

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
 Data File : BG061001.D
 Acq On : 22 Apr 2024 21:34
 Operator : MA/JU
 Sample : P2194-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CL-01-041824

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-BG042024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061001.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.165	25	30	43	rVB	19470	35784	2.16%	0.417%
2	3.682	112	118	124	rBV	10322	17319	1.04%	0.202%
3	5.533	426	433	441	rBV	375821	594806	35.87%	6.927%
4	7.113	694	702	711	rBV	388899	668834	40.34%	7.790%
5	7.941	837	843	849	rBV	105584	174386	10.52%	2.031%
6	9.093	1029	1039	1049	rBV	252568	453272	27.34%	5.279%
7	10.503	1273	1279	1290	rBV	21688	37980	2.29%	0.442%
8	10.738	1312	1319	1324	rBV	126472	230445	13.90%	2.684%
9	10.785	1324	1327	1333	rVB2	11963	16897	1.02%	0.197%
10	13.194	1730	1737	1743	rBV	672191	1006450	60.70%	11.722%
11	14.569	1965	1971	1979	rVB	211252	330910	19.96%	3.854%
12	14.792	2000	2009	2018	rBV2	122921	290175	17.50%	3.380%
13	16.061	2218	2225	2232	rBV	664657	1021260	61.59%	11.894%
14	16.291	2258	2264	2267	rBV7	12031	20048	1.21%	0.233%
15	16.320	2267	2269	2277	rVB2	13235	17347	1.05%	0.202%
16	17.319	2433	2439	2444	rBV	276977	425649	25.67%	4.957%
17	17.354	2444	2445	2450	rVB	18325	20249	1.22%	0.236%
18	18.000	2550	2555	2559	rVB	79168	99880	6.02%	1.163%
19	18.100	2567	2572	2576	rBV7	12588	26893	1.62%	0.313%
20	18.224	2587	2593	2600	rBV	198727	275132	16.59%	3.204%
21	19.134	2745	2748	2751	rBV2	56012	66147	3.99%	0.770%
22	19.169	2751	2754	2759	rVB	112988	124188	7.49%	1.446%
23	19.305	2773	2777	2781	rBV2	45039	57301	3.46%	0.667%
24	19.375	2784	2789	2794	rVB	60772	90765	5.47%	1.057%
25	19.499	2806	2810	2818	rBV	73805	103515	6.24%	1.206%
26	19.734	2846	2850	2858	rVB	59591	98350	5.93%	1.145%
27	19.939	2880	2885	2892	rVB	1325338	1658030	100.00%	19.310%
28	21.249	3104	3108	3114	rBV2	83883	131159	7.91%	1.528%
29	21.578	3158	3164	3170	rBV2	289200	493096	29.74%	5.743%

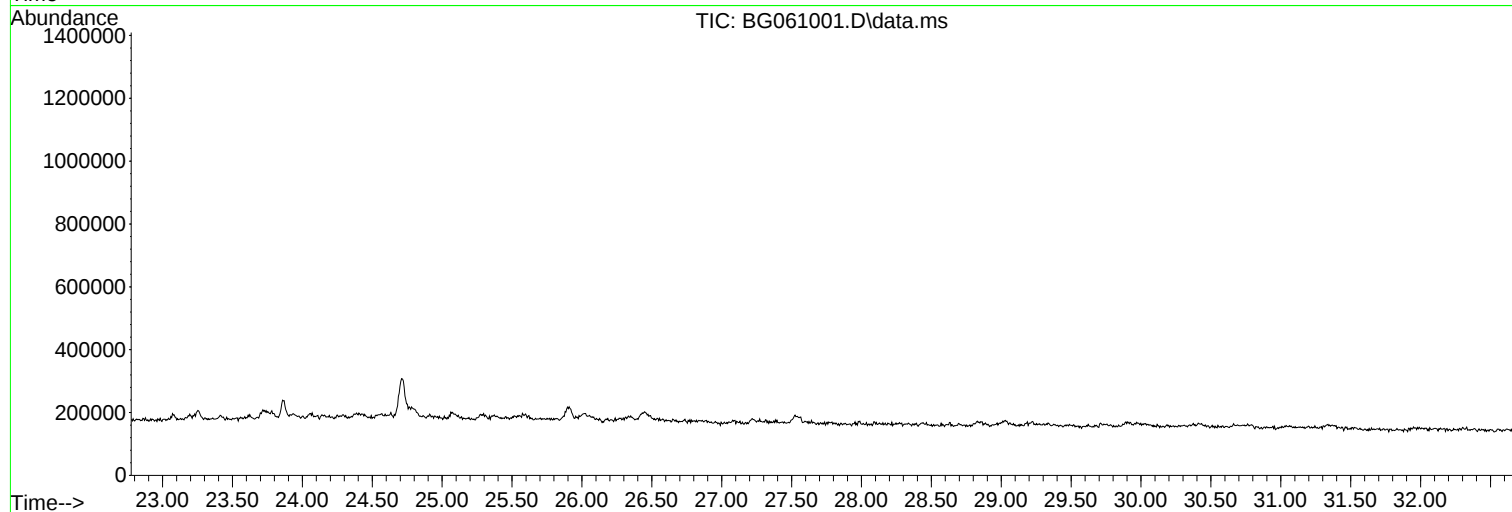
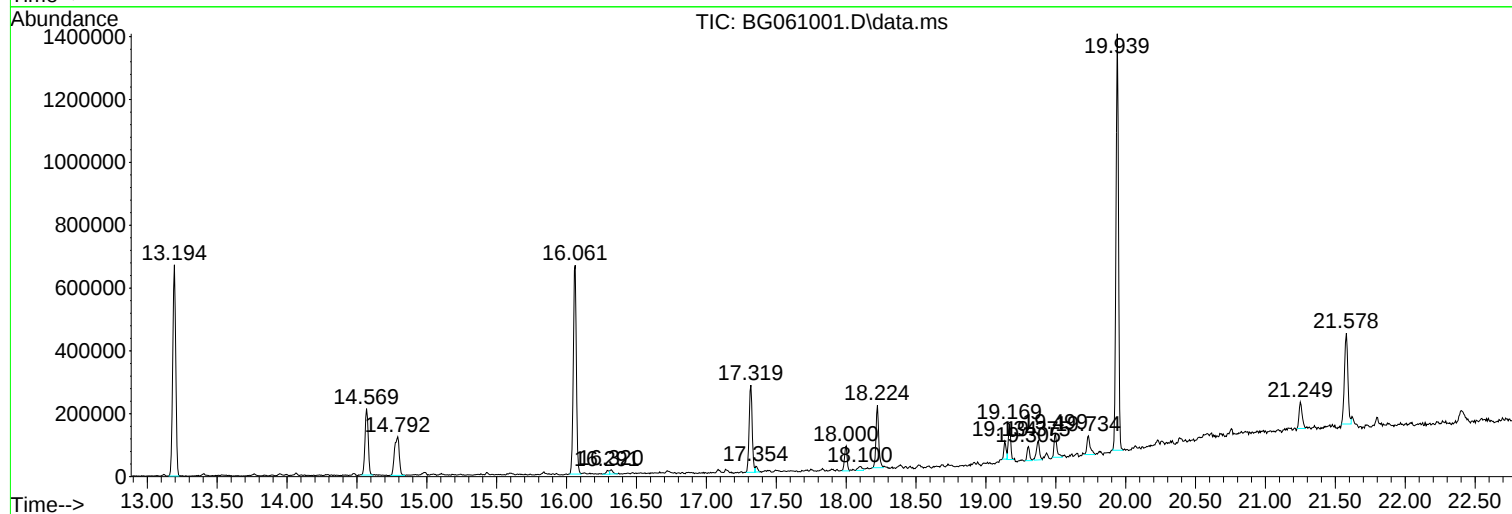
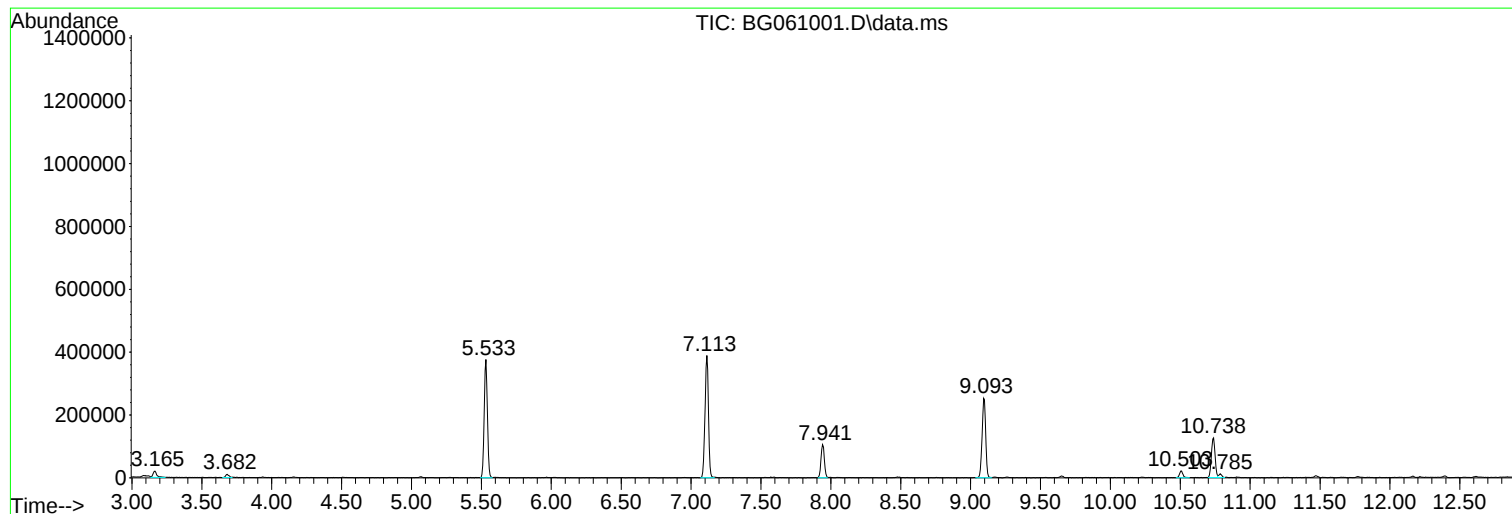
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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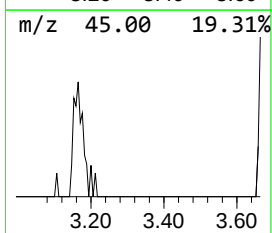
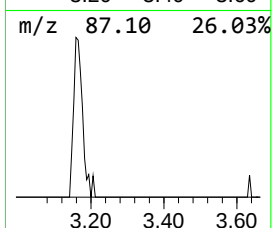
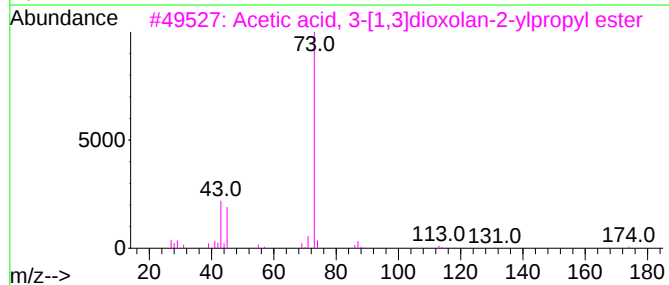
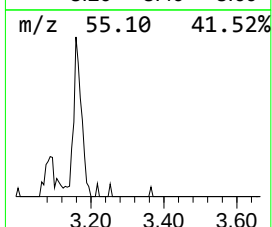
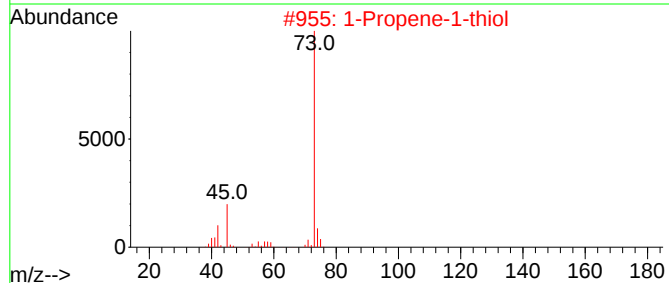
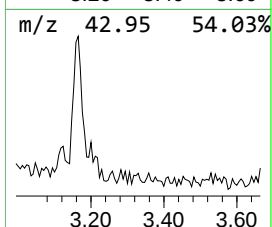
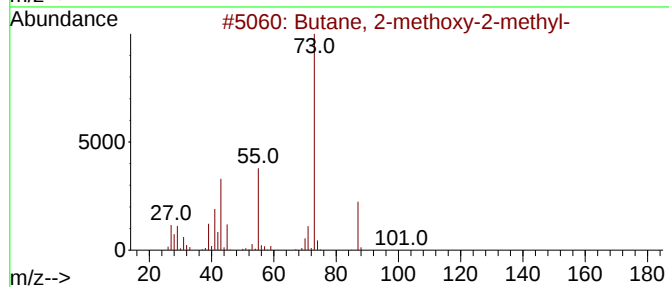
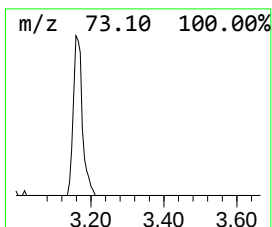
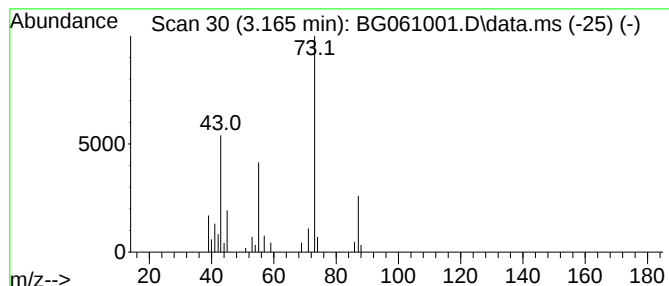
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.165 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.165	4.10 ng	35784	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	32
3			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	25
4			1-Pentanamine	87	C5H13N	000110-58-7	25
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10



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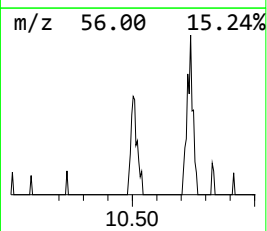
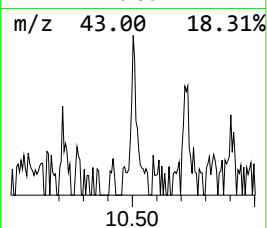
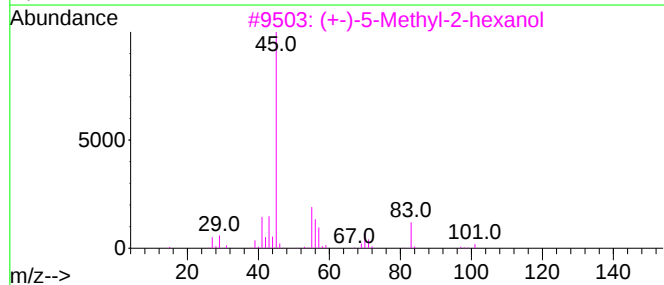
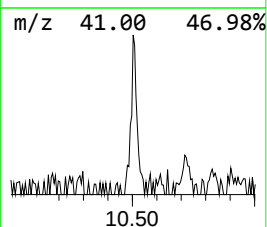
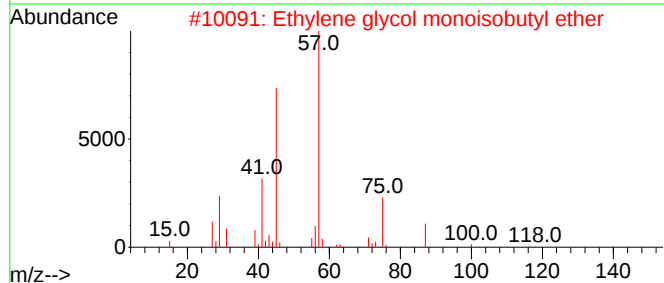
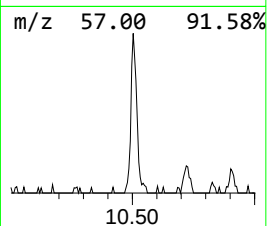
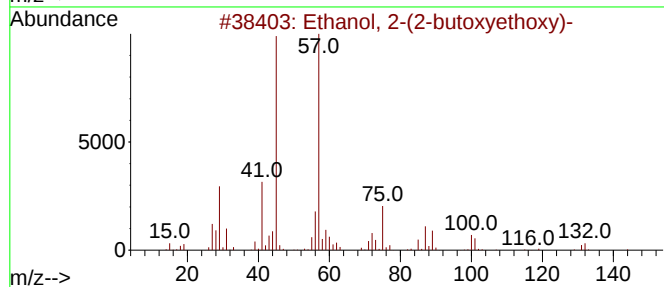
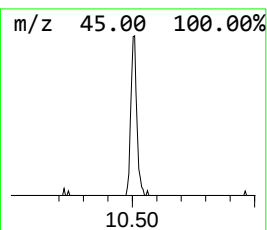
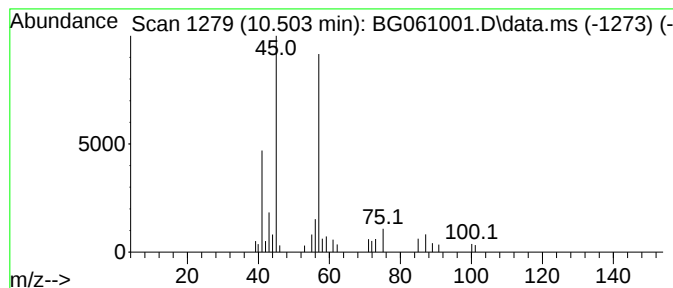
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.503	3.30 ng	37980	Naphthalene-d8	10.738

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
3			(+)-5-Methyl-2-hexanol	116	C7H16O	111768-09-3	47
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45



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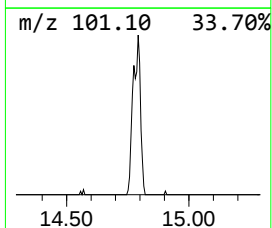
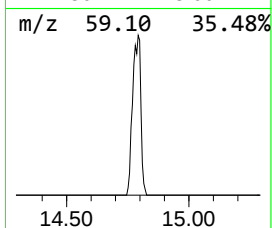
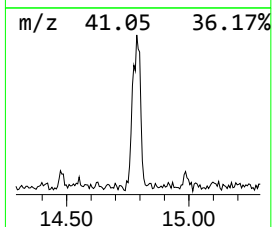
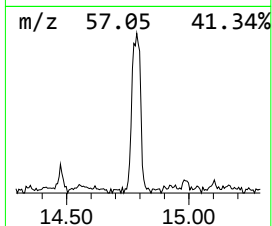
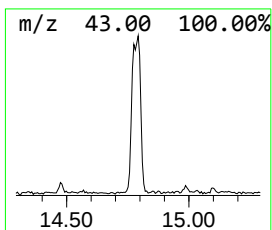
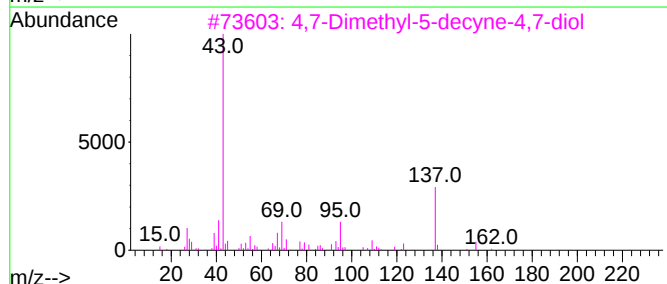
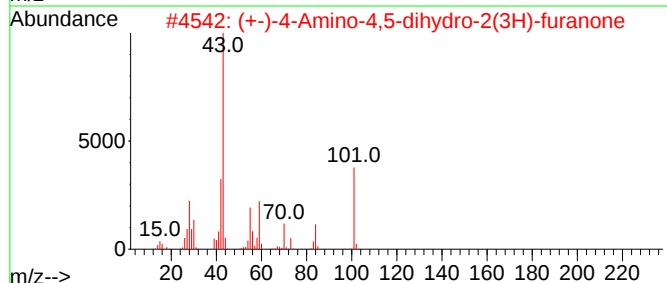
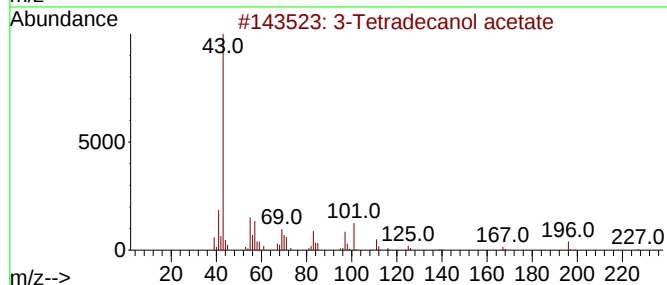
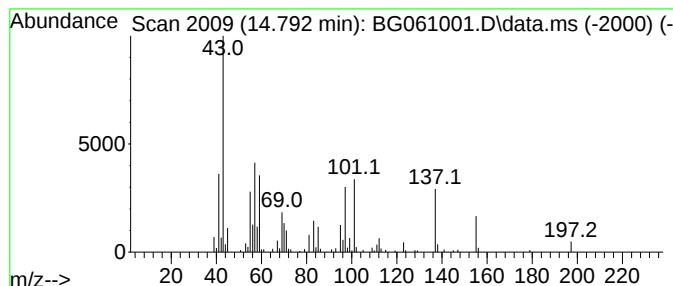
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.792 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	17.54 ng	290175	Acenaphthene-d10	14.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Tetradecanol acetate	256	C16H32O2	051354-23-5	25
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
3			4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	22
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
5			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14



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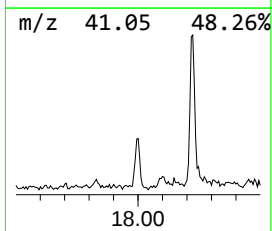
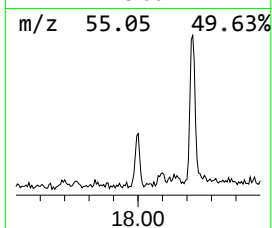
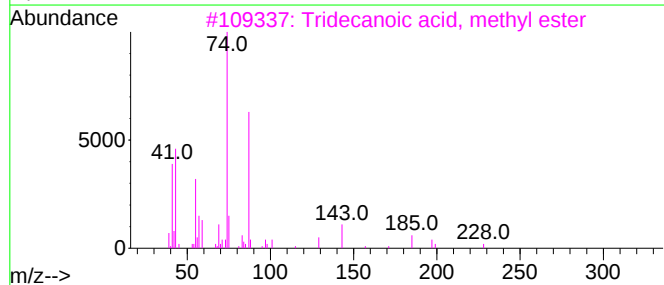
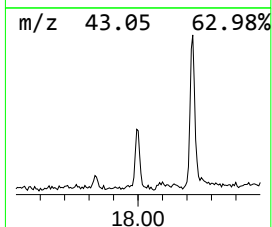
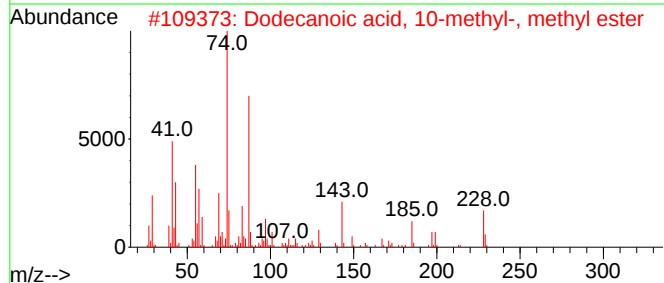
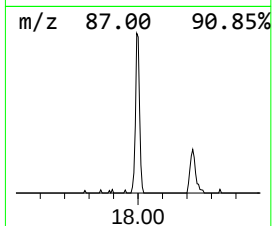
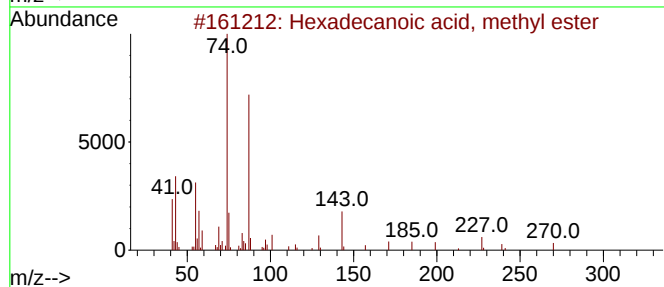
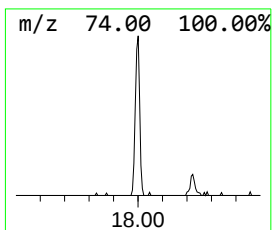
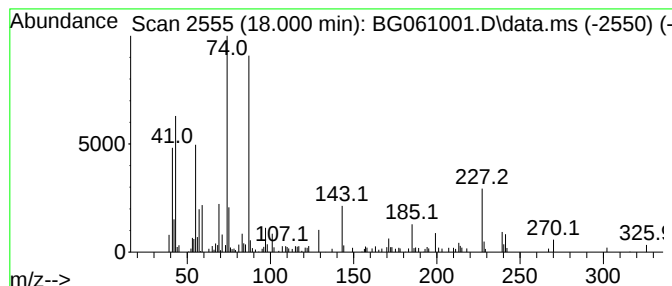
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.000	4.69 ng	99880	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	72
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	70
4			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	68
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	68



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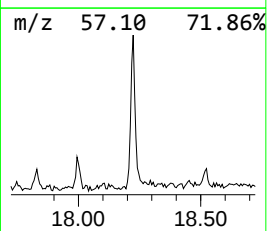
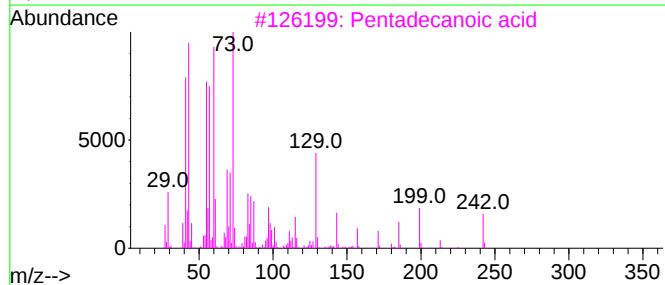
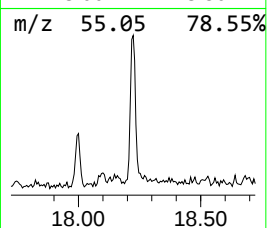
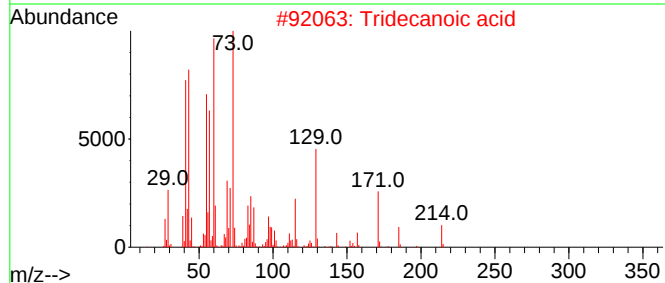
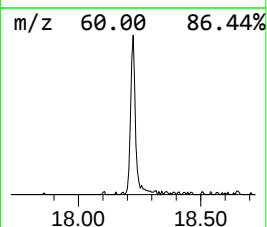
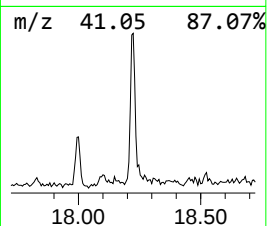
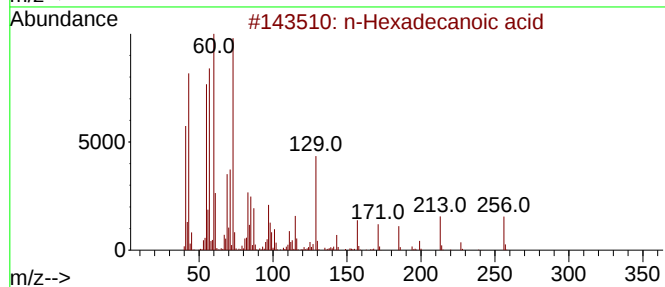
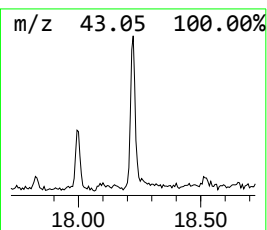
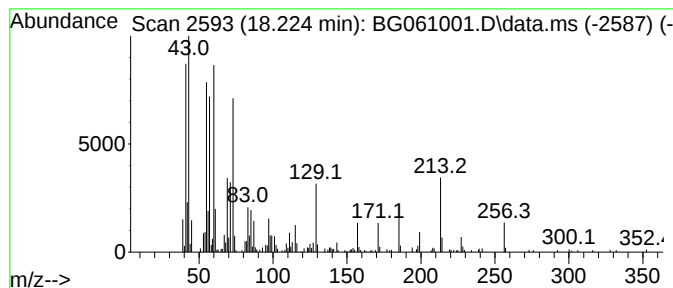
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.224	12.93 ng	275132	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Octadecanoic acid	284	C18H36O2	000057-11-4	55



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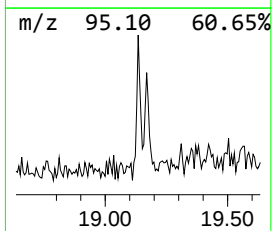
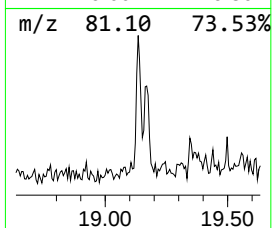
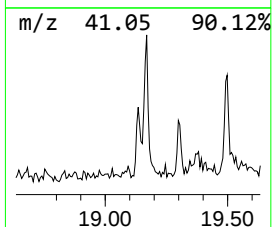
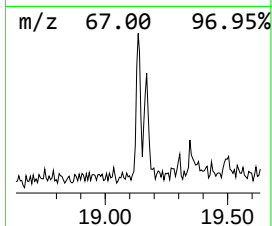
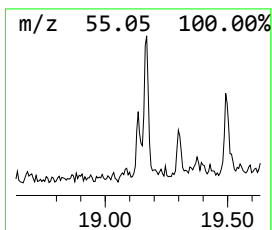
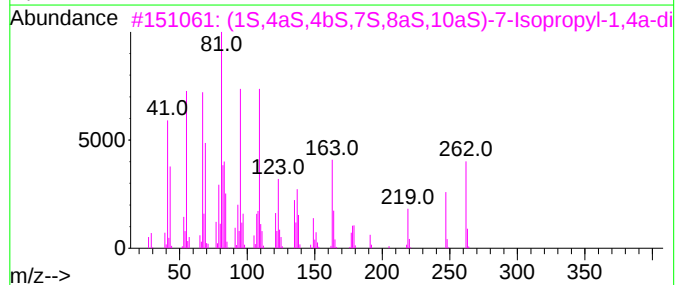
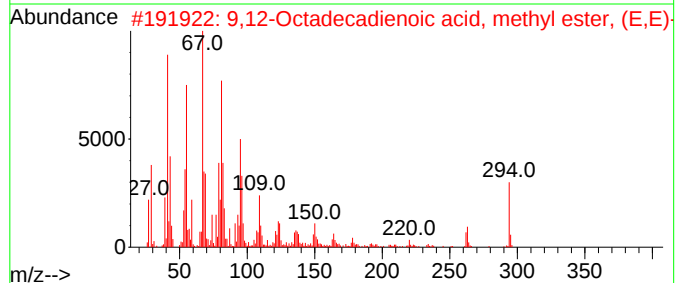
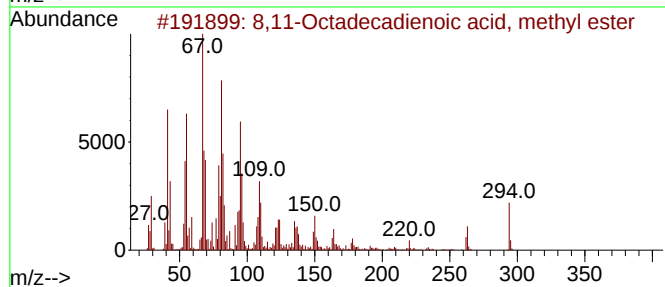
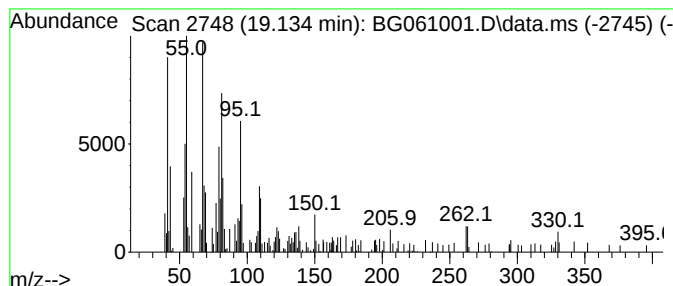
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 8,11-Octadecadienoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.134	3.11 ng	66147	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	89
2			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	80
3			(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	72
4			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	49
5			Cyclodecene, (Z)-	138	C10H18	000935-31-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG061001.D
Acq On : 22 Apr 2024 21:34
Operator : MA/JU
Sample : P2194-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

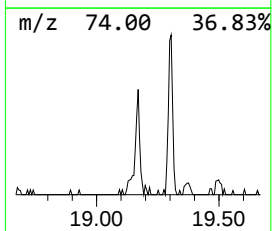
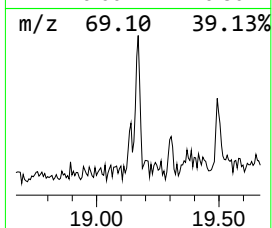
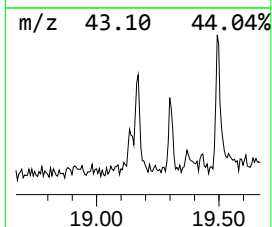
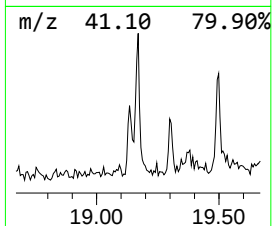
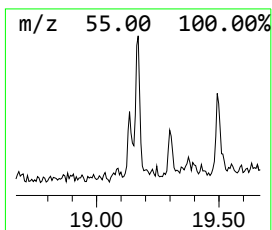
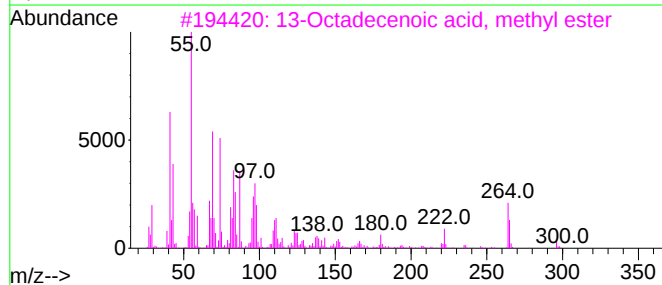
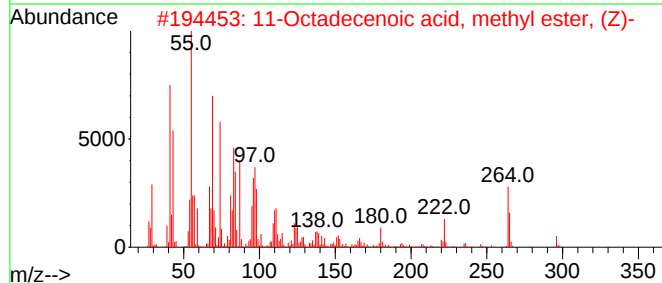
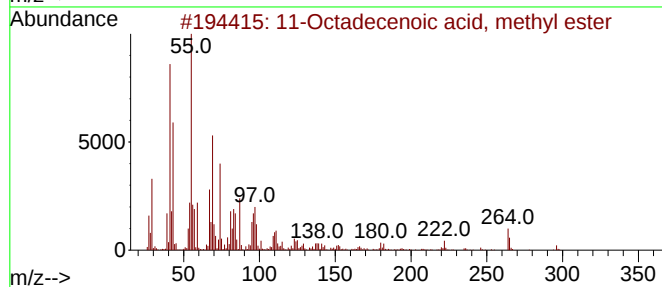
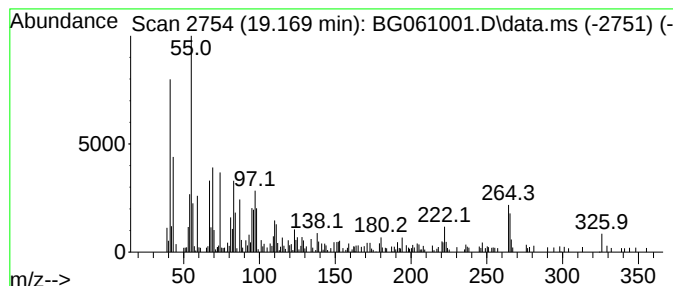
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ClientSampleId :
CL-01-041824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.169	5.84 ng	124188	Phenanthrene-d10	17.319	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	87
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	83
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	83
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG061001.D
Acq On : 22 Apr 2024 21:34
Operator : MA/JU
Sample : P2194-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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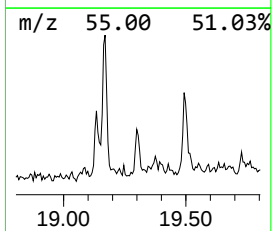
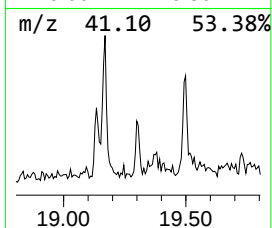
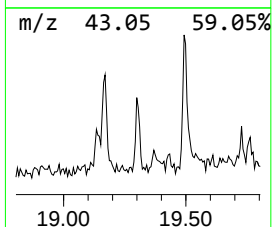
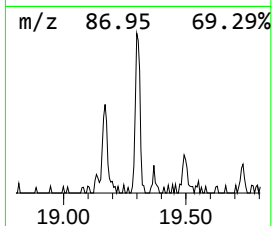
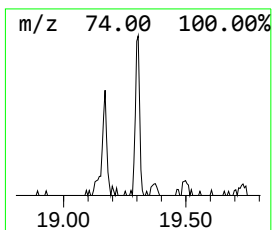
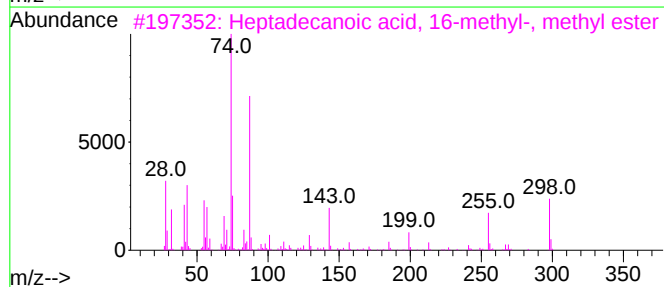
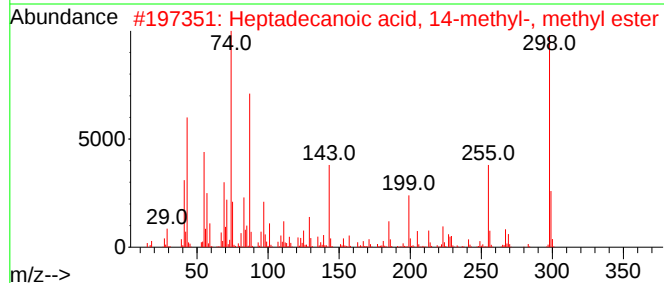
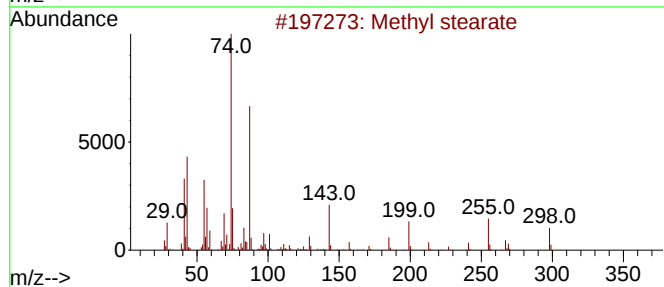
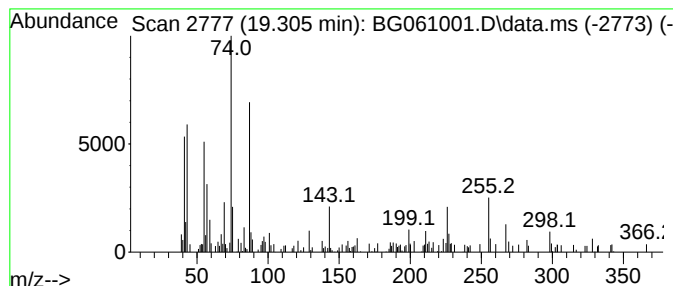
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.305	2.69 ng	57301	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	93
2			Heptadecanoic acid, 14-methyl-, ...	298	C19H38O2	002490-23-5	86
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	68
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	64
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG061001.D
Acq On : 22 Apr 2024 21:34
Operator : MA/JU
Sample : P2194-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-041824

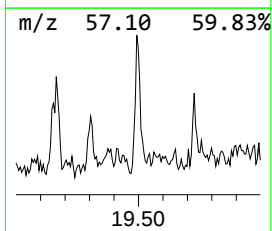
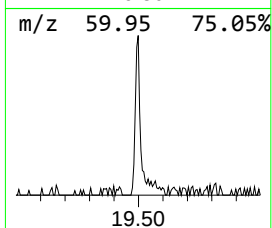
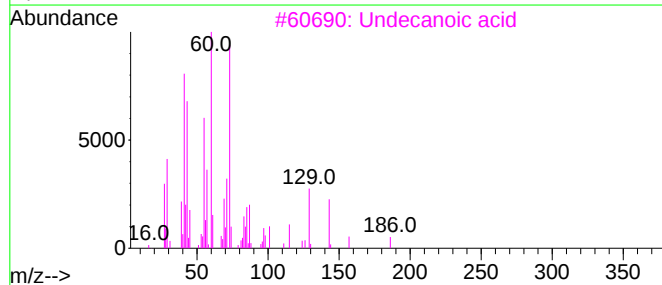
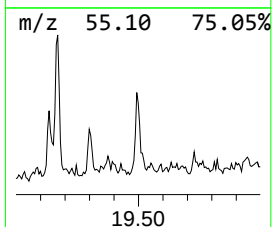
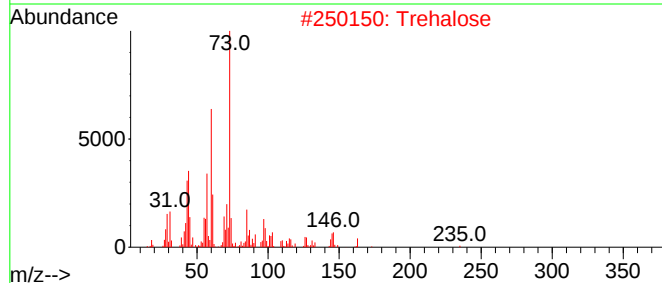
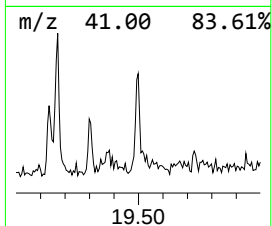
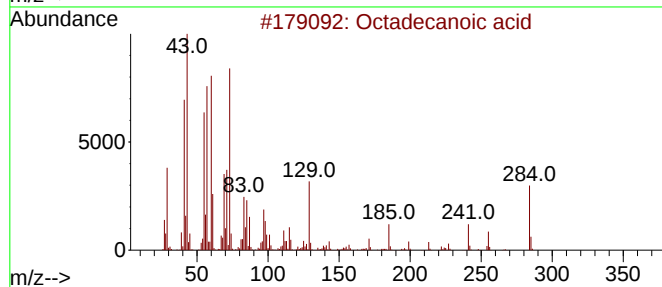
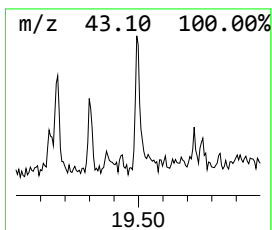
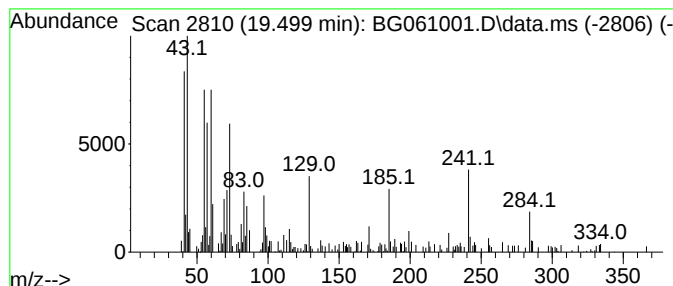
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.499	4.20 ng	103515	Chrysene-d12	21.578

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Trehalose	342	C12H22O11	000099-20-7	43
3			Undecanoic acid	186	C11H22O2	000112-37-8	41
4			9-Bromononanoic acid	236	C9H17BrO2	041059-02-3	38
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG061001.D
Acq On : 22 Apr 2024 21:34
Operator : MA/JU
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Misc :
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Instrument :
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ClientSampleId :
CL-01-041824

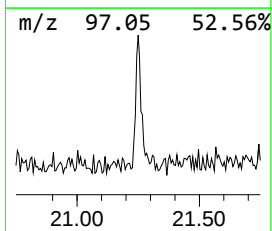
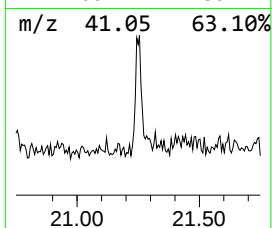
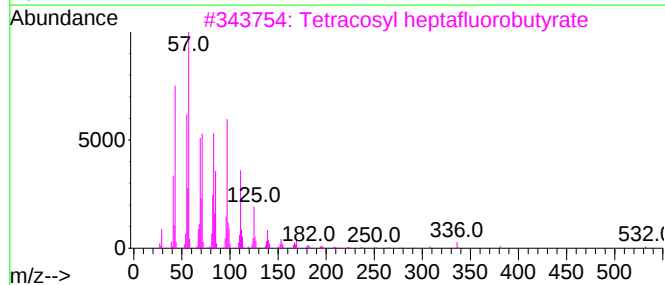
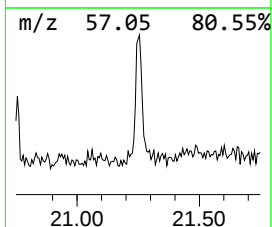
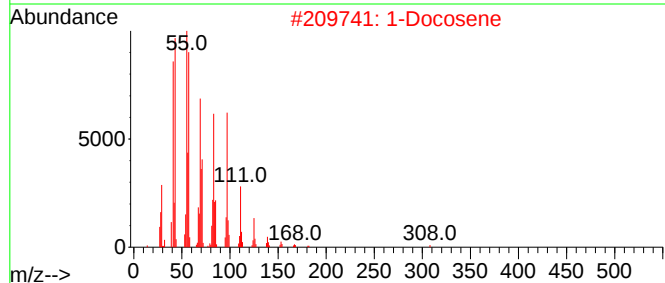
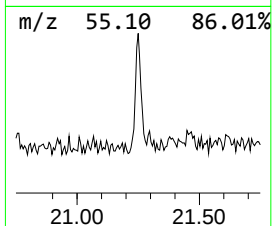
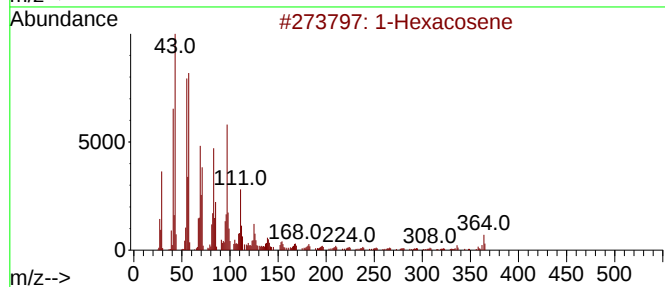
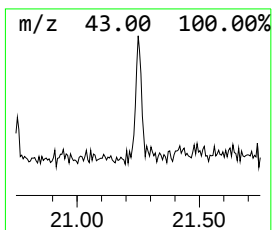
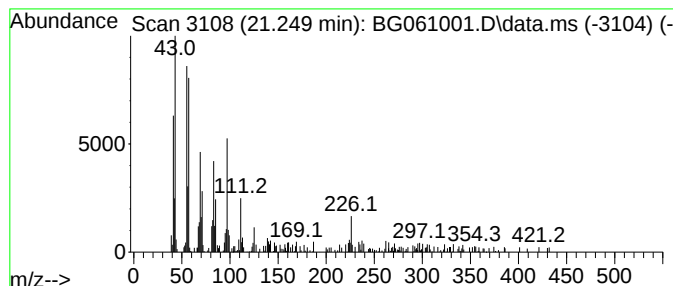
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.249	5.32 ng	131159	Chrysene-d12	21.578

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	90
2	1-Docosene		308	C22H44	001599-67-3	90
3	Tetracosyl heptafluorobutyrate		550	C28H49F7O2	1000351-83-7	87
4	Triacosyl pentafluoropropionate		584	C33H61F5O2	1000351-80-0	83
5	Octacosyl propyl ether		452	C31H64O	1000406-28-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG061001.D
Acq On : 22 Apr 2024 21:34
Operator : MA/JU
Sample : P2194-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-041824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.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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Ethanol, 2-(2-b...	10.503	3.3	ng	37980	2	10.738	230445	20.0
unknown14.792	14.792	17.5	ng	290175	3	14.569	330910	20.0
Hexadecanoic ac...	18.000	4.7	ng	99880	4	17.319	425649	20.0
n-Hexadecanoic ...	18.224	12.9	ng	275132	4	17.319	425649	20.0
8,11-Octadecadi...	19.134	3.1	ng	66147	4	17.319	425649	20.0
11-Octadecenoic...	19.169	5.8	ng	124188	4	17.319	425649	20.0
Methyl stearate	19.305	2.7	ng	57301	4	17.319	425649	20.0
Octadecanoic acid	19.499	4.2	ng	103515	5	21.578	493096	20.0
1-Hexacosene	21.249	5.3	ng	131159	5	21.578	493096	20.0