

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
 Data File : BG055597.D
 Acq On : 12 Nov 2022 20:08
 Operator : CG/JU
 Sample : N5583-01 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NB-08-111022

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.797	420	427	442	rBV	582597	976482	2.34%	0.872%
2	7.407	692	701	710	rBV	584841	1065106	2.55%	0.951%
3	8.270	840	848	857	rBV	250238	438959	1.05%	0.392%
4	9.440	1039	1047	1054	rBV	350829	634484	1.52%	0.567%
5	11.096	1323	1329	1336	rBV	339731	599229	1.44%	0.535%
6	13.517	1733	1741	1752	rVB	949864	1503769	3.60%	1.343%
7	14.886	1962	1974	1981	rBV	534941	911498	2.18%	0.814%
8	16.367	2220	2226	2234	rVB	764690	1136315	2.72%	1.015%
9	17.630	2435	2441	2445	rBV	649631	1004509	2.41%	0.897%
10	18.282	2545	2552	2557	rBV	8229457	11589034	27.76%	10.348%
11	18.511	2584	2591	2602	rBV2	1204475	2062772	4.94%	1.842%
12	19.434	2737	2748	2750	rBV3	15748362	41741664	100.00%	37.272%
13	19.463	2750	2753	2760	rVV3	16105196	28008486	67.10%	25.009%
14	19.522	2760	2763	2766	rVV	400717	536480	1.29%	0.479%
15	19.569	2766	2771	2775	rVV	5472303	6898462	16.53%	6.160%
16	19.628	2775	2781	2783	rVV	2257094	3164931	7.58%	2.826%
17	19.651	2783	2785	2796	rVV2	1422814	2874870	6.89%	2.567%
18	19.757	2800	2803	2809	rVB	314445	427491	1.02%	0.382%
19	20.033	2846	2850	2858	rVB	421594	701760	1.68%	0.627%
20	20.221	2877	2882	2887	rVB	1505228	1922089	4.60%	1.716%
21	20.538	2933	2936	2943	rVB2	433775	608039	1.46%	0.543%
22	20.644	2951	2954	2958	rBV	492848	496186	1.19%	0.443%
23	21.702	3130	3134	3140	rVB	442384	617820	1.48%	0.552%
24	21.931	3166	3173	3178	rBV3	603451	1238524	2.97%	1.106%
25	25.368	3751	3758	3769	rVB2	273250	834430	2.00%	0.745%

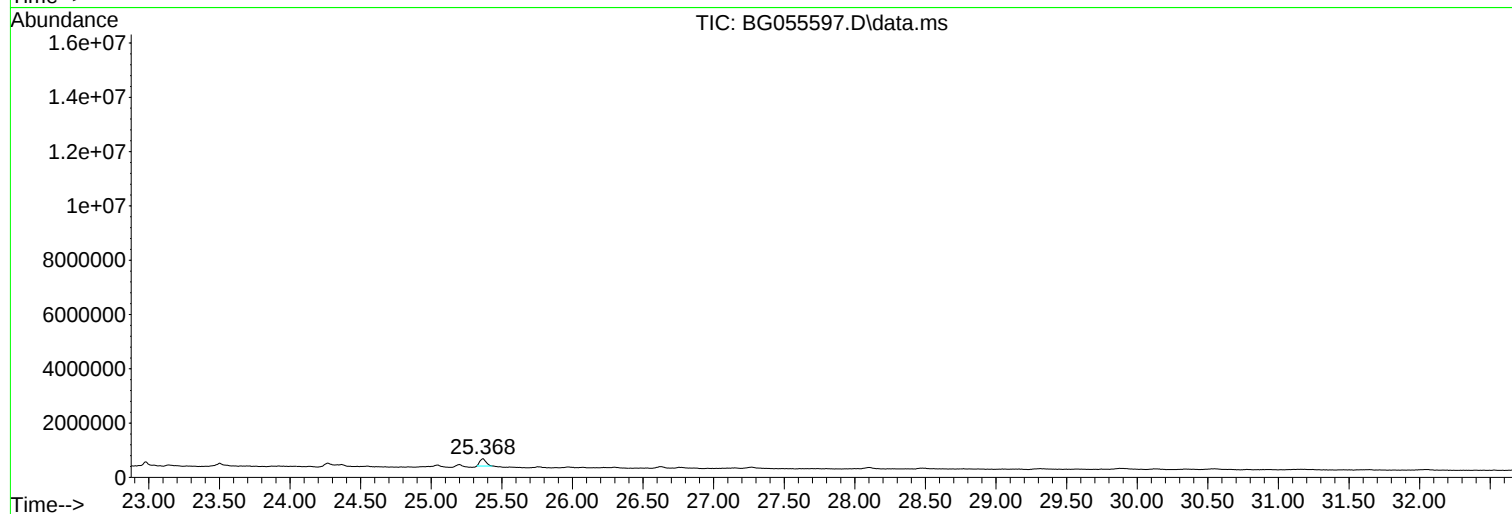
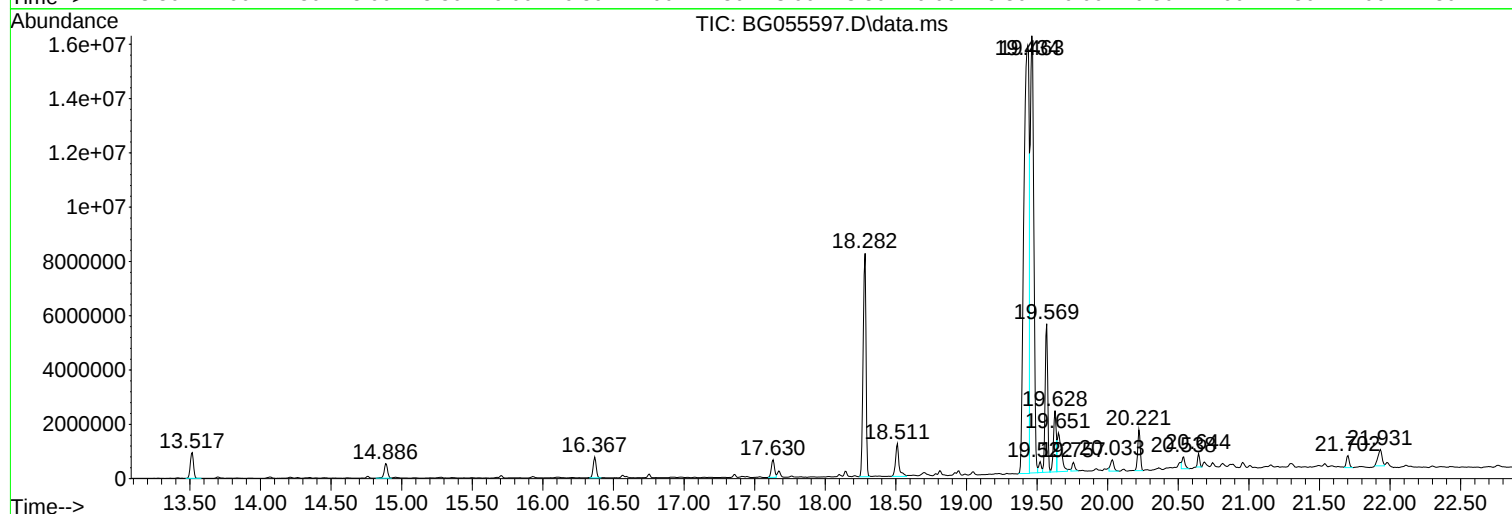
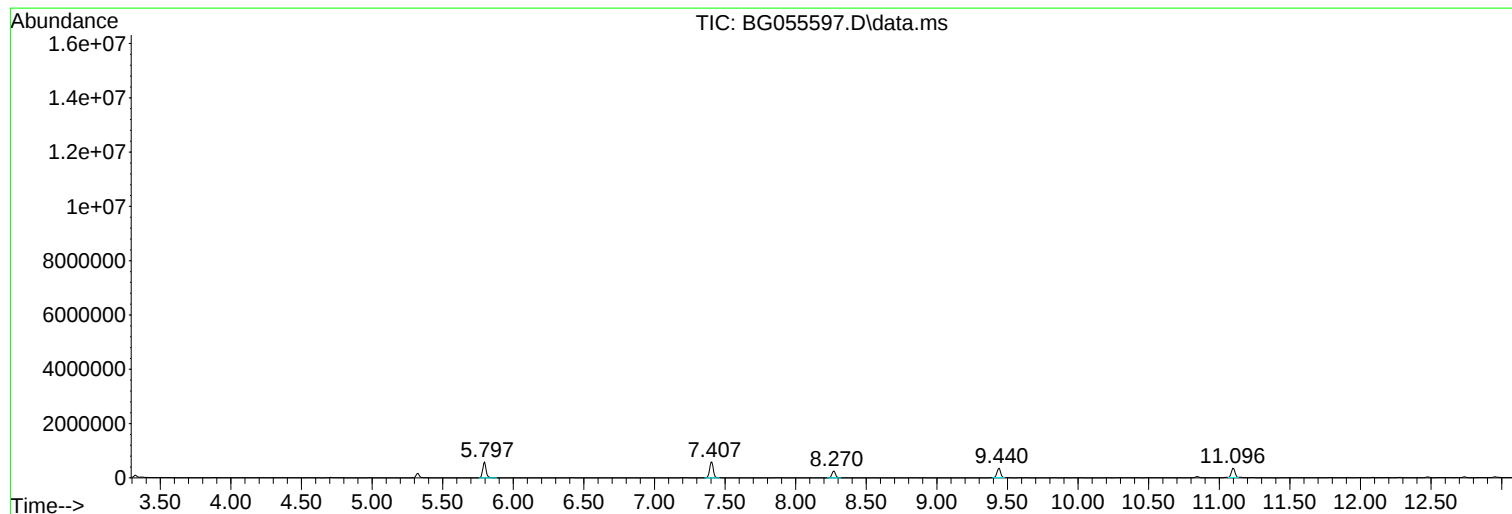
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Instrument :
BNA_G
ClientSampleId :
NB-08-111022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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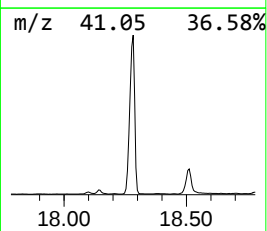
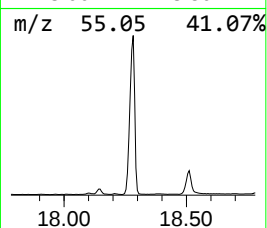
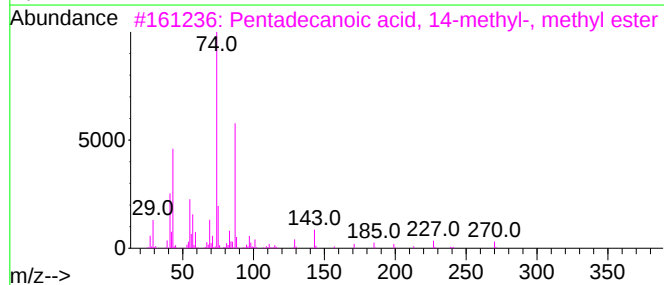
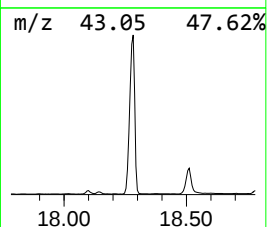
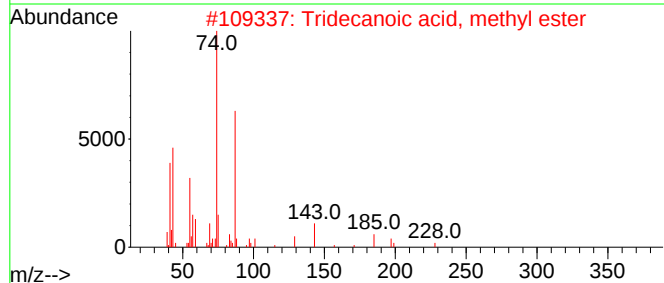
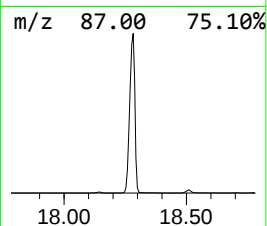
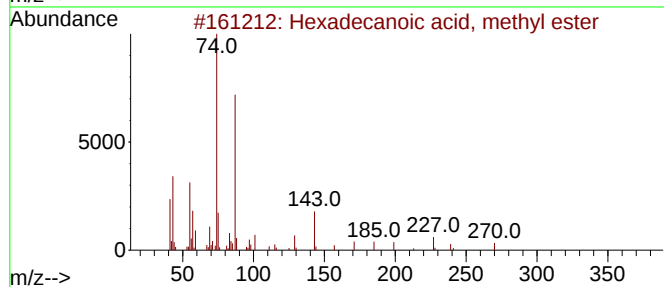
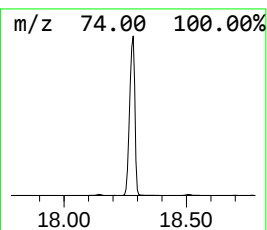
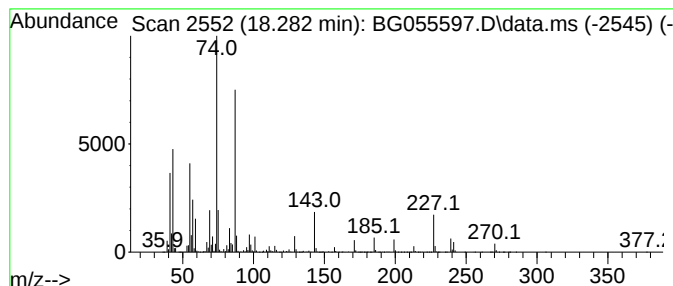
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.282	230.74 ng	11589000	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	81



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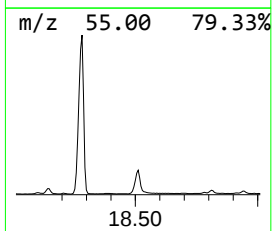
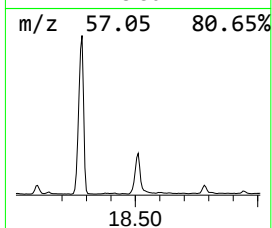
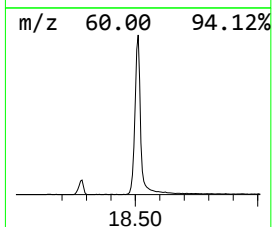
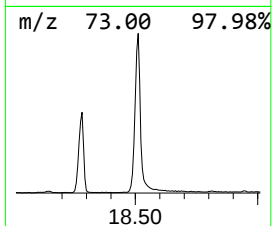
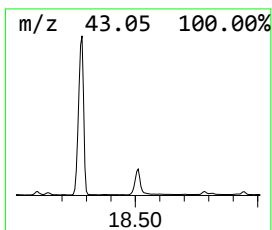
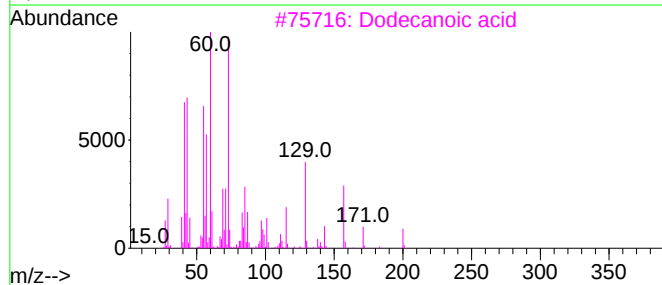
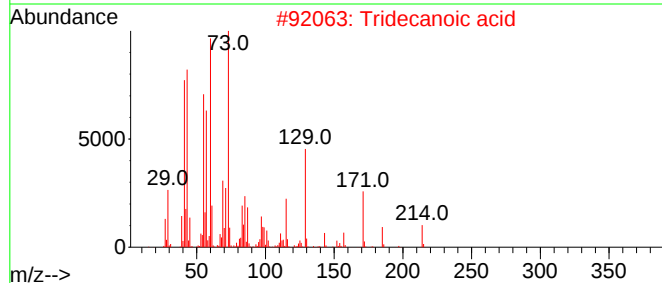
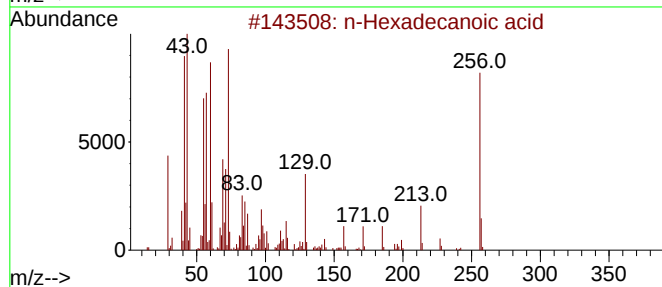
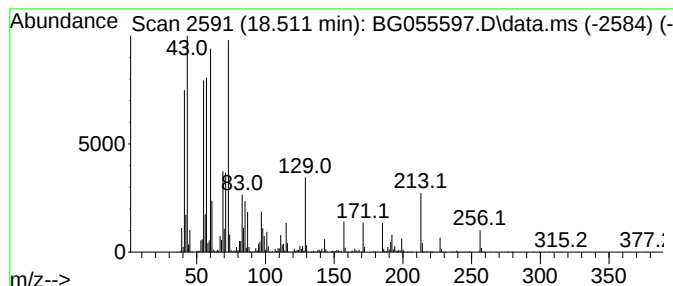
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	41.07 ng	2062770	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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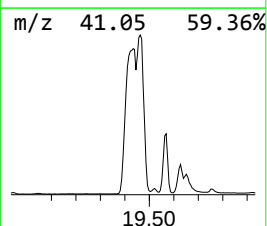
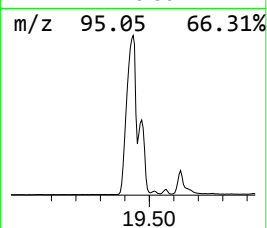
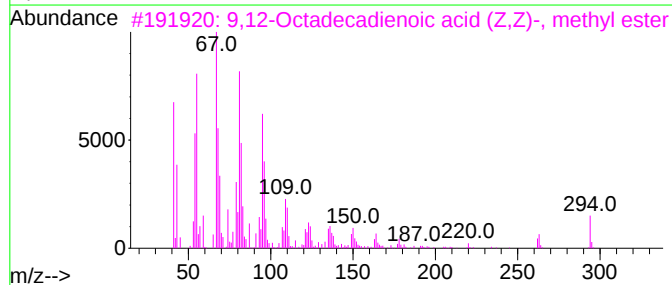
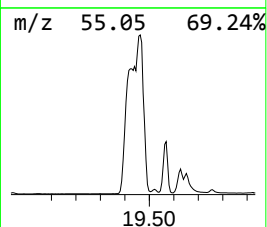
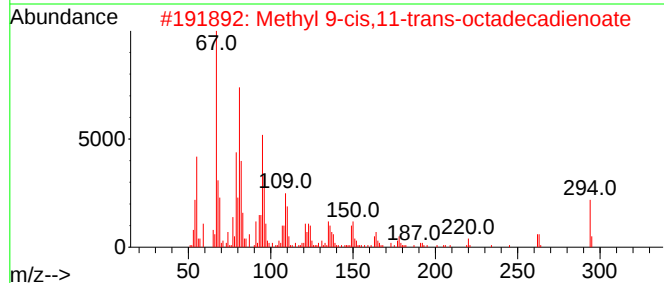
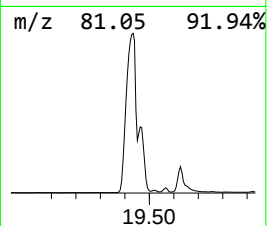
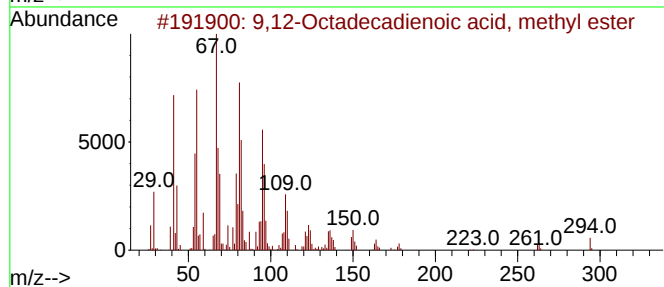
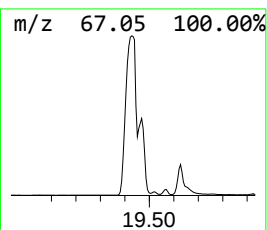
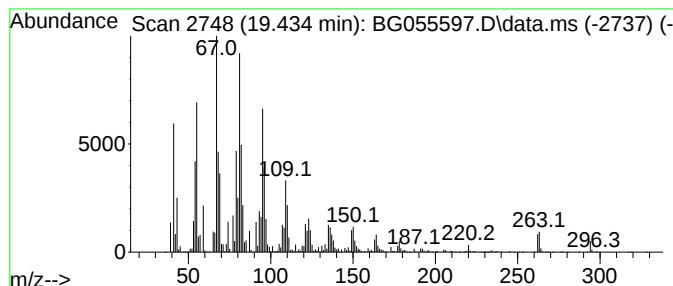
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.434	831.09 ng	41741700	Phenanthrene-d10	17.630	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	97



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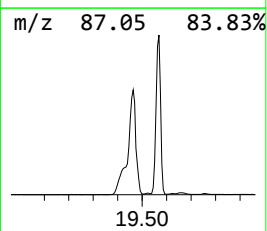
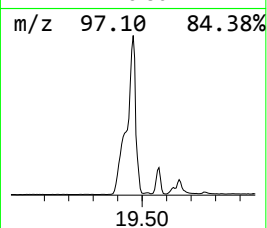
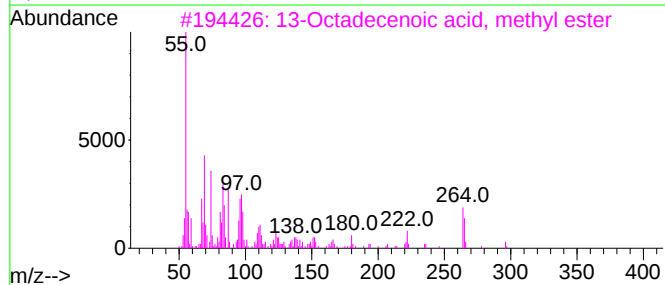
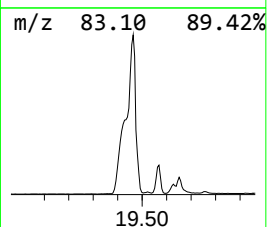
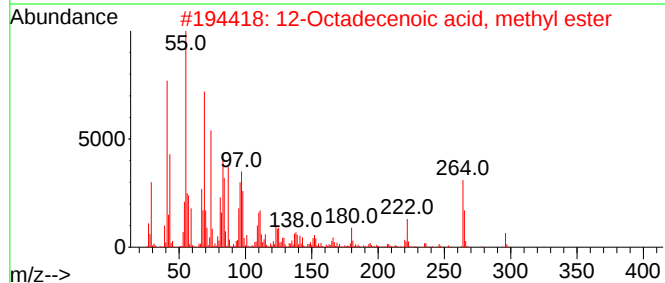
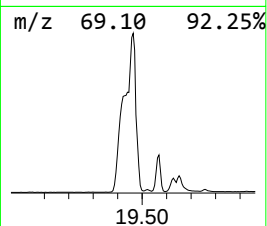
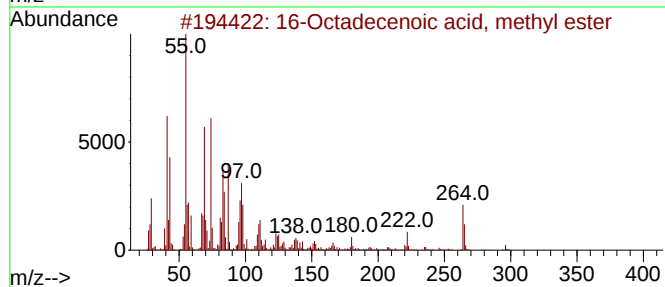
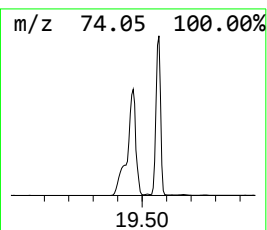
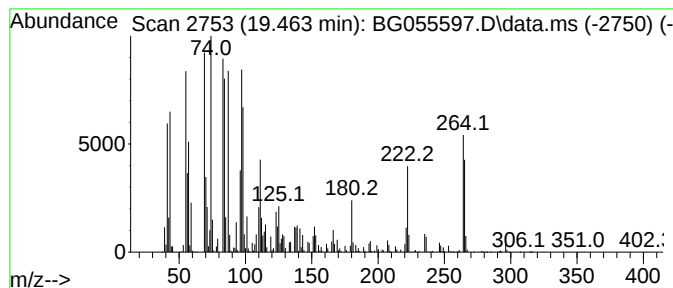
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 16-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.463	557.65 ng	28008500	Phenanthrene-d10	17.630	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	87
5	cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	87



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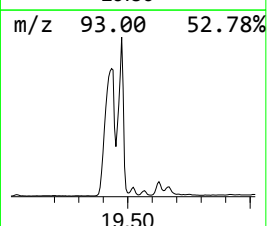
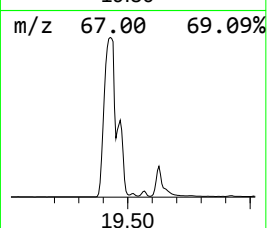
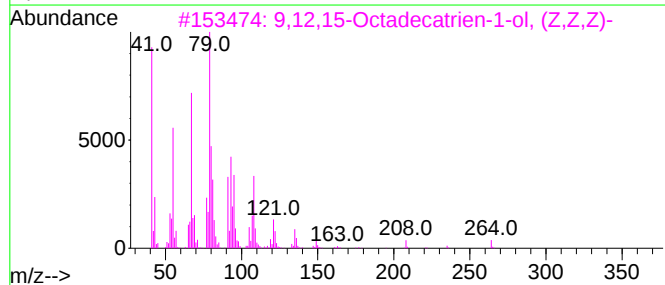
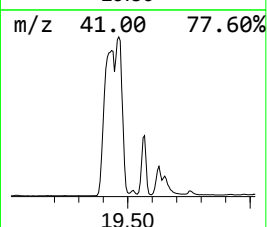
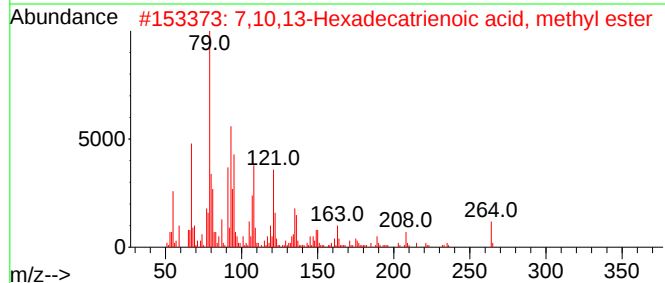
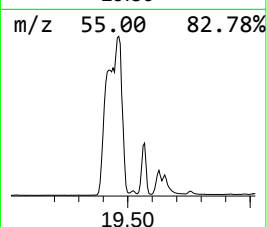
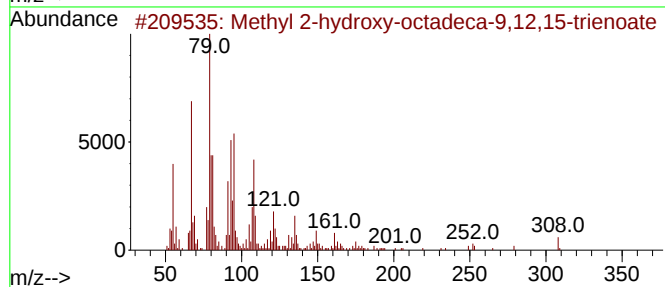
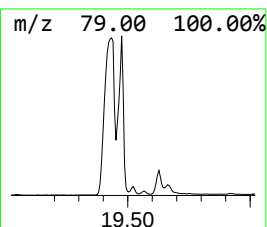
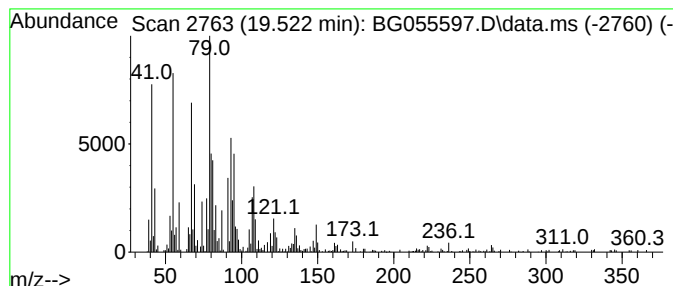
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Peak Number 5 Methyl 2-hydroxy-octadeca-9... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.522	10.68 ng	536480	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2-hydroxy-octadeca-9,12,1...	308	C19H32O3	1000336-39-1	97
2			7,10,13-Hexadecatrienoic acid, m...	264	C17H28O2	056554-30-4	95
3			9,12,15-Octadecatrien-1-ol, (Z,Z...	264	C18H32O	000506-44-5	94
4			1,8,11,14-Heptadecatetraene, (Z...	232	C17H28	010482-53-8	92
5			9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	91



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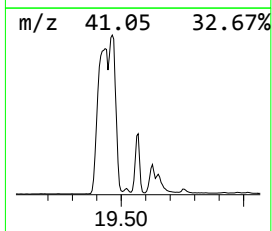
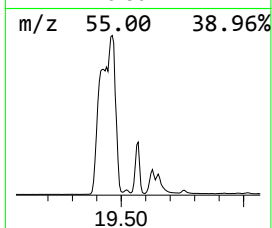
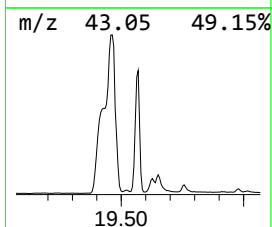
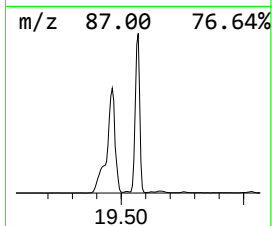
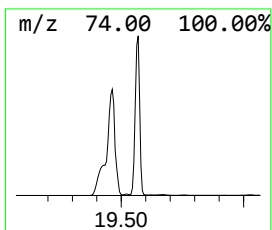
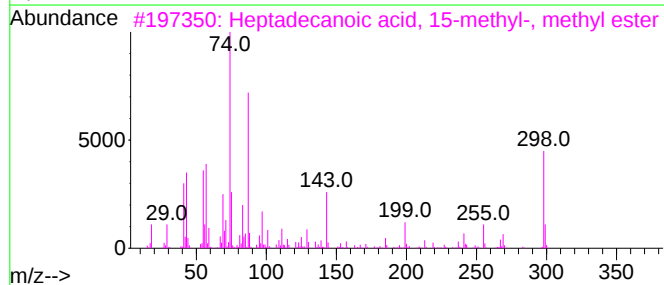
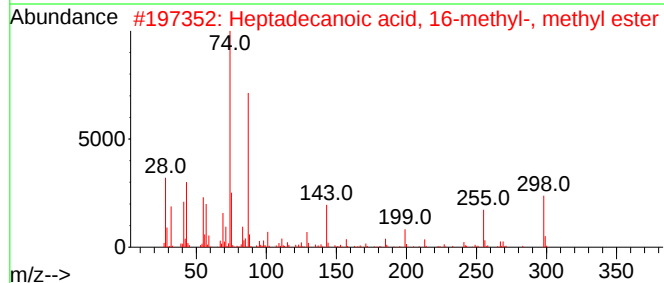
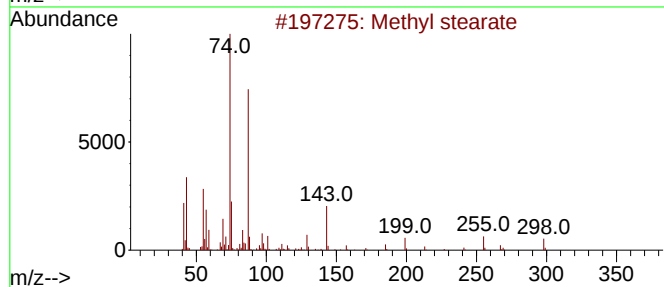
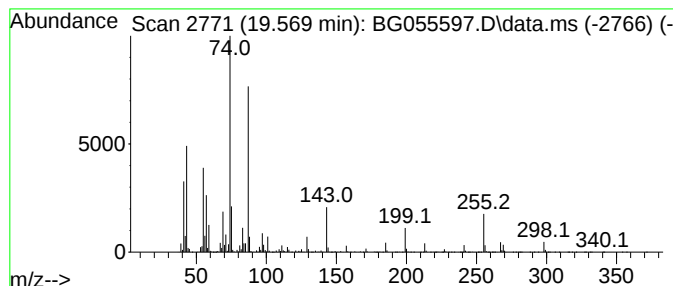
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
19.569	137.35 ng	6898460	Phenanthrene-d10	17.630

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	92
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055597.D
Acq On : 12 Nov 2022 20:08
Operator : CG/JU
Sample : N5583-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-111022

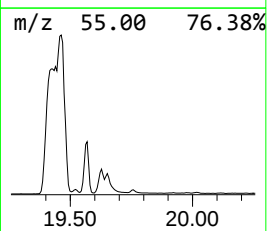
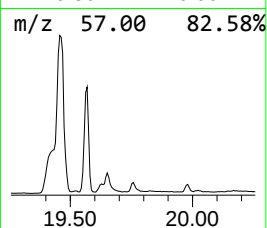
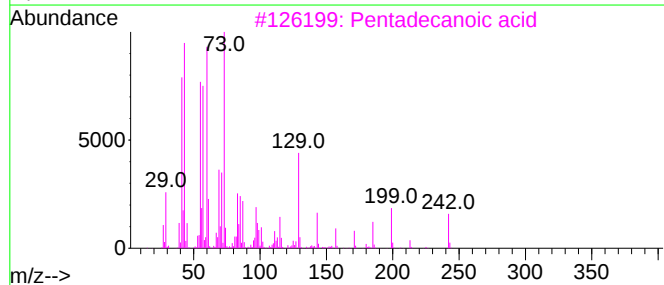
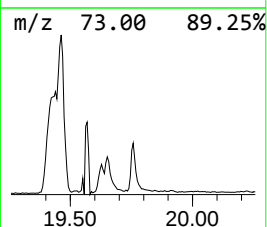
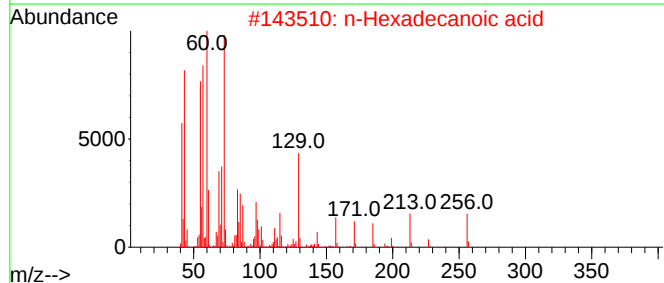
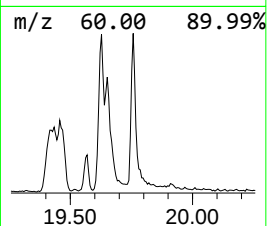
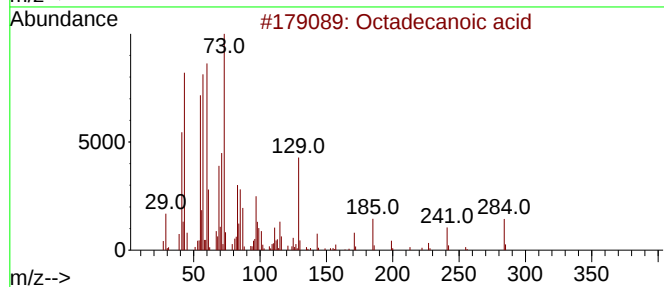
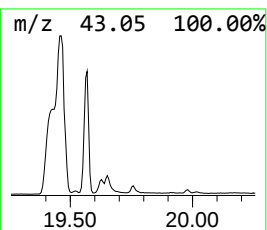
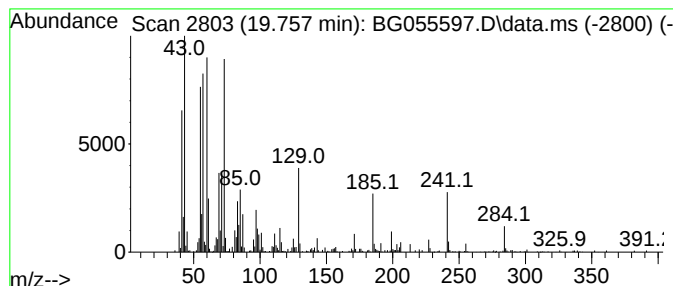
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.757	8.51 ng	427491	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055597.D
Acq On : 12 Nov 2022 20:08
Operator : CG/JU
Sample : N5583-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

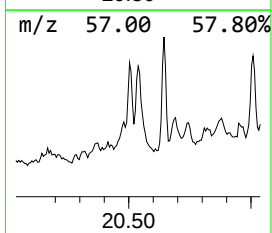
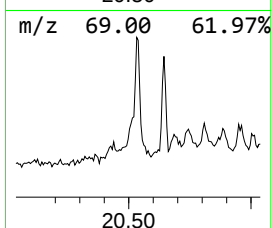
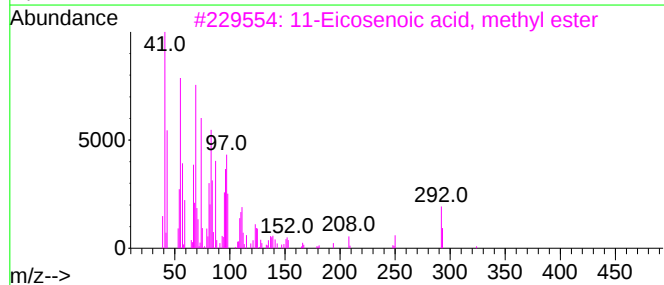
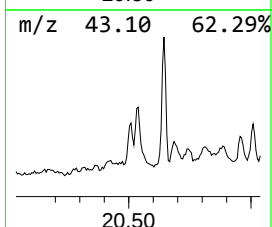
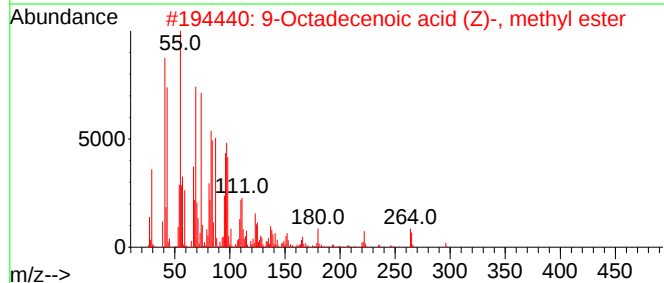
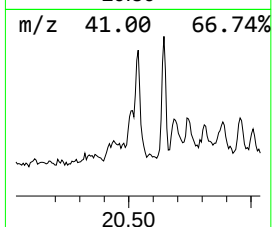
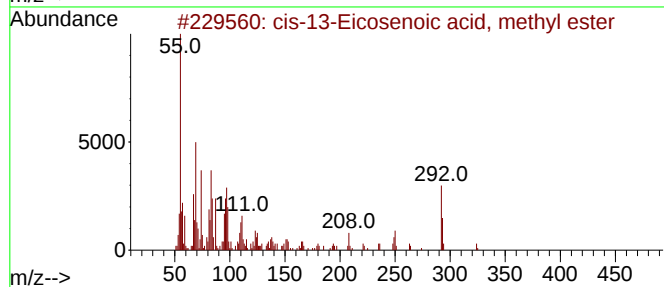
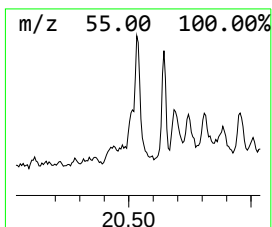
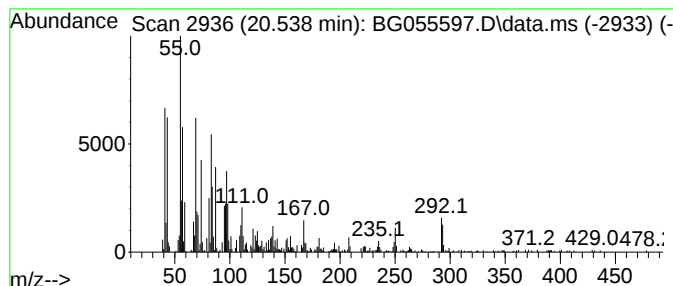
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BNA_G
ClientSampleId :
NB-08-111022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 cis-13-Eicosenoic acid, met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.538	9.82 ng	608039	Chrysene-d12	21.931	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	93
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	86
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	83
4	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	78
5	Oleic Acid	282	C18H34O2	000112-80-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055597.D
Acq On : 12 Nov 2022 20:08
Operator : CG/JU
Sample : N5583-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-111022

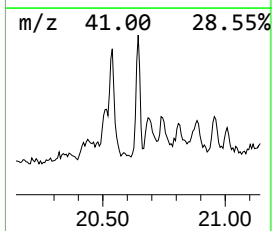
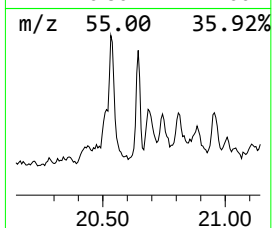
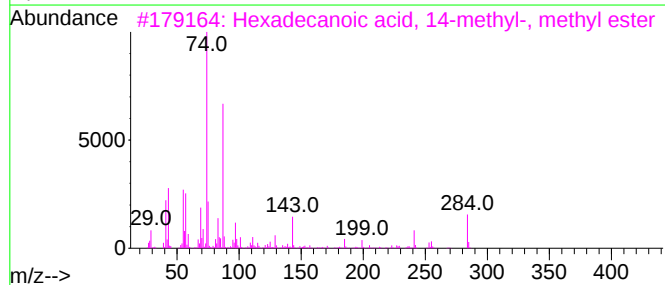
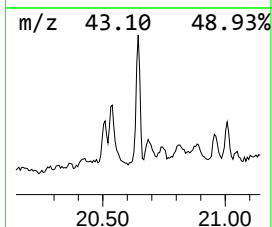
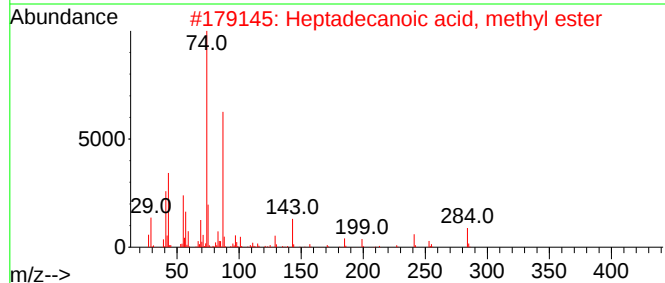
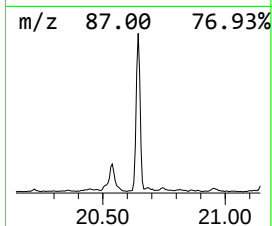
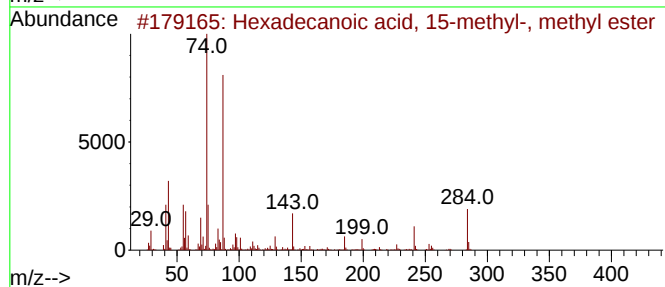
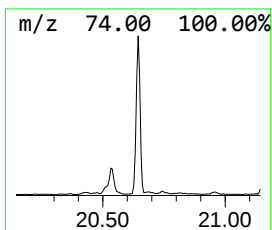
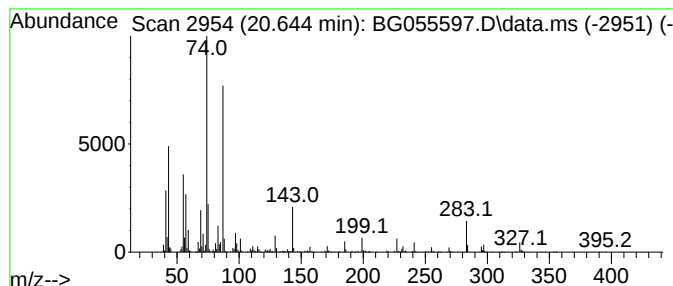
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, 15-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.644	8.01 ng	496186	Chrysene-d12	21.931

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	97
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
3			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	90
4			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
5			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055597.D
Acq On : 12 Nov 2022 20:08
Operator : CG/JU
Sample : N5583-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-08-111022

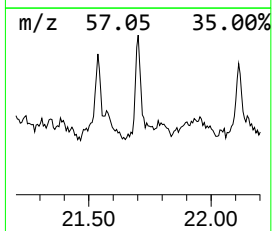
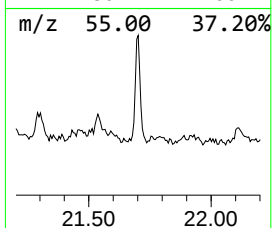
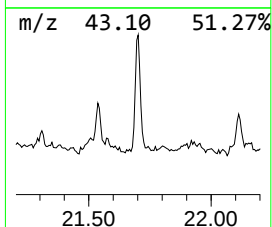
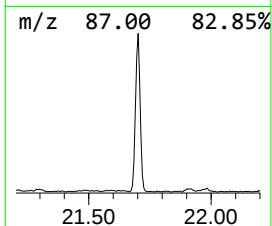
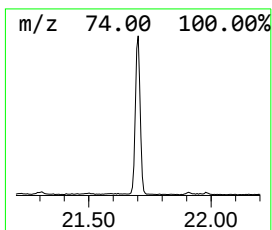
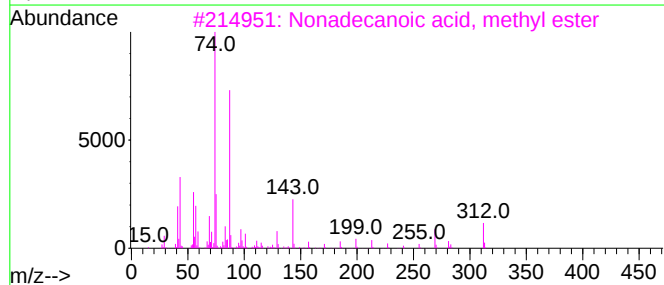
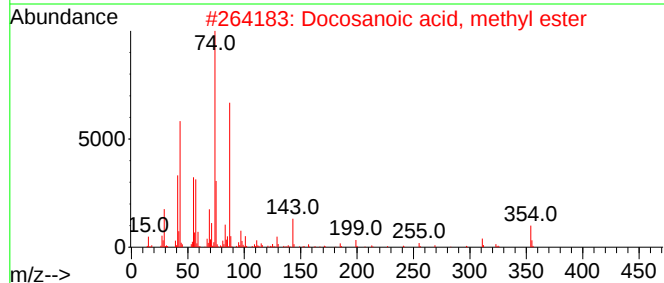
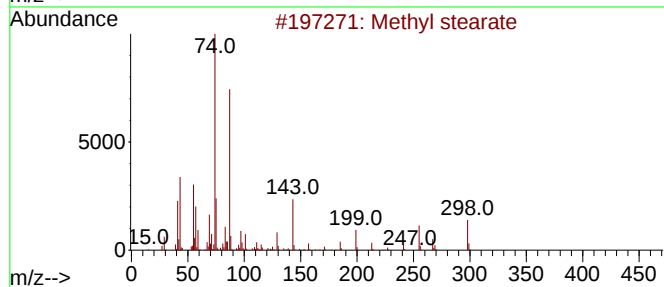
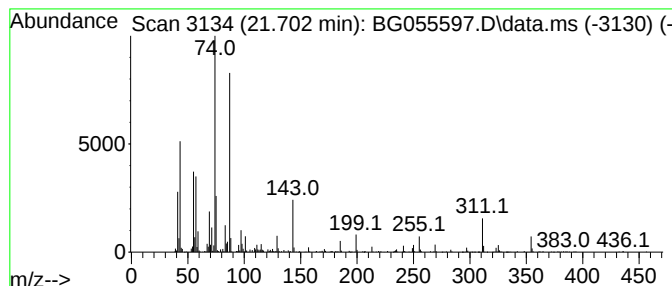
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.702	9.98 ng	617820	Chrysene-d12	21.931

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	97
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
4			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90
5			Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055597.D
Acq On : 12 Nov 2022 20:08
Operator : CG/JU
Sample : N5583-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-111022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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n-Hexadecanoic ...	18.511	41.1	ng	2062770	4	17.630	1004510	20.0
9,12-Octadecadi...	19.434	831.1	ng	41741700	4	17.630	1004510	20.0
16-Octadecenoic...	19.463	557.6	ng	28008500	4	17.630	1004510	20.0
Methyl 2-hydrox...	19.522	10.7	ng	536480	4	17.630	1004510	20.0
Methyl stearate	19.569	137.3	ng	6898460	4	17.630	1004510	20.0
Octadecanoic acid	19.757	8.5	ng	427491	4	17.630	1004510	20.0
cis-13-Eicoseno...	20.538	9.8	ng	608039	5	21.931	1238520	20.0
Hexadecanoic ac...	20.644	8.0	ng	496186	5	21.931	1238520	20.0
Docosanoic acid...	21.702	10.0	ng	617820	5	21.931	1238520	20.0