

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
 Data File : BG056993.D
 Acq On : 5 Apr 2023 16:35
 Operator : CG/JU
 Sample : 02109-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-30-SB02

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056993.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.441	317	324	331	rVB	82943	126194	14.59%	2.853%
2	5.922	399	406	416	rBB	207041	339770	39.29%	7.682%
3	7.544	674	682	691	rBV	213060	378869	43.81%	8.566%
4	8.413	824	830	836	rBB	45151	73832	8.54%	1.669%
5	9.588	1021	1030	1037	rBB2	125221	222715	25.75%	5.035%
6	11.250	1307	1313	1320	rBV	55503	102871	11.89%	2.326%
7	13.653	1715	1722	1731	rVB	343082	524924	60.69%	11.868%
8	15.028	1949	1956	1963	rVB	105837	163334	18.89%	3.693%
9	16.502	2200	2207	2216	rBV	336967	535563	61.92%	12.109%
10	17.765	2416	2422	2430	rBV2	151512	227001	26.25%	5.132%
11	18.558	2546	2557	2558	rBV5	9456	20509	2.37%	0.464%
12	18.605	2558	2565	2576	rVB4	35183	88938	10.28%	2.011%
13	19.804	2765	2769	2770	rBV4	7972	8717	1.01%	0.197%
14	19.851	2770	2777	2786	rVB3	44017	90718	10.49%	2.051%
15	19.986	2797	2800	2803	rVB3	9374	10722	1.24%	0.242%
16	20.332	2854	2859	2866	rVB	707247	864877	100.00%	19.554%
17	20.673	2913	2917	2922	rBV7	8660	18959	2.19%	0.429%
18	21.648	3078	3083	3093	rBV3	43955	78947	9.13%	1.785%
19	22.083	3150	3157	3167	rVB2	138571	240756	27.84%	5.443%
20	22.236	3178	3183	3189	rVB7	14743	27410	3.17%	0.620%
21	22.905	3289	3297	3298	rBV8	11173	23151	2.68%	0.523%
22	23.657	3418	3425	3430	rBV8	9550	23562	2.72%	0.533%
23	25.631	3750	3761	3770	rVB3	75108	230601	26.66%	5.214%

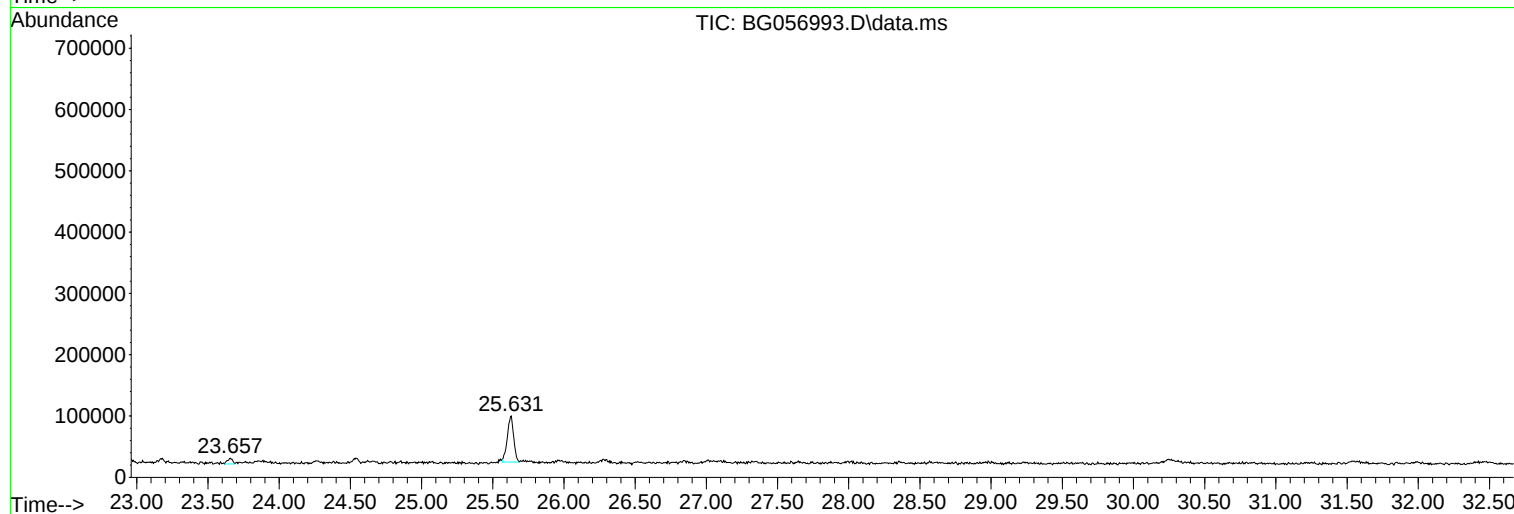
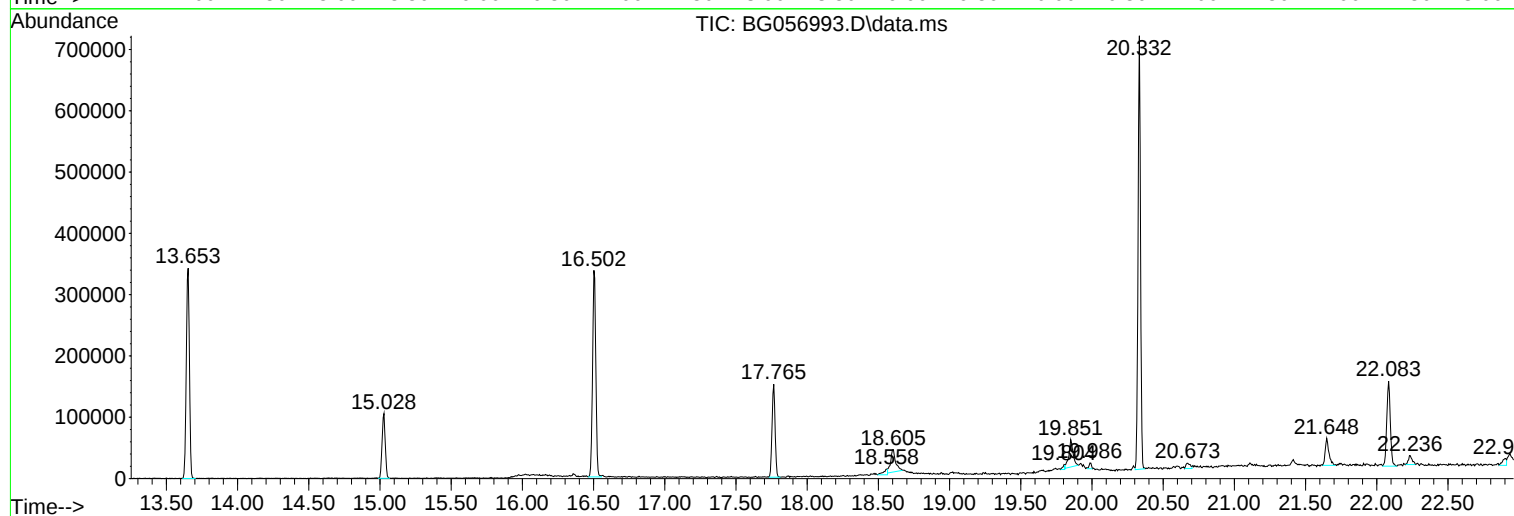
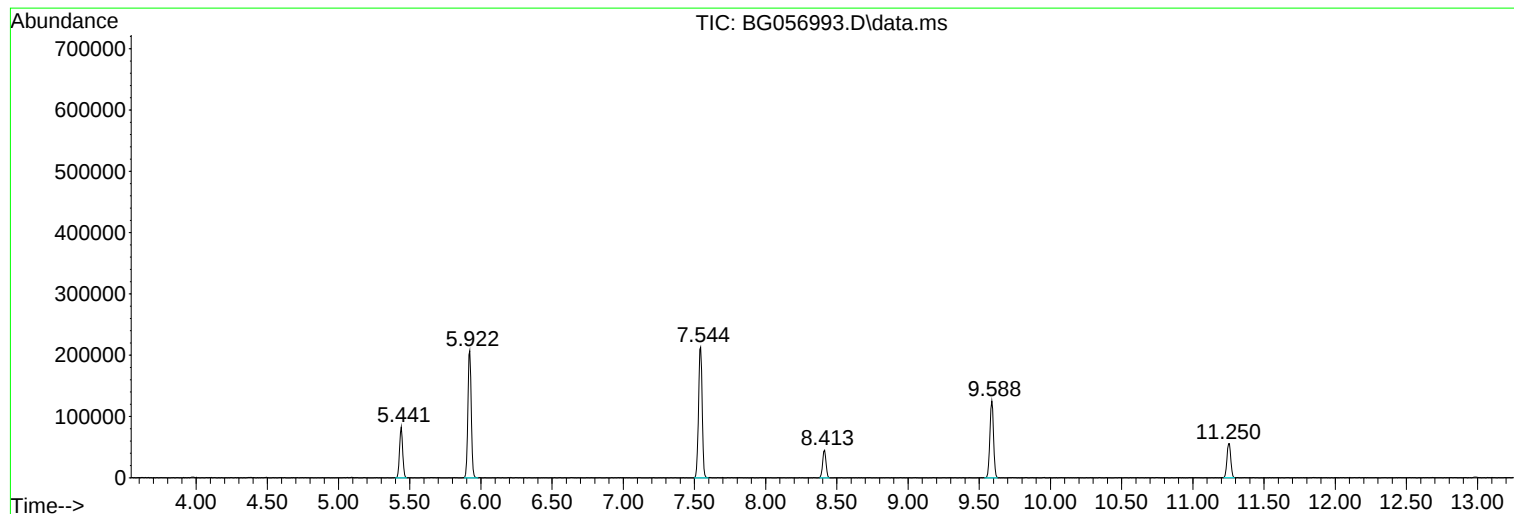
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Instrument :
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ClientSampleId :
B-30-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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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Data File : BG056993.D
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Operator : CG/JU
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Misc :
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Instrument :
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ClientSampleId :
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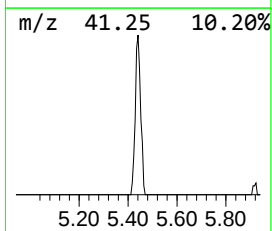
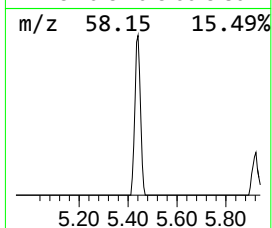
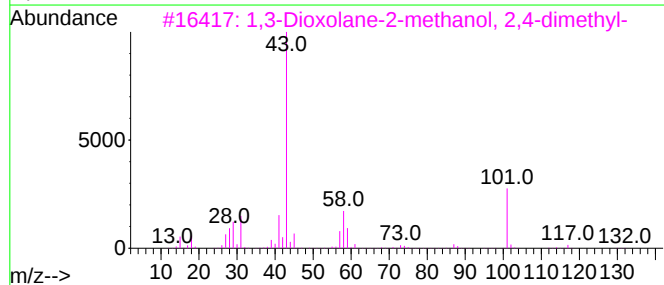
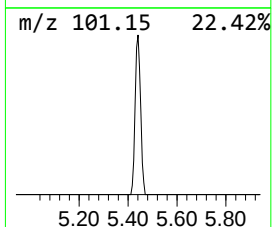
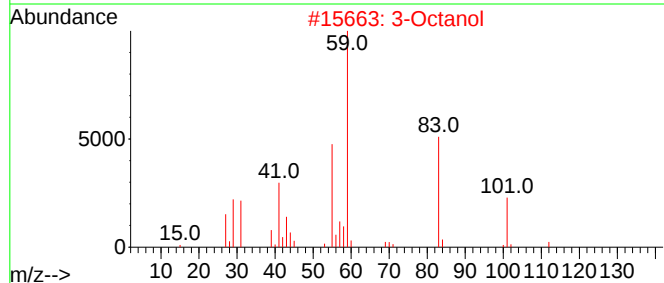
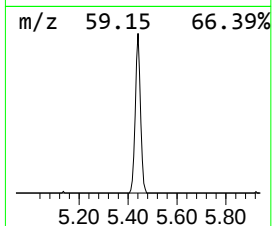
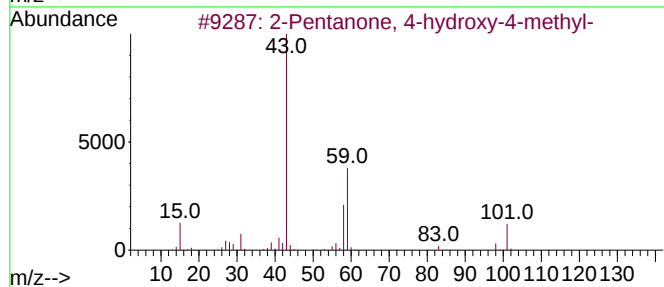
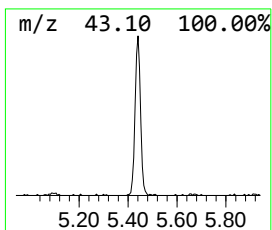
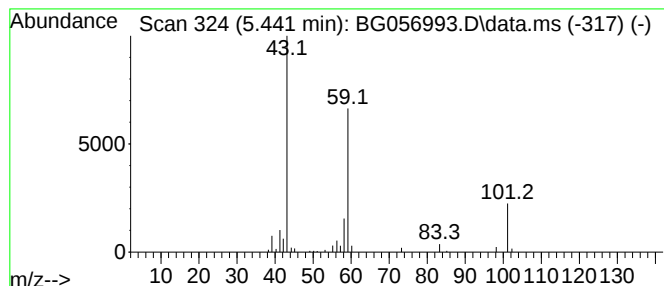
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.441	34.18 ng	126194	1,4-Dichlorobenzene-d4	8.413

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Octanol	130	C8H18O	000589-98-0	33
3			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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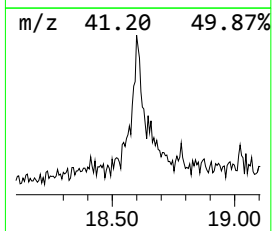
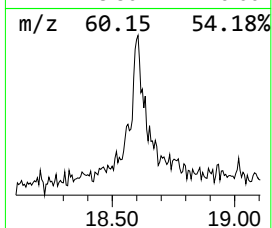
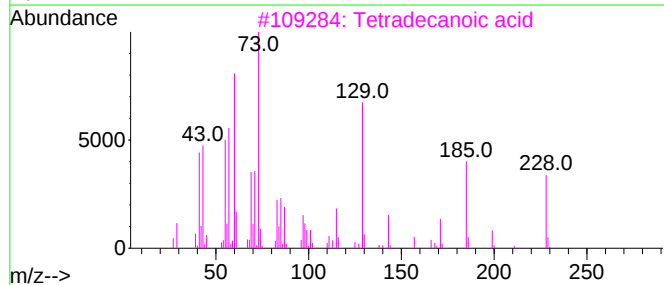
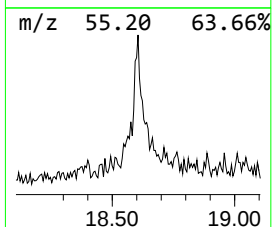
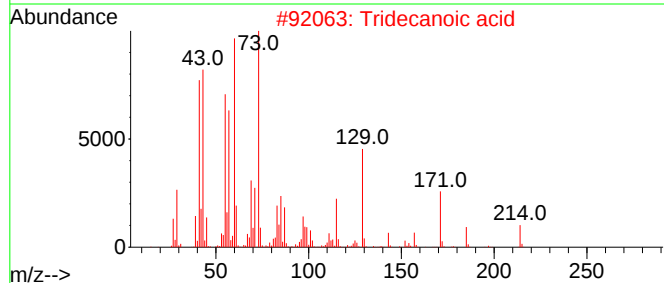
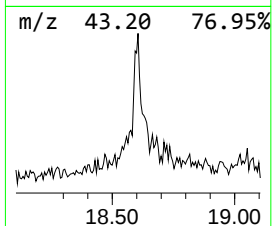
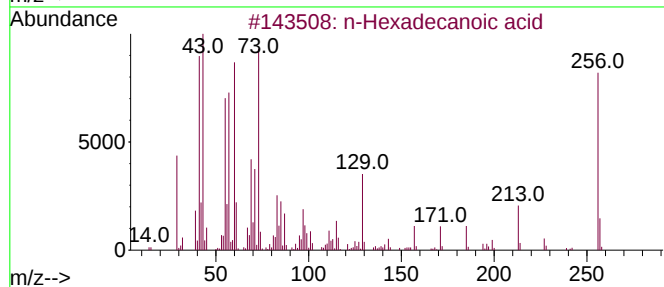
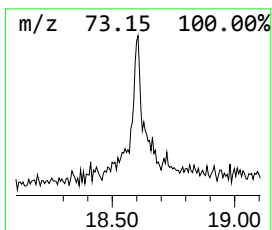
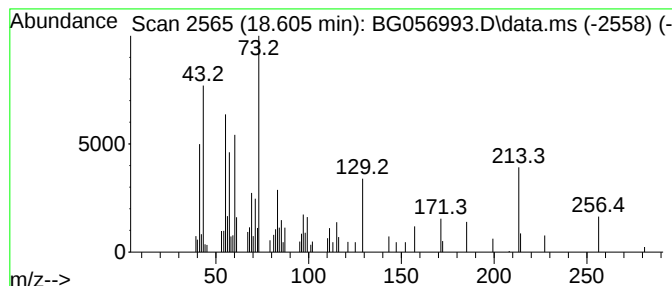
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.605	7.84 ng	88938	Phenanthrene-d10	17.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4			n-Decanoic acid	172	C10H20O2	000334-48-5	38
5			Carbamic acid, (4-chlorophenyl)-...	213	C10H12ClNO2	002239-92-1	27



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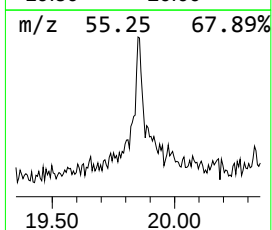
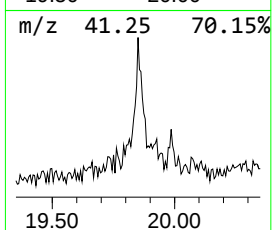
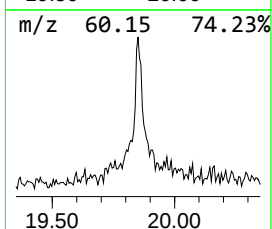
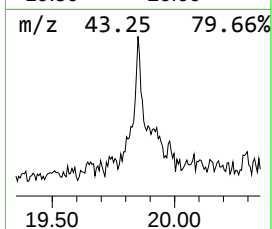
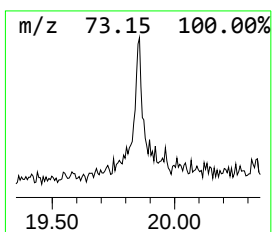
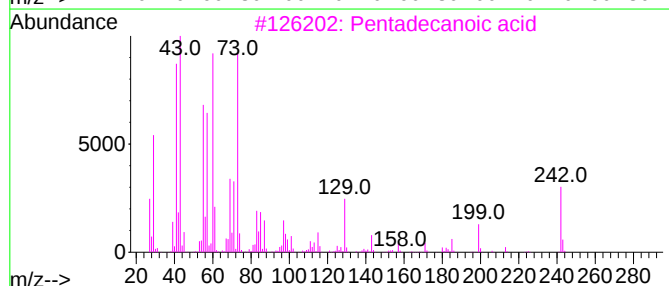
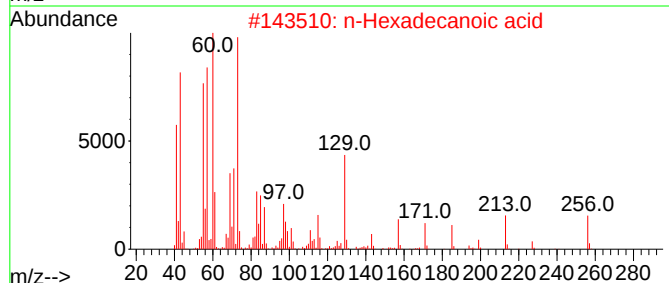
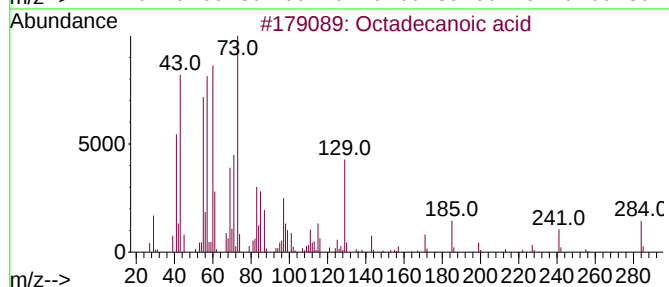
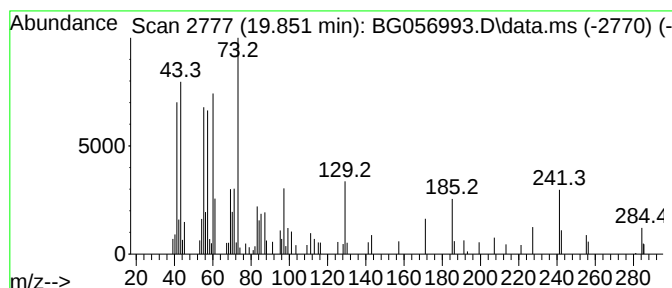
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.851	7.99 ng	90718	Phenanthrene-d10	17.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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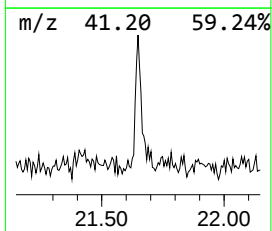
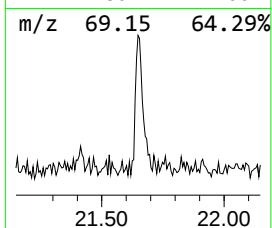
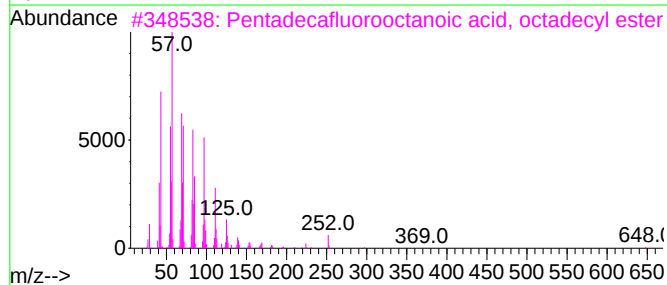
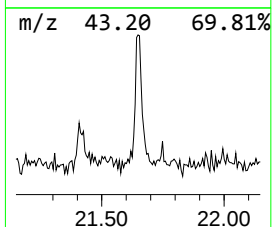
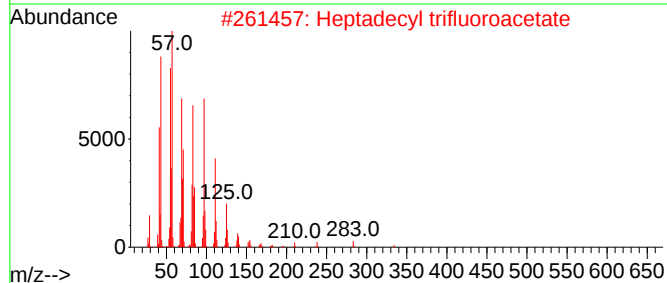
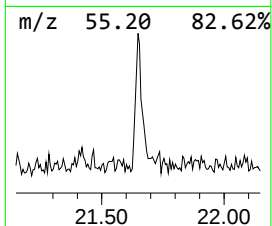
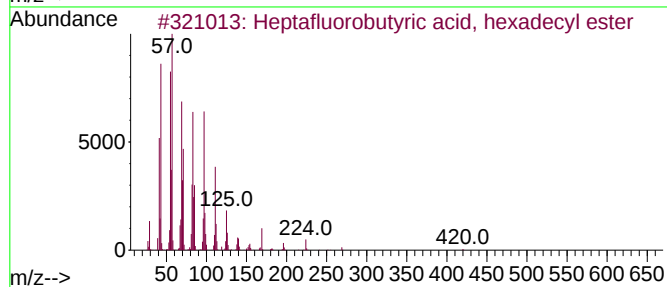
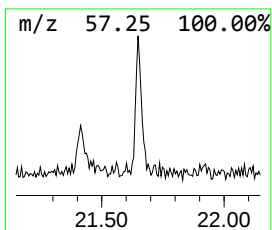
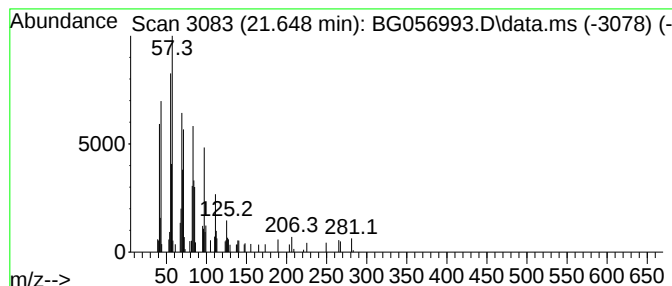
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.648	6.56 ng	78947	Chrysene-d12	22.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5			1-Octadecene	252	C18H36	000112-88-9	87



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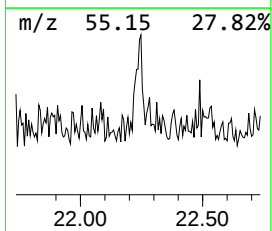
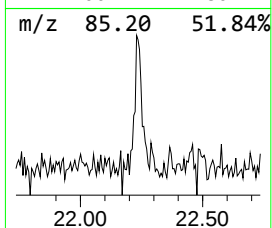
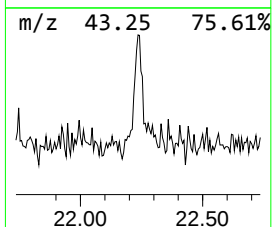
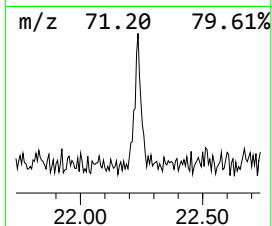
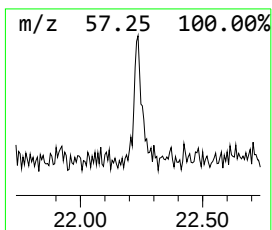
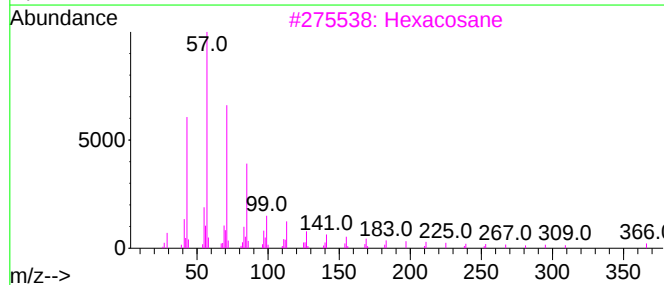
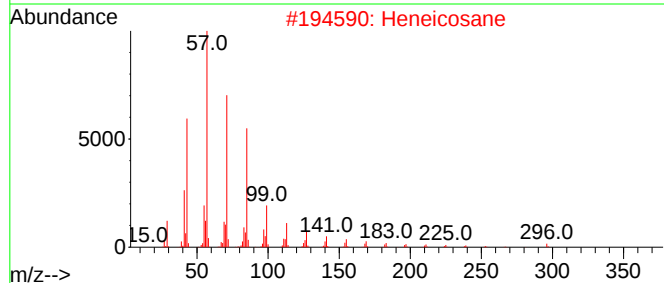
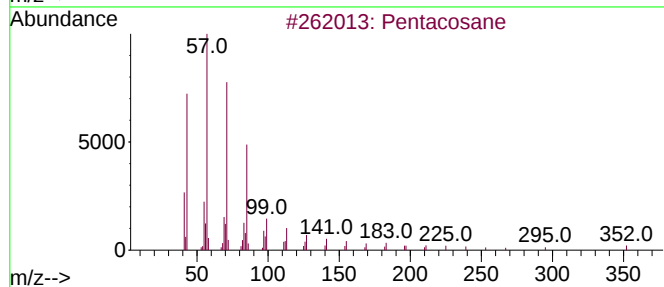
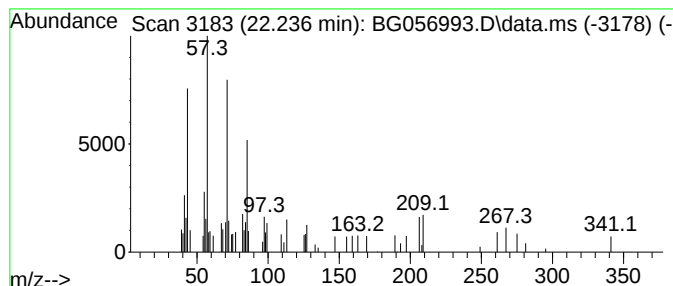
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.236	2.28 ng	27410	Chrysene-d12	22.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	58
2			Heneicosane	296	C21H44	000629-94-7	58
3			Hexacosane	366	C26H54	000630-01-3	58
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	58
5			Hentriacontane	437	C31H64	000630-04-6	58



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.441	34.2	ng	126194	1	8.413	73832	20.0
n-Hexadecanoic ...	18.605	7.8	ng	88938	4	17.765	227001	20.0
Octadecanoic acid	19.851	8.0	ng	90718	4	17.765	227001	20.0
Heptafluorobuty...	21.648	6.6	ng	78947	5	22.083	240756	20.0
Pentacosane	22.236	2.3	ng	27410	5	22.083	240756	20.0