

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
 Data File : BG053298.D
 Acq On : 23 Apr 2022 18:17
 Operator : CG/JU
 Sample : N2525-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HR-02-042122

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.679	382	390	404	rBV	491527	839207	23.23%	4.542%
2	7.271	652	661	676	rBV	529913	962608	26.64%	5.210%
3	8.111	797	804	810	rBV	135459	235842	6.53%	1.276%
4	9.268	991	1001	1009	rBV	333382	627351	17.36%	3.395%
5	10.925	1271	1283	1291	rBV	184902	354532	9.81%	1.919%
6	13.357	1689	1697	1704	rBV	895130	1392451	38.54%	7.537%
7	14.731	1922	1931	1938	rBV	286224	476858	13.20%	2.581%
8	16.223	2177	2185	2193	rBV	616267	1001517	27.72%	5.421%
9	17.480	2392	2399	2403	rBV	326329	524208	14.51%	2.837%
10	17.522	2403	2406	2410	rVB	66535	92517	2.56%	0.501%
11	18.133	2504	2510	2515	rBV	728689	915094	25.33%	4.953%
12	18.362	2544	2549	2554	rBV3	152991	255272	7.07%	1.382%
13	18.544	2575	2580	2585	rBV6	23720	49827	1.38%	0.270%
14	19.266	2697	2703	2706	rBV	2741769	3612891	100.00%	19.554%
15	19.296	2706	2708	2720	rVB2	1894225	2460634	68.11%	13.318%
16	19.425	2726	2730	2735	rBV	503221	598362	16.56%	3.239%
17	19.484	2736	2740	2743	rBV	148335	220594	6.11%	1.194%
18	19.525	2743	2747	2757	rVB	164716	335830	9.30%	1.818%
19	19.672	2769	2772	2777	rVB7	48204	61587	1.70%	0.333%
20	19.889	2805	2809	2817	rVB	121449	190388	5.27%	1.030%
21	20.083	2836	2842	2847	rVB	1253031	1634535	45.24%	8.847%
22	20.377	2889	2892	2895	rBV2	59391	65938	1.83%	0.357%
23	20.412	2895	2898	2904	rVB4	50583	73371	2.03%	0.397%
24	20.518	2912	2916	2919	rBV2	56325	77457	2.14%	0.419%
25	20.676	2940	2943	2948	rVB2	89975	106301	2.94%	0.575%
26	20.876	2974	2977	2981	rVB	51086	54221	1.50%	0.293%
27	21.387	3060	3064	3070	rBV	127295	200500	5.55%	1.085%
28	21.546	3088	3091	3095	rVB2	50596	63894	1.77%	0.346%
29	21.763	3122	3128	3133	rBV2	284151	477912	13.23%	2.587%
30	25.064	3682	3690	3699	rVB2	184527	514354	14.24%	2.784%

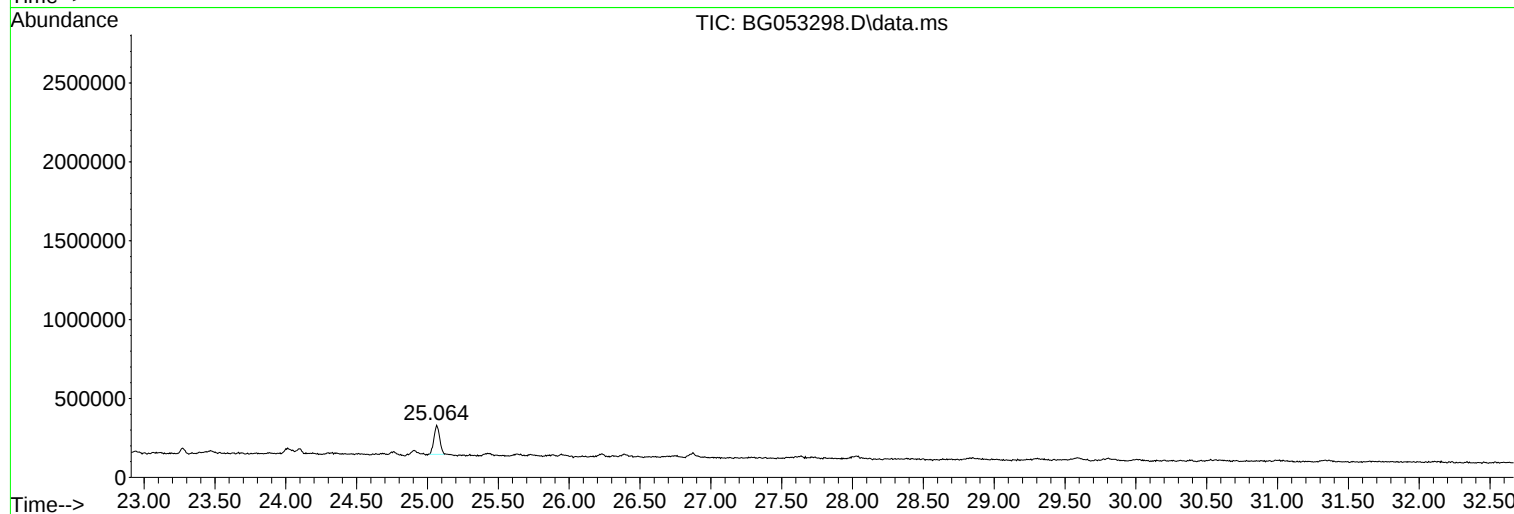
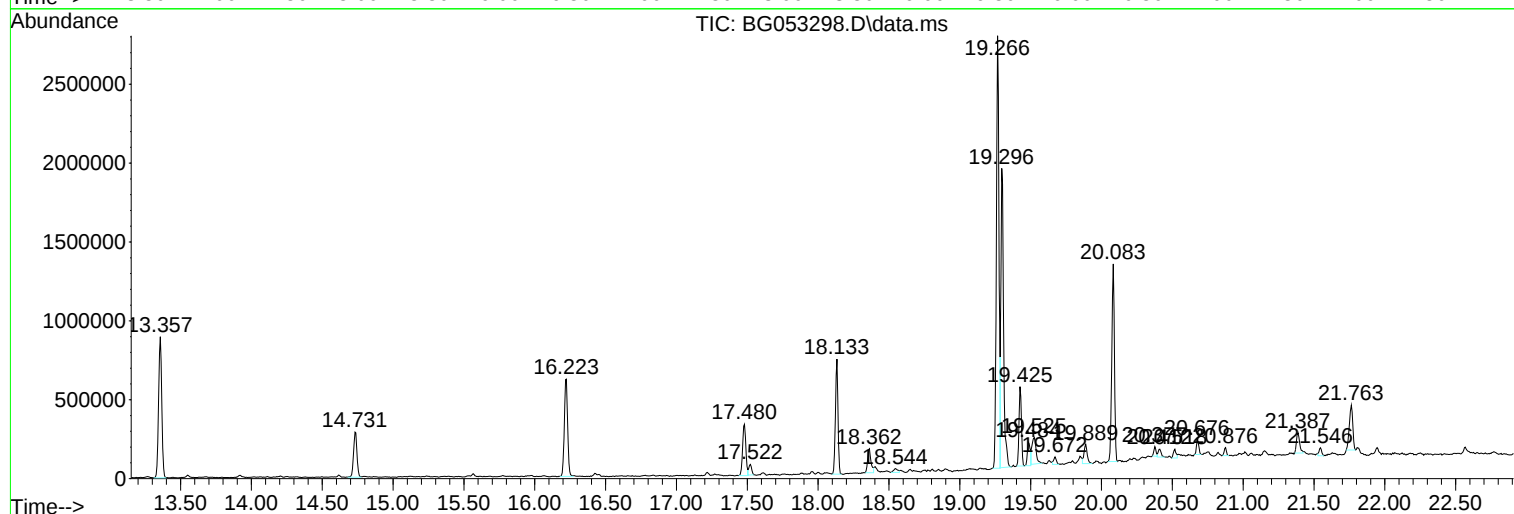
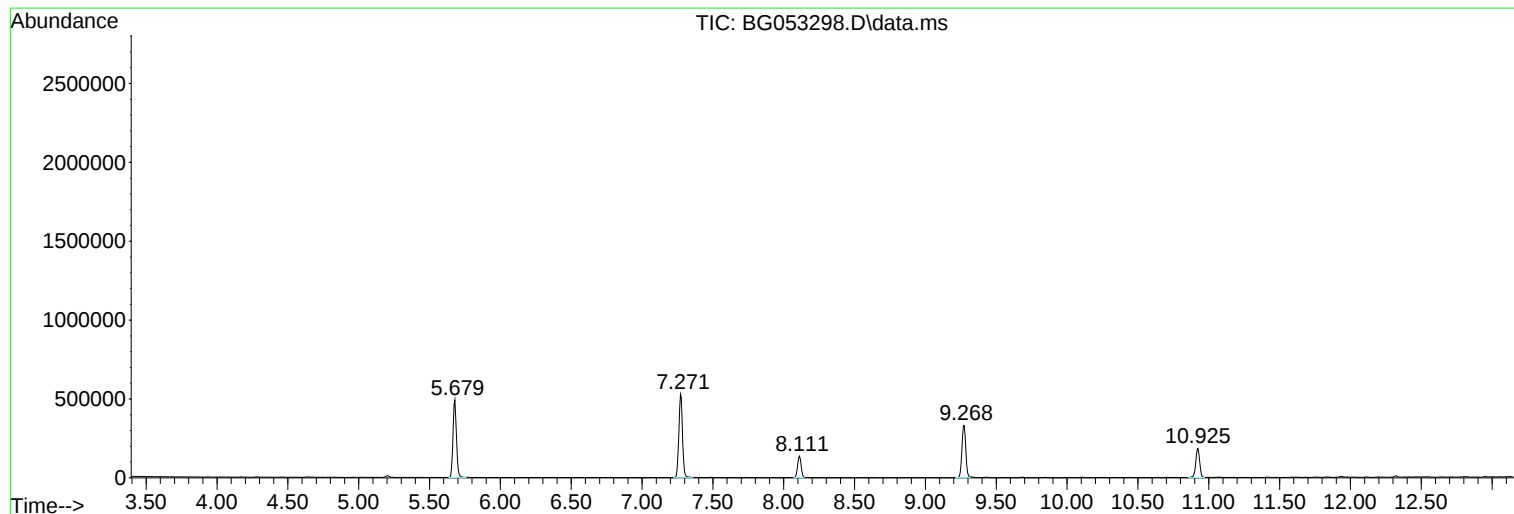
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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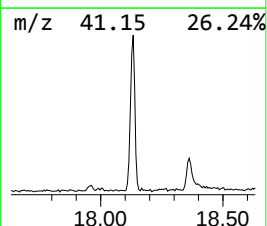
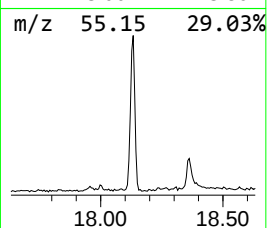
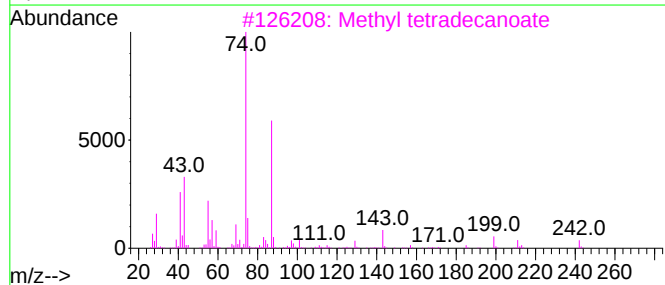
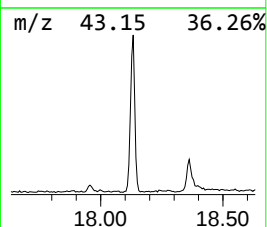
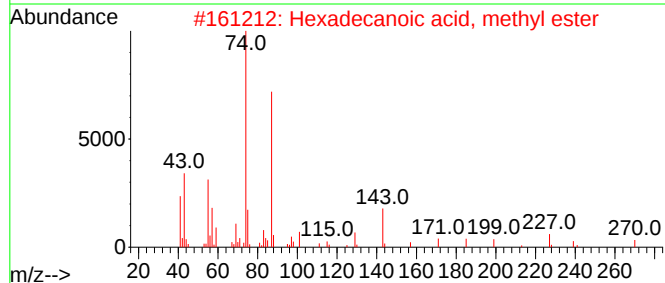
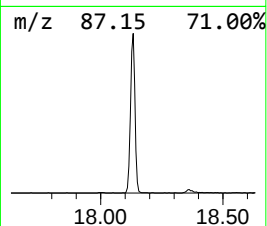
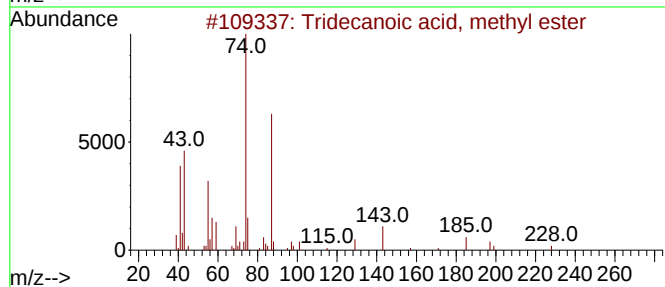
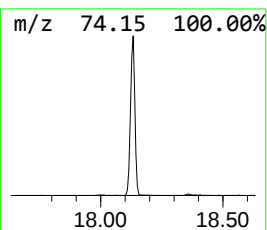
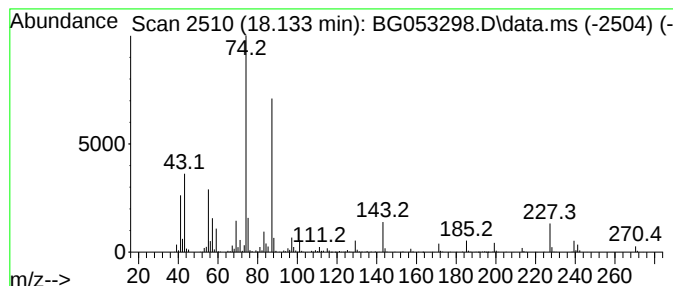
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tridecanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.133	34.91 ng	915094	Phenanthrene-d10	17.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	98
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



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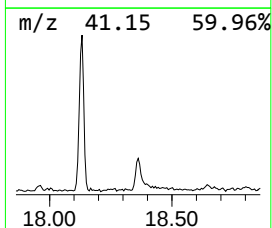
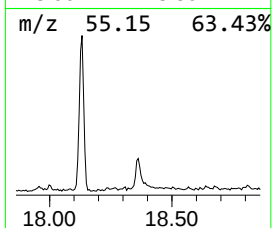
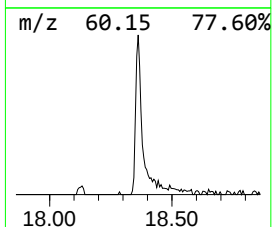
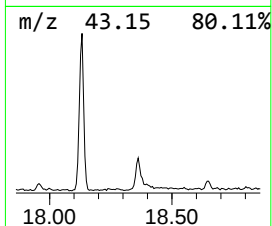
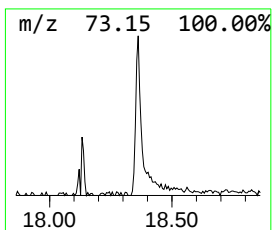
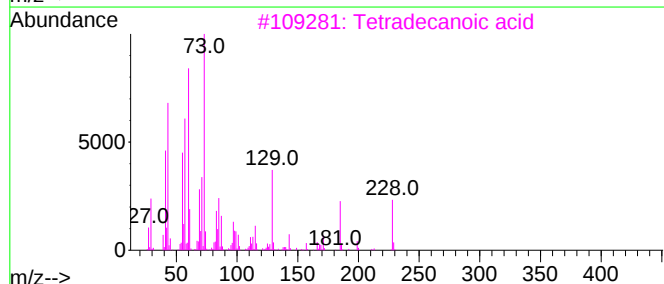
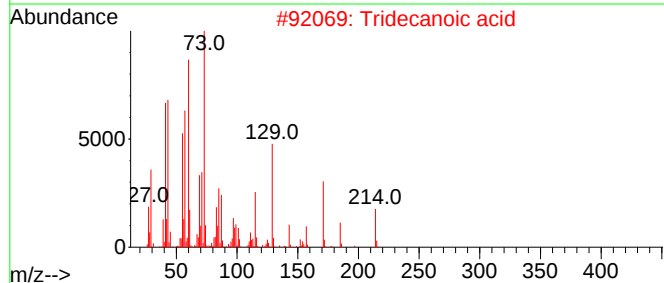
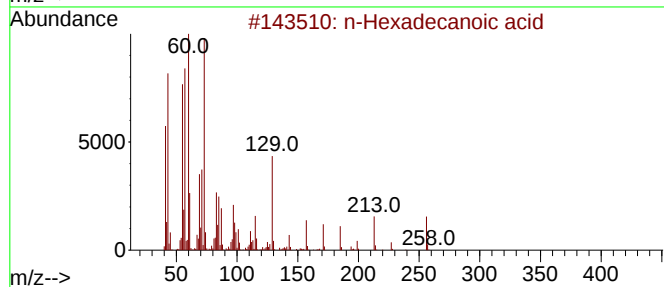
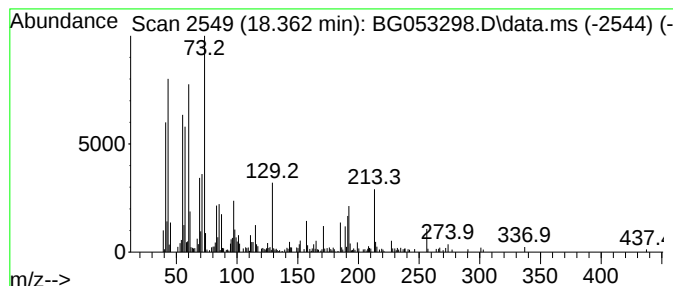
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	9.74 ng	255272	Phenanthrene-d10	17.480

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	46



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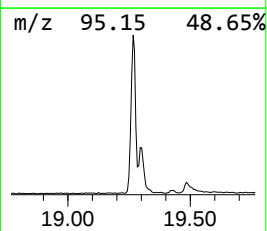
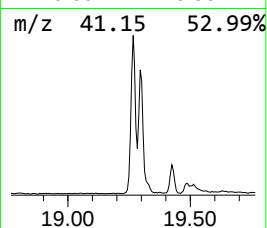
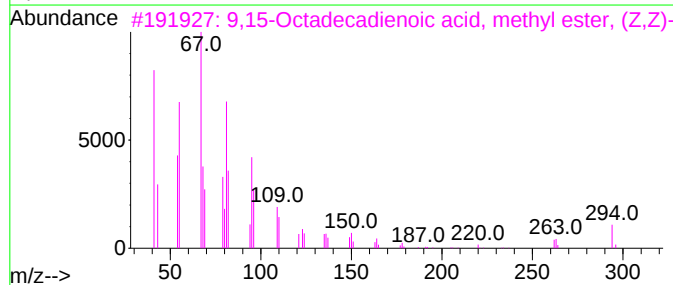
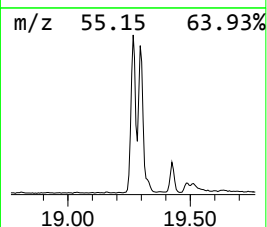
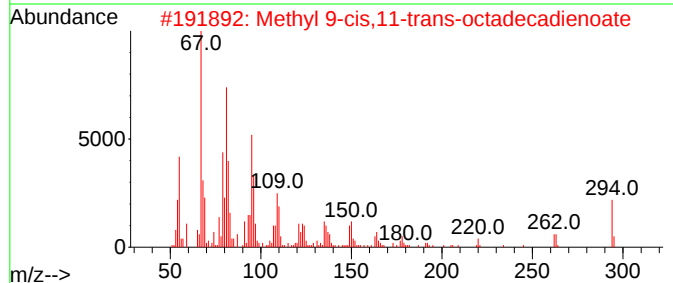
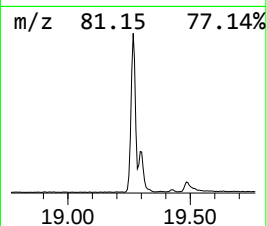
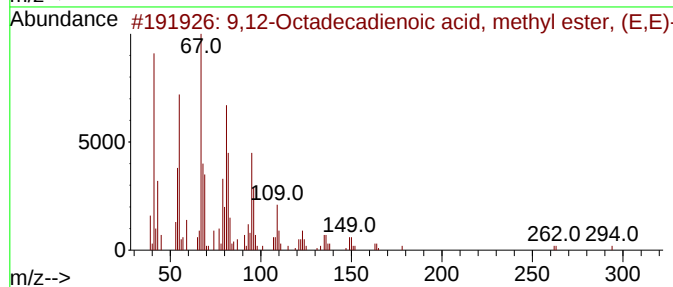
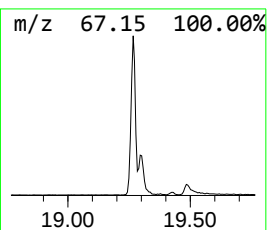
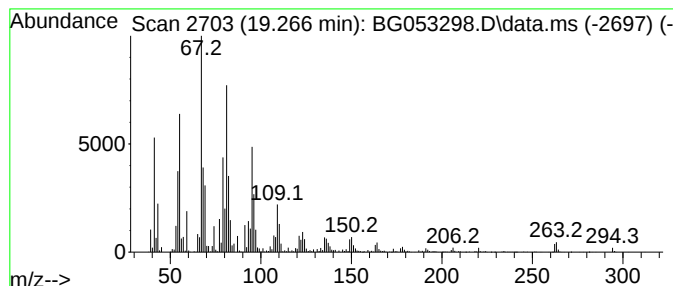
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.266	137.84 ng	3612890	Phenanthrene-d10	17.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93



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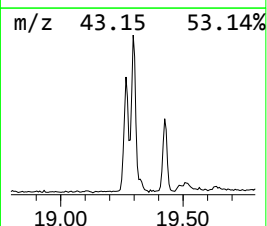
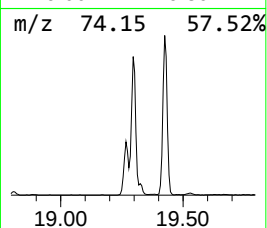
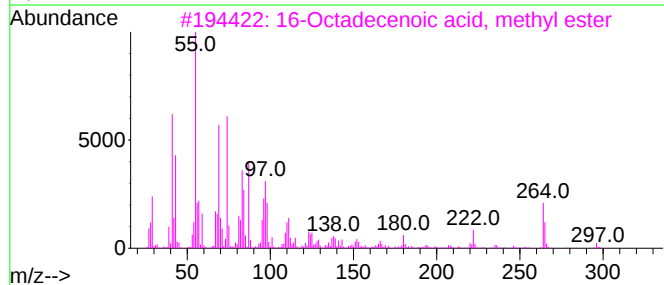
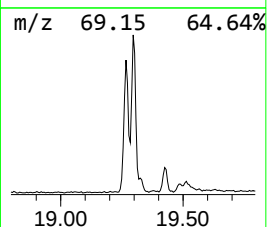
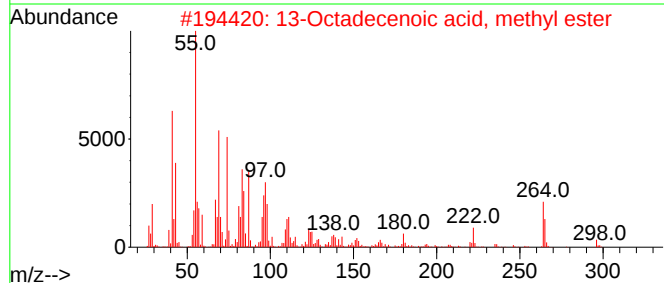
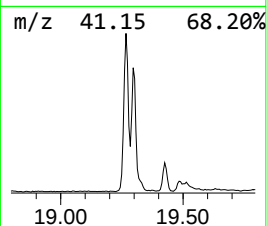
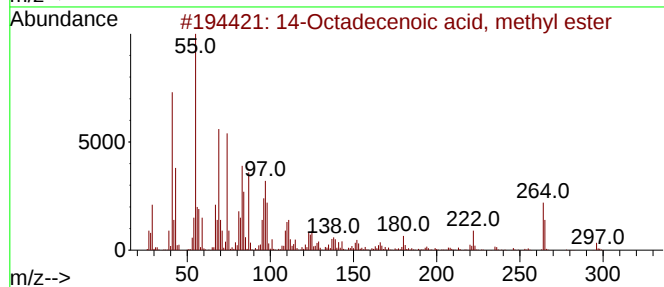
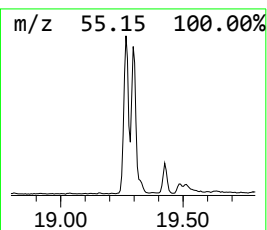
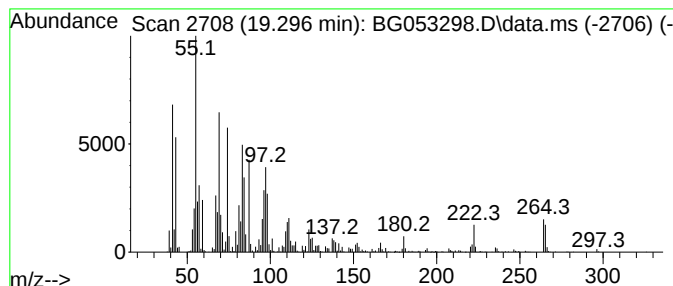
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Peak Number 4 14-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.296	93.88 ng	2460630	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98



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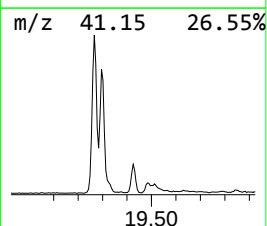
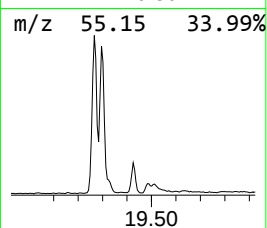
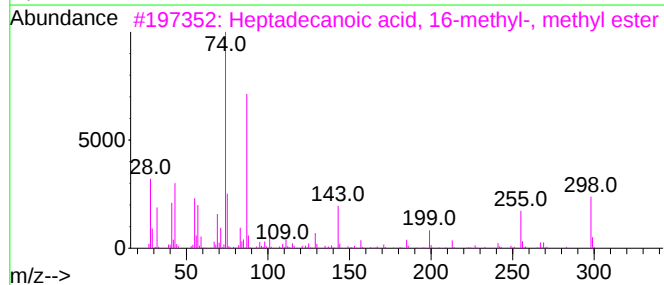
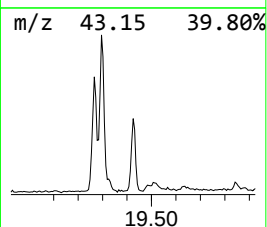
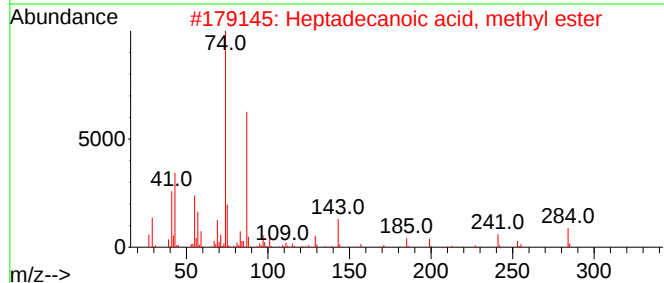
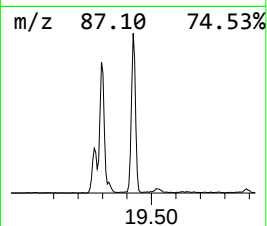
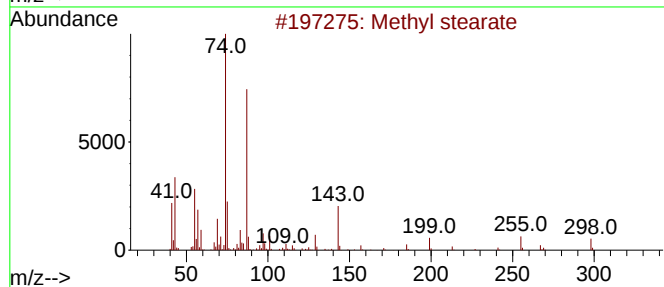
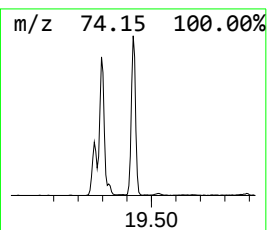
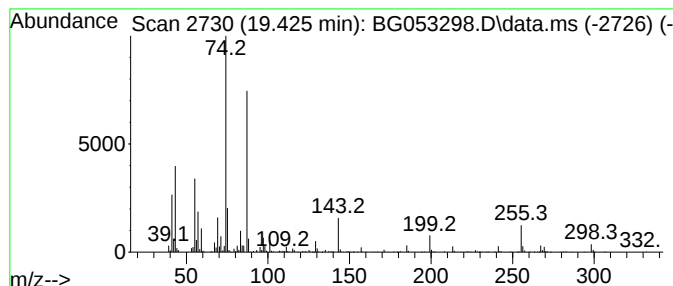
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Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.425	22.83 ng	598362	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87



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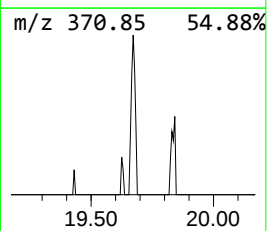
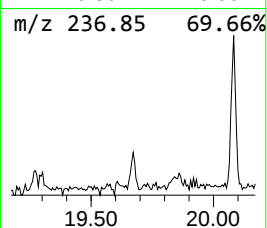
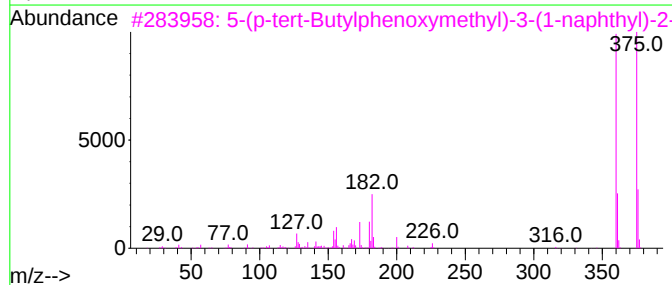
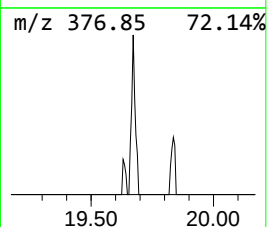
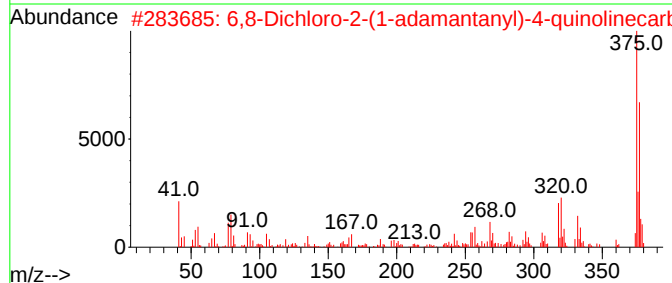
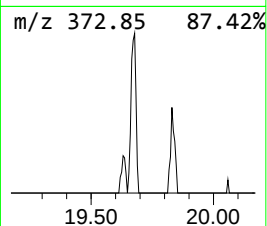
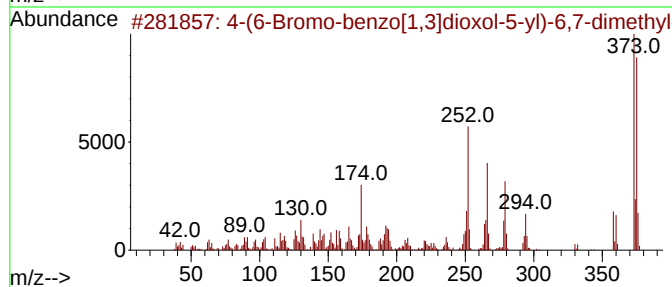
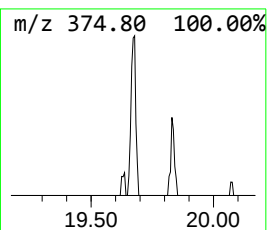
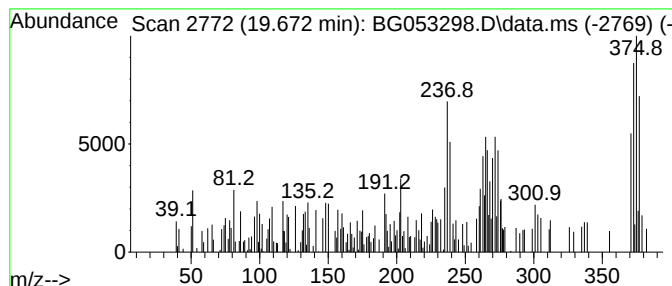
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ClientSampleId :
HR-02-042122

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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 unknown19.672 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.672	2.58 ng	61587	Chrysene-d12	21.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(6-Bromo-benzo[1,3]dioxol-5-yl)...	373	C18H16BrNO3	1000296-27-0	23
2	6,8-Dichloro-2-(1-adamantanyl)-4...	375	C20H19Cl2NO2	049647-91-8	18
3	5-(p-tert-Butylphenoxy)methyl)-3-...	375	C24H25NO3	005256-24-6	15
4	Benzoic acid, 2-(2'-bromophenyla...	369	C13H9Br2NO2	209460-12-8	14
5	Nicotinamide, N-(4-fluorophenyl)...	375	C19H13F4N3O	1000302-13-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-042122

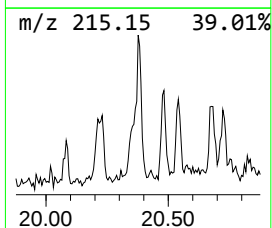
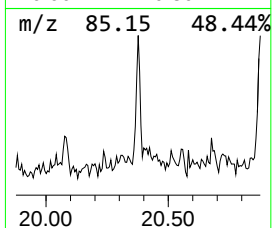
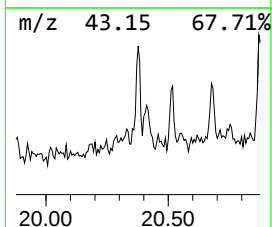
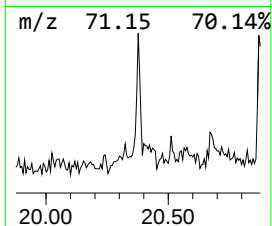
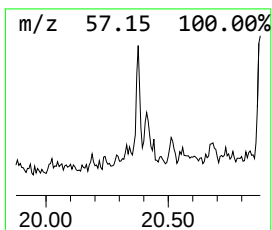
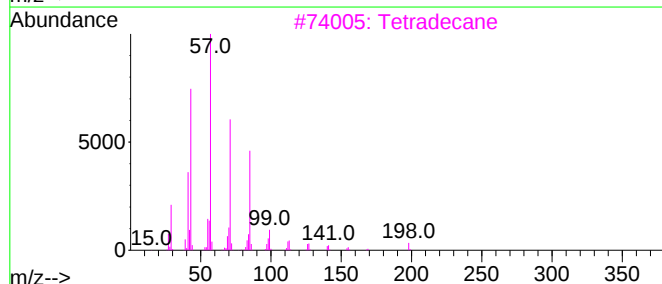
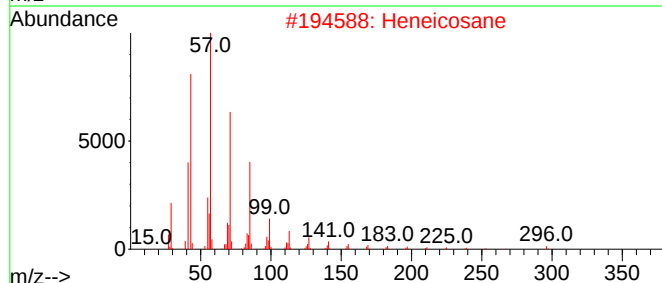
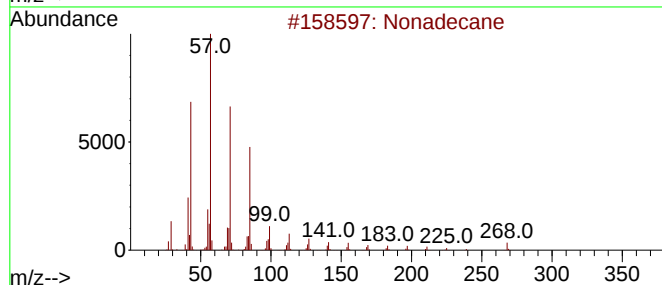
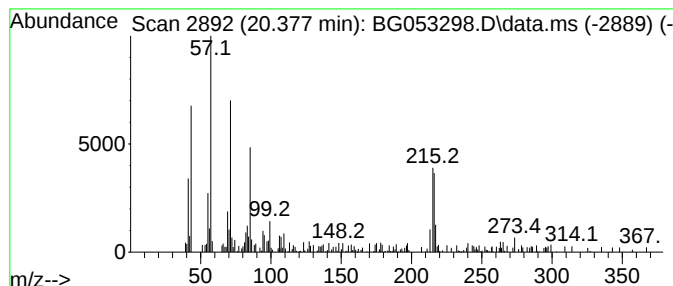
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.377	2.76 ng	65938	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	60
2			Heneicosane	296	C21H44	000629-94-7	60
3			Tetradecane	198	C14H30	000629-59-4	46
4			Hexacosane	366	C26H54	000630-01-3	38
5			Docosane	310	C22H46	000629-97-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-02-042122

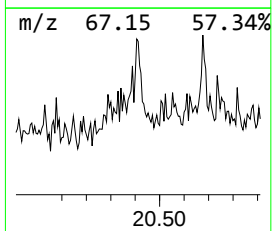
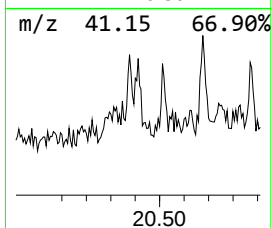
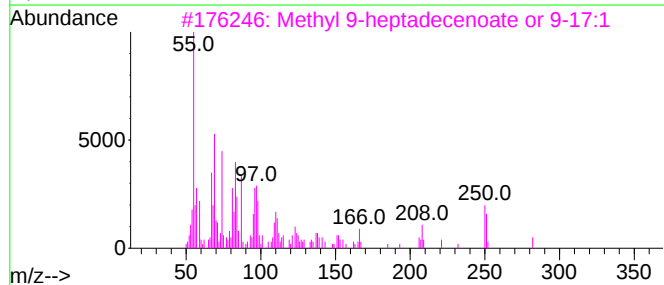
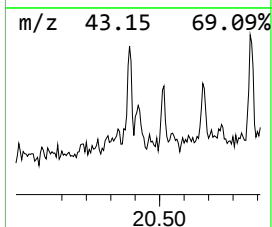
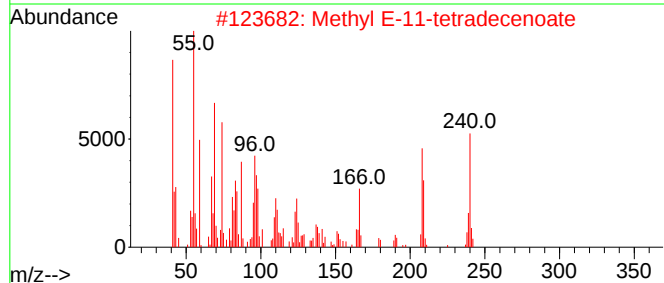
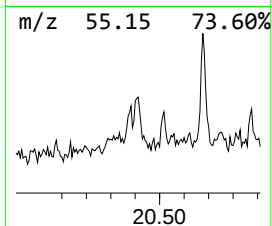
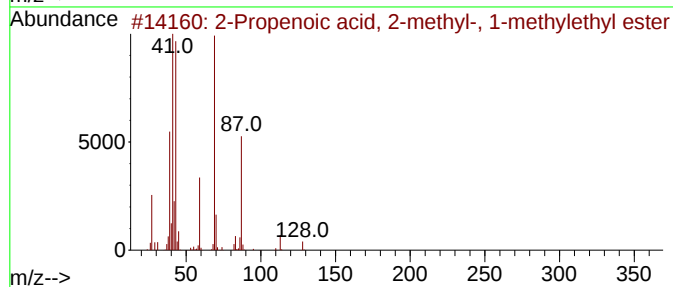
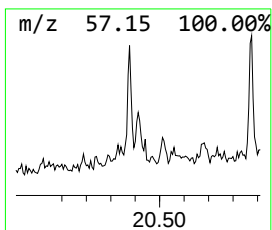
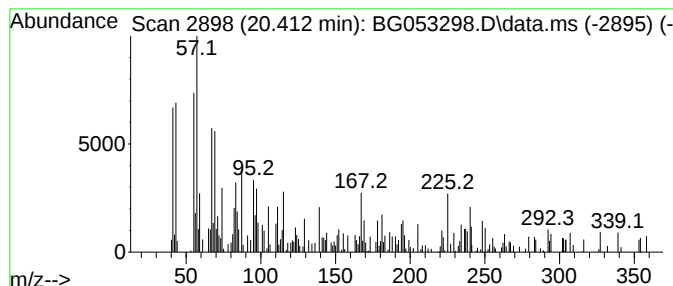
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.412 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.412	3.07 ng	73371	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	15
2			Methyl E-11-tetradecenoate	240	C15H28O2	1000130-82-9	11
3			Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	11
4			Cyclopropanenonanoic acid, methy...	212	C13H24O2	010152-60-0	11
5			2-Hexanol, acetate	144	C8H16O2	005953-49-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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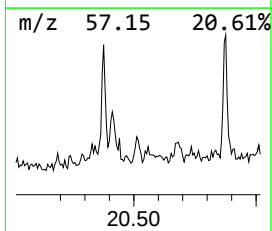
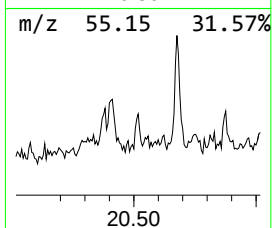
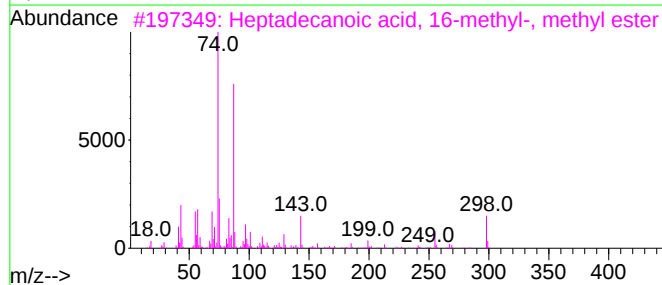
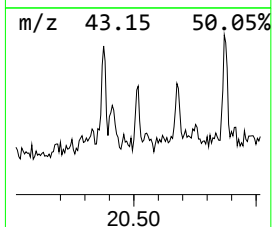
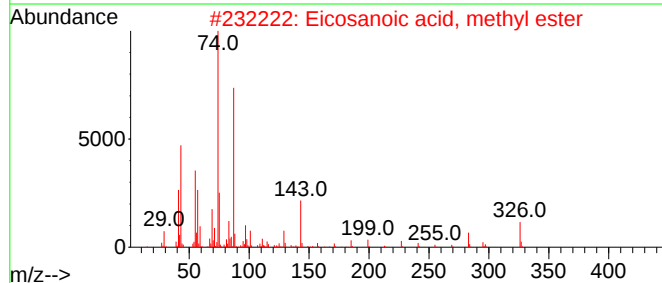
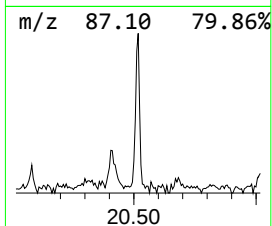
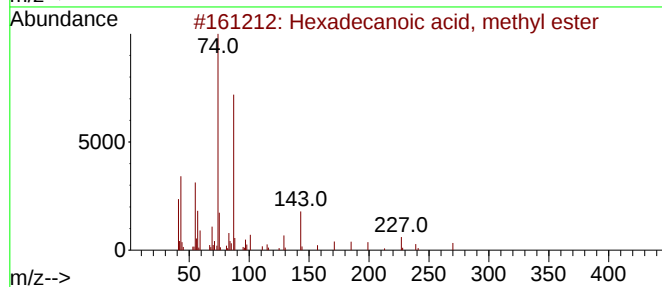
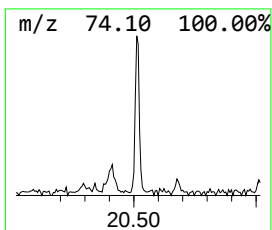
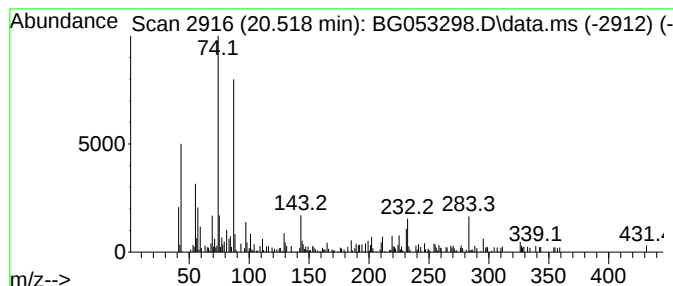
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.518	3.24 ng	77457	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	76
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
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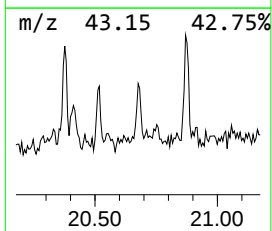
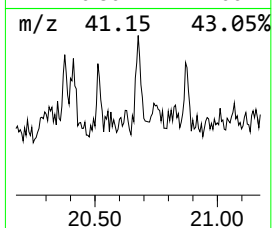
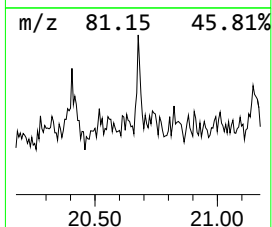
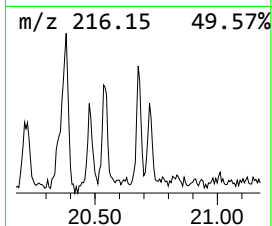
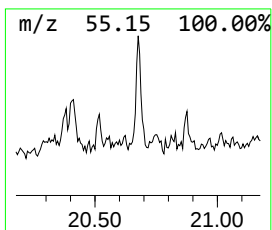
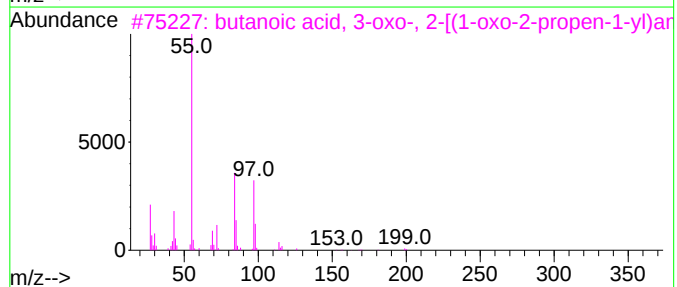
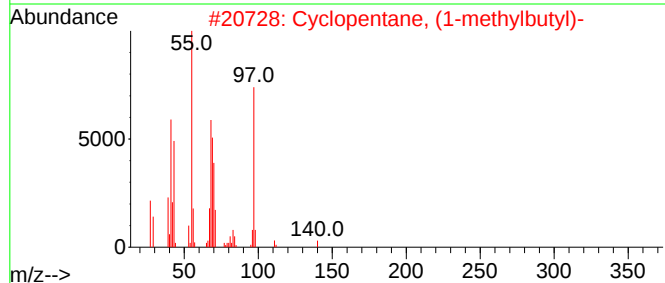
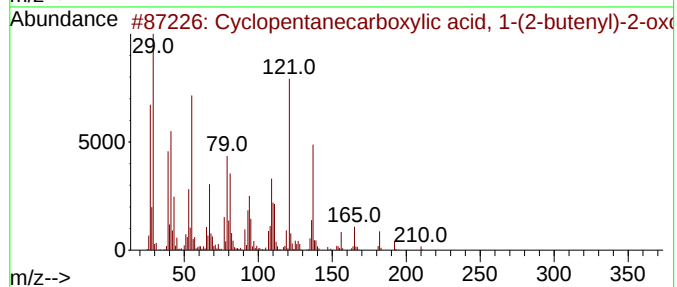
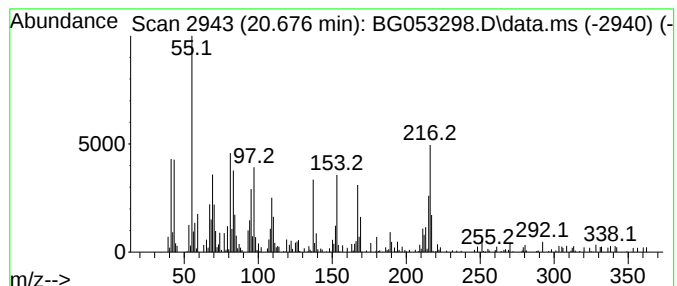
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.676 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.676	4.45 ng	106301	Chrysene-d12	21.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentanecarboxylic acid, 1-(...	210	C12H18O3	112825-89-5	11
2		Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	10
3		butanoic acid, 3-oxo-, 2-[(1-oxo...	199	C9H13NO4	1000400-37-9	10
4		(4-Bromobutan-2-yl)cyclopropane	176	C7H13Br	1000444-18-1	10
5		Cyclopropane, 1-bromo-2,2-diethyl-	176	C7H13Br	343926-55-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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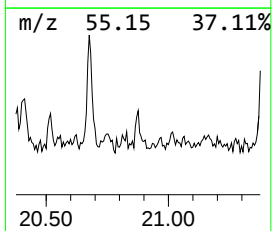
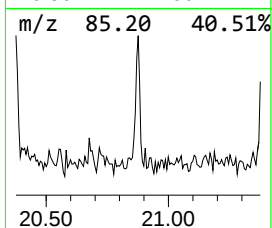
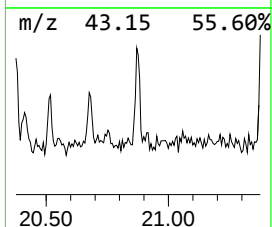
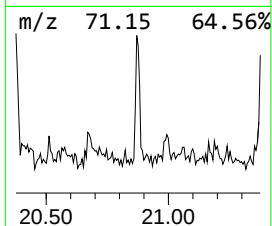
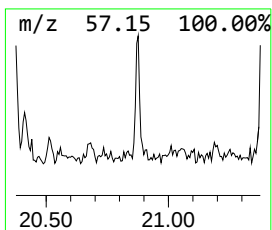
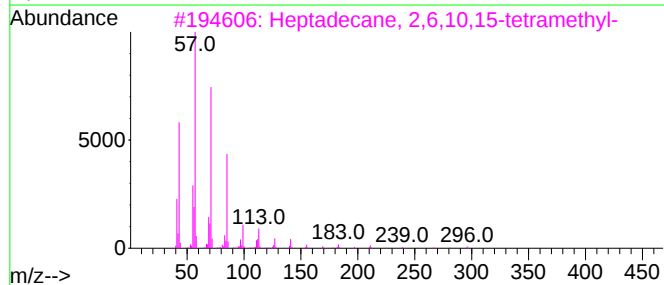
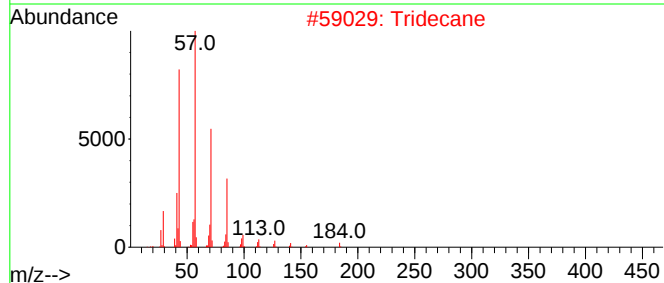
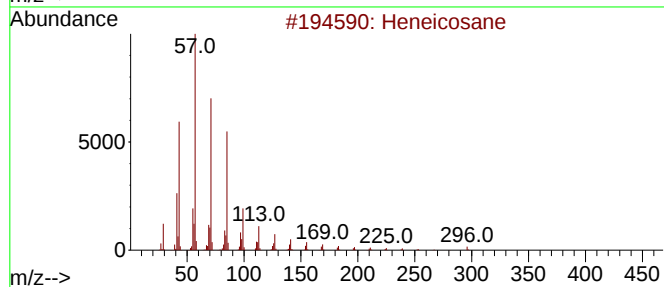
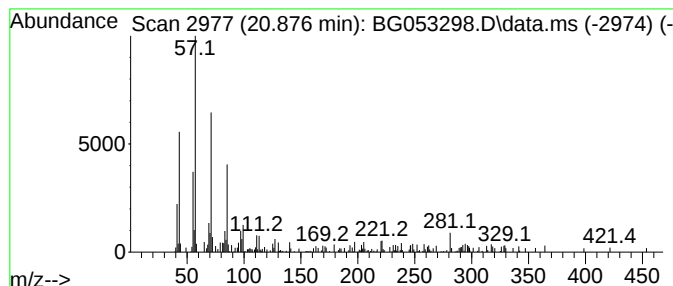
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.876	2.27 ng	54221	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	86
2			Tridecane	184	C13H28	000629-50-5	70
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	70
4			Octadecane	254	C18H38	000593-45-3	70
5			Eicosane	282	C20H42	000112-95-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

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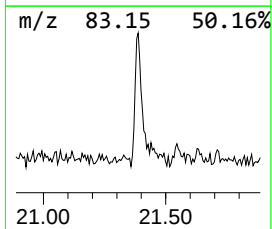
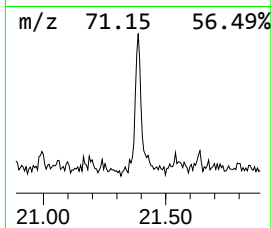
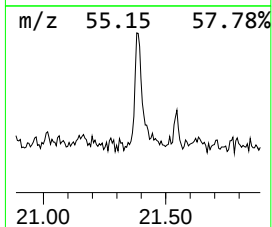
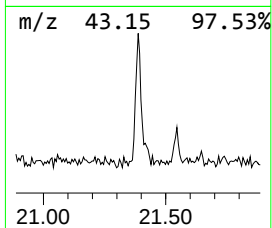
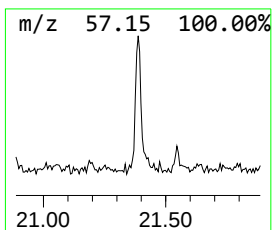
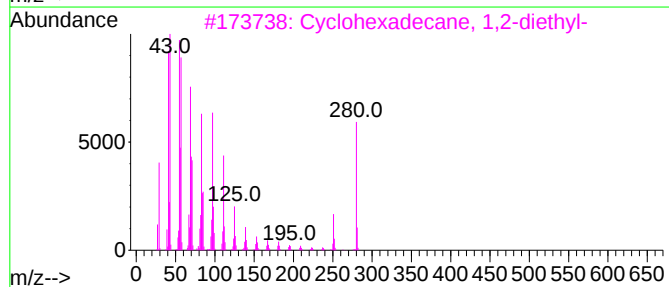
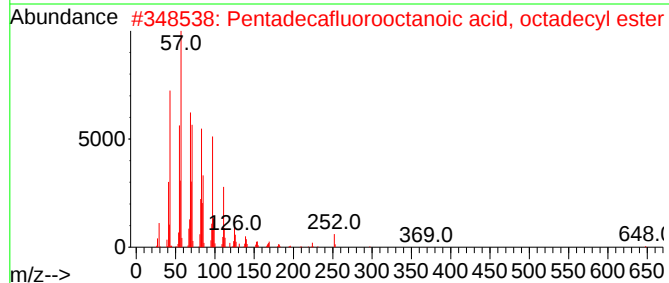
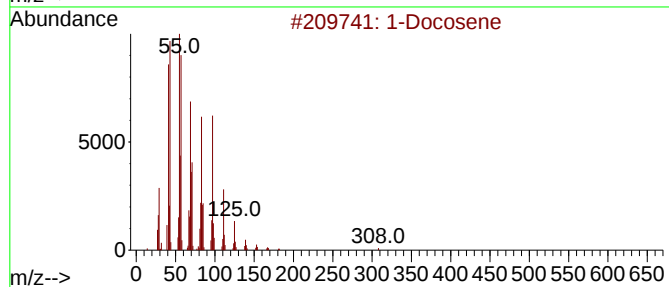
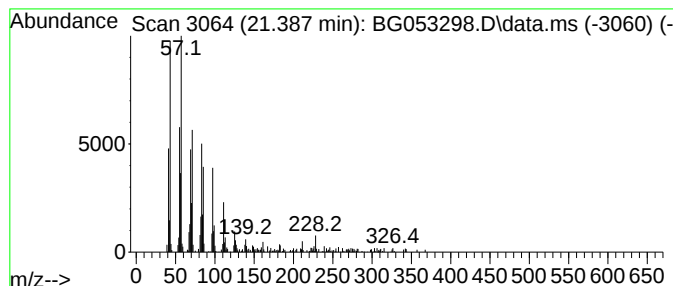
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.387	8.39 ng	200500	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	98
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	92
4			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
5			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

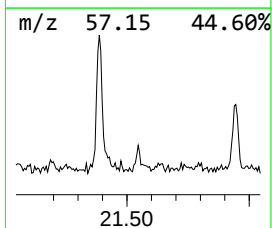
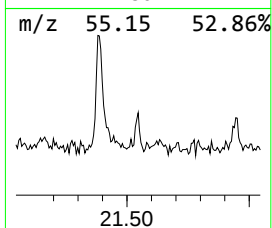
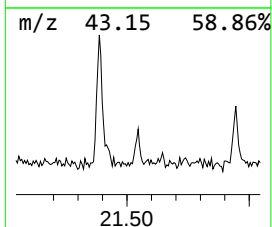
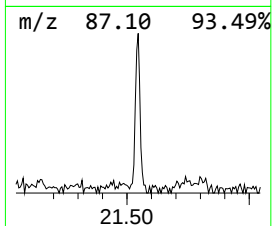
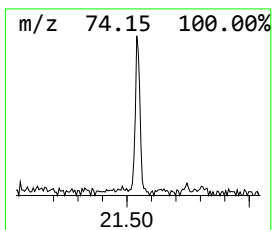
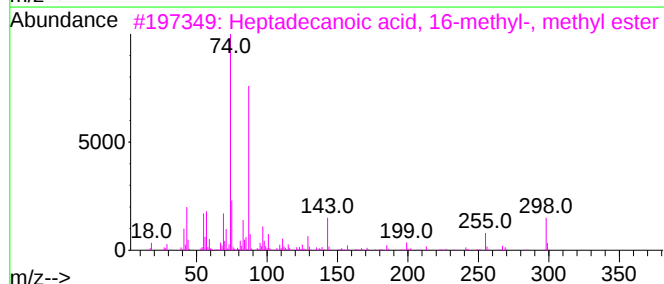
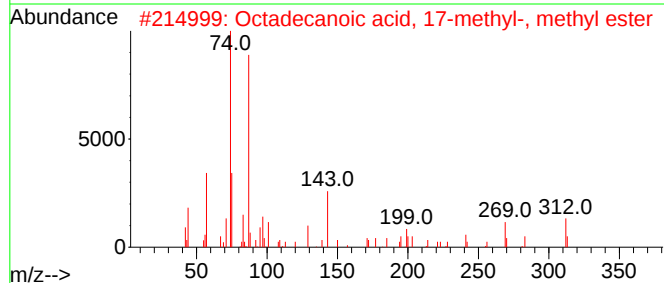
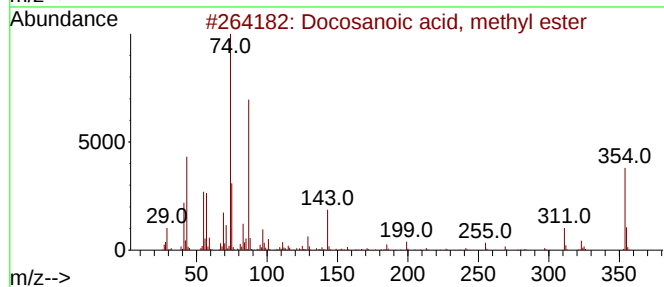
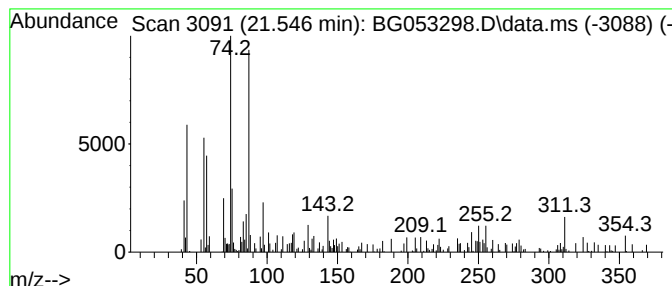
Instrument :
BNA_G
ClientSampleId :
HR-02-042122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.546	2.67 ng	63894	Chrysene-d12	21.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	81
2	Octadecanoic acid, 17-methyl-, m...	312	C20H40O2	055124-97-5	70
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	62
4	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	58
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042322\
Data File : BG053298.D
Acq On : 23 Apr 2022 18:17
Operator : CG/JU
Sample : N2525-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-042122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
Tridecanoic aci...	18.133	34.9	ng	915094	4	17.480	524208	20.0
n-Hexadecanoic ...	18.362	9.7	ng	255272	4	17.480	524208	20.0
9,12-Octadecadi...	19.266	137.8	ng	3612890	4	17.480	524208	20.0
14-Octadecenoic...	19.296	93.9	ng	2460630	4	17.480	524208	20.0
Methyl stearate	19.425	22.8	ng	598362	4	17.480	524208	20.0
unknown19.672	19.672	2.6	ng	61587	5	21.763	477912	20.0
Nonadecane	20.377	2.8	ng	65938	5	21.763	477912	20.0
unknown20.412	20.412	3.1	ng	73371	5	21.763	477912	20.0
Hexadecanoic ac...	20.518	3.2	ng	77457	5	21.763	477912	20.0
unknown20.676	20.676	4.5	ng	106301	5	21.763	477912	20.0
Heneicosane	20.876	2.3	ng	54221	5	21.763	477912	20.0
1-Docosene	21.387	8.4	ng	200500	5	21.763	477912	20.0
Docosanoic acid...	21.546	2.7	ng	63894	5	21.763	477912	20.0