

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
 Data File : BG050786.D
 Acq On : 29 Oct 2021 20:44
 Operator : CG/JU
 Sample : M4392-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 N41924

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.779	384	390	400	rBV	332893	563983	21.60%	4.218%
2	7.389	656	664	677	rBV	204368	379755	14.54%	2.840%
3	8.246	803	810	816	rBV	123583	208722	7.99%	1.561%
4	9.416	1001	1009	1019	rBV	469407	875452	33.53%	6.548%
5	10.814	1240	1247	1262	rBV	199648	360357	13.80%	2.695%
6	11.073	1282	1291	1298	rBV	160806	297362	11.39%	2.224%
7	13.493	1693	1703	1711	rBV	1130296	1802721	69.04%	13.483%
8	14.868	1929	1937	1946	rVB	260974	417060	15.97%	3.119%
9	16.355	2183	2190	2199	rBV	871020	1340056	51.32%	10.023%
10	16.977	2289	2296	2303	rBV6	15576	28123	1.08%	0.210%
11	17.612	2398	2404	2411	rBV	323254	504838	19.33%	3.776%
12	18.247	2508	2512	2517	rVB3	43439	59656	2.28%	0.446%
13	18.346	2524	2529	2535	rBV8	18673	33713	1.29%	0.252%
14	18.476	2546	2551	2559	rBV	136918	206741	7.92%	1.546%
15	19.733	2762	2765	2773	rBV6	17710	26233	1.00%	0.196%
16	19.992	2806	2809	2817	rVB2	21384	27563	1.06%	0.206%
17	20.209	2839	2846	2851	rBV	1883432	2611095	100.00%	19.529%
18	20.479	2887	2892	2896	rBV	30674	44558	1.71%	0.333%
19	20.984	2974	2978	2982	rBV	51678	59449	2.28%	0.445%
20	21.513	3063	3068	3082	rBV2	124999	295567	11.32%	2.211%
21	21.919	3130	3137	3144	rVB	310883	550545	21.08%	4.118%
22	22.083	3160	3165	3170	rBV	53993	78279	3.00%	0.585%
23	22.724	3269	3274	3280	rVB	46002	77152	2.95%	0.577%
24	23.458	3393	3399	3406	rVB	42712	80233	3.07%	0.600%
25	23.664	3425	3434	3442	rVB	829326	1668164	63.89%	12.477%
26	24.310	3539	3544	3554	rVB2	39511	86427	3.31%	0.646%
27	25.332	3708	3718	3731	rVB2	200953	620197	23.75%	4.639%
28	26.531	3917	3922	3931	rVB3	25216	66201	2.54%	0.495%

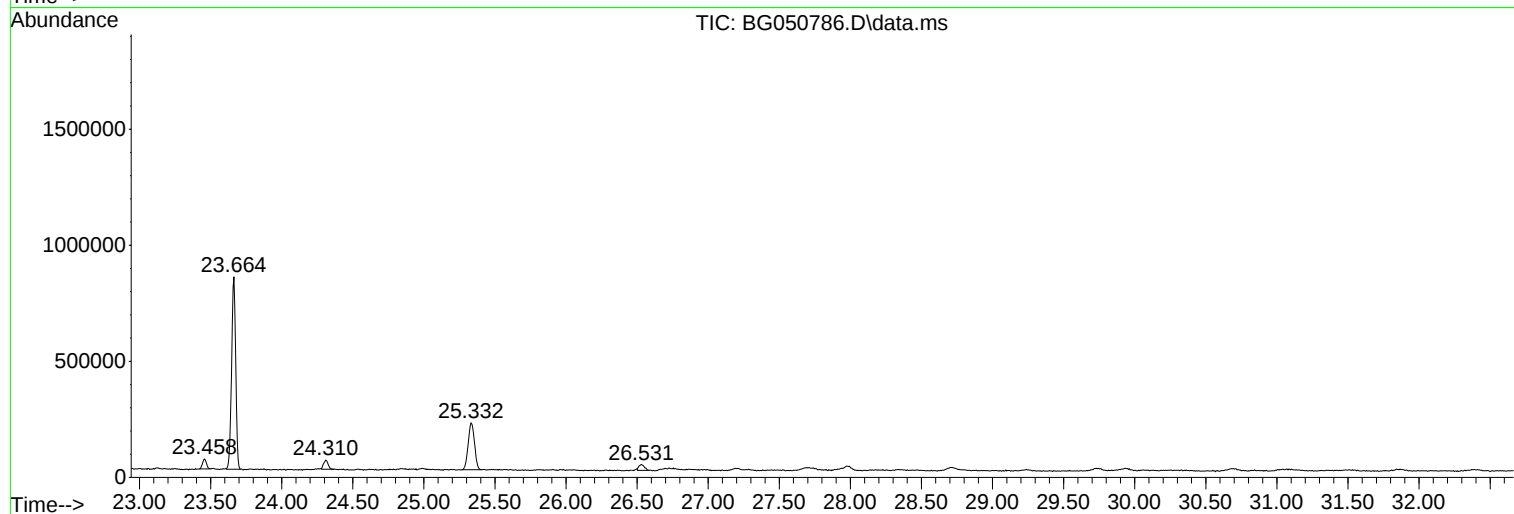
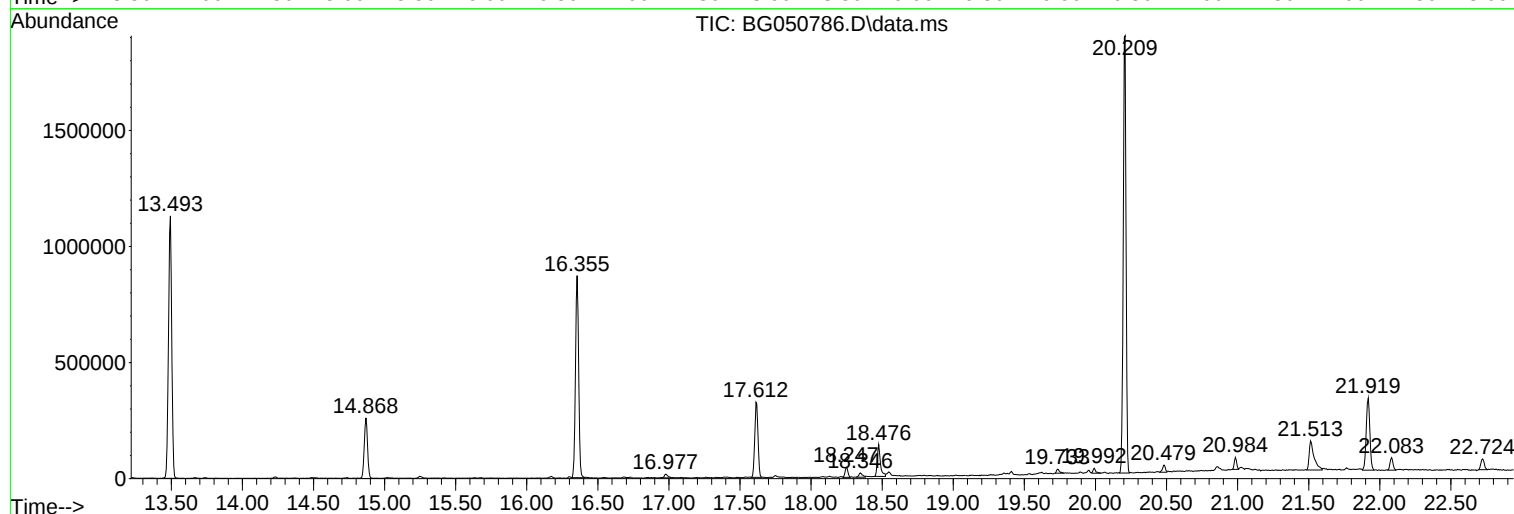
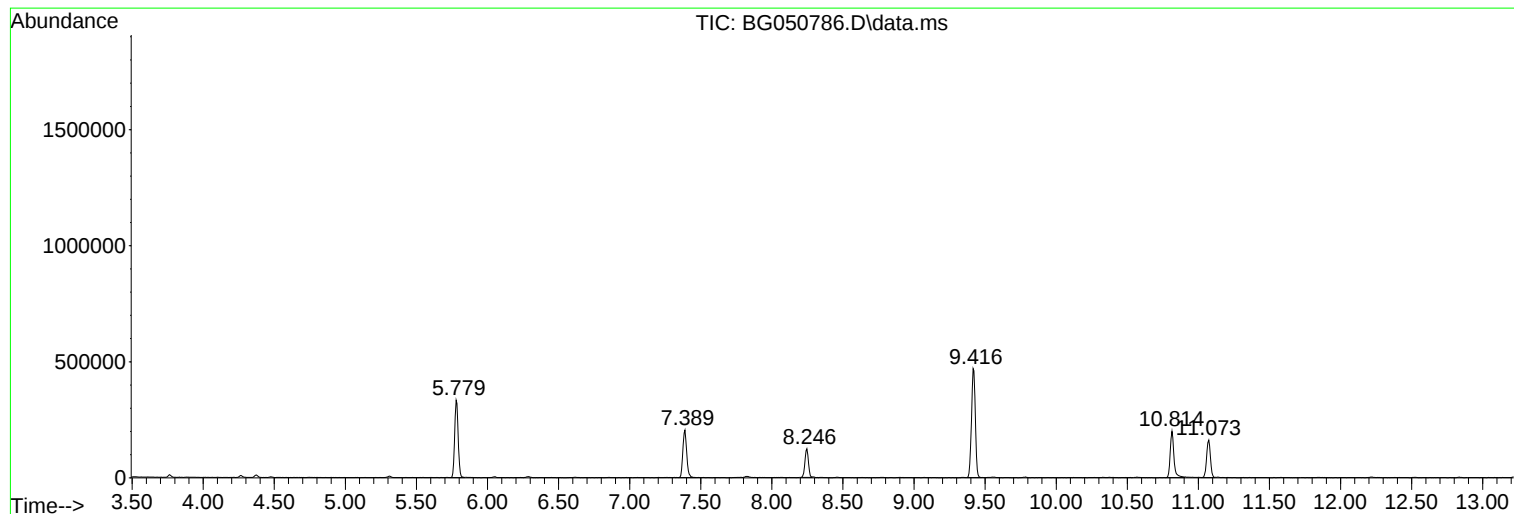
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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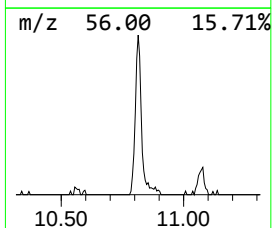
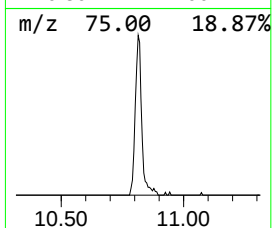
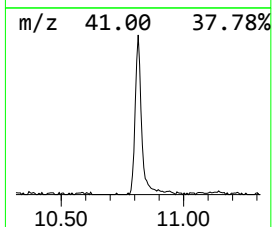
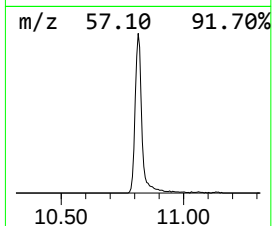
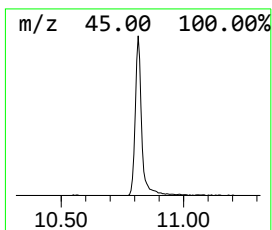
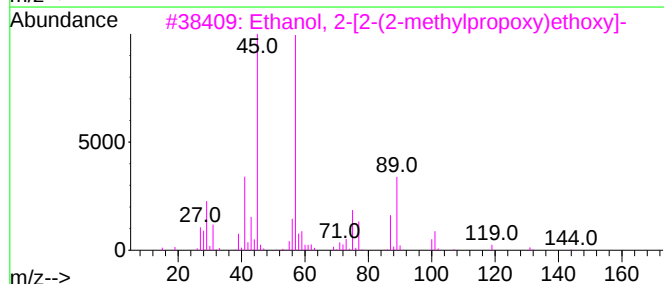
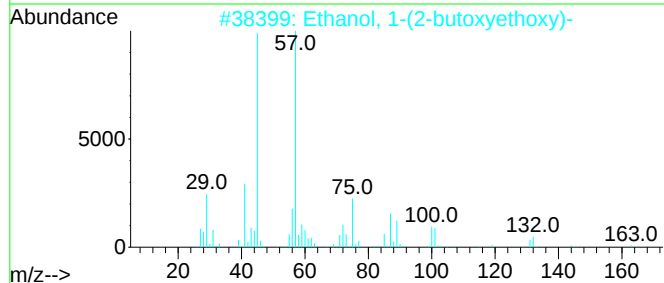
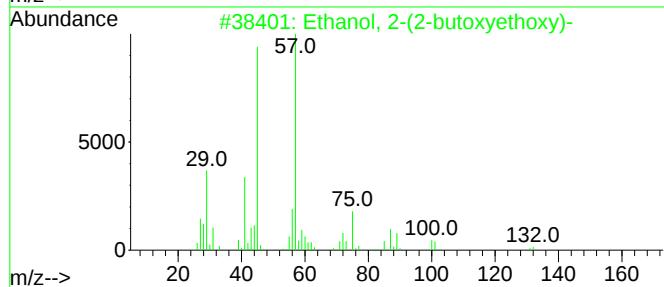
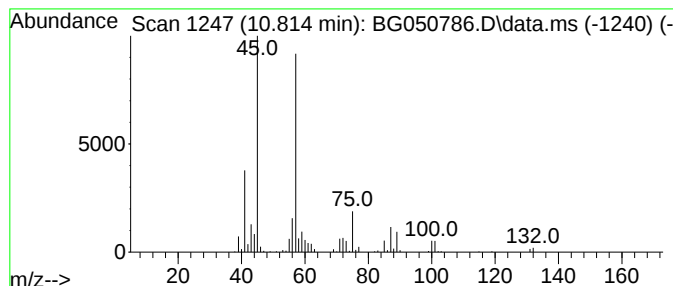
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.814	24.24 ng	360357	Naphthalene-d8	11.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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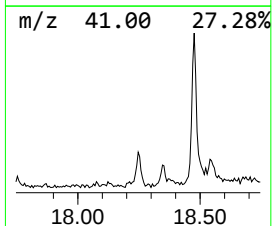
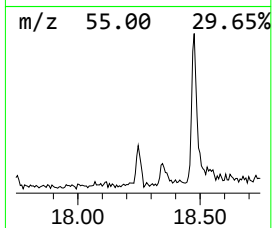
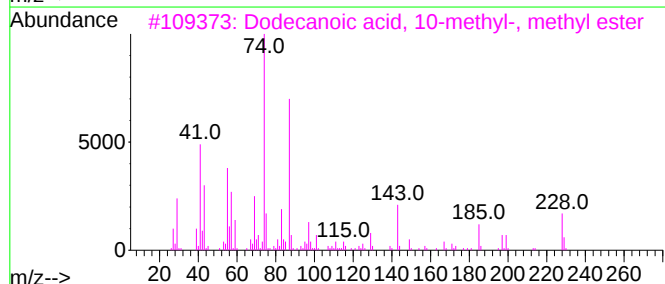
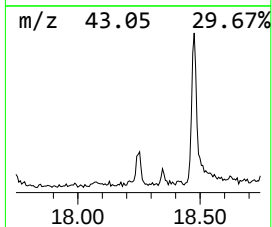
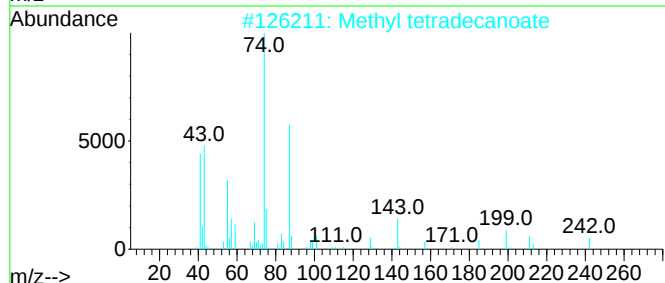
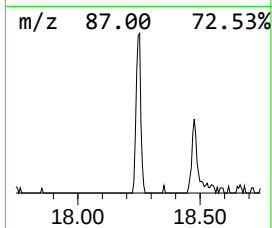
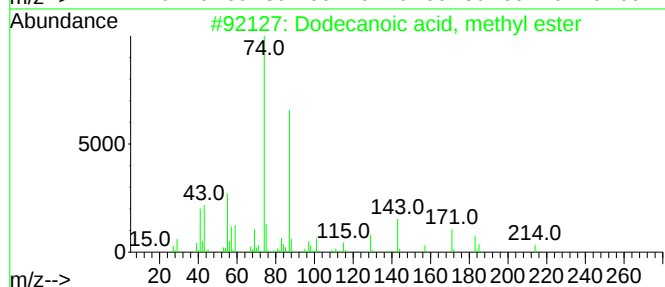
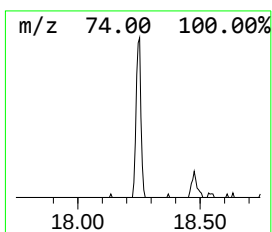
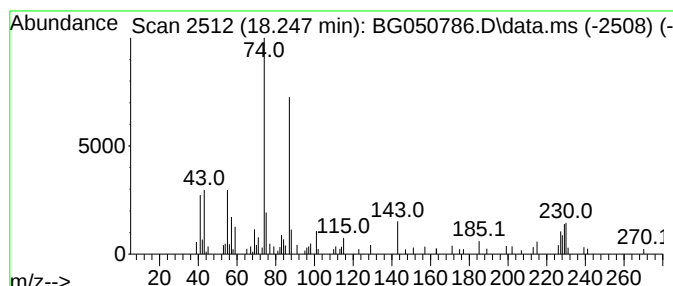
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Peak Number 2 Dodecanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.247	2.36 ng	59656	Phenanthrene-d10	17.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
3	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	76
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	74
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	74



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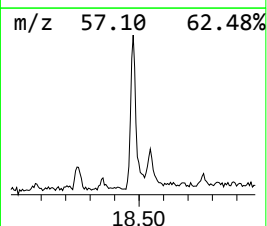
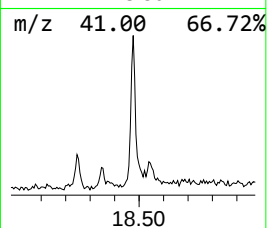
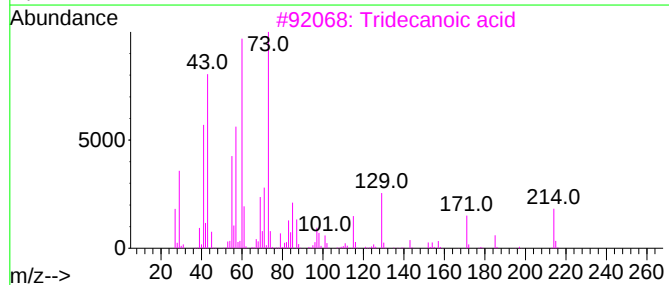
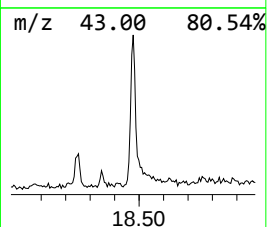
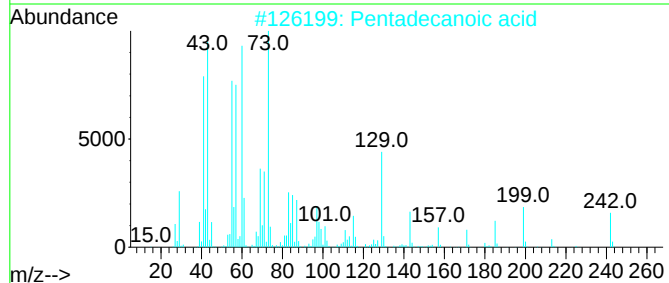
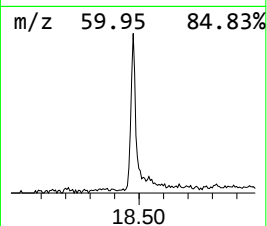
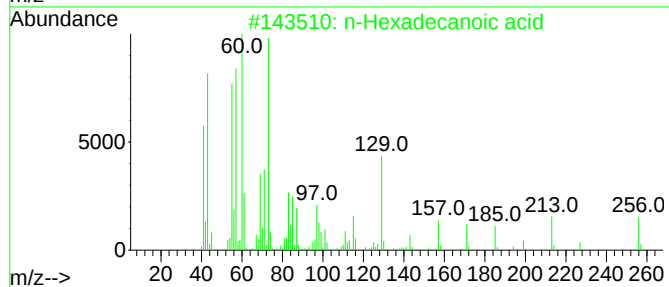
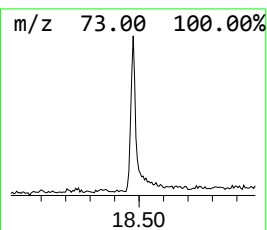
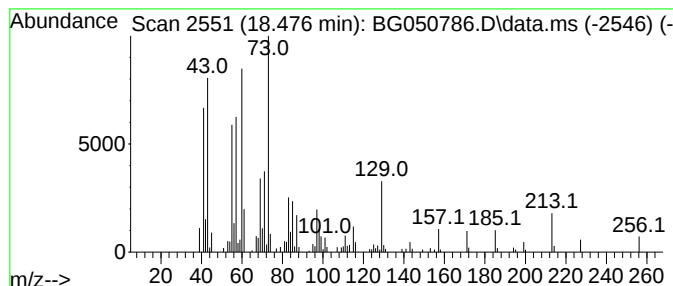
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.476	8.19 ng	206741	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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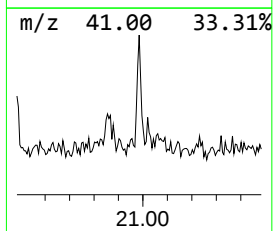
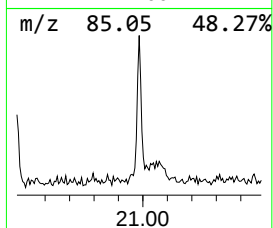
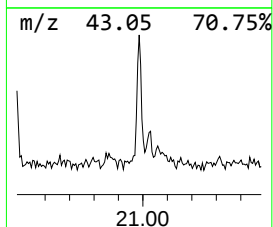
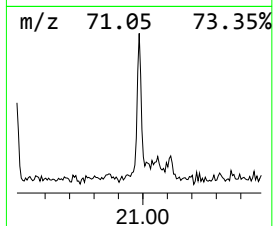
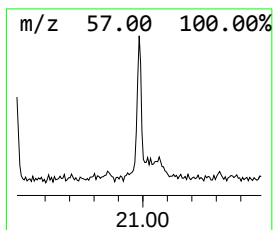
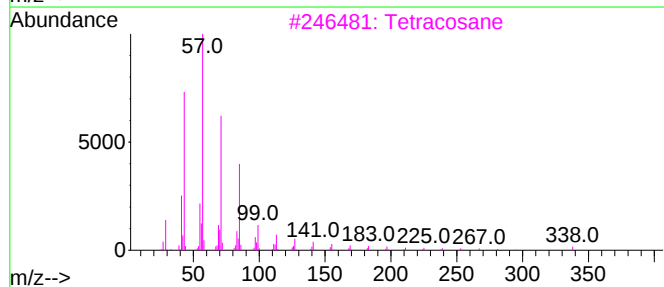
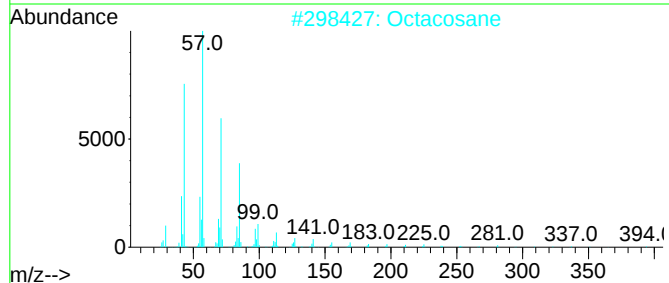
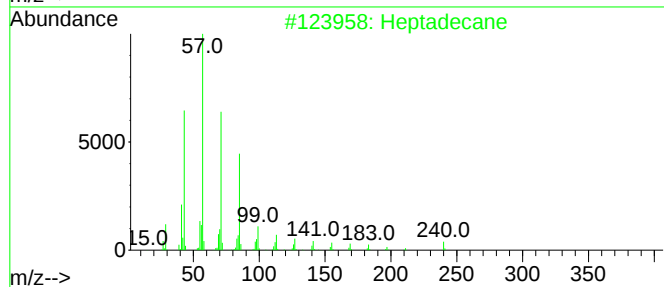
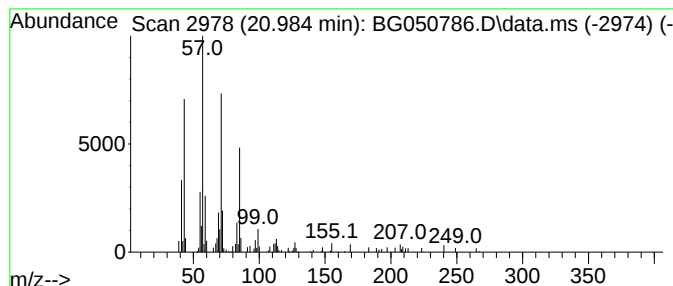
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Peak Number 4 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.985	2.16 ng	59449	Chrysene-d12	21.919

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	93
2		Octacosane	394	C28H58	000630-02-4	64
3		Tetracosane	338	C24H50	000646-31-1	64
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5		Tetradecane	198	C14H30	000629-59-4	59



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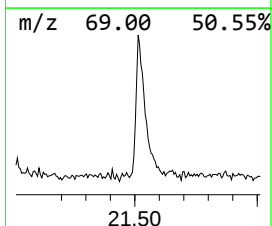
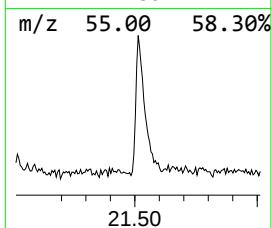
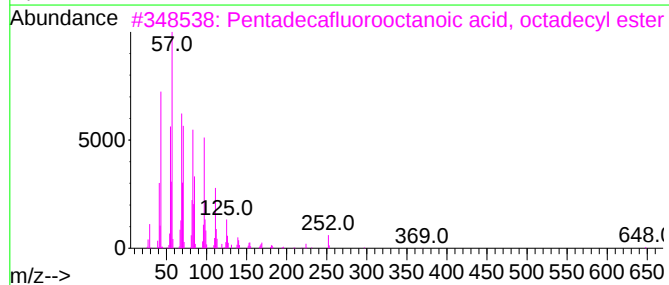
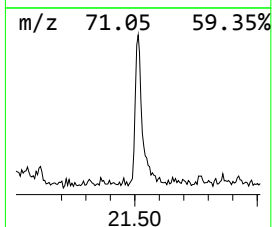
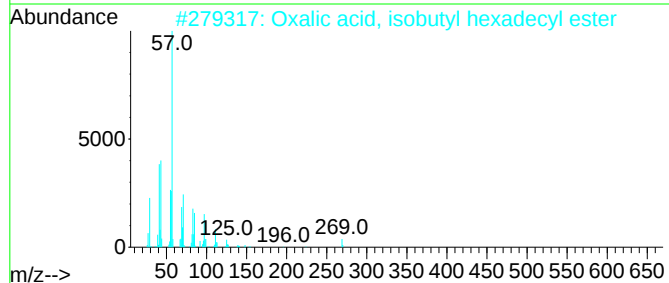
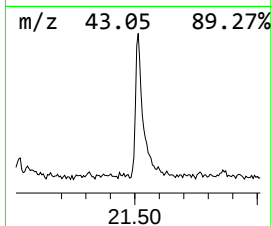
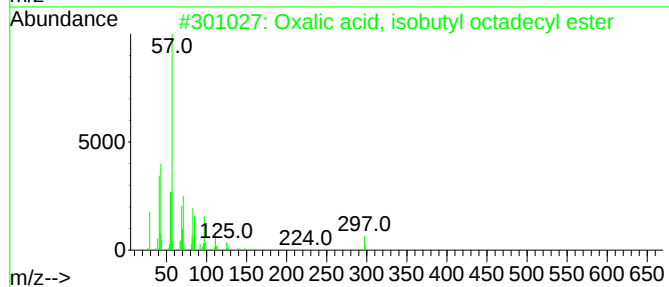
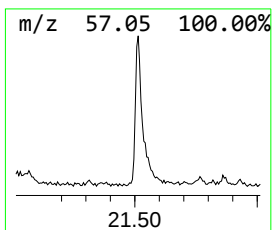
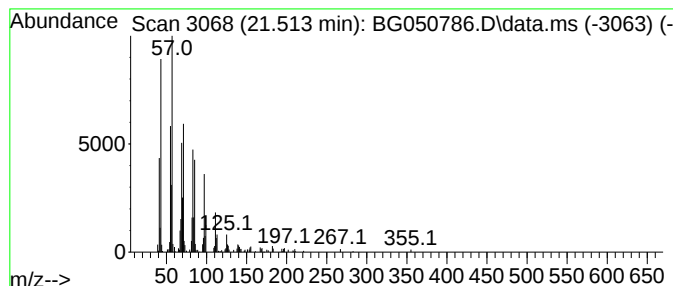
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Peak Number 5 Oxalic acid, isobutyl octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.513	10.74 ng	295567	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	81
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
4			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	74
5			Cyclotetradecane	196	C14H28	000295-17-0	70



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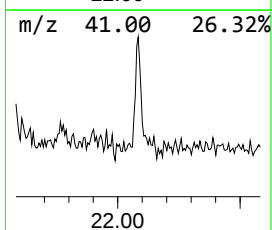
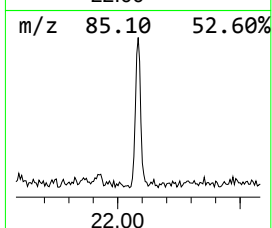
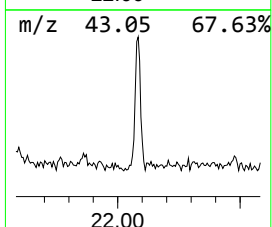
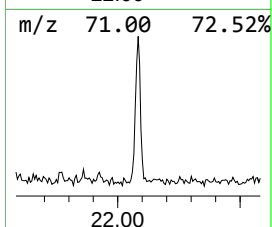
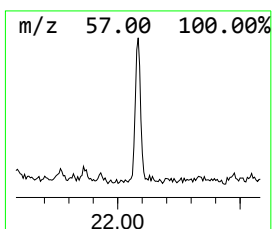
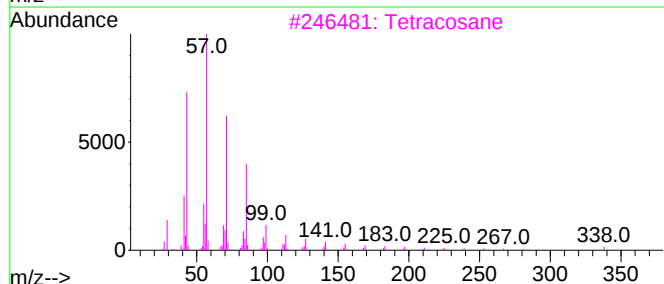
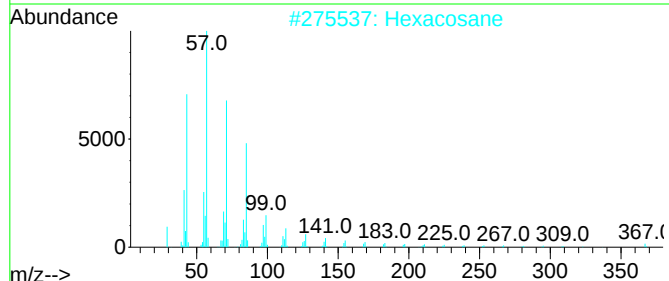
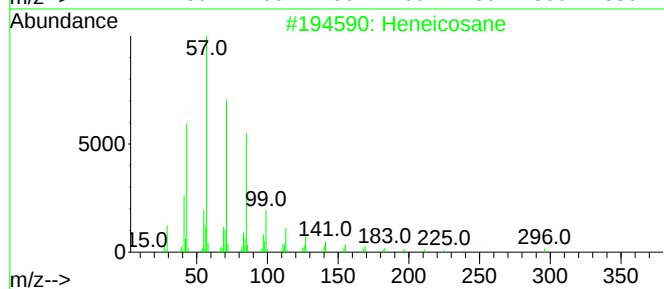
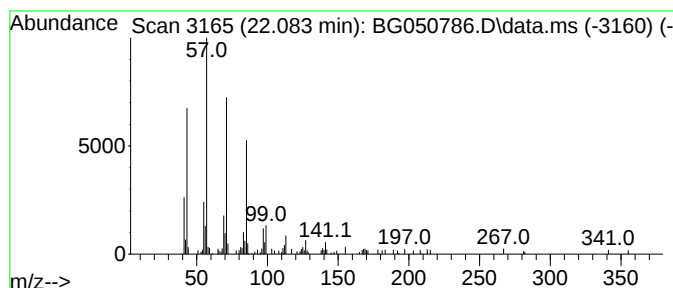
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.083	2.84 ng	78279	Chrysene-d12	21.919

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Tetracosane	338	C24H50	000646-31-1	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N41924

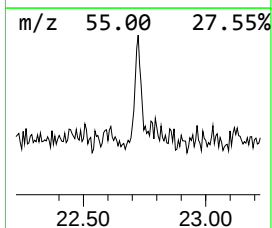
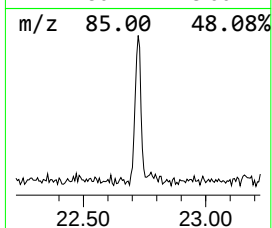
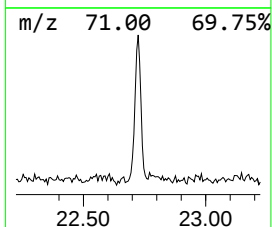
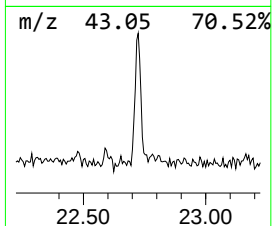
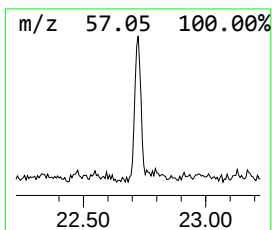
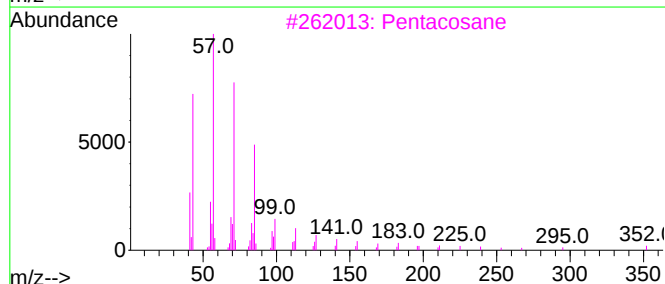
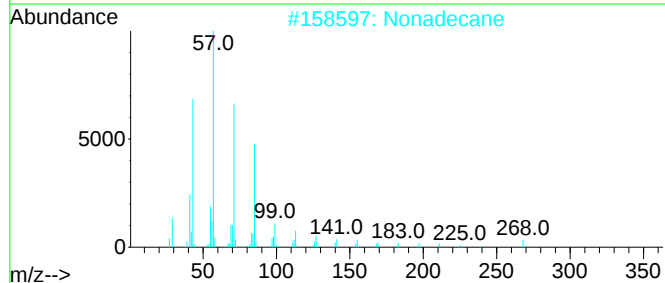
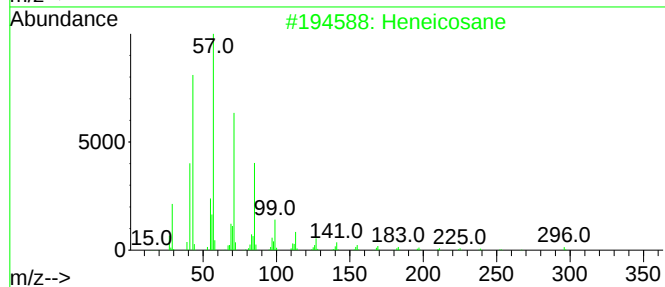
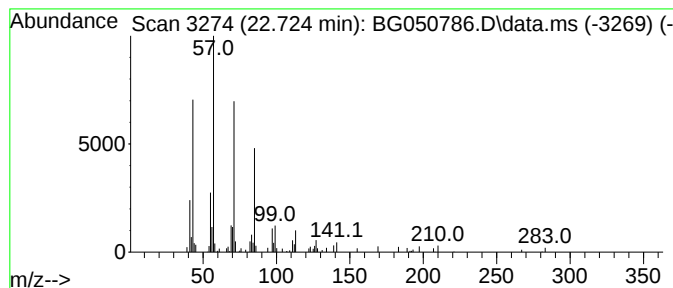
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.724	2.80 ng	77152	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Nonadecane	268	C19H40	000629-92-5	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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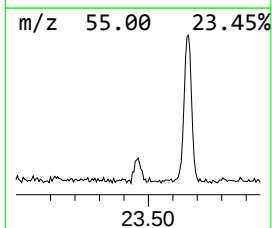
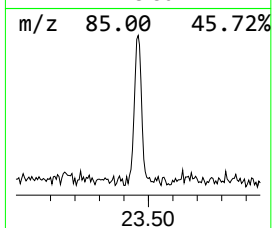
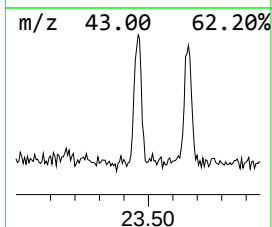
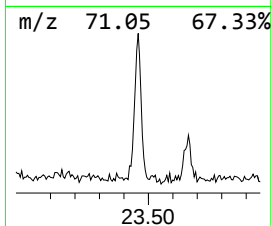
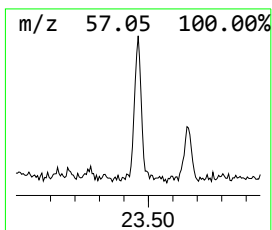
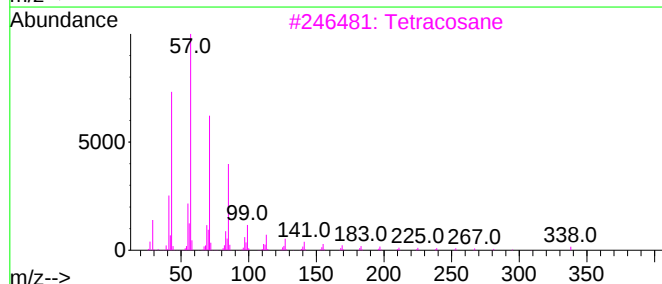
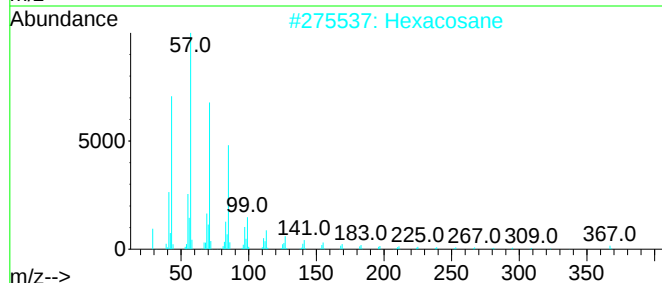
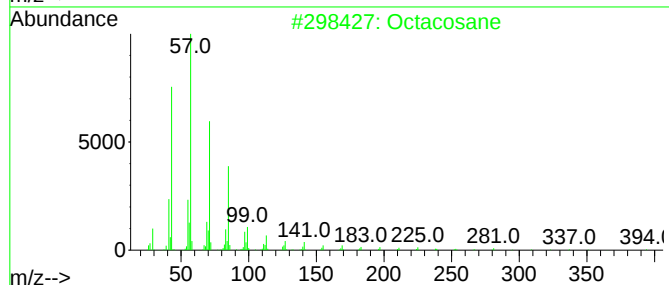
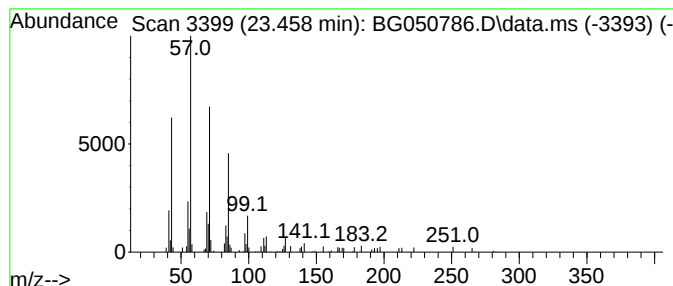
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.458	2.91 ng	80233	Chrysene-d12	21.919

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Tetracosane	338	C24H50	000646-31-1	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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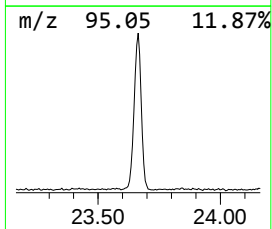
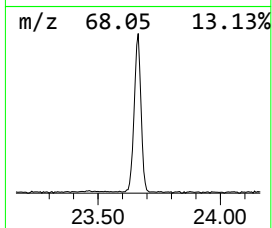
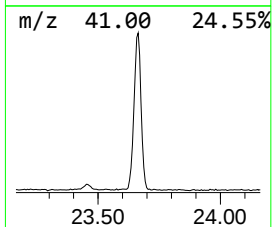
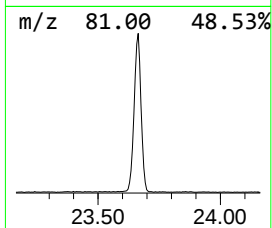
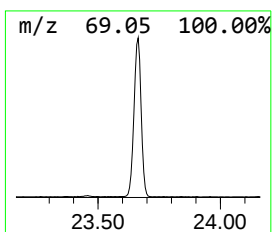
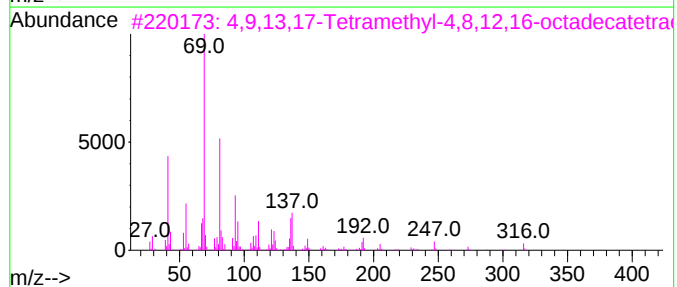
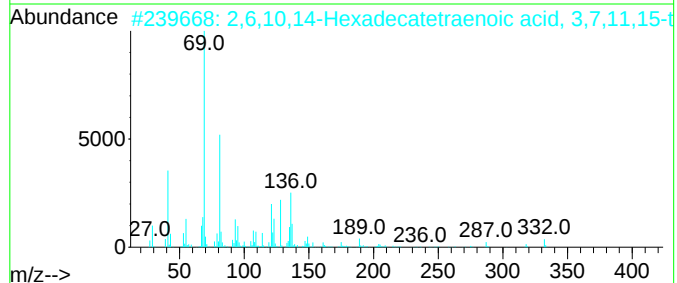
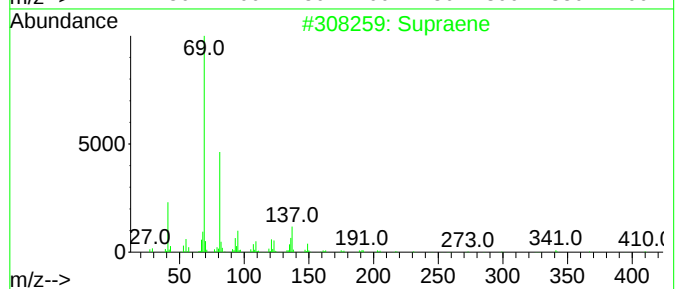
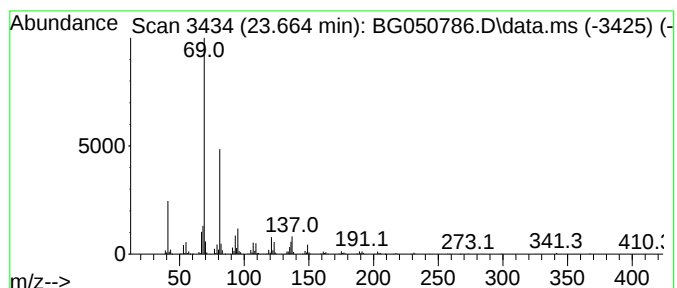
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.664	53.79 ng	1668160	Perylene-d12	25.332

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	83
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			Squalene	410	C30H50	000111-02-4	83
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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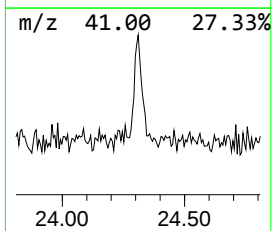
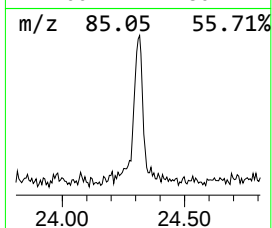
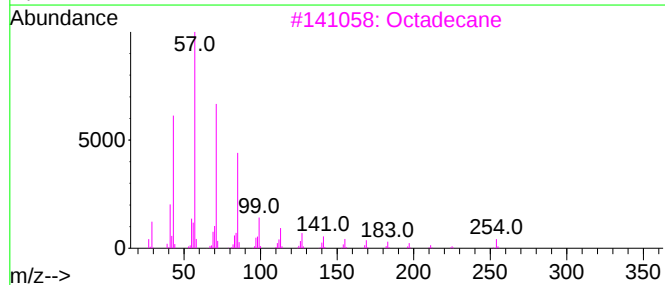
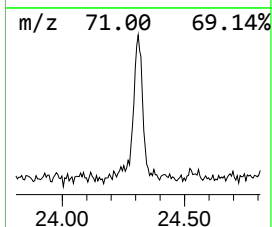
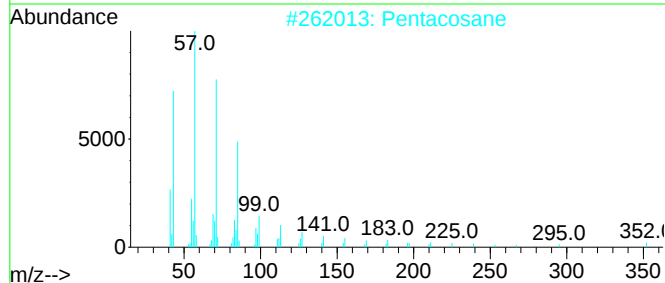
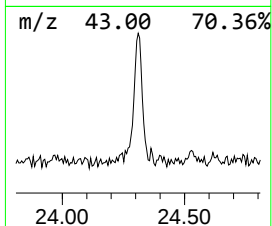
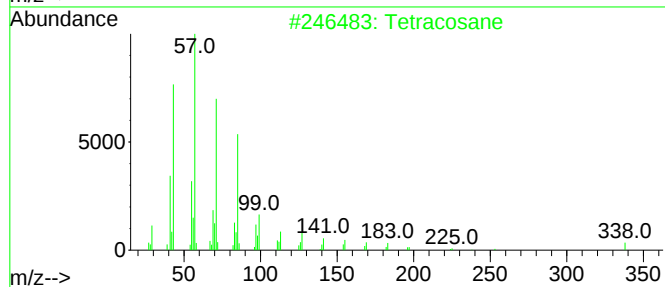
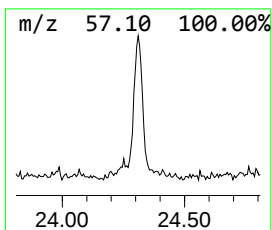
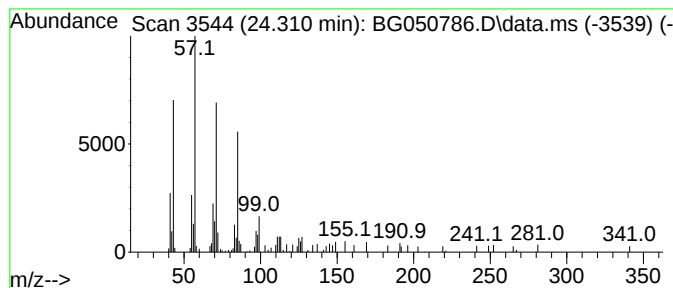
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.310	2.79 ng	86427	Perylene-d12	25.332

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	87
2		Pentacosane	352	C25H52	000629-99-2	87
3		Octadecane	254	C18H38	000593-45-3	83
4		Heptadecane	240	C17H36	000629-78-7	83
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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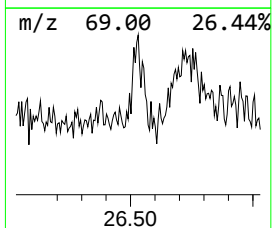
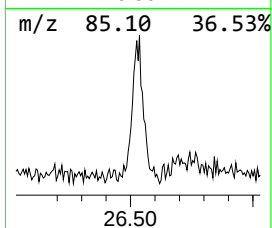
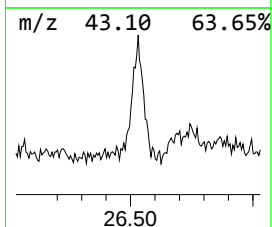
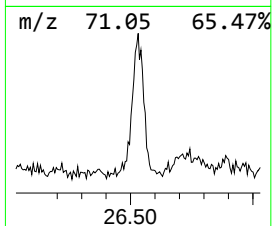
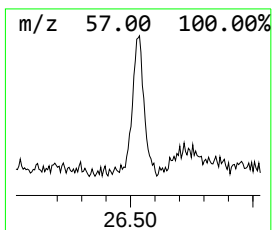
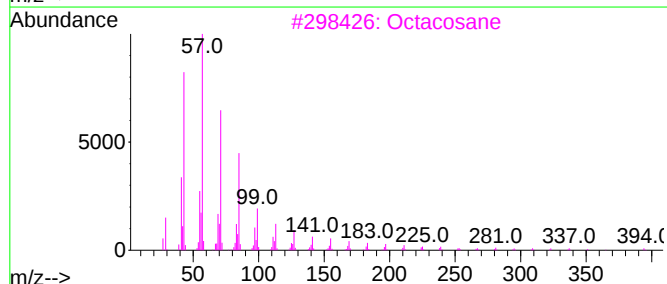
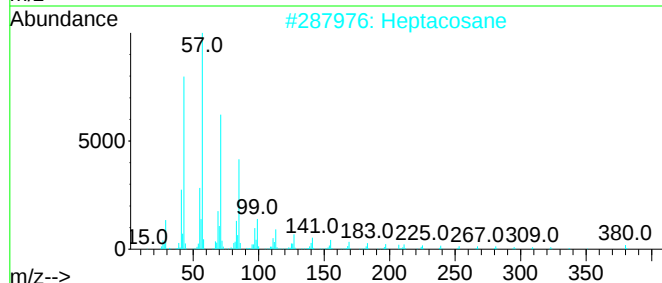
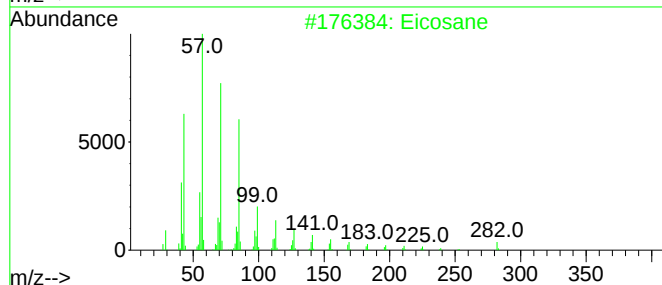
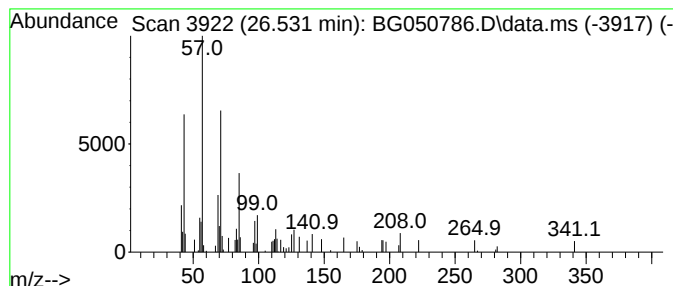
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.531	2.13 ng	66201	Perylene-d12	25.332

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	70
2	Heptacosane		380	C27H56	000593-49-7	62
3	Octacosane		394	C28H58	000630-02-4	62
4	Pentacosane		352	C25H52	000629-99-2	62
5	Hexacosane		366	C26H54	000630-01-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050786.D
Acq On : 29 Oct 2021 20:44
Operator : CG/JU
Sample : M4392-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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Dodecanoic acid...	18.247	2.4	ng	59656	4	17.612	504838	20.0
n-Hexadecanoic ...	18.476	8.2	ng	206741	4	17.612	504838	20.0
Heptadecane	20.985	2.2	ng	59449	5	21.919	550545	20.0
Oxalic acid, is...	21.513	10.7	ng	295567	5	21.919	550545	20.0
Heneicosane	22.083	2.8	ng	78279	5	21.919	550545	20.0
Nonadecane	22.724	2.8	ng	77152	5	21.919	550545	20.0
Octacosane	23.458	2.9	ng	80233	5	21.919	550545	20.0
Supraene	23.664	53.8	ng	1668160	6	25.332	620197	20.0
Tetracosane	24.310	2.8	ng	86427	6	25.332	620197	20.0
Eicosane	26.531	2.1	ng	66201	6	25.332	620197	20.0