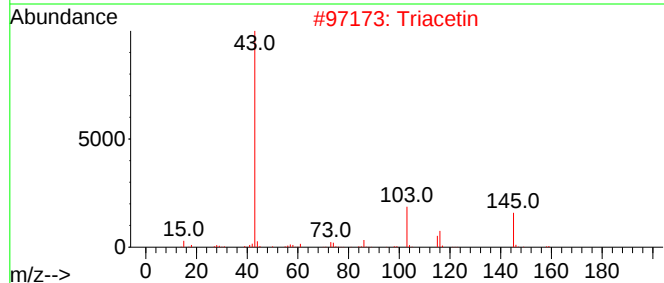
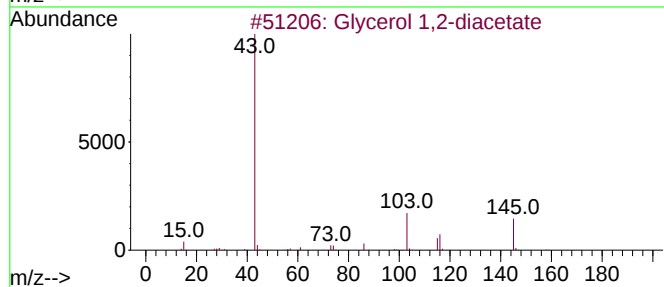
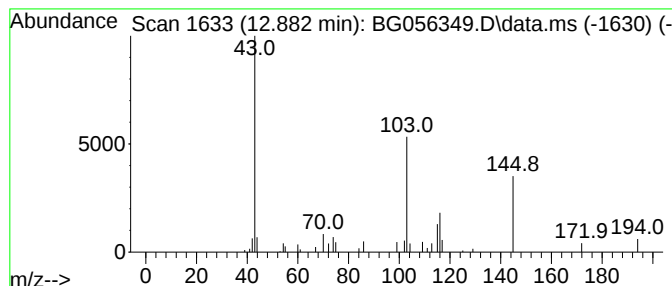
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Glycerol 1,2-diacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.882	2.70 ng	37829	Naphthalene-d8	11.137

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	50
2			Triacetin	218	C9H14O6	000102-76-1	50
3			Dimethyl (S)-(-)-malate	162	C6H10O5	000617-55-0	35
4			3-Acetoxy-3-hydroxypropionic aci...	162	C6H10O5	1000190-19-0	17
5			Dimethyl (R)-(+)-malate	162	C6H10O5	070681-41-3	17



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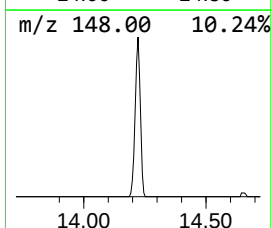
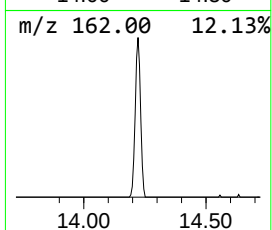
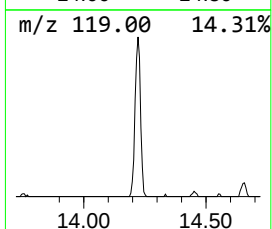
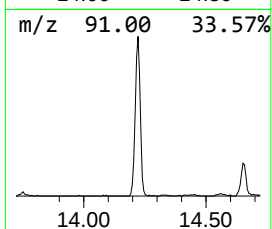
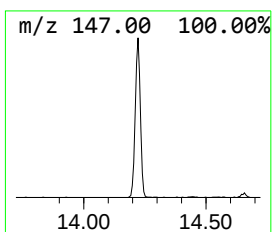
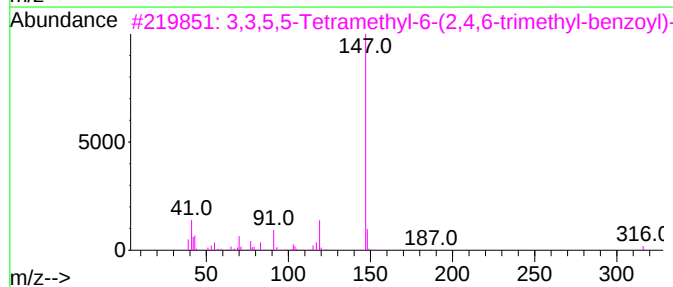
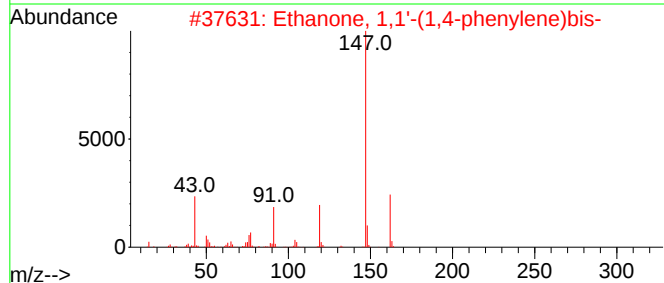
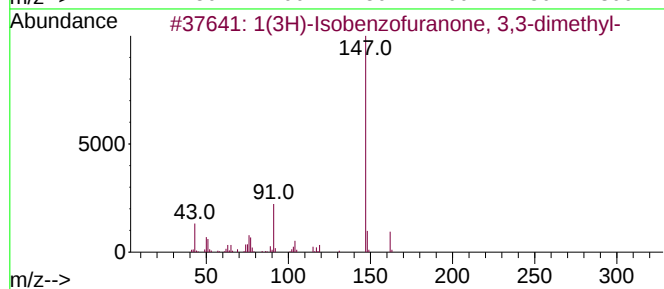
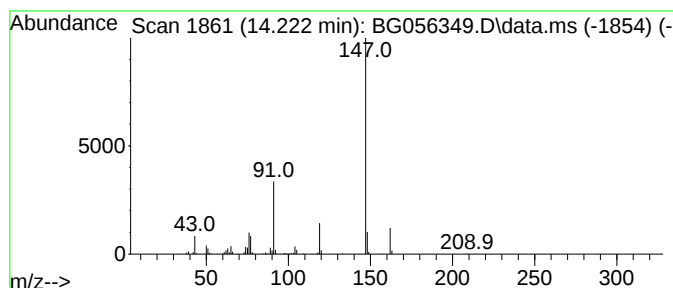
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Peak Number 4 1(3H)-Isobenzofuranone, 3,3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.222	17.81 ng	407620	Acenaphthene-d10	14.921	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone, 3,3-dime...	162	C10H10O2	001689-09-4	86
2	Ethanone, 1,1'-(1,4-phenylene)bis-	162	C10H10O2	001009-61-6	76
3	3,3,5,5-Tetramethyl-6-(2,4,6-tri...	316	C19H24O4	1000300-11-3	72
4	o-Diacetylbenzene	162	C10H10O2	000704-00-7	72
5	Ethanone, 1,1'-(1,3-phenylene)bis-	162	C10H10O2	006781-42-6	70



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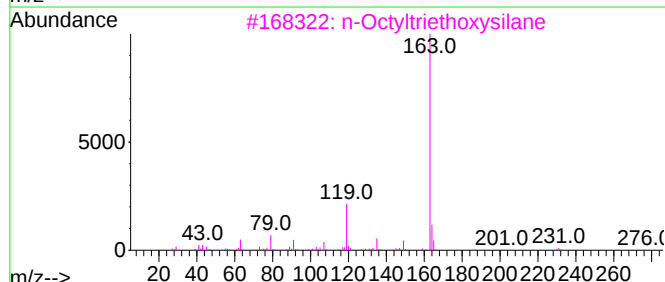
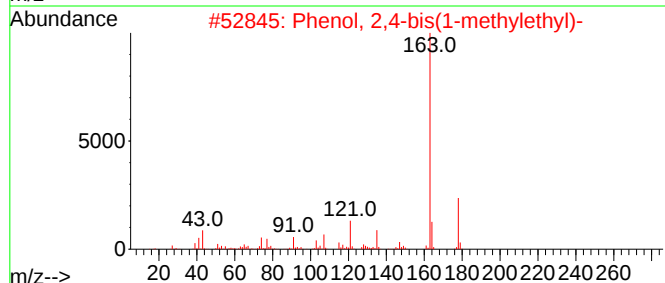
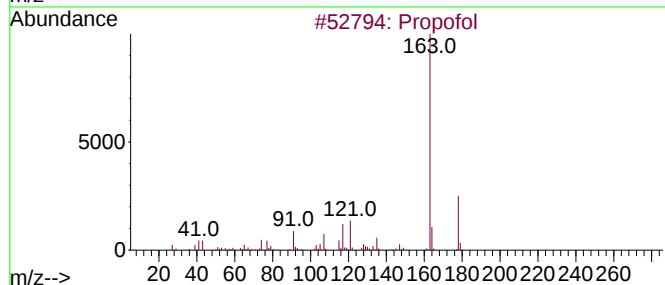
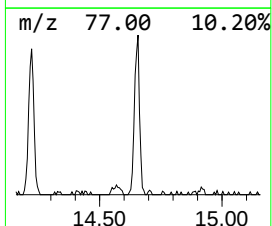
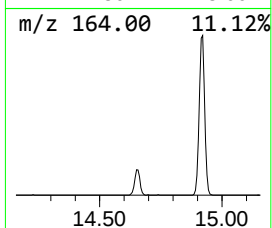
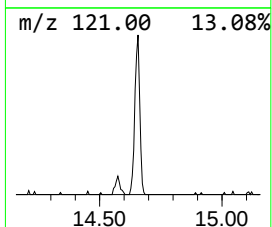
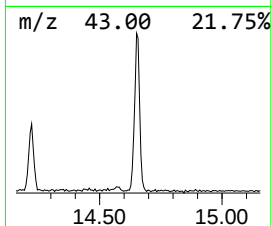
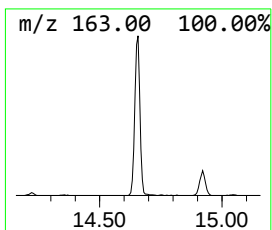
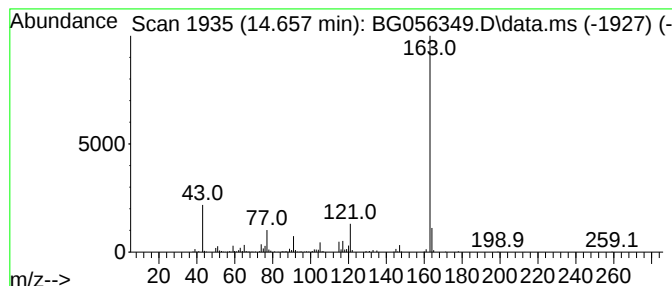
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Peak Number 5 Propofol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	15.61 ng	357402	Acenaphthene-d10	14.921

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propofol	178	C12H18O	002078-54-8	72
2			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	64
3			n-Octyltriethoxysilane	276	C14H32O3Si	002943-75-1	59
4			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	59
5			Phthalic acid, 2-isopropylphenyl...	298	C18H18O4	1000315-52-2	50



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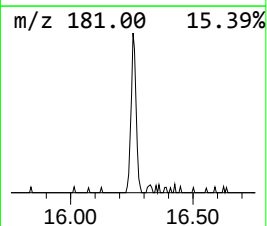
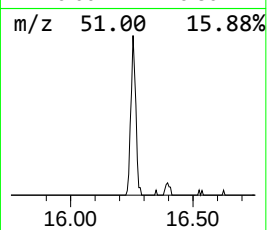
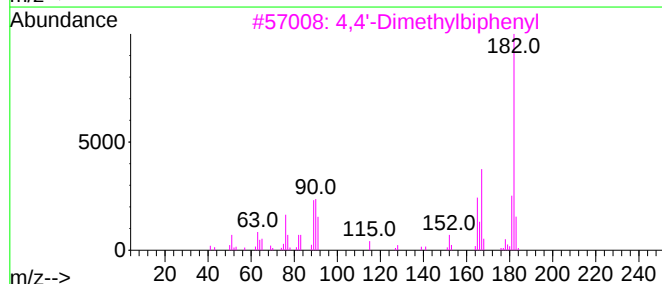
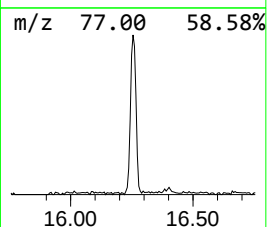
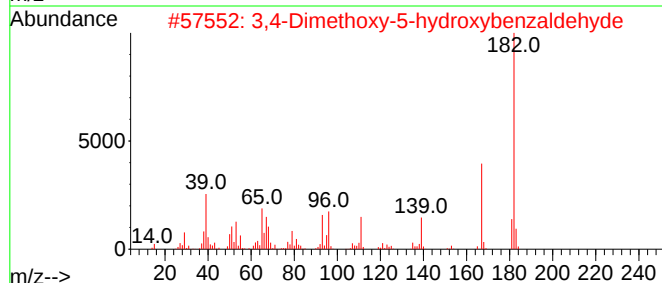
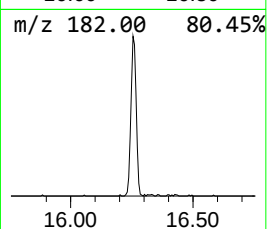
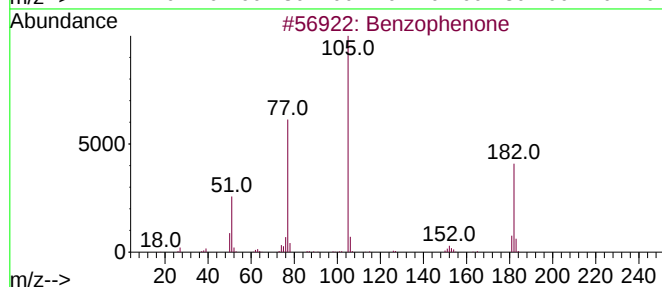
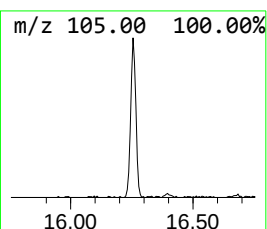
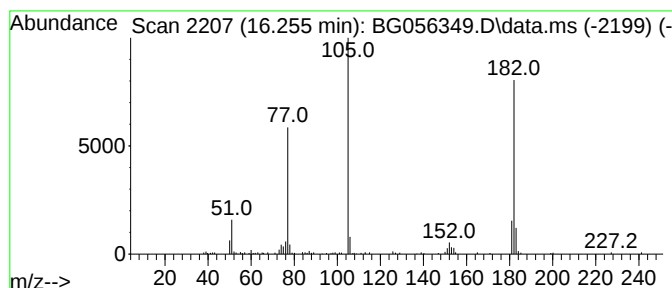
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.255	9.28 ng	212347	Acenaphthene-d10	14.921

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	47
3			4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	46
4			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
5			1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

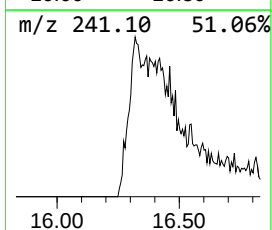
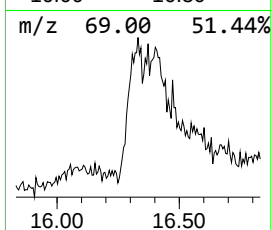
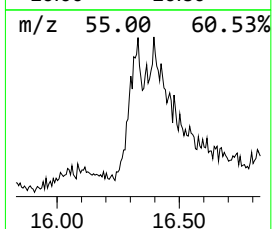
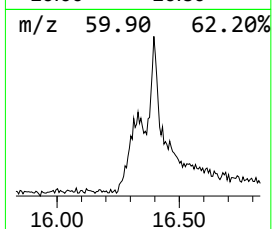
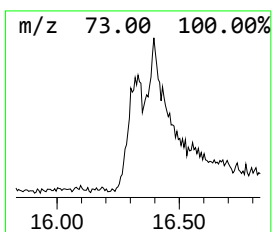
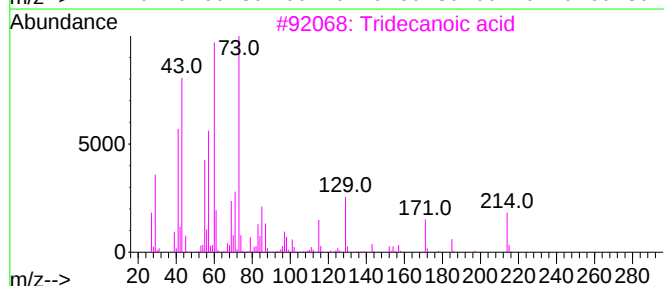
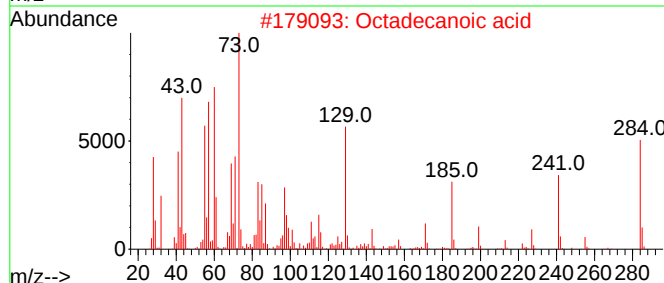
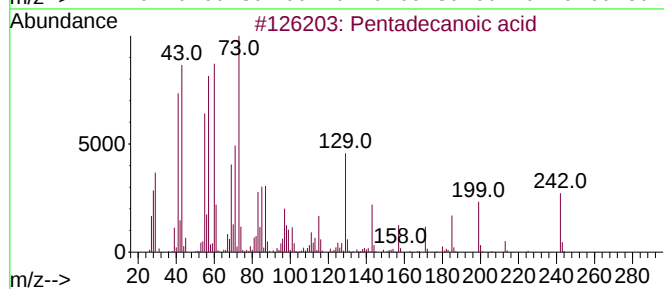
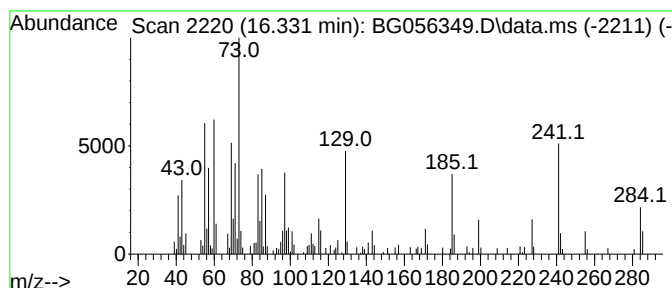
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ClientSampleId :
TWP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.331	11.27 ng	346395	Phenanthrene-d10	17.653	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
2	Octadecanoic acid	284	C18H36O2	000057-11-4	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	45
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP-03

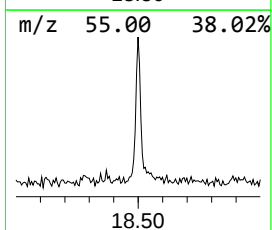
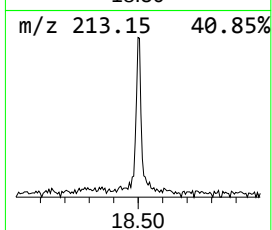
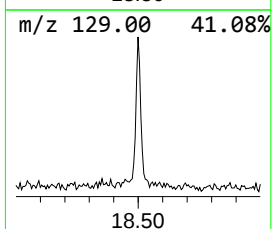
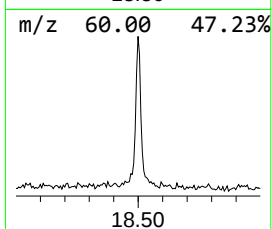
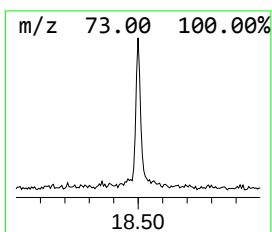
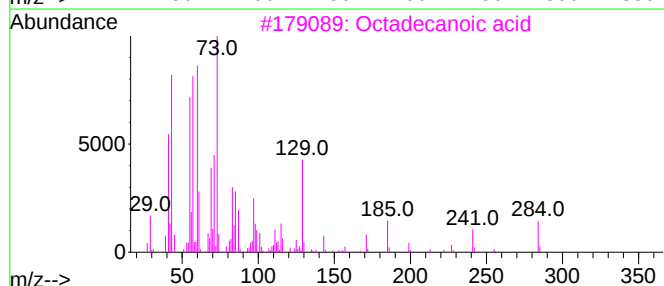
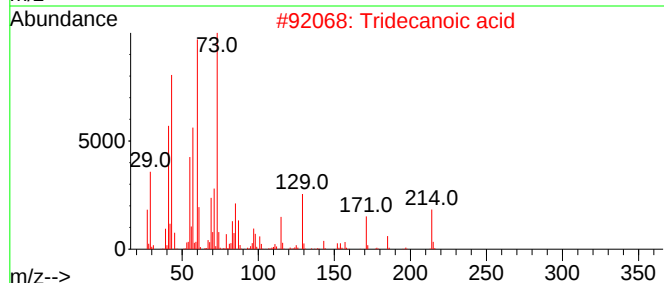
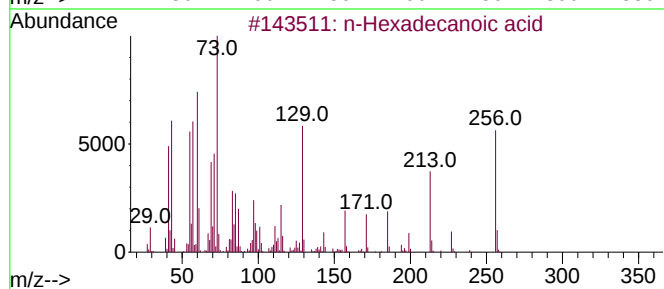
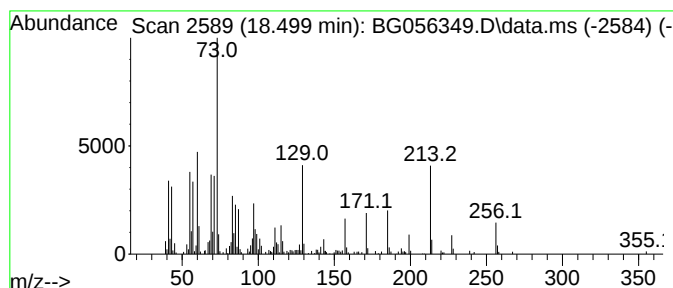
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	8.88 ng	272888	Phenanthrene-d10	17.653

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Octadecanoic acid	284	C18H36O2	000057-11-4	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP-03

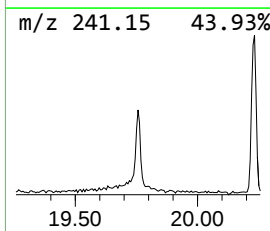
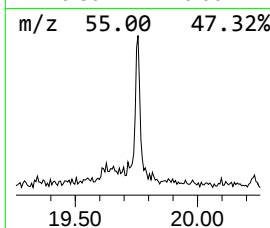
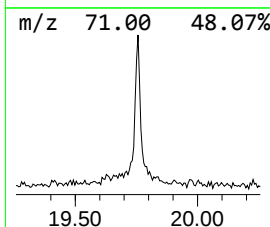
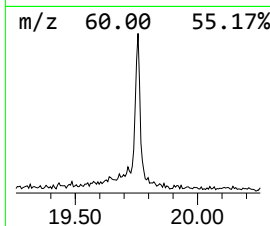
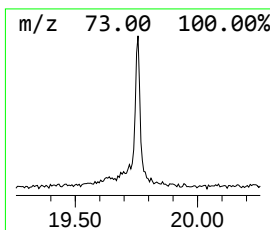
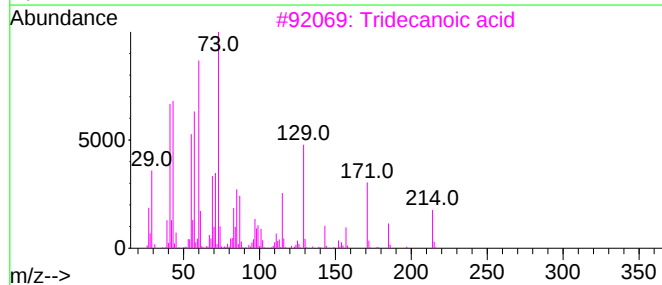
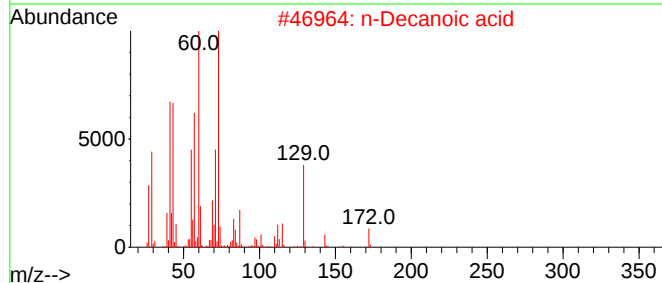
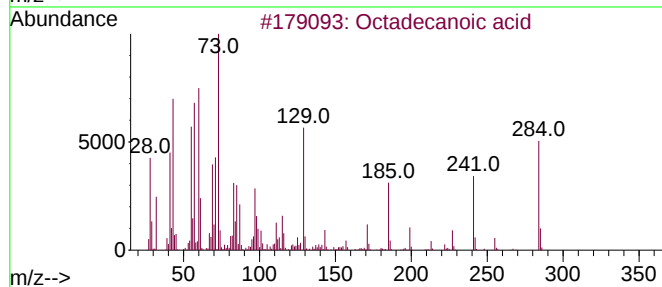
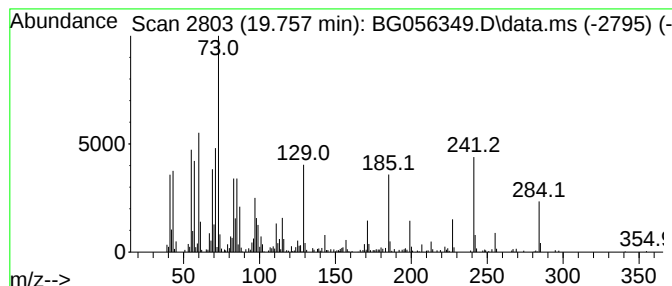
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.757	15.05 ng	462612	Phenanthrene-d10	17.653

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Decanoic acid	172	C10H20O2	000334-48-5	55
3			Tridecanoic acid	214	C13H26O2	000638-53-9	50
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TWP-03

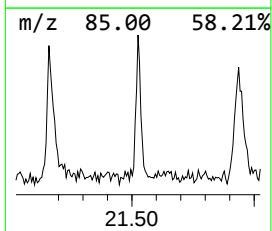
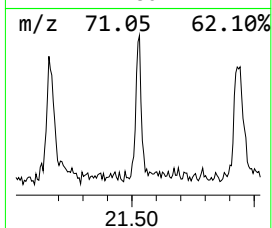
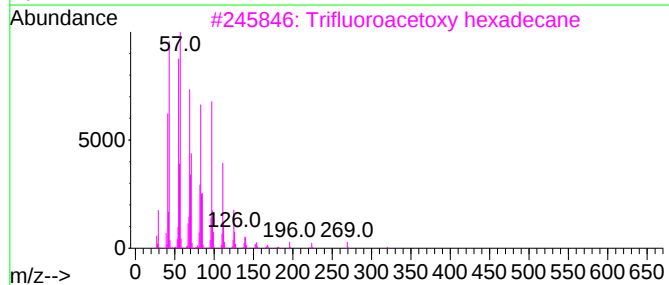
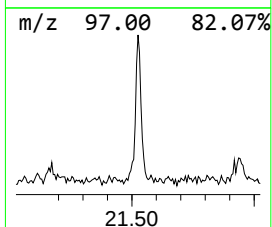
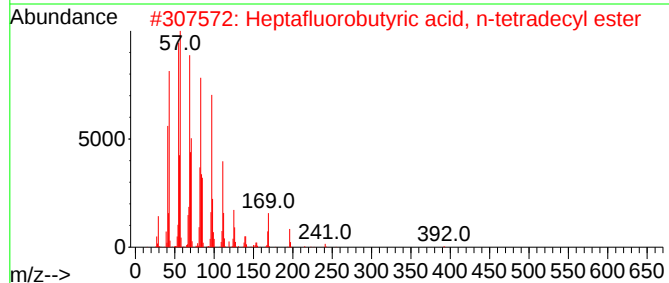
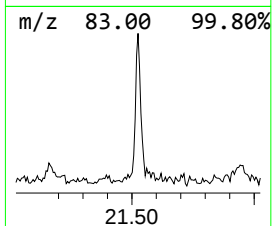
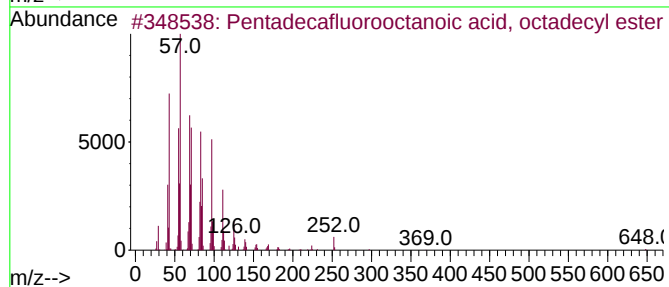
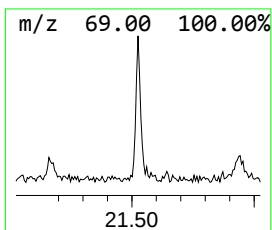
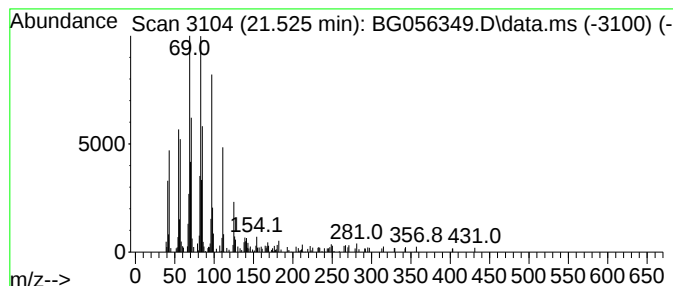
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	3.62 ng	143679	Chrysene-d12	21.948

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP-03

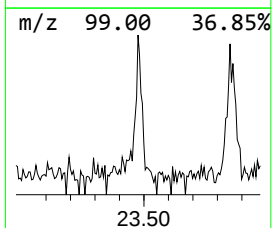
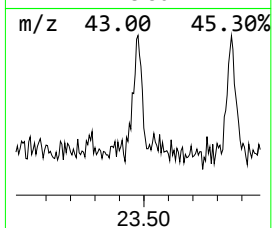
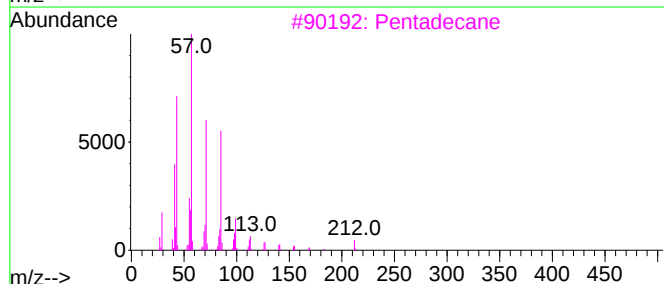
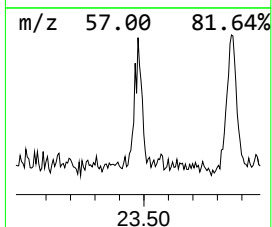
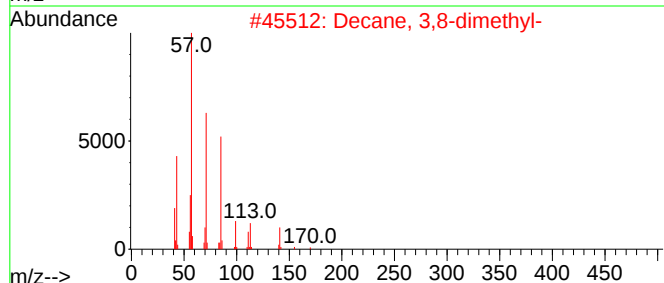
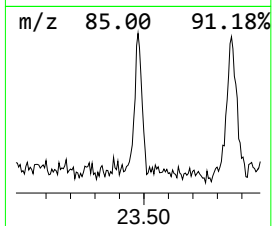
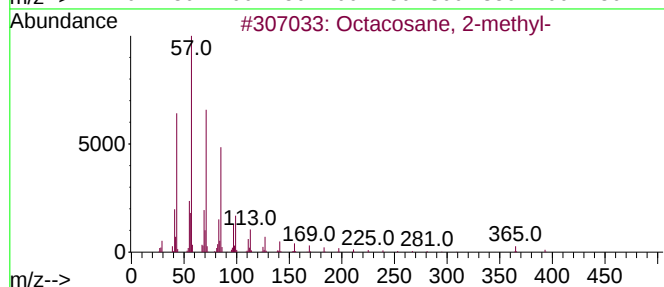
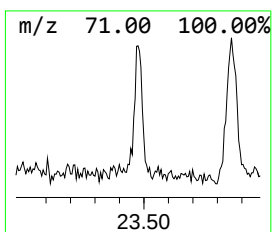
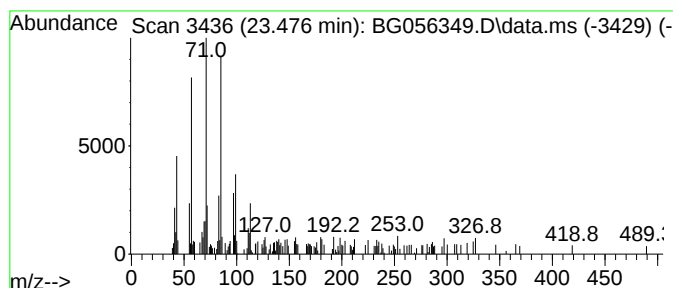
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.476	2.45 ng	97507	Chrysene-d12	21.948

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	64
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
3			Pentadecane	212	C15H32	000629-62-9	62
4			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	59
5			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
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Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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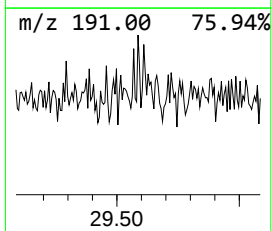
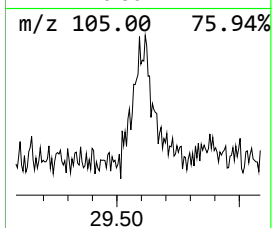
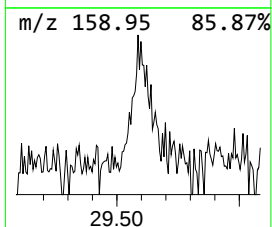
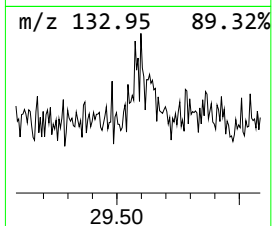
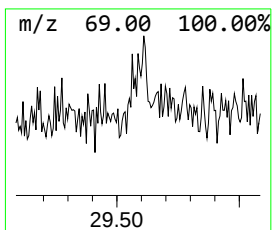
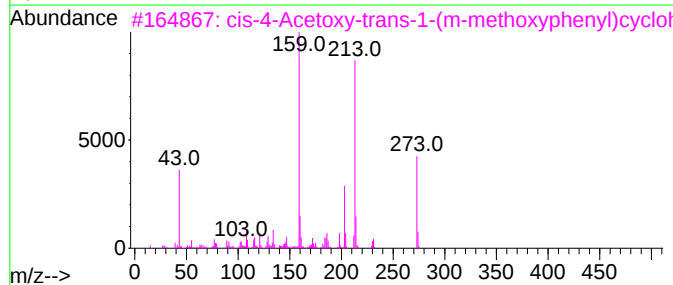
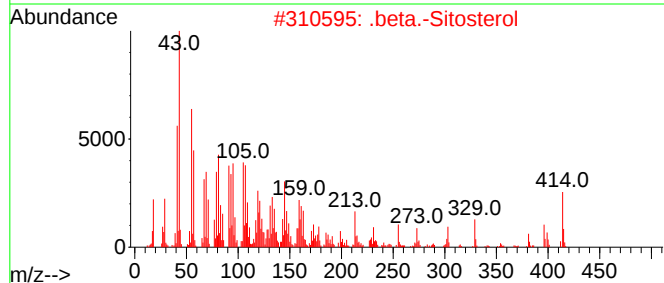
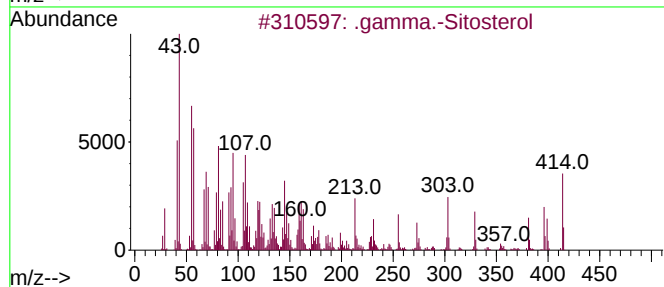
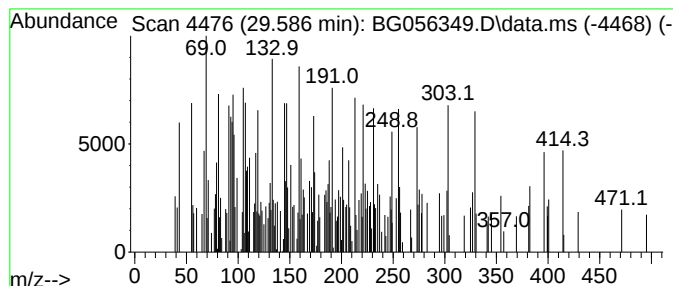
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown29.586 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.586	2.16 ng	82112	Perylene-d12	25.385

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-	Sitosterol	414	C29H50O	000083-47-6	35
2	.	beta.-	Sitosterol	414	C29H50O	000083-46-5	11
3	cis-4-	Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	11	
4	Propenone, 3-(4-chlorophenylthio...	302	C17H15ClO5	275802-49-8	10		
5	D-Arabinose, diethyl mercaptal, ...	424	C17H28O8S2	005329-45-3	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056349.D
Acq On : 19 Jan 2023 16:20
Operator : CG/JU
Sample : 01209-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.317	51.9	ng	533237	1	8.305	205557	20.0
unknown5.344	5.344	7.1	ng	72929	1	8.305	205557	20.0
Glycerol 1,2-di...	12.882	2.7	ng	37829	2	11.137	280018	20.0
1(3H)-Isobenzof...	14.222	17.8	ng	407620	3	14.921	457834	20.0
Propofol	14.657	15.6	ng	357402	3	14.921	457834	20.0
Benzophenone	16.255	9.3	ng	212347	3	14.921	457834	20.0
Pentadecanoic acid	16.331	11.3	ng	346395	4	17.653	614736	20.0
n-Hexadecanoic ...	18.499	8.9	ng	272888	4	17.653	614736	20.0
Octadecanoic acid	19.757	15.1	ng	462612	4	17.653	614736	20.0
Pentadecafluoro...	21.525	3.6	ng	143679	5	21.948	794441	20.0
Octacosane, 2-m...	23.476	2.5	ng	97507	5	21.948	794441	20.0
unknown29.586	29.586	2.2	ng	82112	6	25.385	761725	20.0