

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010424\
 Data File : BG060249.D
 Acq On : 4 Jan 2024 17:40
 Operator : MA/JU
 Sample : 06038-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 T-703

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060249.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	10	rVB	280809	300834	2.31%	0.386%
2	5.038	327	332	337	rBV	317406	460998	3.54%	0.592%
3	5.508	406	412	431	rBV	2569079	4345789	33.35%	5.579%
4	7.100	676	683	700	rBV	2808875	4848635	37.21%	6.224%
5	7.940	818	826	830	rBV	602052	1073983	8.24%	1.379%
6	7.993	830	835	842	rVB	1858523	2865018	21.98%	3.678%
7	9.098	1016	1023	1039	rBV	1580012	2849448	21.86%	3.658%
8	10.743	1293	1303	1309	rBV	908818	1648872	12.65%	2.117%
9	13.199	1713	1721	1733	rBV	5141310	8109054	62.22%	10.410%
10	14.574	1948	1955	1963	rBV	1852491	2811869	21.58%	3.610%
11	14.785	1981	1991	2001	rBV	1447524	3067081	23.53%	3.937%
12	15.966	2186	2192	2197	rVB	116350	169022	1.30%	0.217%
13	16.060	2200	2208	2224	rBV	3959676	6341238	48.66%	8.141%
14	17.323	2415	2423	2430	rBV	2495655	3850297	29.54%	4.943%
15	18.211	2570	2574	2578	rBV4	127243	175587	1.35%	0.225%
16	18.516	2622	2626	2629	rBV5	118341	209780	1.61%	0.269%
17	18.757	2663	2667	2672	rBV2	224870	462369	3.55%	0.594%
18	18.969	2700	2703	2706	rVV2	191401	269316	2.07%	0.346%
19	19.139	2728	2732	2736	rBV	417488	705752	5.42%	0.906%
20	19.362	2766	2770	2774	rBV3	561147	1036460	7.95%	1.331%
21	19.715	2827	2830	2833	rBV	273391	349391	2.68%	0.449%
22	19.944	2864	2869	2878	rVB	9234505	13032077	100.00%	16.730%
23	21.231	3084	3088	3102	rVB2	298598	562919	4.32%	0.723%
24	21.589	3142	3149	3162	rVB	2379111	3976140	30.51%	5.104%
25	22.752	3339	3347	3359	rBV	5568213	9803574	75.23%	12.585%
26	23.252	3427	3432	3439	rVB4	82519	175079	1.34%	0.225%
27	24.762	3679	3689	3707	rVB	1526279	4395814	33.73%	5.643%

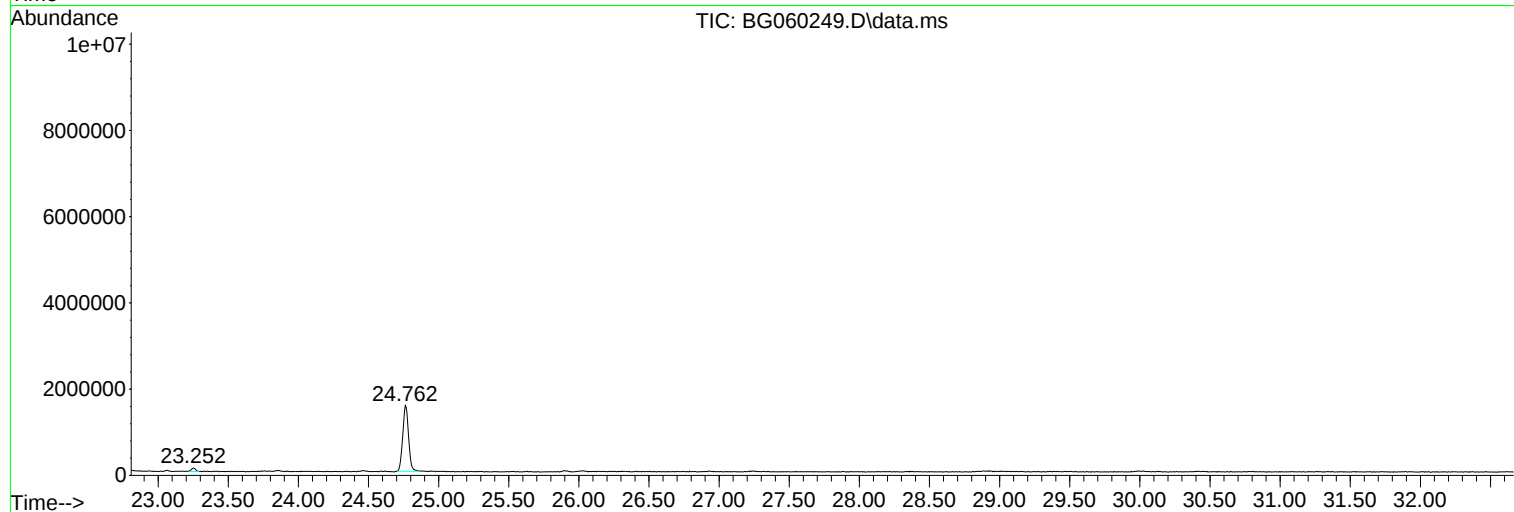
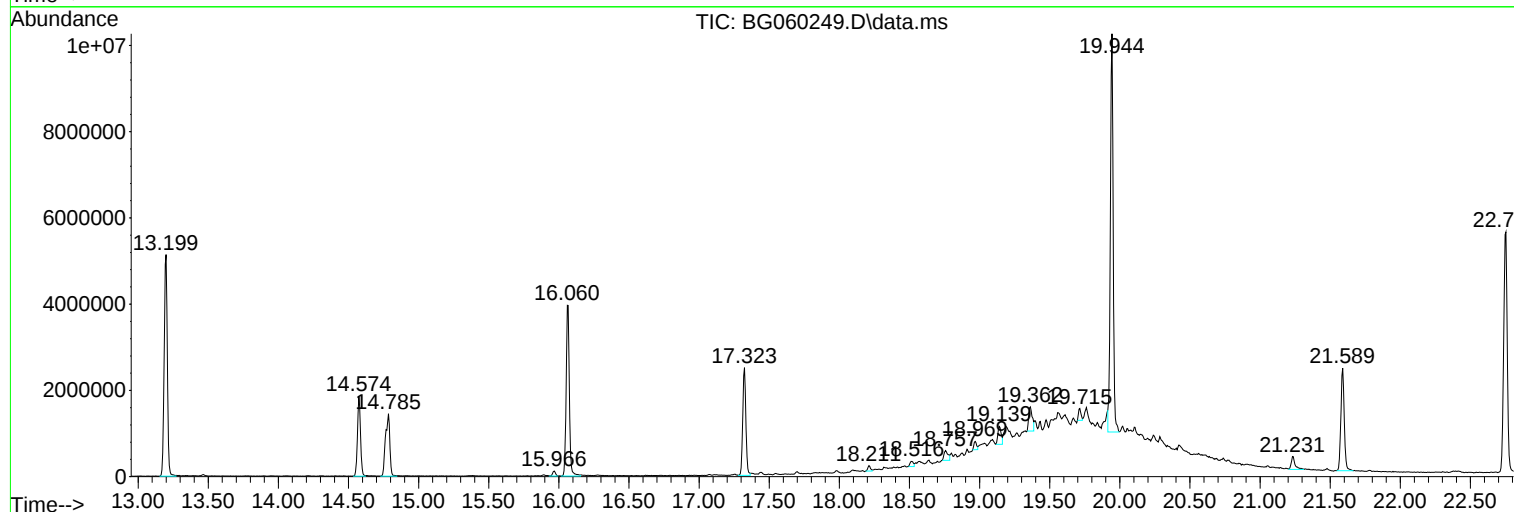
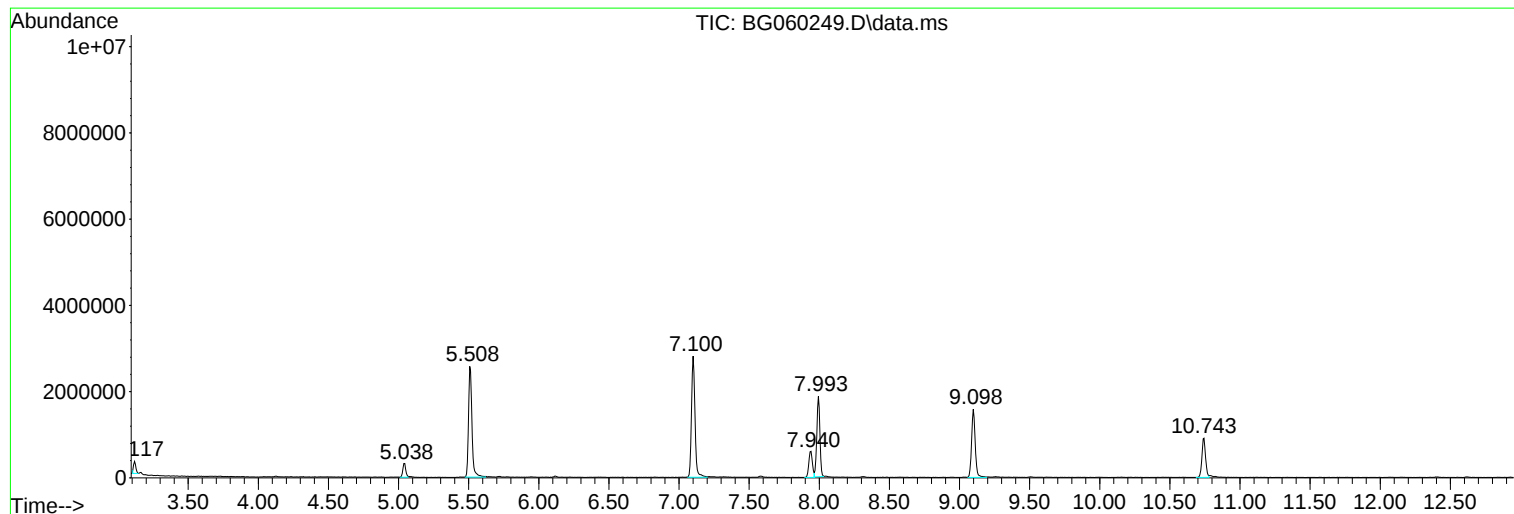
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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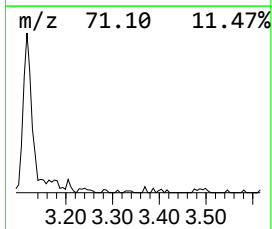
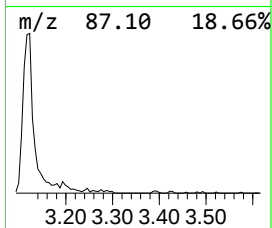
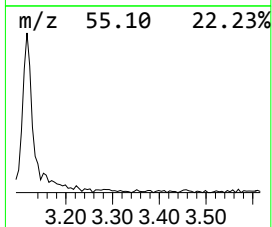
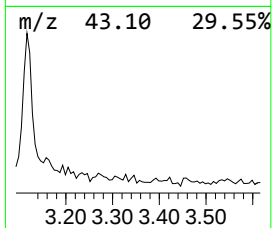
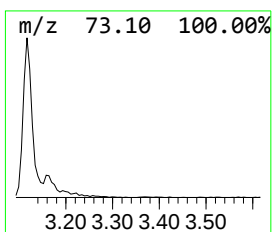
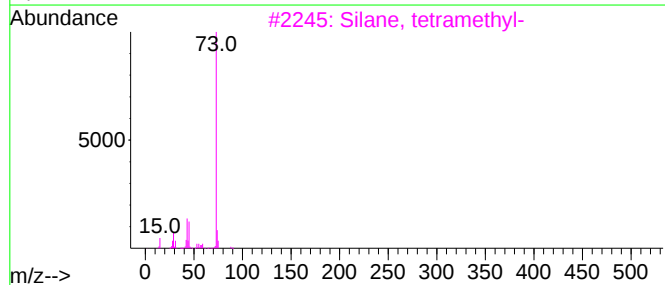
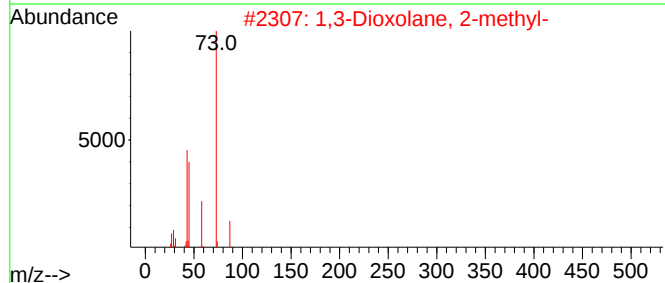
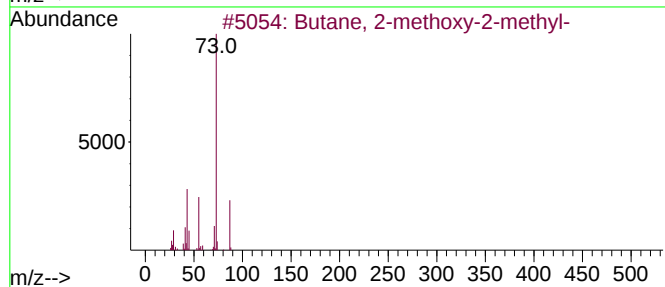
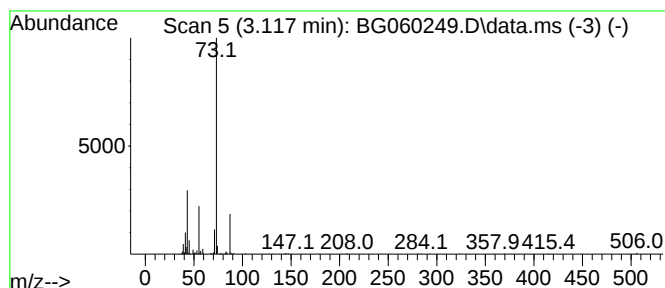
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.117 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	5.60 ng	300834	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	43
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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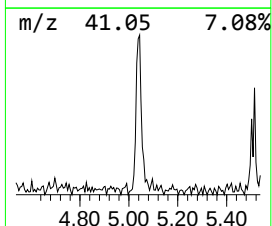
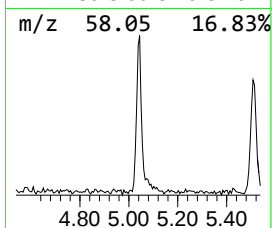
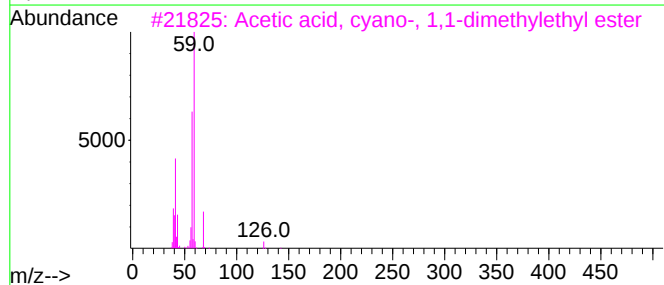
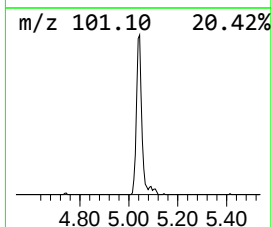
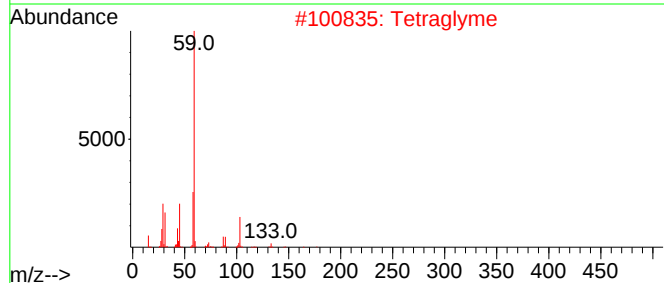
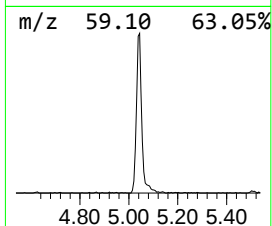
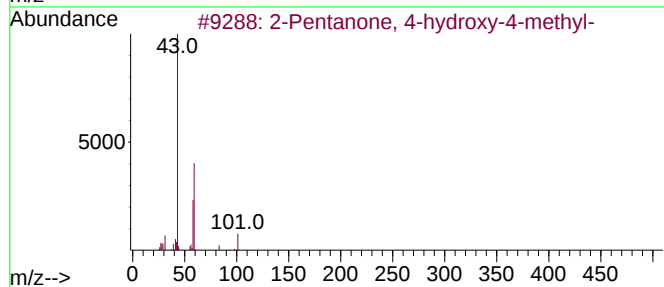
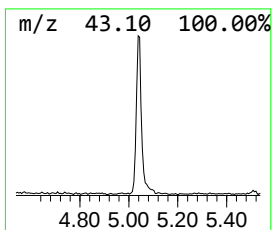
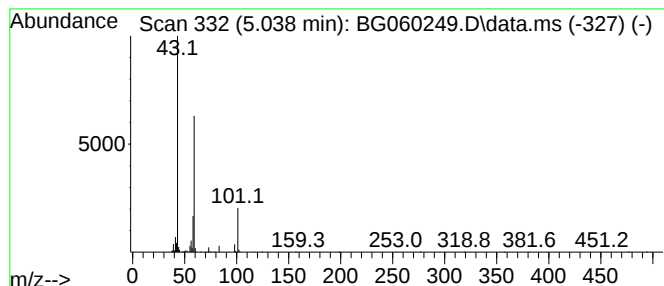
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.038	8.58 ng	460998	1,4-Dichlorobenzene-d4	7.940	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Tetraglyme	222	C10H22O5	000143-24-8	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16
4	Hexanamide	115	C6H13NO	000628-02-4	12
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12



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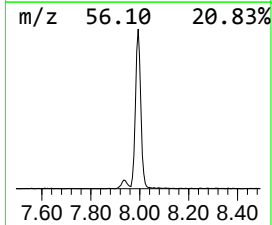
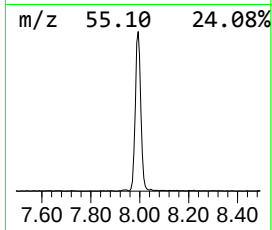
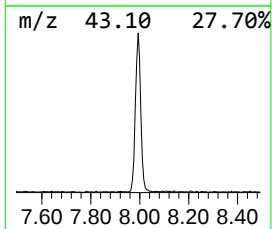
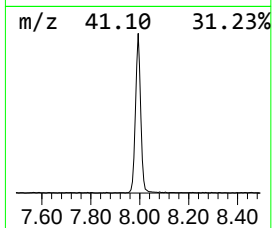
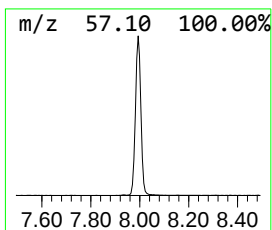
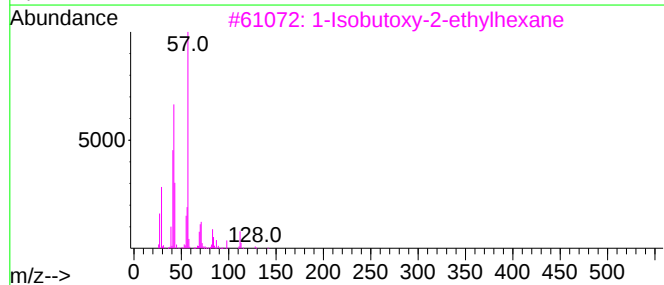
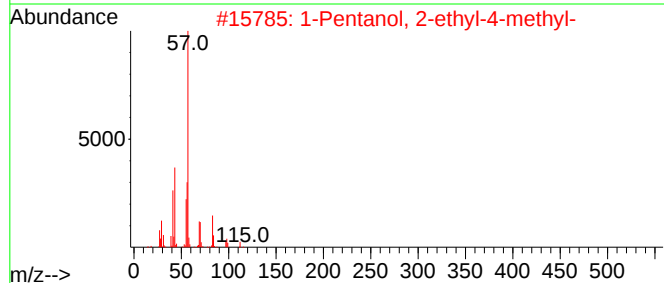
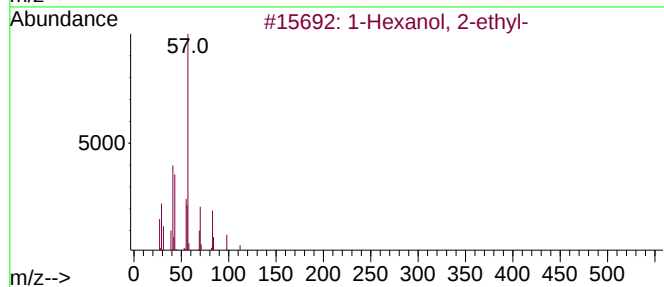
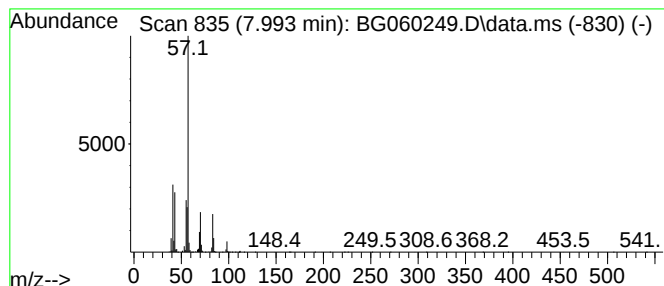
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.993	53.35 ng	2865020	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	78
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53



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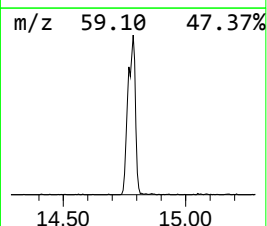
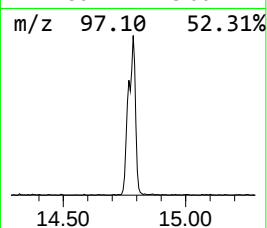
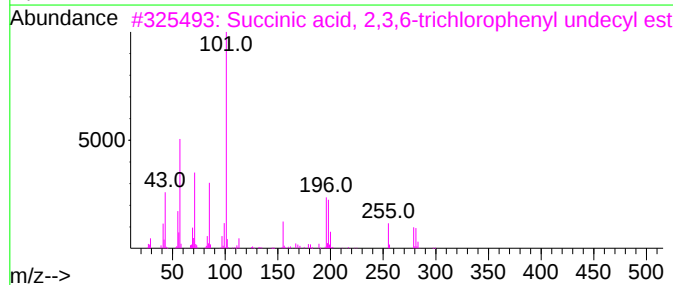
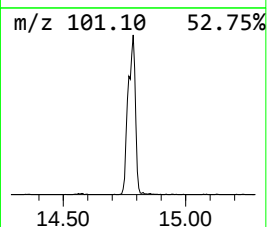
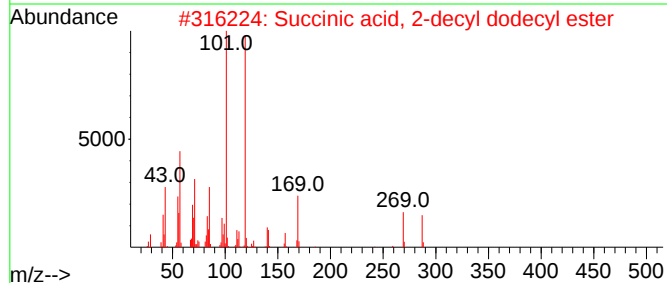
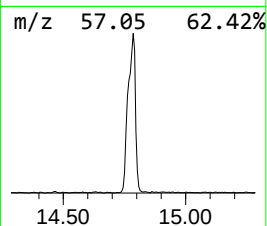
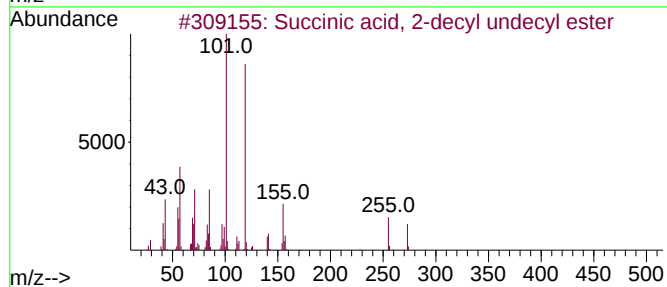
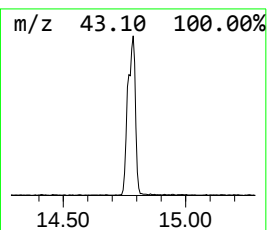
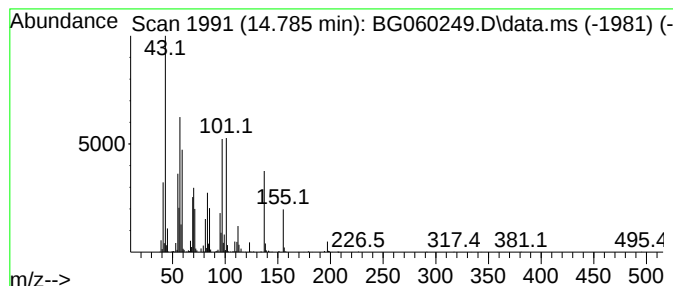
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Peak Number 4 unknown14.785 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.785	21.82 ng	3067080	Acenaphthene-d10	14.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-decyl undecyl e...	412	C25H48O4	1000349-43-1	27
2			Succinic acid, 2-decyl dodecyl e...	426	C26H50O4	1000349-43-2	22
3			Succinic acid, 2,3,6-trichloroph...	450	C21H29Cl3O4	1010349-71-2	22
4			Succinic acid, decyl 2-decyl ester	398	C24H46O4	1000349-43-0	22
5			meso-3,4-Dicyclohexyl-2,2,5,5-te...	306	C22H42	065149-86-2	22



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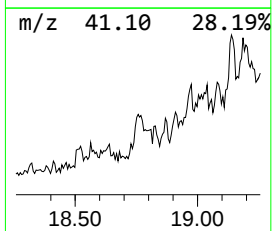
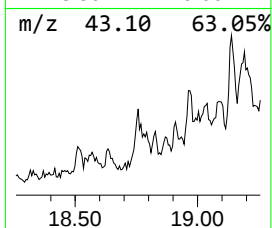
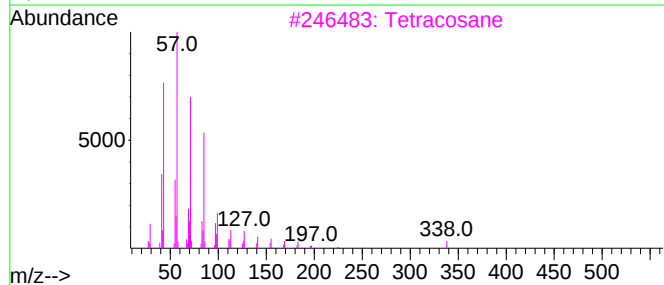
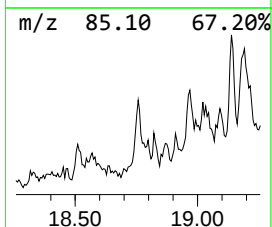
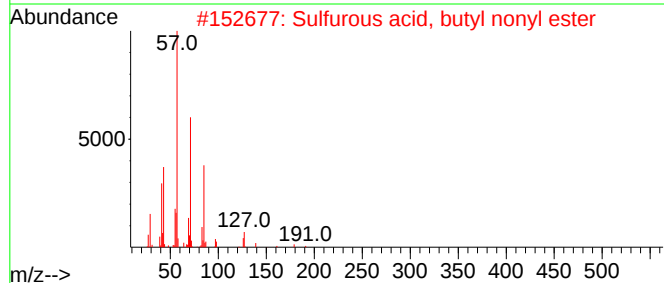
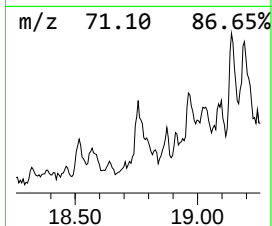
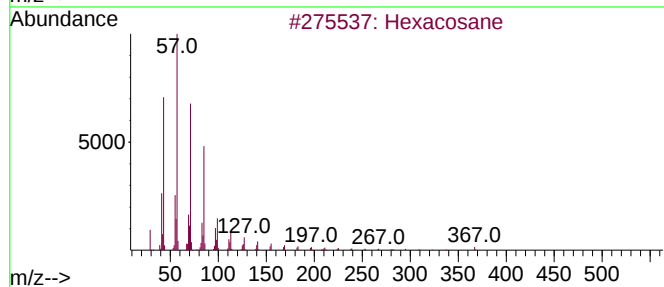
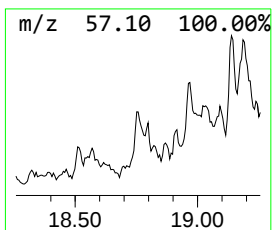
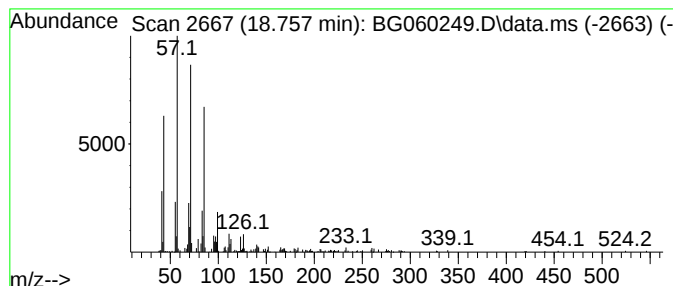
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Peak Number 5 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.757	2.40 ng	462369	Phenanthrene-d10	17.323

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	80
2			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
3			Tetracosane	338	C24H50	000646-31-1	72
4			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	64
5			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64



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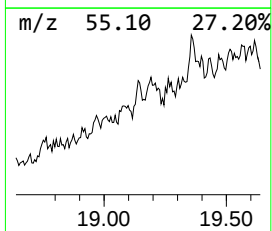
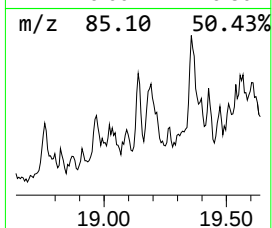
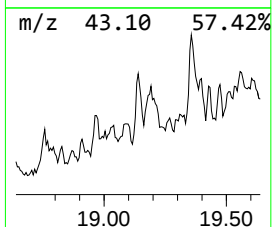
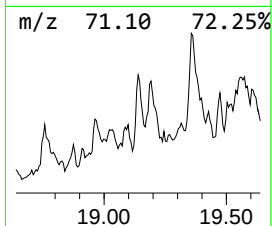
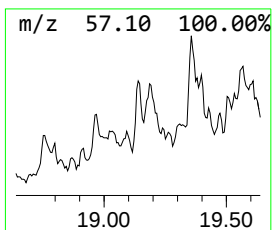
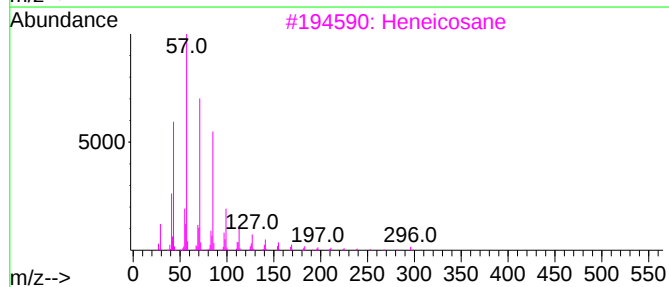
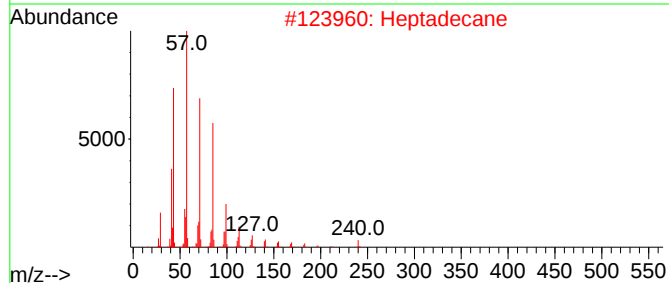
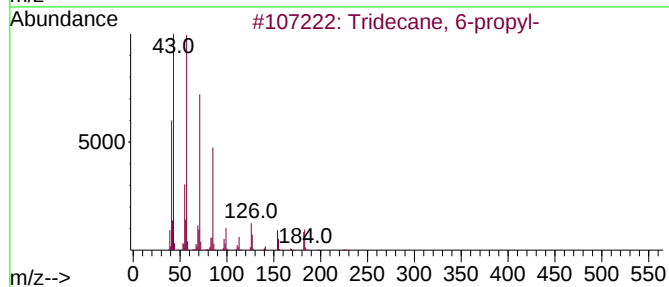
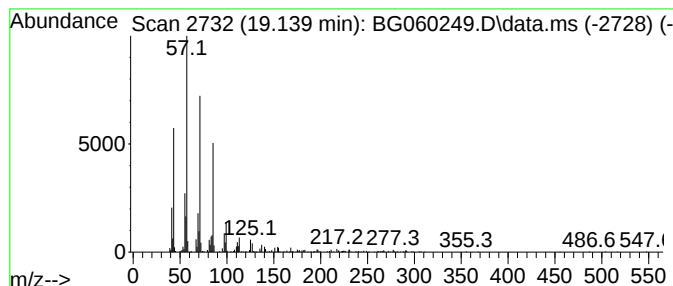
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane, 6-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.139	3.67 ng	705752	Phenanthrene-d10	17.323

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
2			Heptadecane	240	C17H36	000629-78-7	80
3			Heneicosane	296	C21H44	000629-94-7	80
4			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	80
5			Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010424\
Data File : BG060249.D
Acq On : 4 Jan 2024 17:40
Operator : MA/JU
Sample : 06038-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

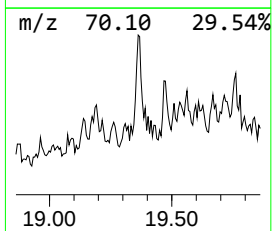
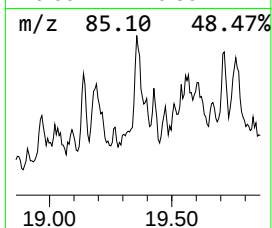
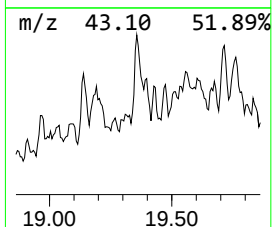
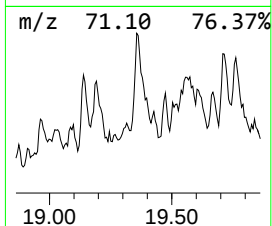
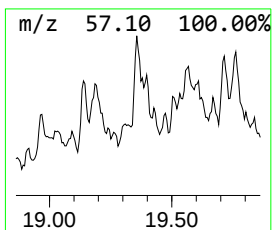
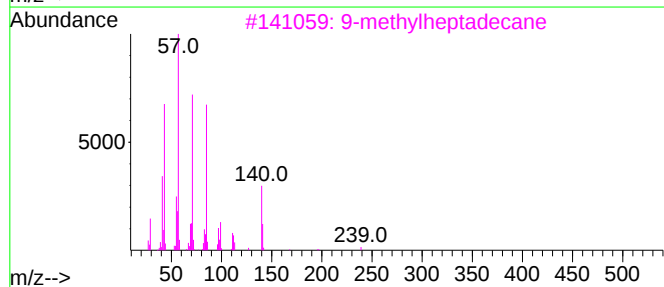
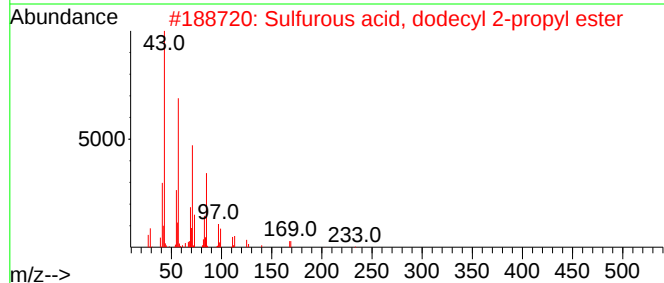
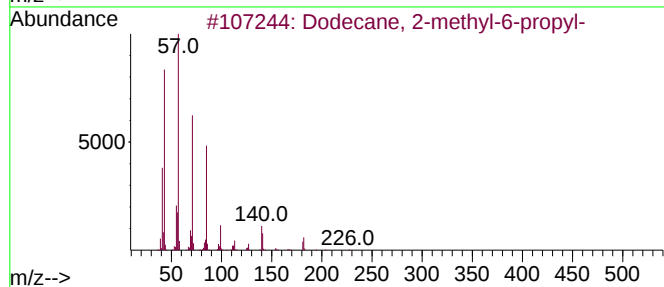
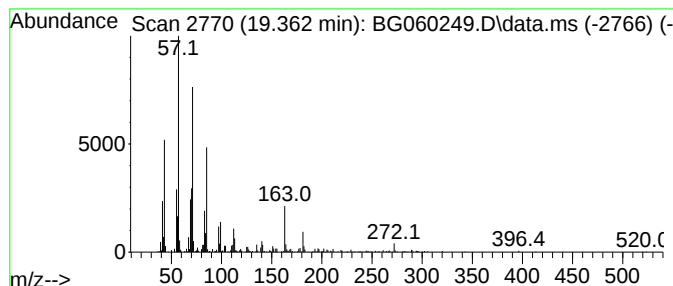
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ClientSampleId :
T-703

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2-methyl-6-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.362	5.38 ng	1036460	Phenanthrene-d10	17.323	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	60
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	58
3	9-methylheptadecane	254	C18H38	026741-18-4	53
4	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	53
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010424\
Data File : BG060249.D
Acq On : 4 Jan 2024 17:40
Operator : MA/JU
Sample : 06038-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-703

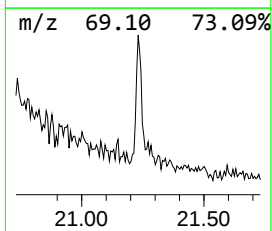
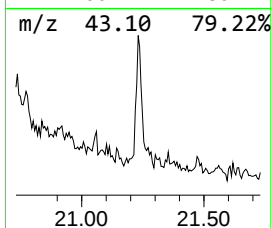
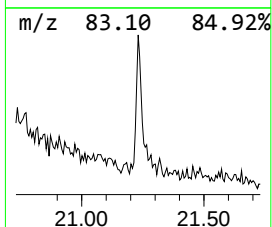
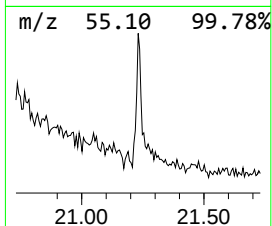
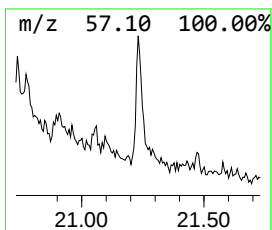
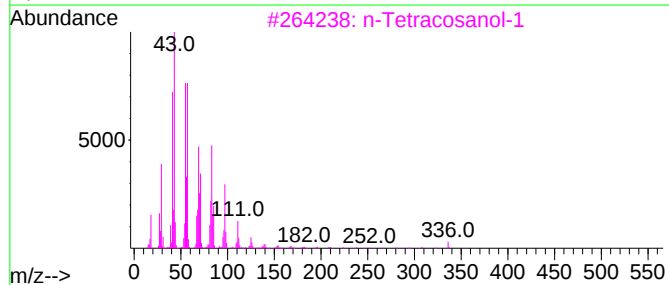
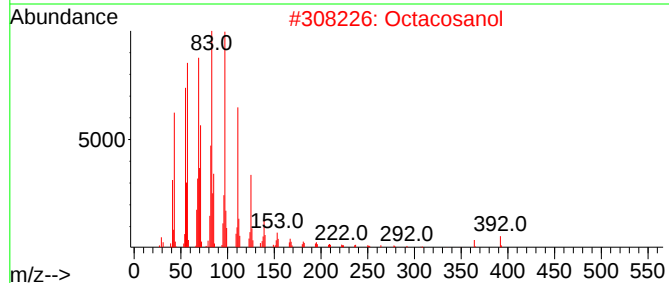
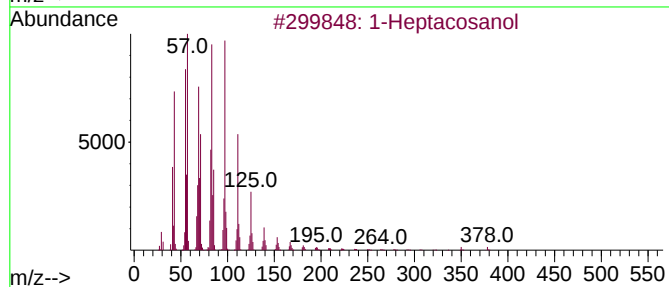
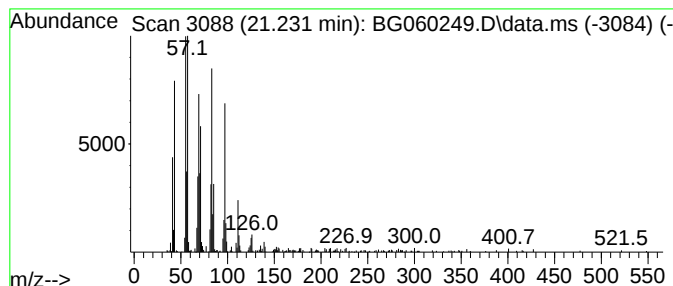
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.231	2.83 ng	562919	Chrysene-d12	21.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			Octacosanol	410	C28H58O	000557-61-9	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	87
5			1-Hexacosene	364	C26H52	018835-33-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010424\
Data File : BG060249.D
Acq On : 4 Jan 2024 17:40
Operator : MA/JU
Sample : 06038-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-703

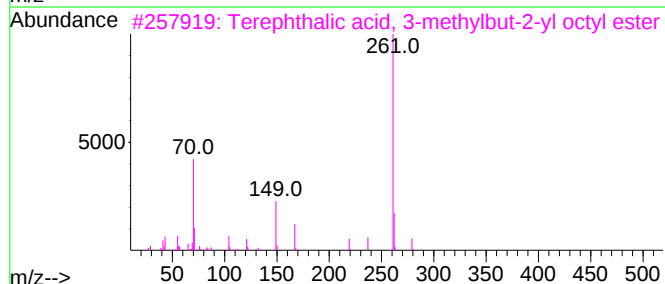
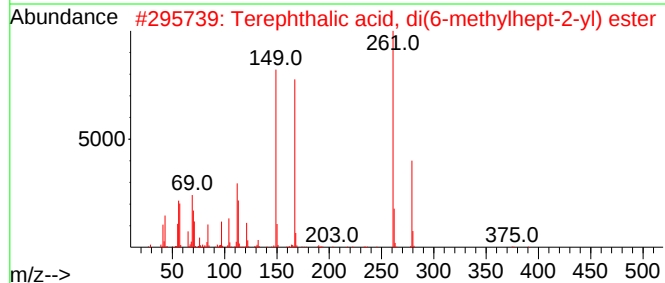
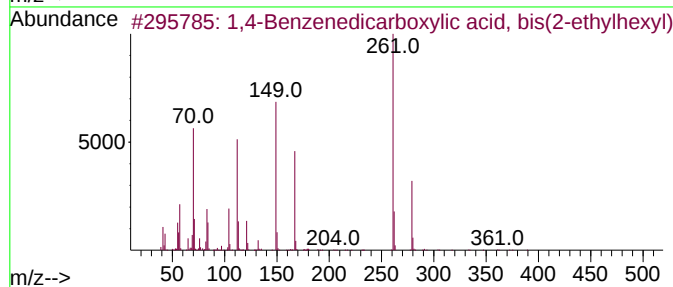
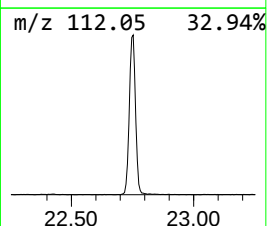
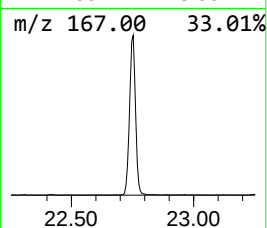
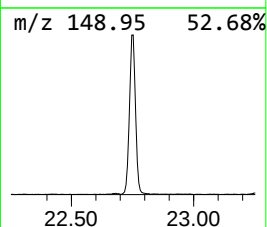
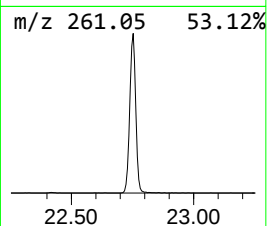
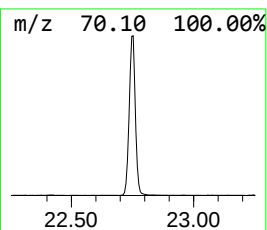
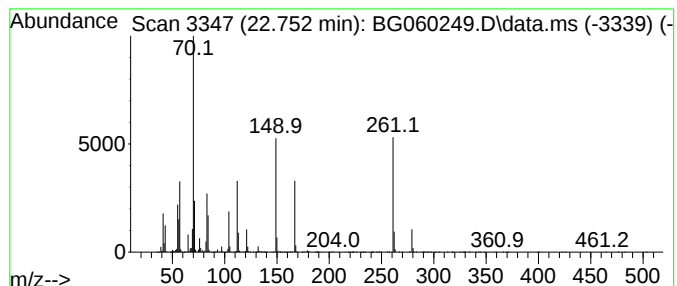
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.752	49.31 ng	9803570	Chrysene-d12	21.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	58
2			Terephthalic acid, di(6-methylhe...	390	C24H3804	1000416-00-0	53
3			Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	52
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	46
5			Isophthalic acid, 3-methylbut-2...	348	C21H3204	1000344-72-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010424\
Data File : BG060249.D
Acq On : 4 Jan 2024 17:40
Operator : MA/JU
Sample : 06038-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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
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2-Pentanone, 4-...	5.038	8.6	ng	460998	1	7.940	1073980	20.0
1-Hexanol, 2-et...	7.993	53.4	ng	2865020	1	7.940	1073980	20.0
unknown14.785	14.785	21.8	ng	3067080	3	14.574	2811870	20.0
Hexacosane	18.757	2.4	ng	462369	4	17.323	3850300	20.0
Tridecane, 6-pr...	19.139	3.7	ng	705752	4	17.323	3850300	20.0
Dodecane, 2-met...	19.362	5.4	ng	1036460	4	17.323	3850300	20.0
1-Heptacosanol	21.231	2.8	ng	562919	5	21.589	3976140	20.0
1,4-Benzenedica...	22.752	49.3	ng	9803570	5	21.589	3976140	20.0