

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
 Data File : BG055867.D
 Acq On : 1 Dec 2022 22:46
 Operator : CG/JU
 Sample : N5818-04 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-04-113022

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.262	329	336	345	rBV	91732	151958	1.45%	0.409%
2	5.749	412	419	429	rBV	330409	572962	5.47%	1.542%
3	7.365	684	694	708	rBV	341805	609191	5.82%	1.640%
4	8.211	832	838	852	rVB	195212	343695	3.28%	0.925%
5	9.386	1031	1038	1050	rVB	204005	397006	3.79%	1.069%
6	11.037	1311	1319	1326	rBV	248069	461122	4.40%	1.241%
7	13.458	1724	1731	1740	rVB	562011	853982	8.15%	2.299%
8	14.839	1957	1966	1973	rVB	394413	619284	5.91%	1.667%
9	16.319	2212	2218	2226	rBV	409780	635711	6.07%	1.711%
10	17.577	2426	2432	2437	rBV	454826	716756	6.84%	1.929%
11	18.211	2534	2540	2547	rVB	1706836	2281548	21.79%	6.142%
12	18.446	2574	2580	2587	rBV	720003	1181737	11.28%	3.181%
13	19.345	2726	2733	2736	rBV	6794015	10472941	100.00%	28.193%
14	19.375	2736	2738	2748	rVB2	5706110	7403524	70.69%	19.930%
15	19.498	2754	2759	2764	rBV	1371384	1604709	15.32%	4.320%
16	19.574	2765	2772	2774	rBV	2039243	3578274	34.17%	9.633%
17	19.598	2774	2776	2791	rVV2	1544006	2659717	25.40%	7.160%
18	19.704	2791	2794	2801	rVB	189171	277222	2.65%	0.746%
19	19.862	2817	2821	2827	rBV4	80646	124268	1.19%	0.335%
20	19.980	2839	2841	2848	rVB	100027	126799	1.21%	0.341%
21	20.162	2868	2872	2878	rVB	832525	1073430	10.25%	2.890%
22	20.579	2940	2943	2946	rBV	128877	138918	1.33%	0.374%
23	21.619	3117	3120	3128	rVB	126465	182461	1.74%	0.491%
24	21.872	3158	3163	3168	rVB	417908	680184	6.49%	1.831%

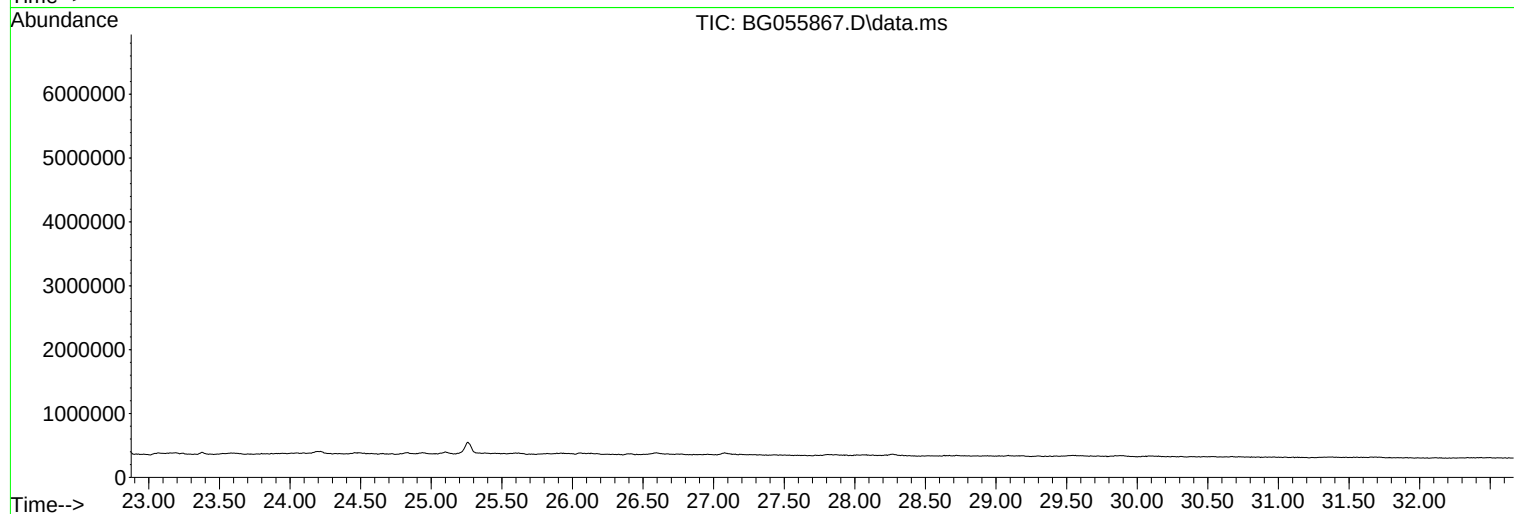
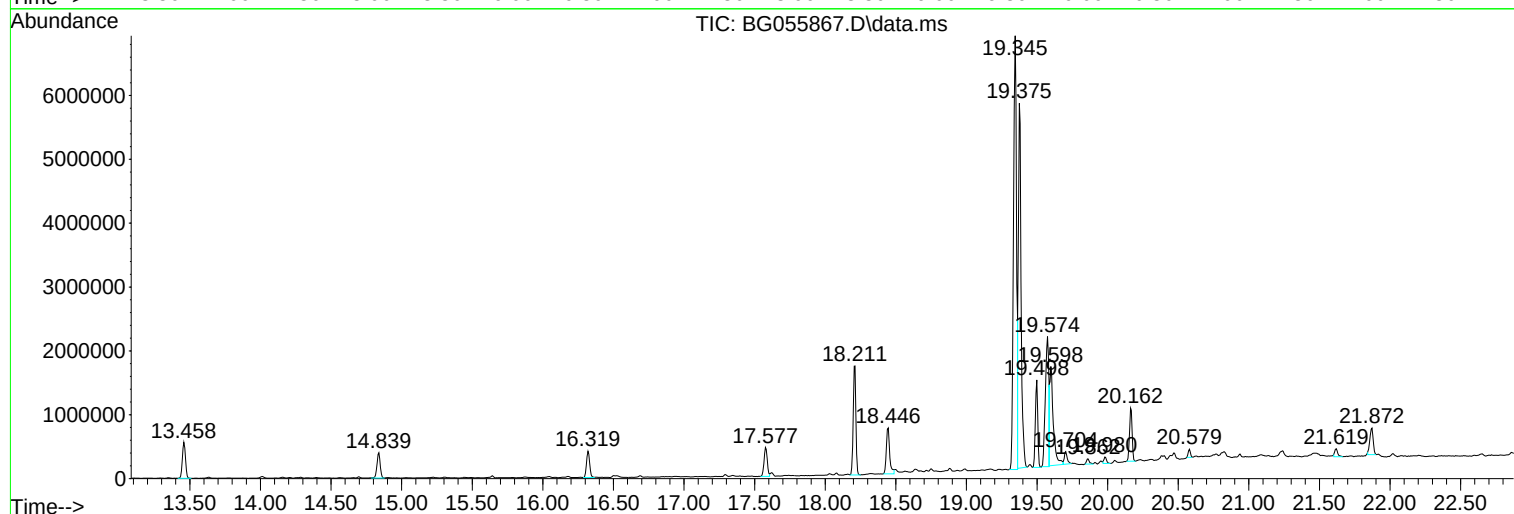
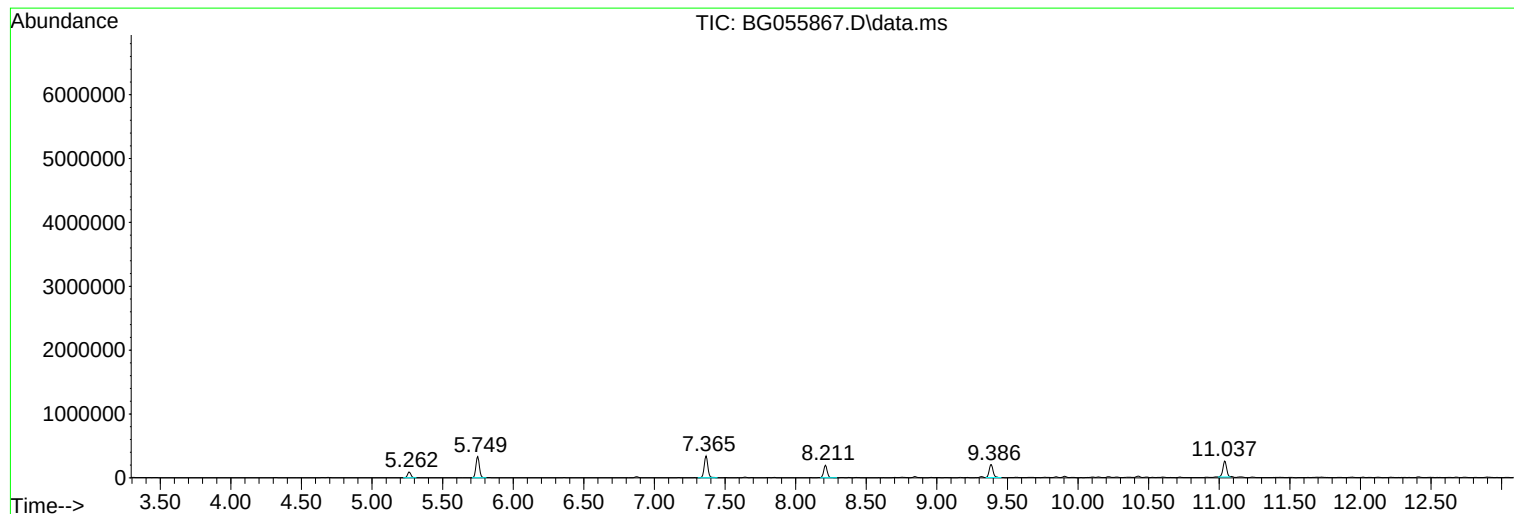
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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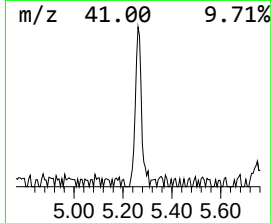
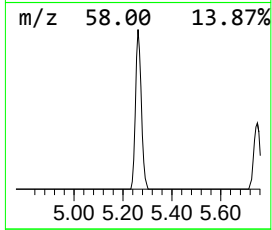
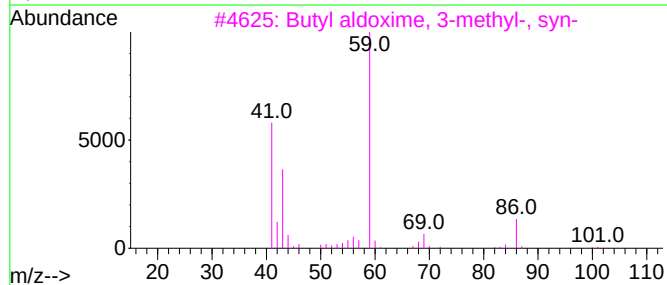
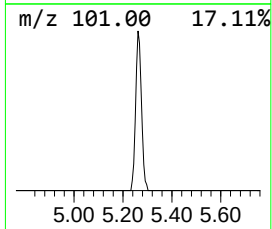
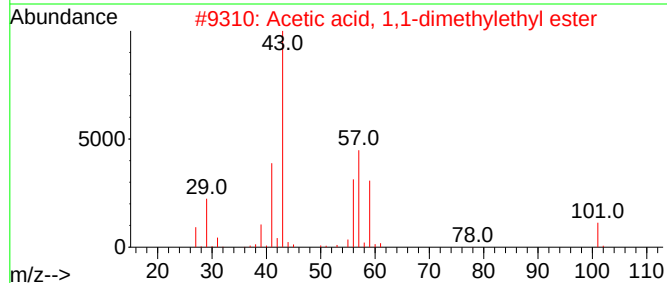
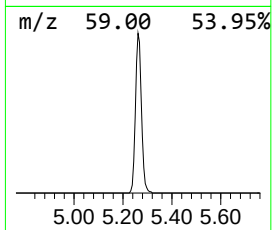
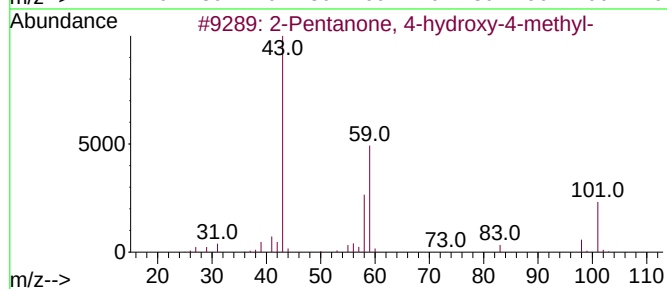
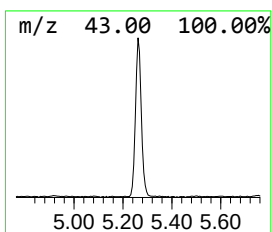
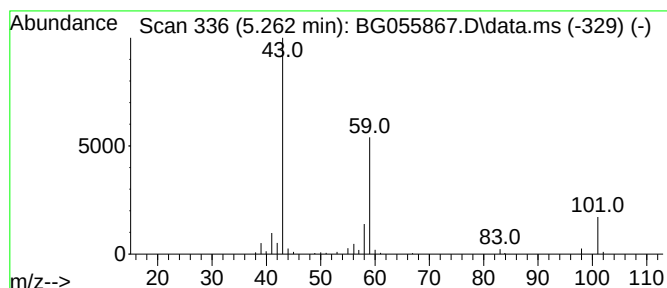
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.262	8.84 ng	151958	1,4-Dichlorobenzene-d4	8.211

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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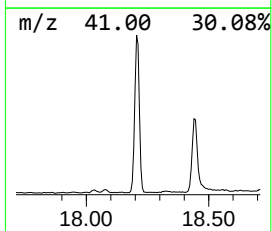
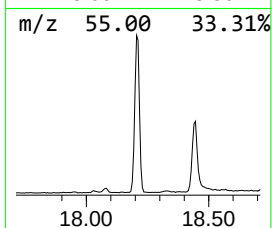
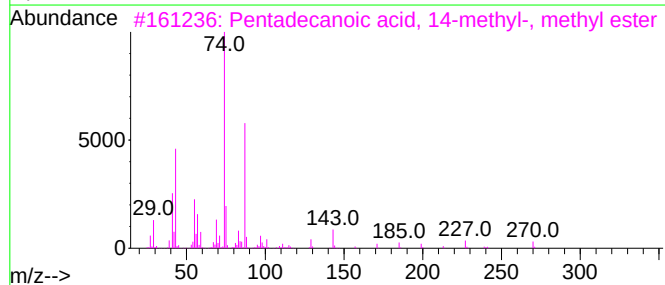
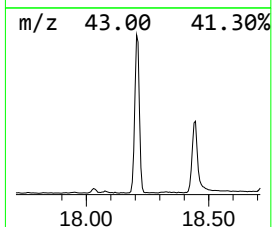
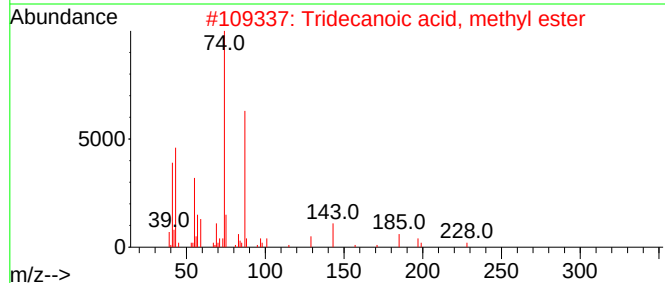
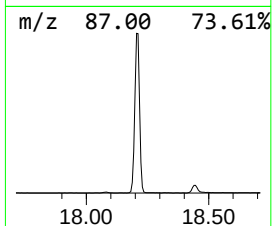
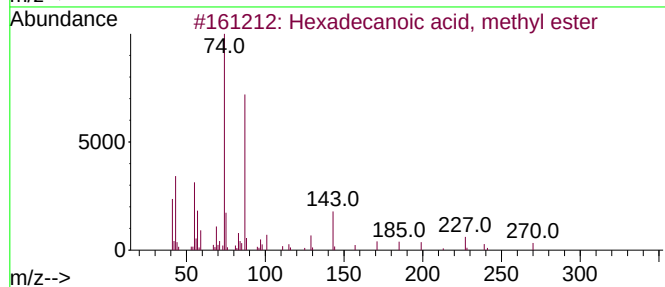
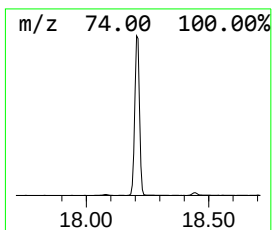
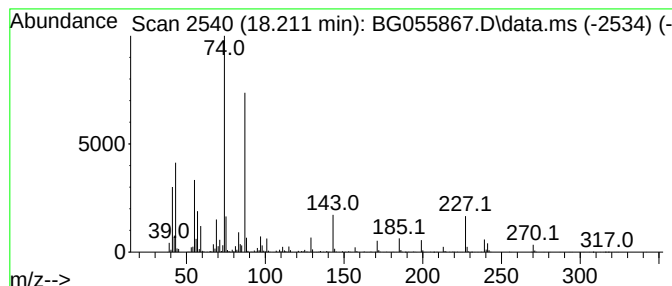
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	63.66 ng	2281550	Phenanthrene-d10	17.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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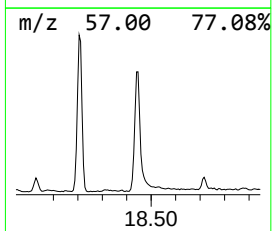
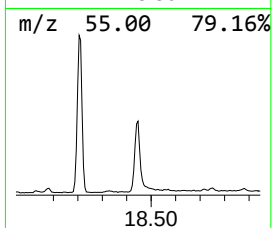
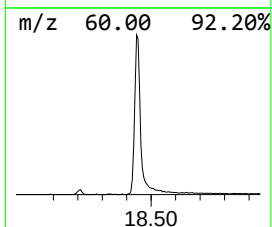
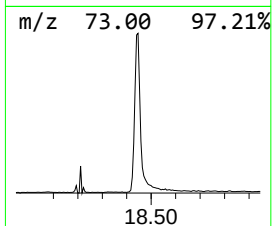
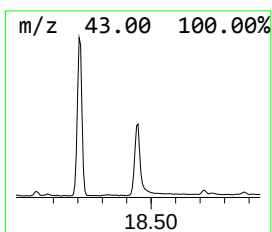
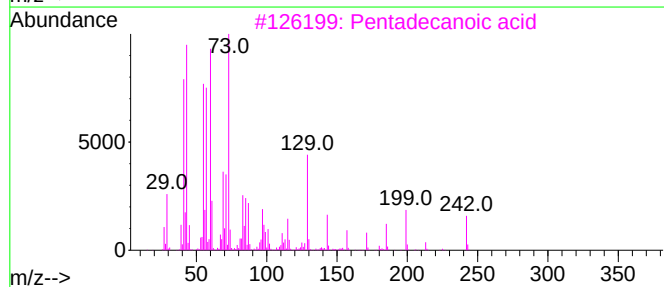
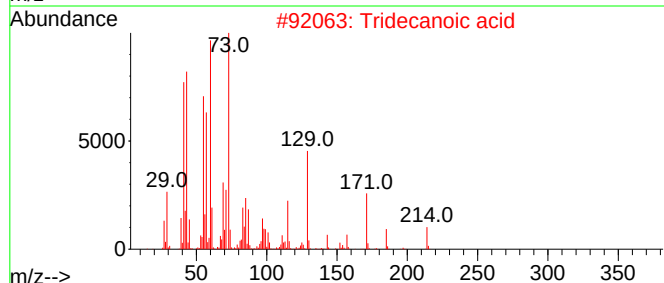
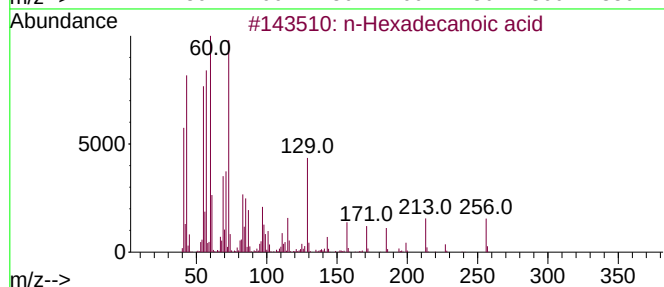
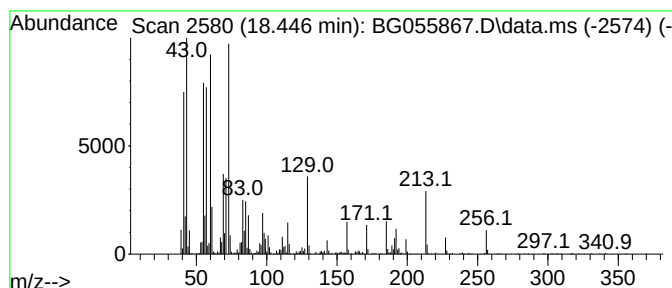
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	32.97 ng	1181740	Phenanthrene-d10	17.577

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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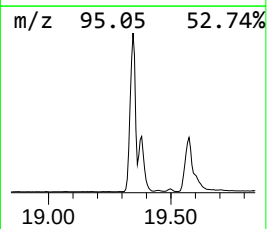
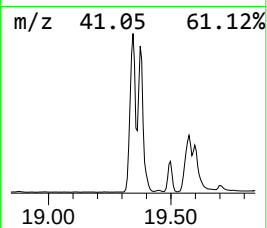
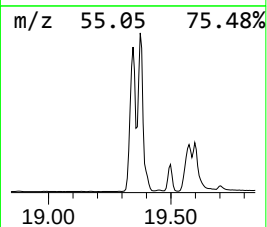
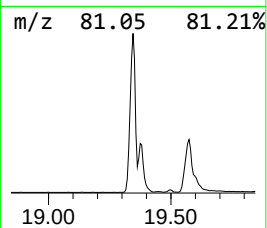
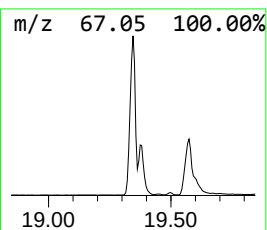
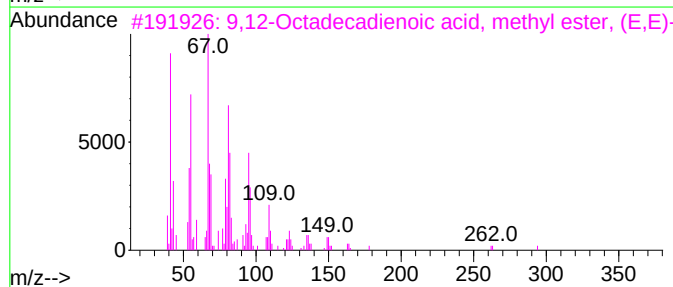
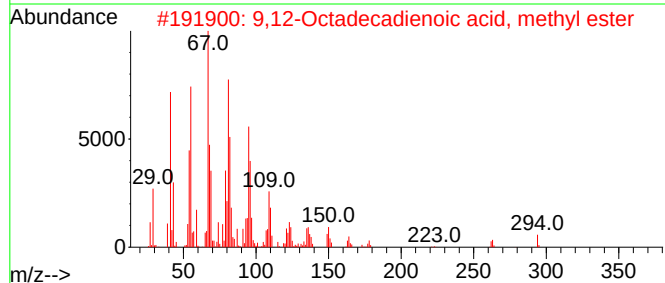
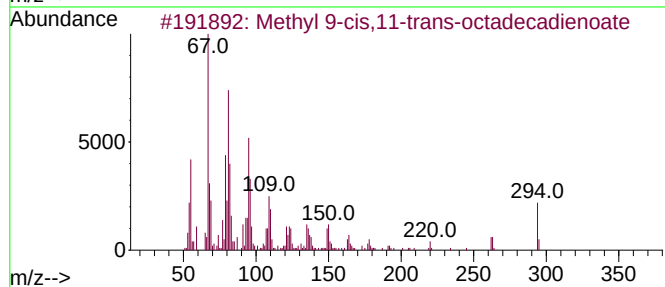
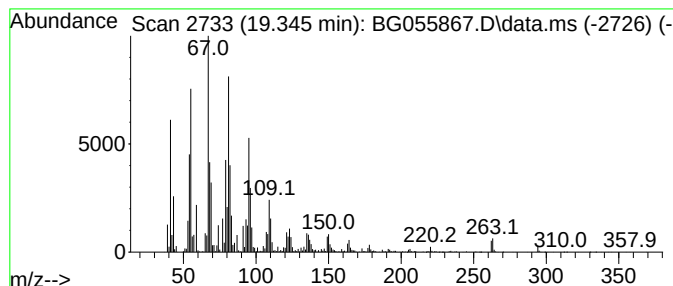
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Peak Number 4 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.345	292.23 ng	10472900	Phenanthrene-d10	17.577	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	97
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95



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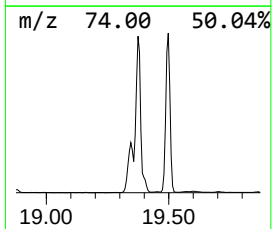
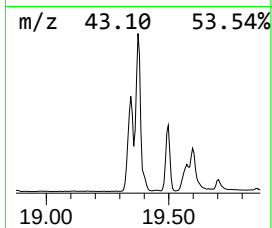
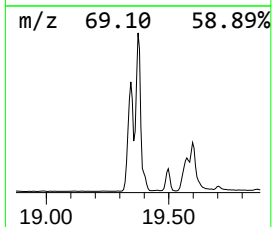
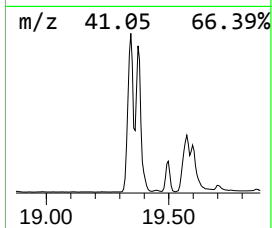
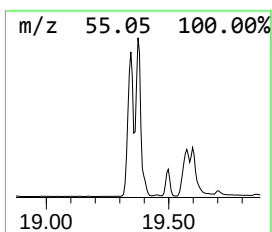
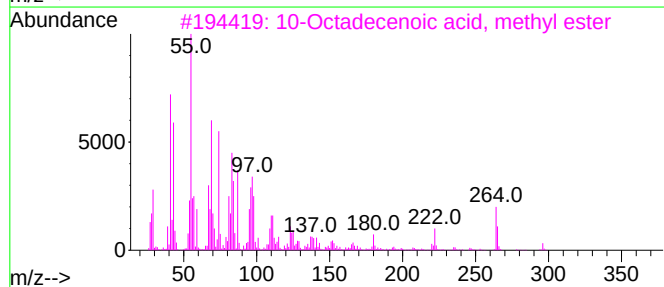
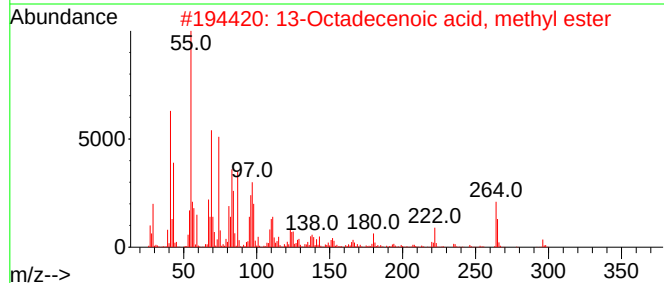
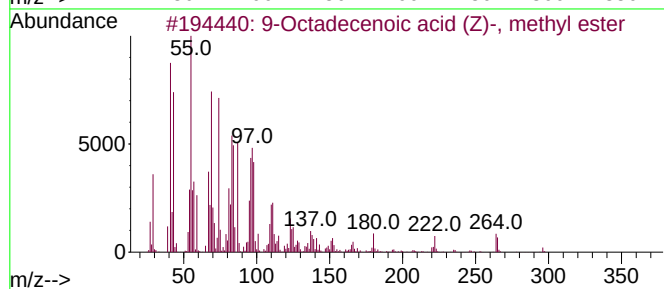
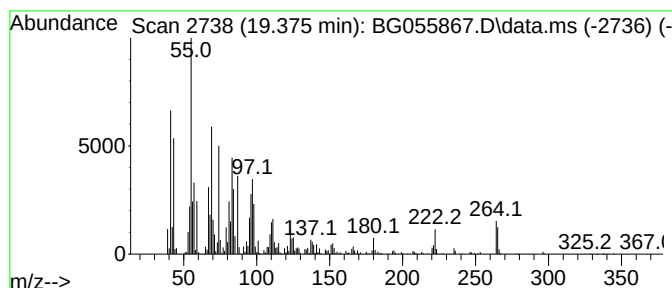
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.375	206.58 ng	7403520	Phenanthrene-d10	17.577	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	93



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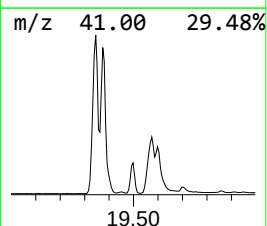
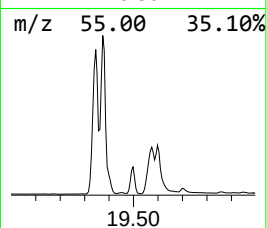
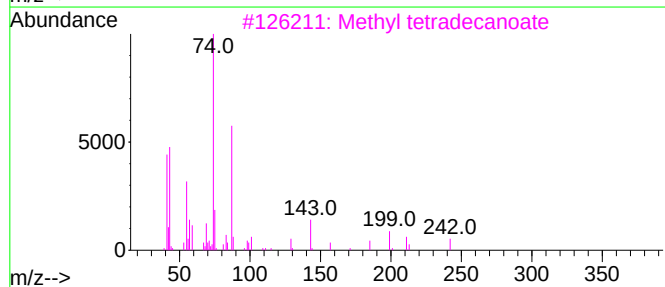
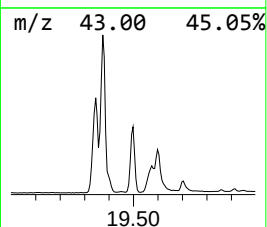
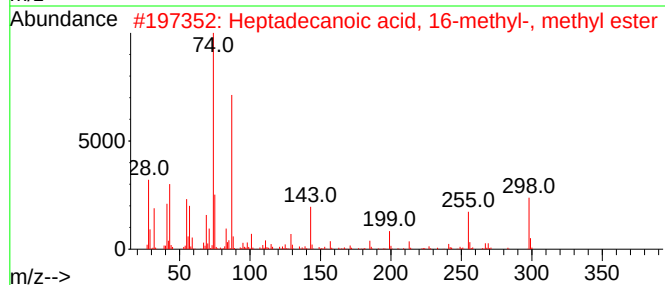
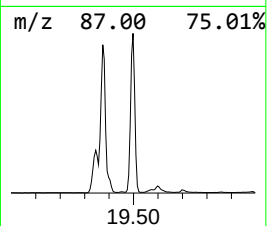
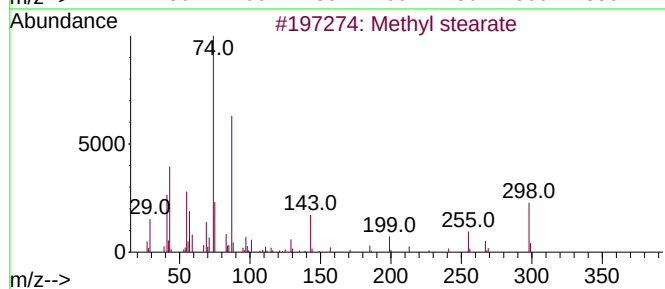
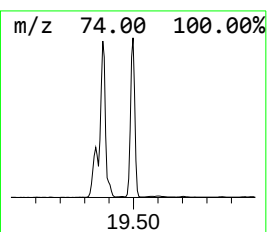
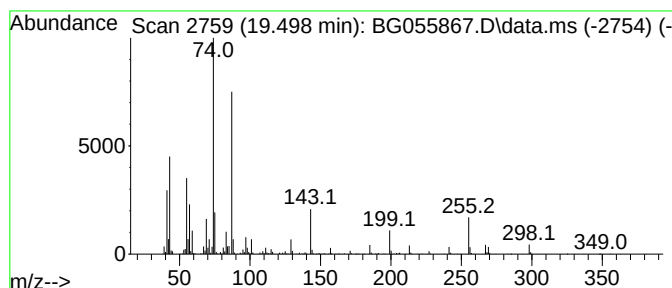
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.498	44.78 ng	1604710	Phenanthrene-d10	17.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83
5			2-Methylpentadecanoic acid	256	C16H32O2	025354-92-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055867.D
Acq On : 1 Dec 2022 22:46
Operator : CG/JU
Sample : N5818-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-113022

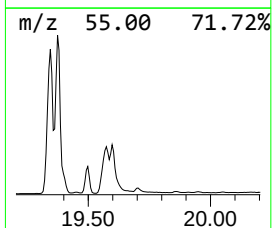
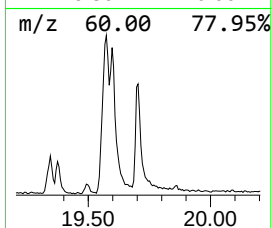
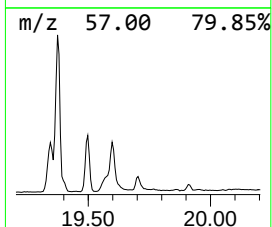
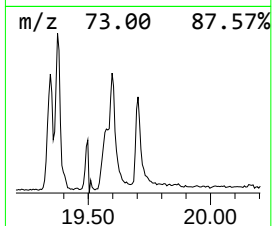
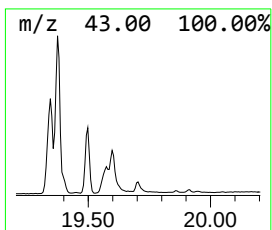
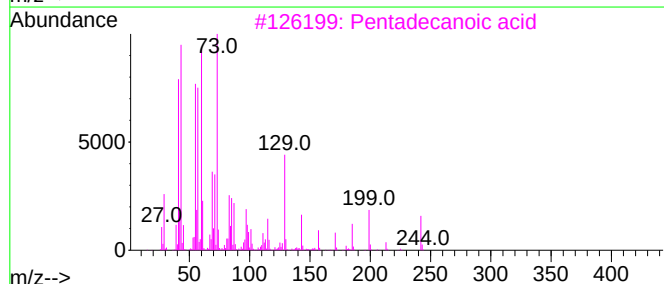
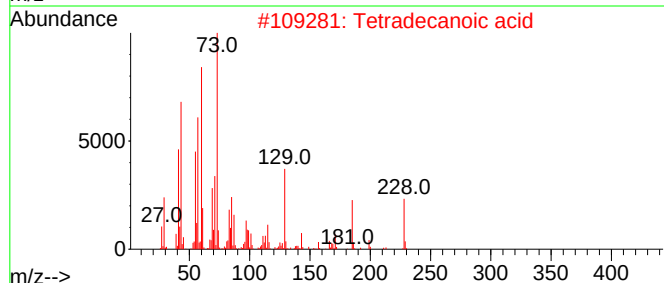
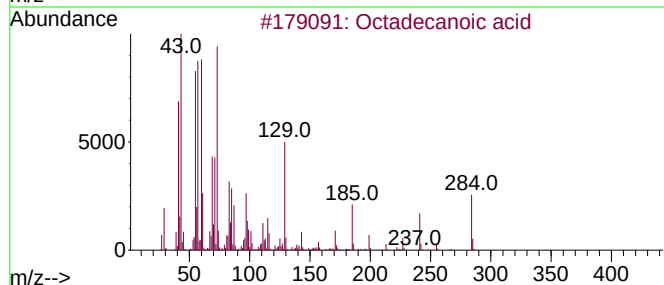
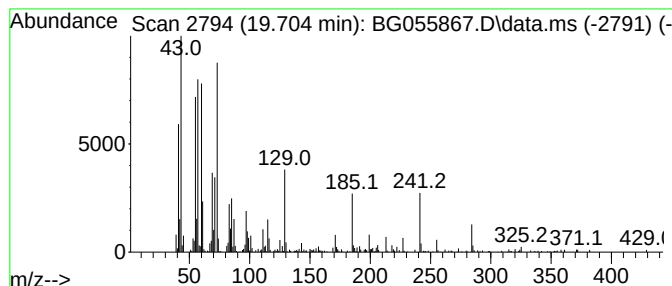
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.703	7.74 ng	277222	Phenanthrene-d10	17.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055867.D
Acq On : 1 Dec 2022 22:46
Operator : CG/JU
Sample : N5818-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

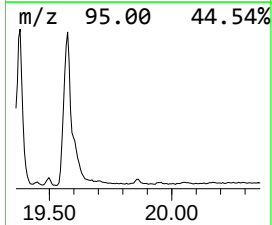
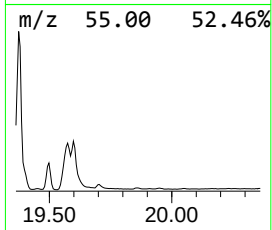
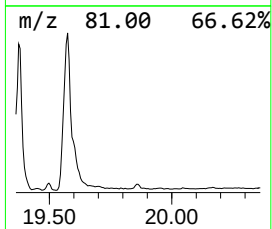
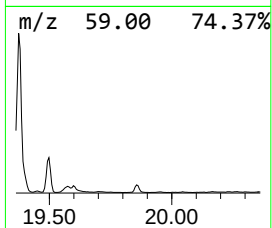
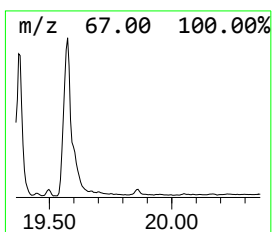
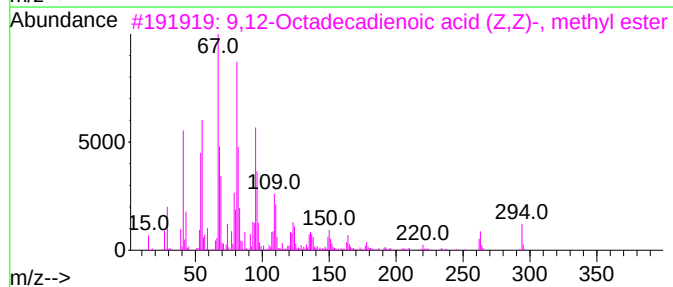
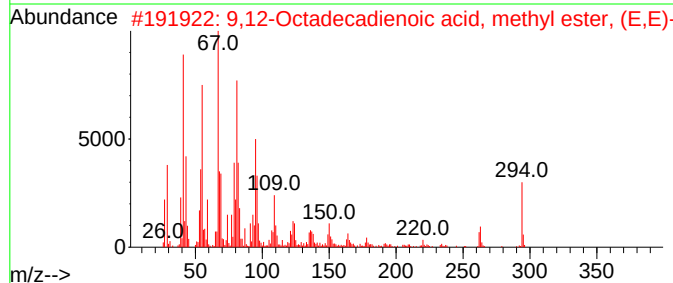
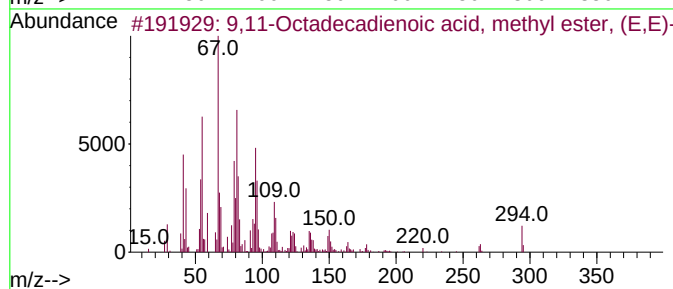
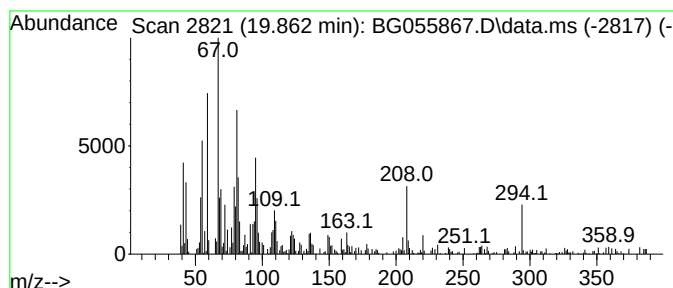
Instrument :
BNA_G
ClientSampleId :
TR-04-113022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,11-Octadecadienoic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.862	3.65 ng	124268	Chrysene-d12	21.872	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	83
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	83
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	60
4	6,9-Octadecadienoic acid, methyl...	294	C19H34O2	056599-55-4	60
5	9,12-Octadecadienoyl chloride, (...	298	C18H31ClO	007459-33-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055867.D
Acq On : 1 Dec 2022 22:46
Operator : CG/JU
Sample : N5818-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

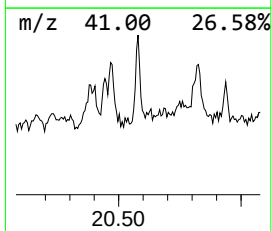
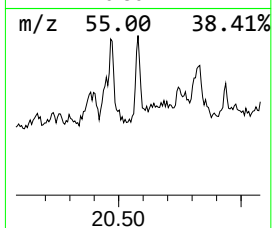
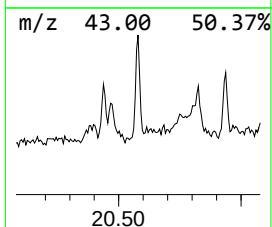
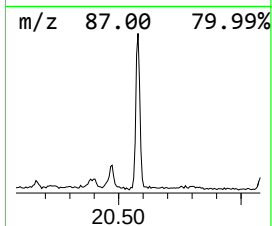
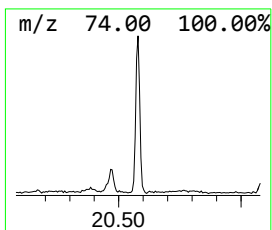
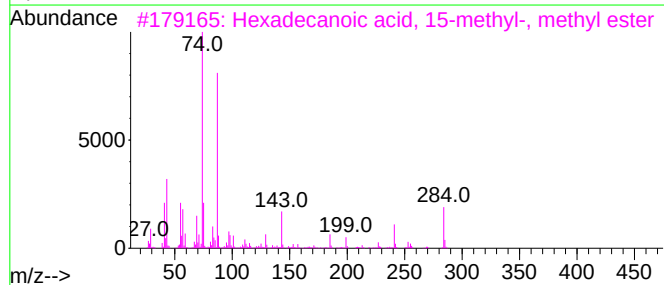
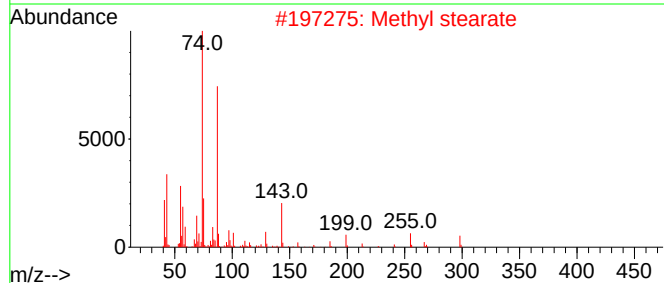
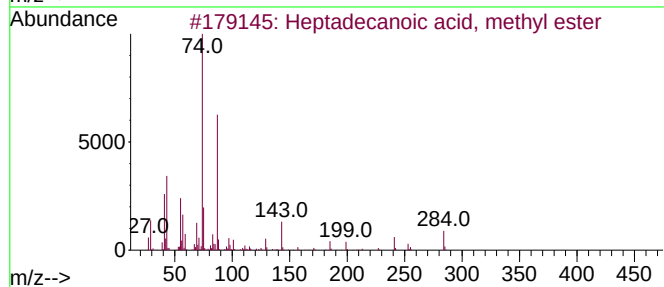
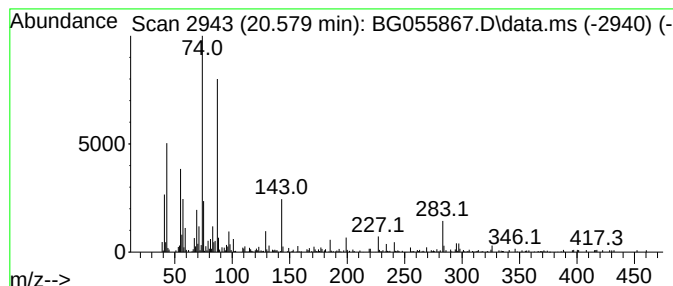
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TR-04-113022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecanoic acid, methyl ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.579	4.08 ng	138918	Chrysene-d12	21.872	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
2	Methyl stearate	298	C19H38O2	000112-61-8	91
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91
5	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055867.D
Acq On : 1 Dec 2022 22:46
Operator : CG/JU
Sample : N5818-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

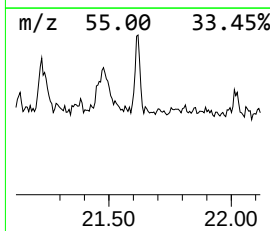
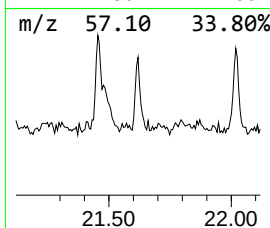
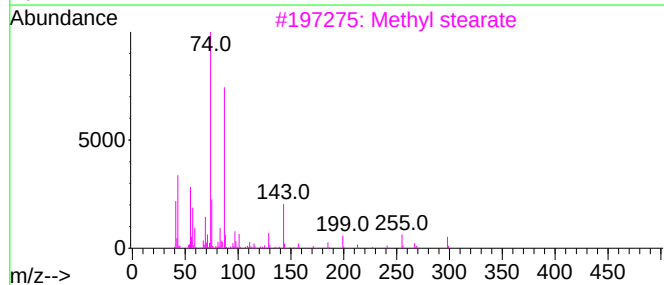
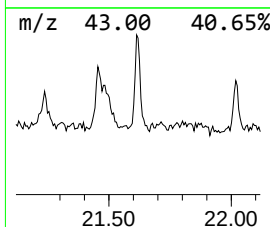
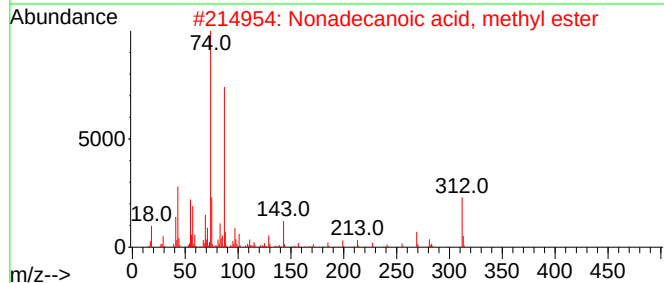
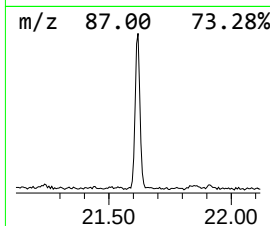
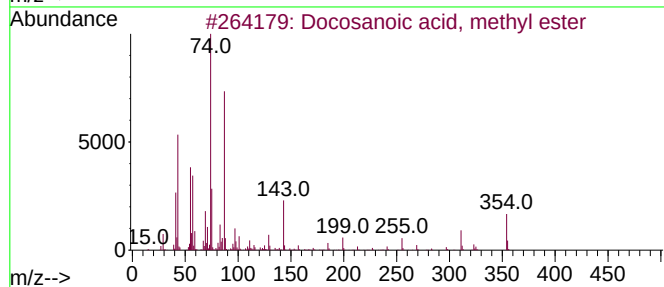
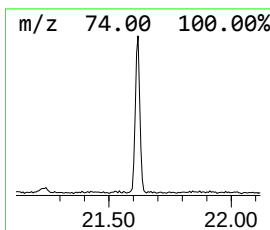
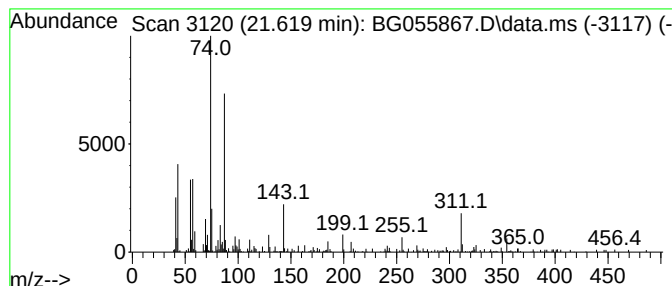
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.619	5.37 ng	182461	Chrysene-d12		21.872	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester		354	C23H46O2	000929-77-1	97
2	Nonadecanoic acid, methyl ester		312	C20H40O2	001731-94-8	95
3	Methyl stearate		298	C19H38O2	000112-61-8	83
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	74
5	Methyl tetradecanoate		242	C15H30O2	000124-10-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055867.D
Acq On : 1 Dec 2022 22:46
Operator : CG/JU
Sample : N5818-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-113022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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Hexadecanoic ac...	18.211	63.7	ng	2281550	4	17.577	716756	20.0
n-Hexadecanoic ...	18.446	33.0	ng	1181740	4	17.577	716756	20.0
Methyl 9-cis,11...	19.345	292.2	ng	10472900	4	17.577	716756	20.0
9-Octadecenoic ...	19.375	206.6	ng	7403520	4	17.577	716756	20.0
Methyl stearate	19.498	44.8	ng	1604710	4	17.577	716756	20.0
Octadecanoic acid	19.703	7.7	ng	277222	4	17.577	716756	20.0
9,11-Octadecadi...	19.862	3.6	ng	124268	5	21.872	680184	20.0
Heptadecanoic a...	20.579	4.1	ng	138918	5	21.872	680184	20.0
Docosanoic acid...	21.619	5.4	ng	182461	5	21.872	680184	20.0