

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
 Data File : BM035392.D
 Acq On : 03 Jun 2022 13:14
 Operator : CG/JU
 Sample : N2987-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P034-SS001-1824-01

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_M\Methods\8270-BM060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	392	399	413	rBV	1624123	2423570	19.23%	4.347%
2	7.034	664	671	682	rBV	1572601	2474987	19.64%	4.439%
3	7.845	800	809	818	rBV	487618	757850	6.01%	1.359%
4	9.010	999	1007	1018	rBV	986324	1662881	13.20%	2.982%
5	10.645	1277	1285	1294	rBV	624230	1054537	8.37%	1.891%
6	13.110	1697	1704	1711	rBV	3044705	4473893	35.50%	8.024%
7	14.486	1932	1938	1944	rBV	1017864	1476305	11.72%	2.648%
8	15.980	2186	2192	2201	rVB	2490022	3579482	28.41%	6.420%
9	16.639	2299	2304	2317	rVB5	148865	335170	2.66%	0.601%
10	17.233	2400	2405	2411	rBV	1288459	1742680	13.83%	3.125%
11	18.145	2546	2560	2568	rBV	2535551	4377940	34.74%	7.852%
12	18.415	2602	2606	2611	rBV	259204	432811	3.43%	0.776%
13	18.462	2611	2614	2622	rVB	233209	367955	2.92%	0.660%
14	19.221	2739	2743	2746	rBV2	128150	201439	1.60%	0.361%
15	19.274	2747	2752	2753	rVV2	385737	573207	4.55%	1.028%
16	19.297	2754	2756	2763	rVV3	480667	1107501	8.79%	1.986%
17	19.427	2765	2778	2800	rVB	6422129	12601047	100.00%	22.600%
18	19.856	2846	2851	2857	rBV	5677805	7239797	57.45%	12.985%
19	20.156	2898	2902	2903	rBV2	121098	159769	1.27%	0.287%
20	20.497	2956	2960	2964	rBV	217171	304955	2.42%	0.547%
21	20.986	3039	3043	3049	rBV2	166772	298511	2.37%	0.535%
22	21.133	3064	3068	3076	rVB	377263	457697	3.63%	0.821%
23	21.415	3112	3116	3125	rBV	1808293	2587246	20.53%	4.640%
24	21.703	3161	3165	3171	rVB2	233957	376144	2.99%	0.675%
25	23.774	3511	3517	3525	rVB2	1191522	2393824	19.00%	4.293%
26	25.232	3759	3765	3786	rVB7	633733	2295867	18.22%	4.118%

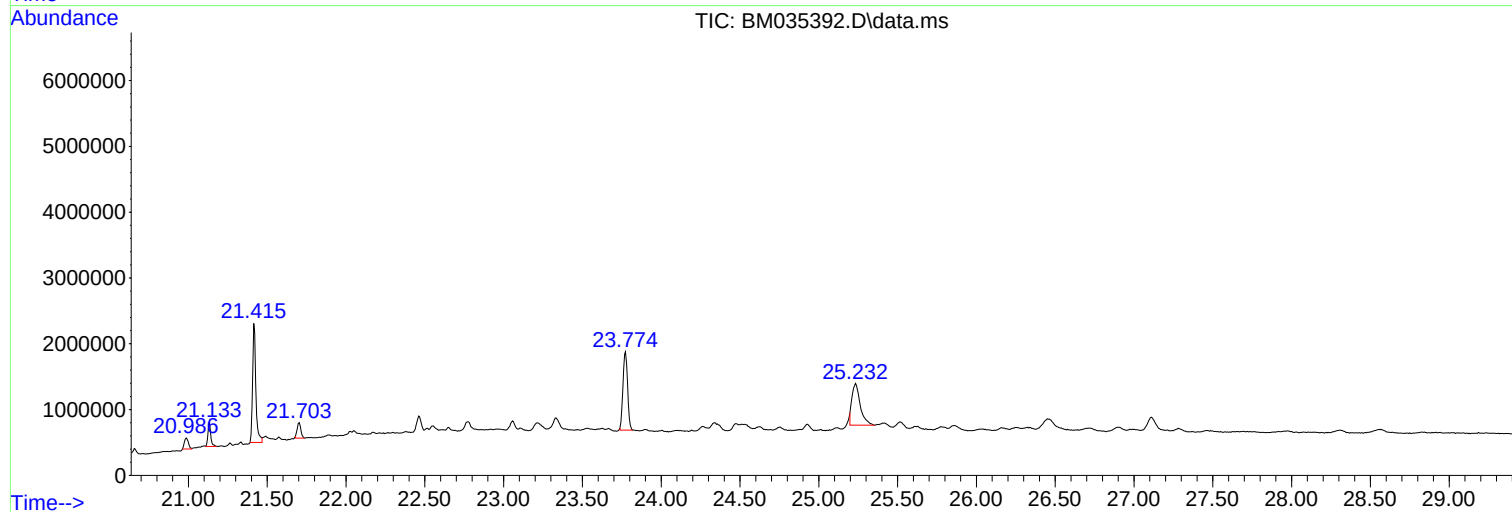
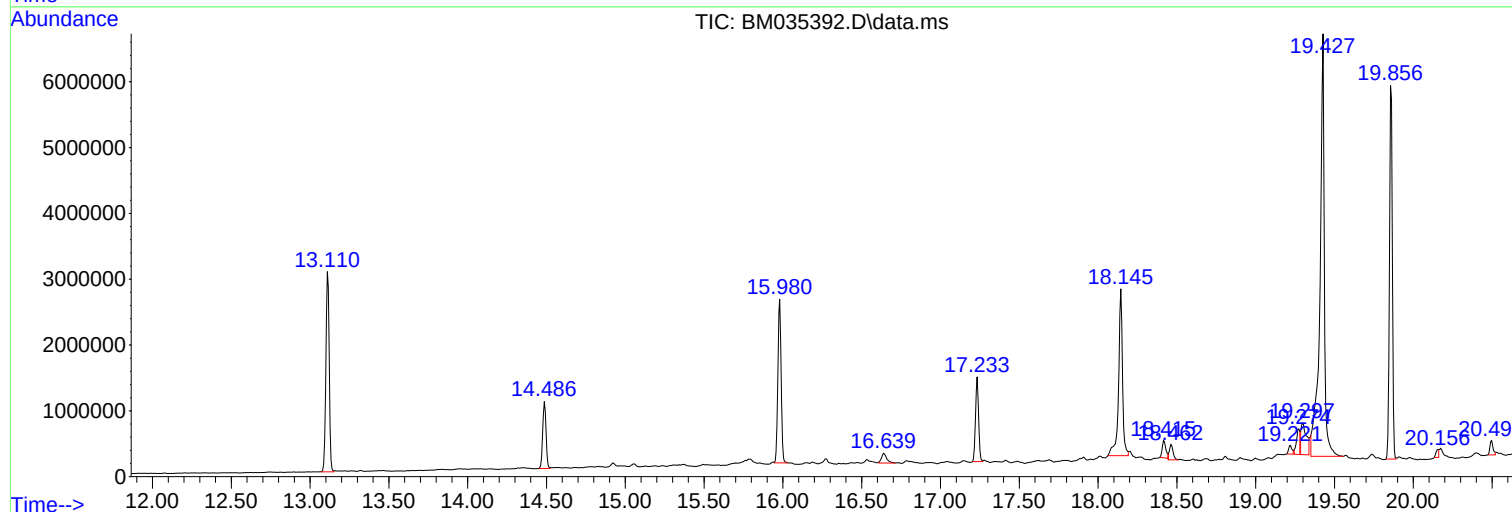
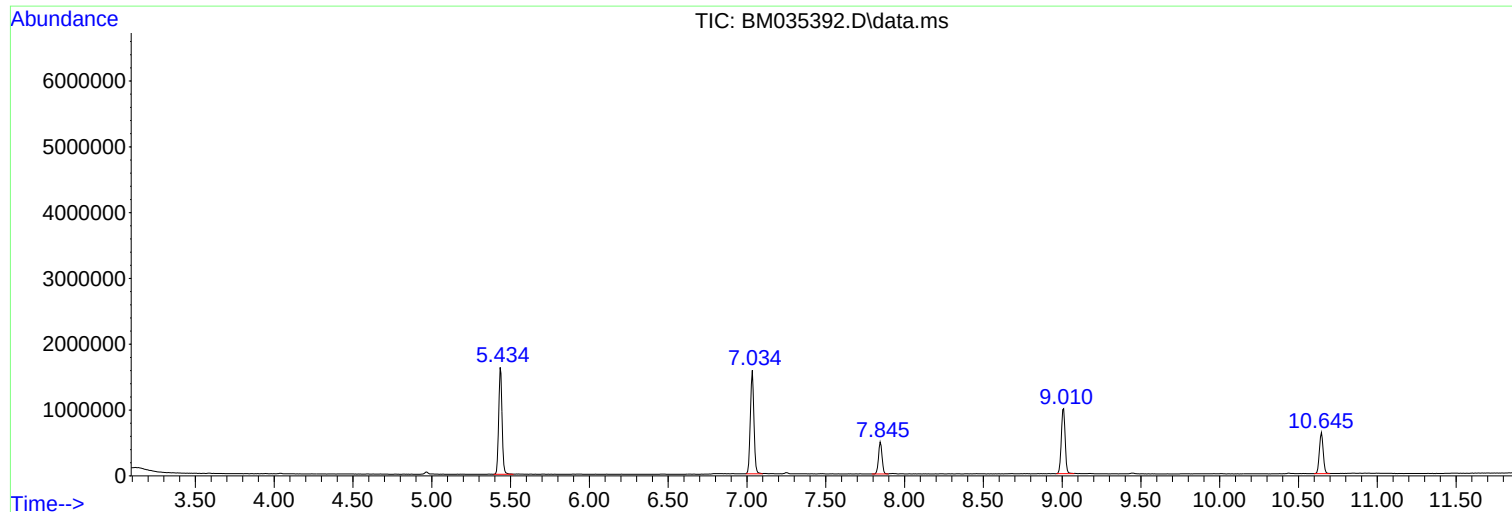
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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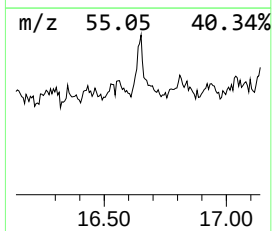
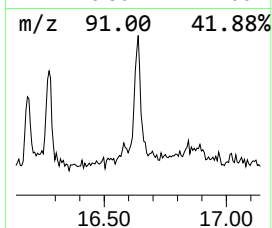
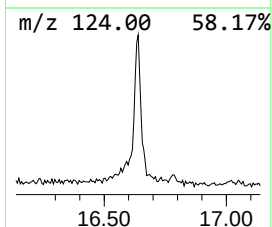
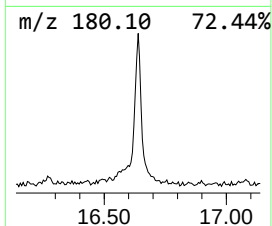
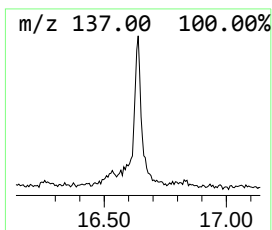
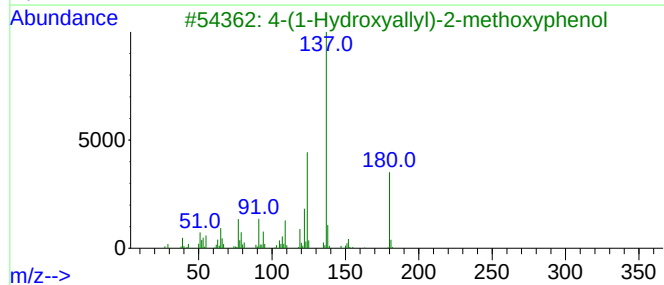
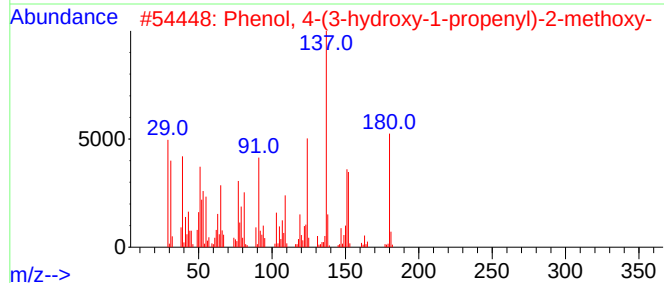
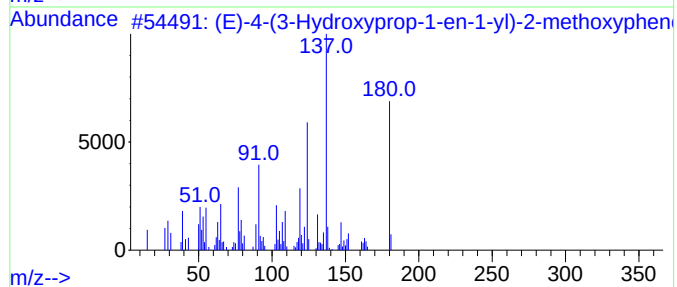
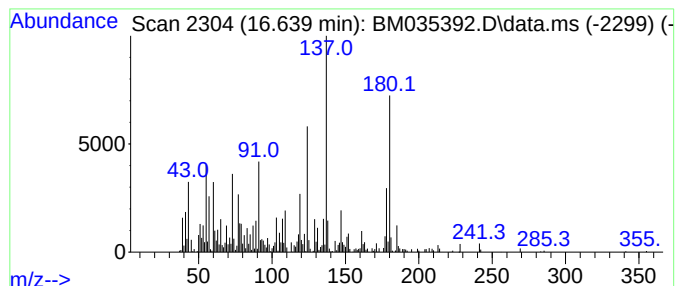
Instrument :
BNA_M
ClientSampleId :
P034-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 1 (E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.639	3.85 ng	335170	Phenanthrene-d10		17.233	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...		180	C10H12O3	032811-40-8	91
2	Phenol, 4-(3-hydroxy-1-propenyl)...		180	C10H12O3	000458-35-5	50
3	4-(1-Hydroxyallyl)-2-methoxyphenol		180	C10H12O3	112465-50-6	47
4	1-Hydroxy-1-(4-methoxyphenyl)pro...		180	C10H12O3	015482-29-8	38
5	Guaiacol, 4-butyl-		180	C11H16O2	059832-96-1	27



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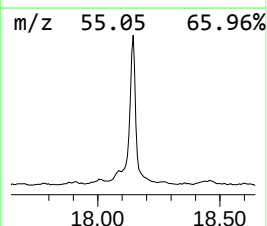
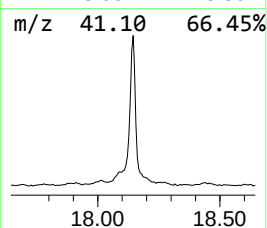
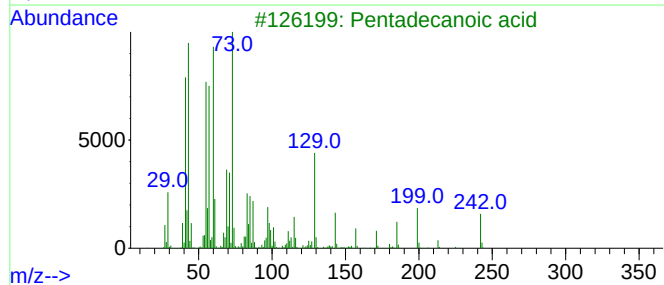
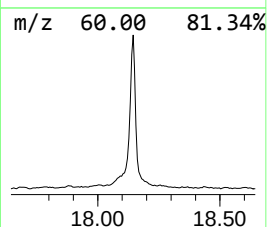
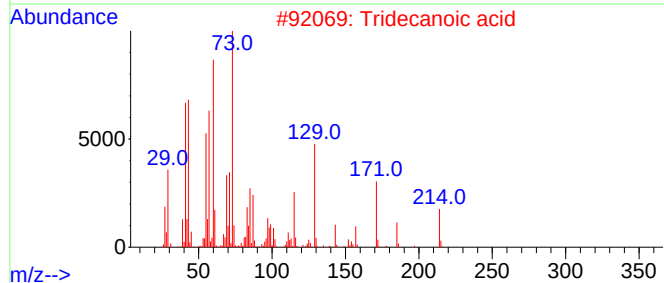
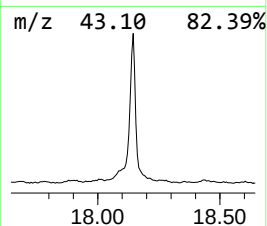
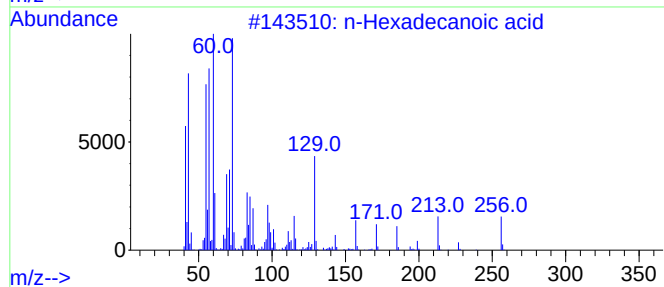
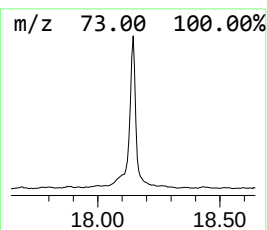
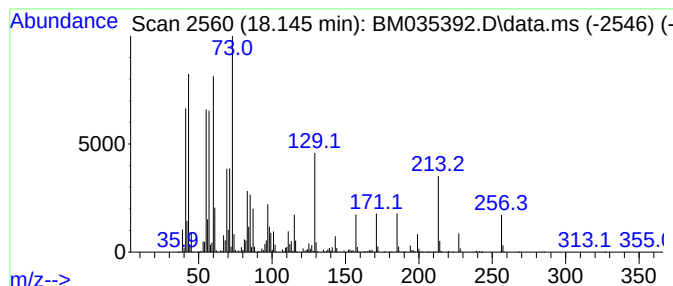
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	50.24 ng	4377940	Phenanthrene-d10	17.233

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	90
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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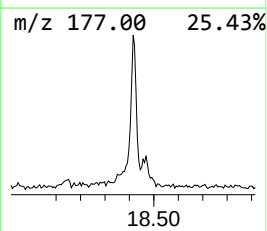
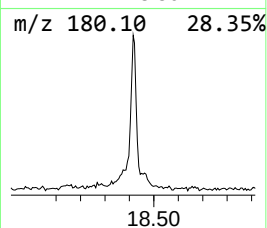
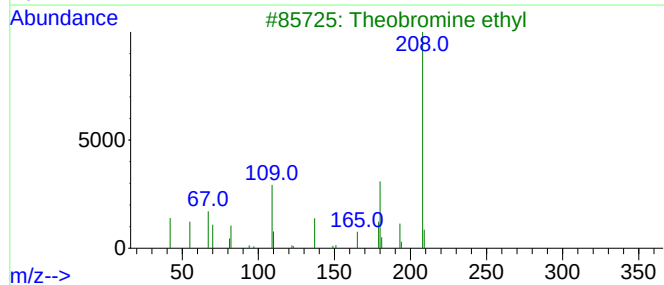
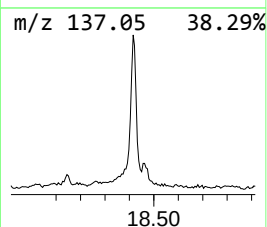
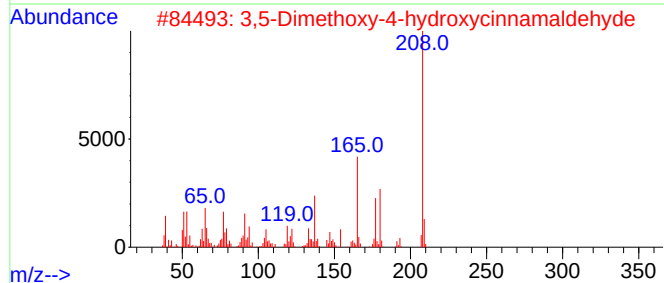
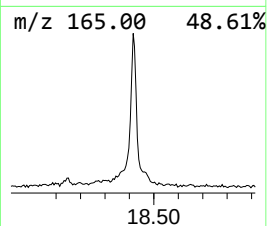
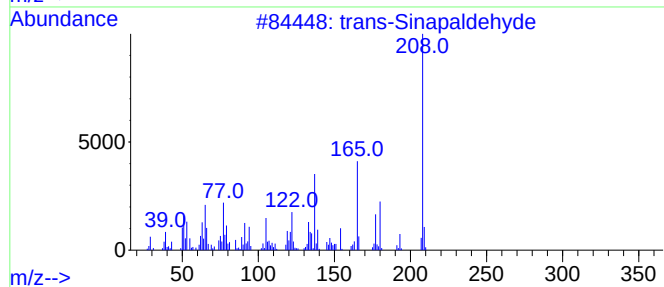
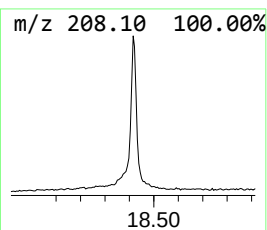
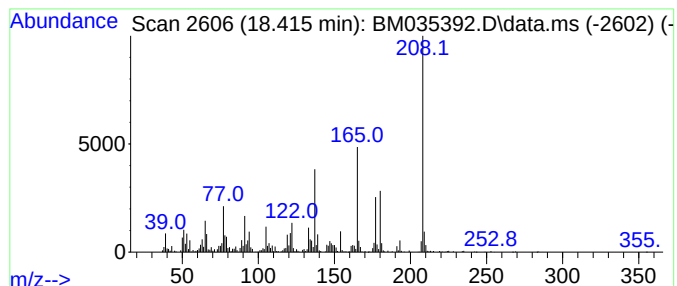
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 trans-Sinapaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.415	4.97 ng	432811	Phenanthrene-d10	17.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapaldehyde	208	C11H12O4	004206-58-0	96
2			3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	C11H12O4	087345-53-7	93
3			Theobromine ethyl	208	C9H12N4O2	007464-74-6	38
4			3,4-Dimethoxy-N-[2-(2-methoxyphenyl)]	331	C18H21NO5	339064-42-5	38
5			2-Propenoic acid, 3-(2,3-dimethoxyphenyl)	208	C11H12O4	007345-82-6	38



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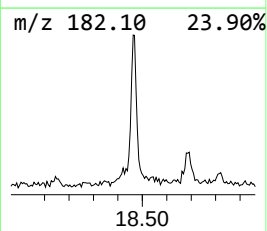
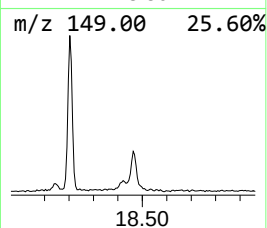
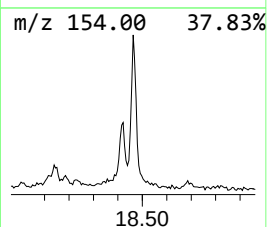
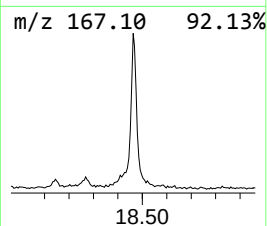
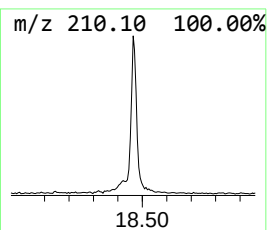
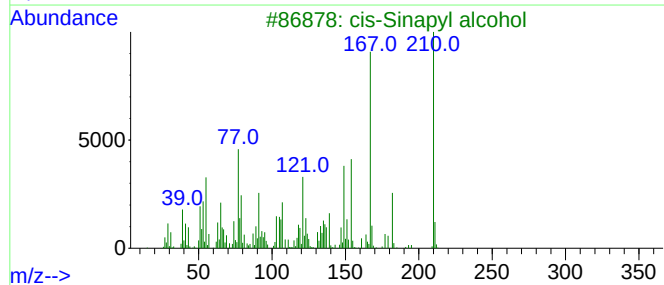
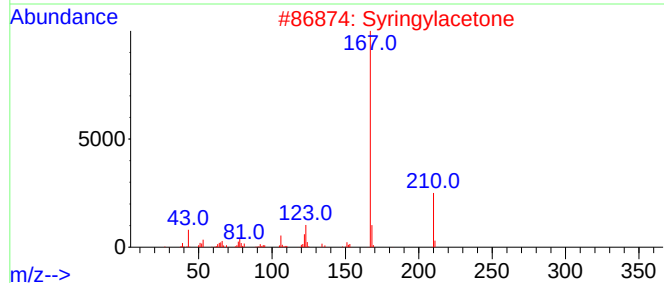
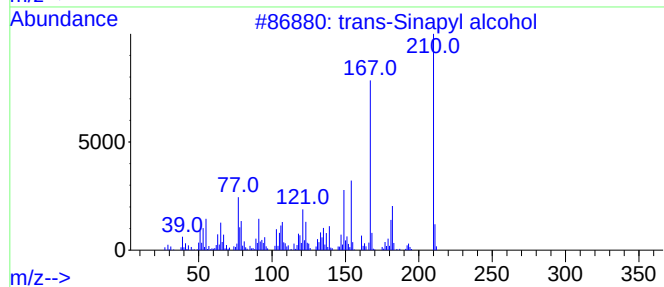
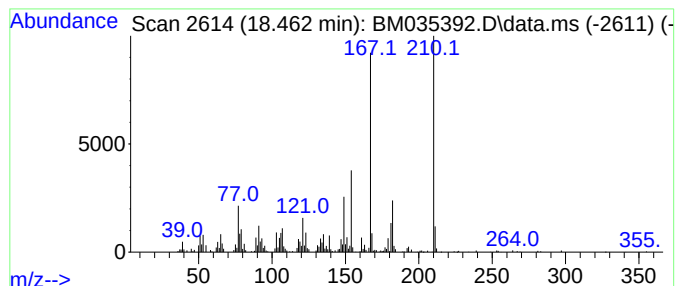
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 trans-Sinapyl alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.462	4.22 ng	367955	Phenanthrene-d10	17.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	97
2			Syringylacetone	210	C11H14O4	019037-58-2	50
3			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	47
4			1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	41
5			9-Methyl-1-phenazinol	210	C13H10N2O	013860-43-0	38



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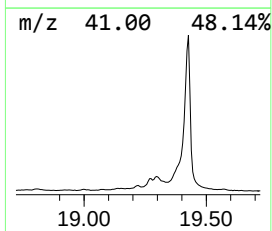
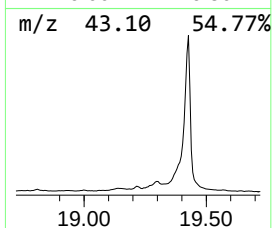
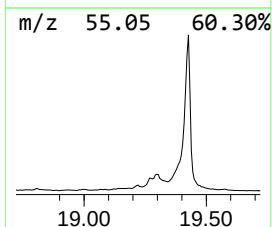
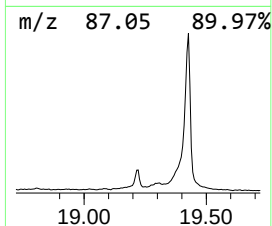
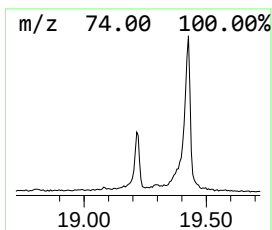
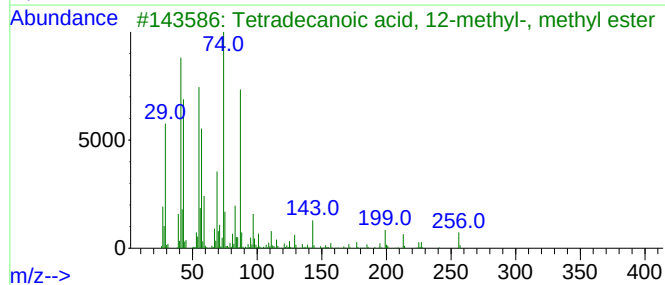
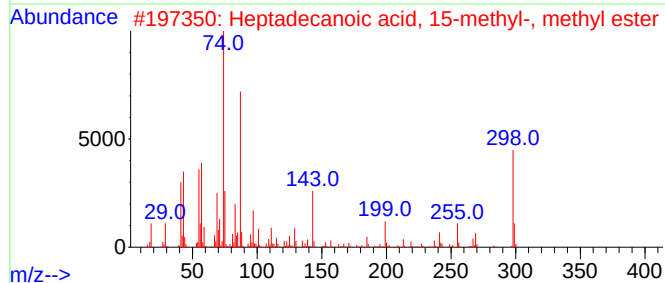
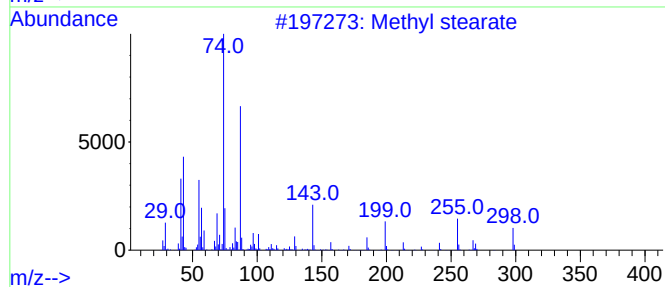
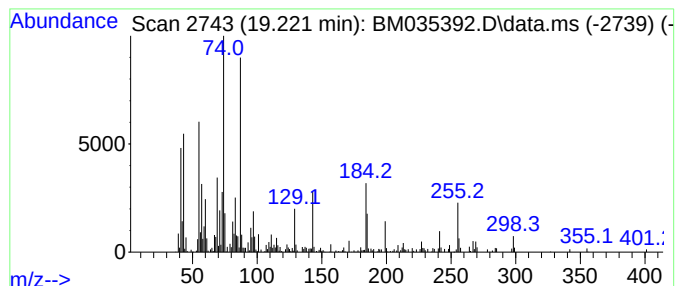
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Methyl stearate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	2.31 ng	201439	Phenanthrene-d10	17.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	86
2			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	83
3			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	005129-66-8	78
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	64
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	64



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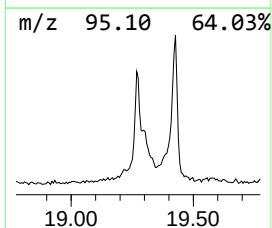
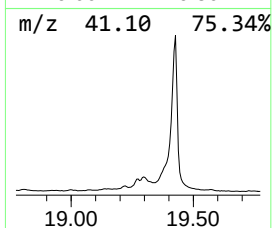
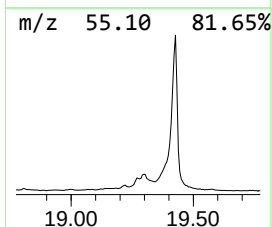
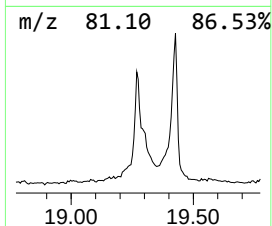
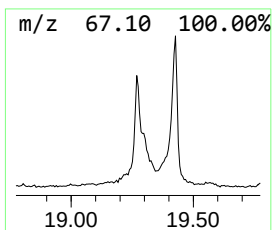
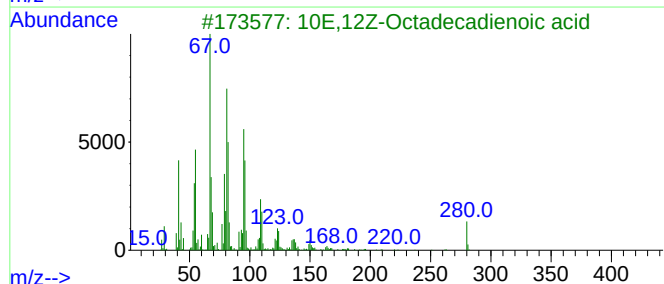
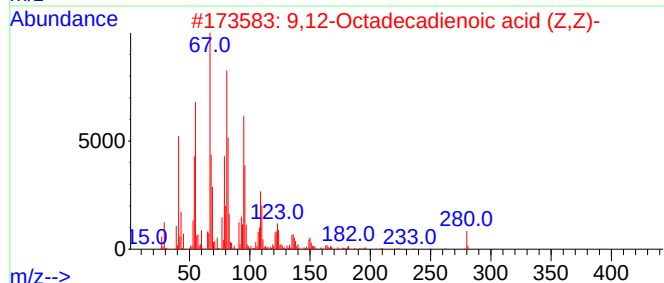
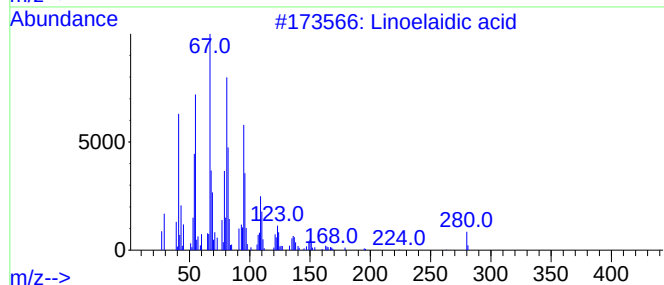
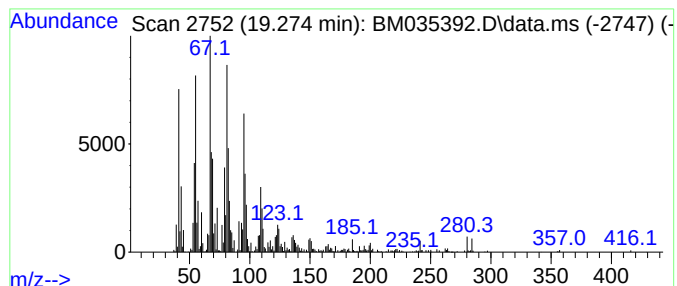
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Linoelaidic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	6.58 ng	573207	Phenanthrene-d10	17.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linoelaidic acid	280	C18H32O2	000506-21-8	95
2			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
3			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	93
4			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	92
5			9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
Acq On : 03 Jun 2022 13:14
Operator : CG/JU
Sample : N2987-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P034-SS001-1824-01

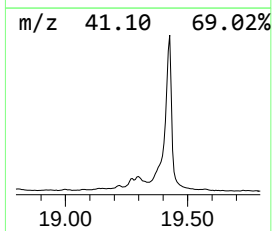
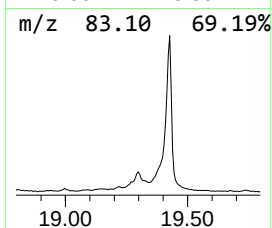
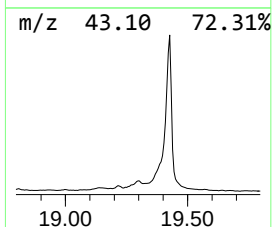
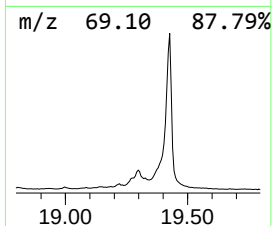
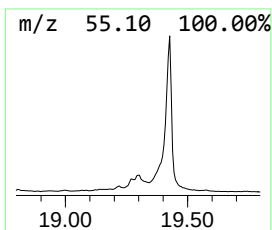
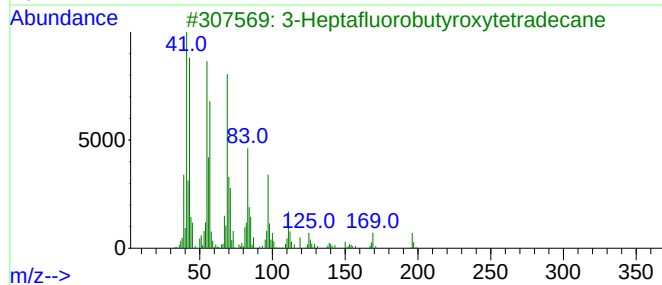
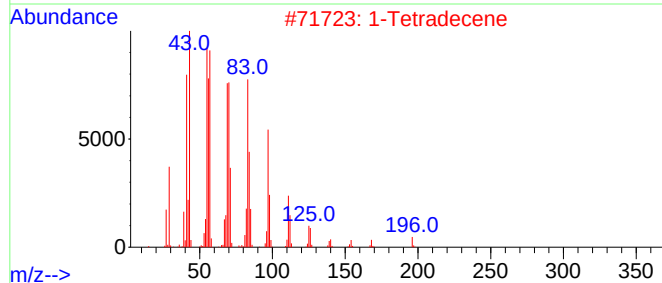
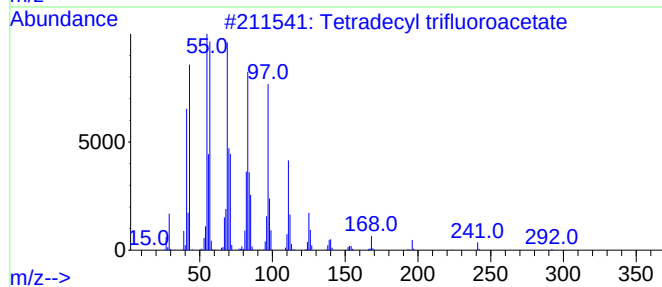
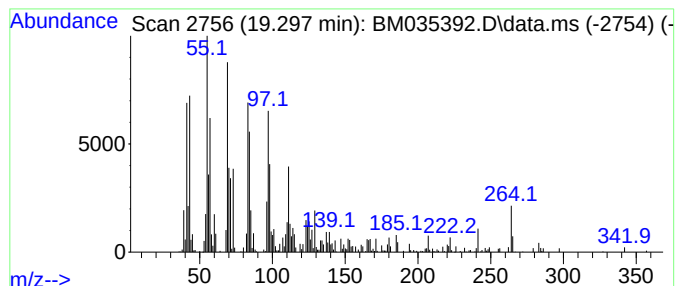
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.297	12.71 ng	1107500	Phenanthrene-d10	17.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	53
2			1-Tetradecene	196	C14H28	001120-36-1	52
3			3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	46
4			1-Undecene, 8-methyl-	168	C12H24	074630-40-3	45
5			1-Tricosene	322	C23H46	018835-32-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
Acq On : 03 Jun 2022 13:14
Operator : CG/JU
Sample : N2987-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P034-SS001-1824-01

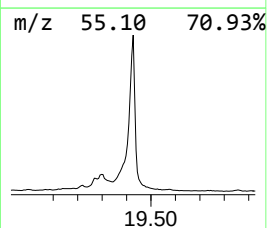
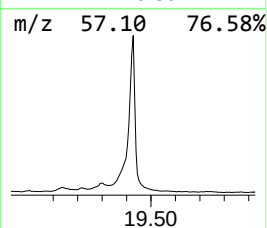
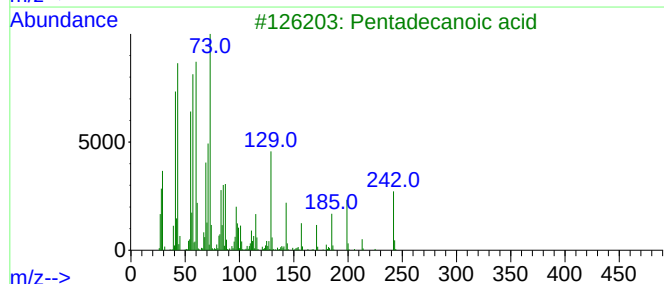
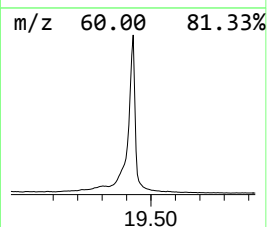
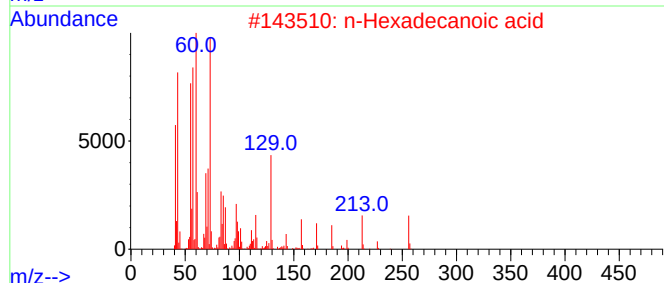
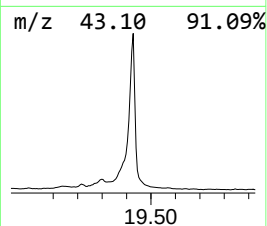
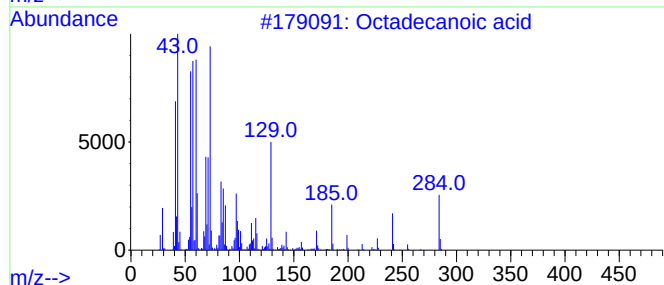
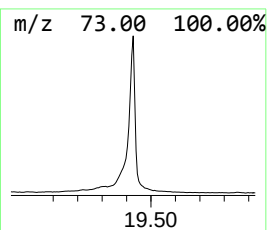
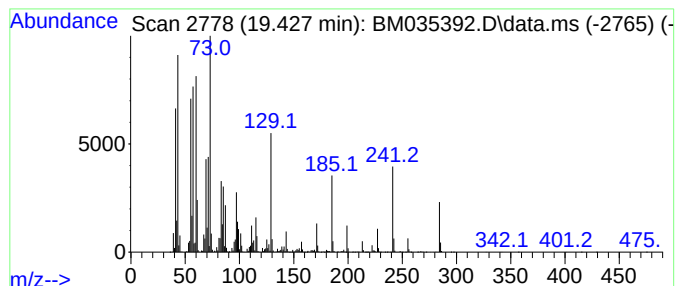
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	97.41 ng	12601000	Chrysene-d12	21.415

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
Acq On : 03 Jun 2022 13:14
Operator : CG/JU
Sample : N2987-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

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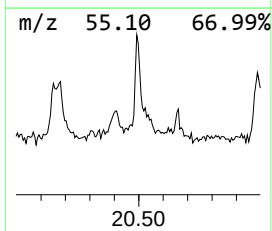
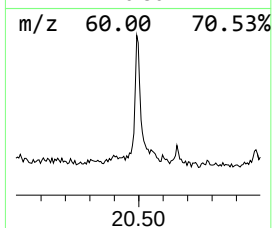
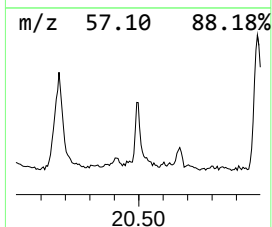
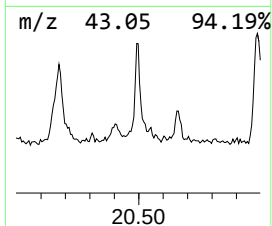
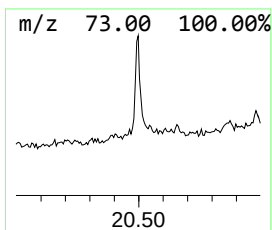
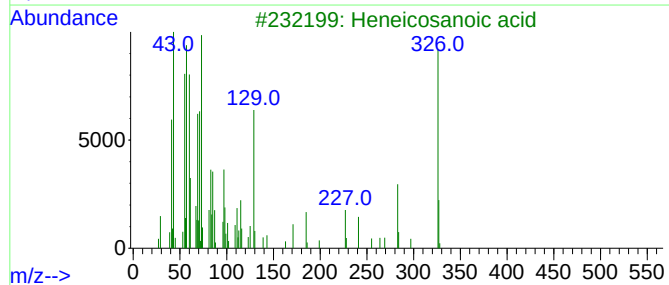
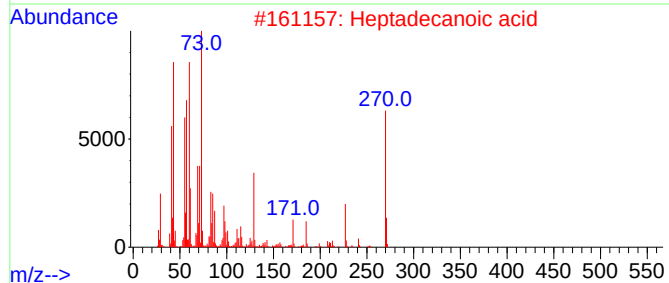
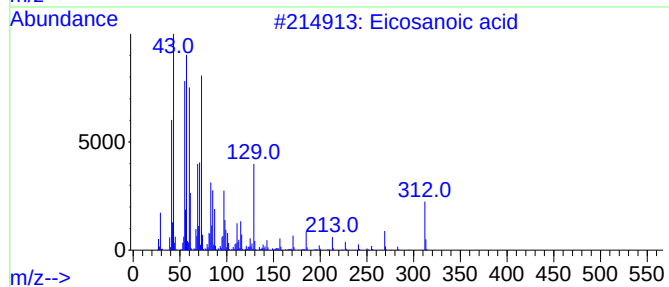
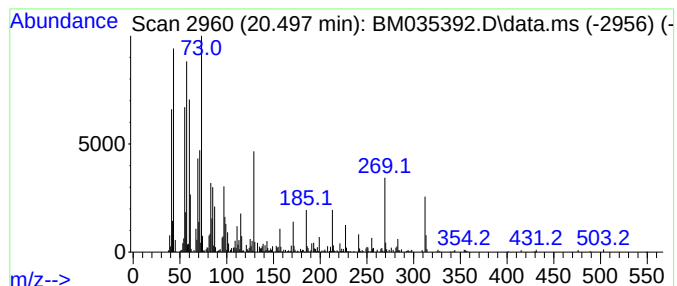
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.497	2.36 ng	304955	Chrysene-d12	21.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid	312	C20H40O2	000506-30-9	99
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	92
3			Heneicosanoic acid	326	C21H42O2	002363-71-5	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tricosanoic acid	354	C23H46O2	002433-96-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
Acq On : 03 Jun 2022 13:14
Operator : CG/JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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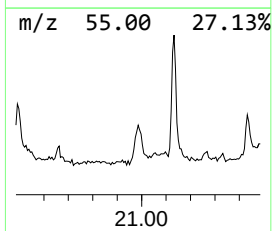
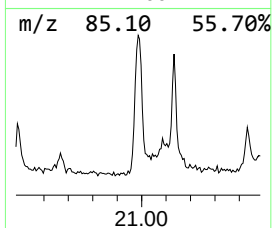
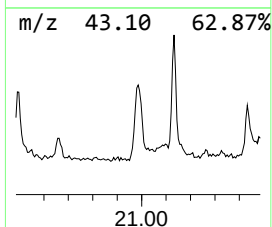
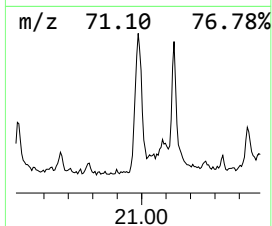
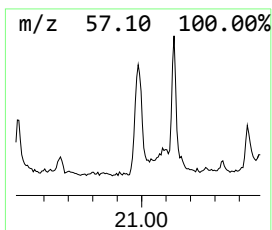
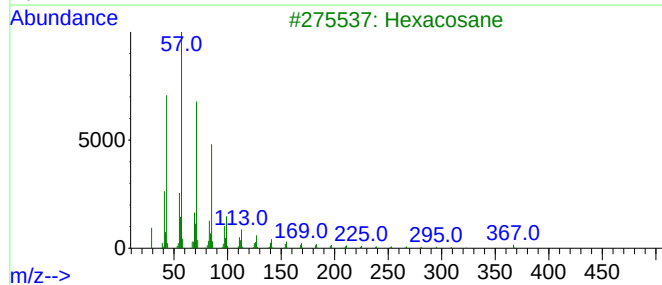
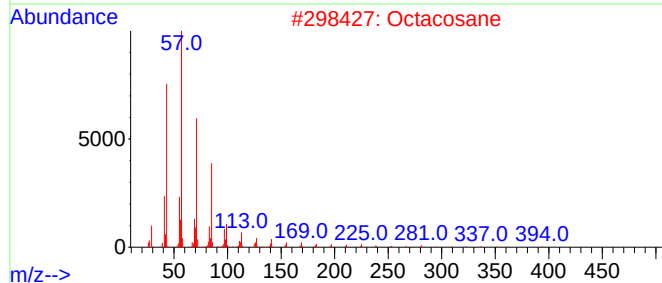
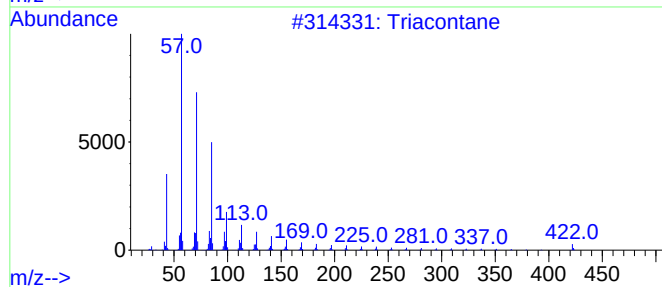
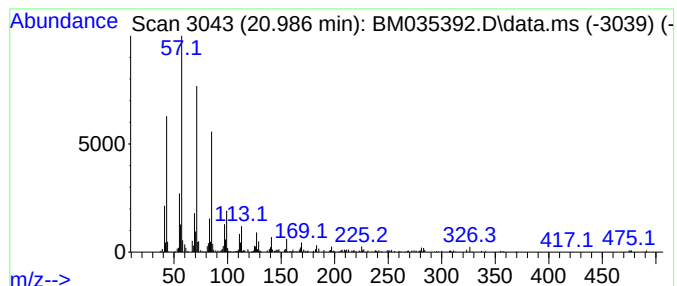
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	2.31 ng	298511	Chrysene-d12	21.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
Acq On : 03 Jun 2022 13:14
Operator : CG/JU
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ALS Vial : 7 Sample Multiplier: 1

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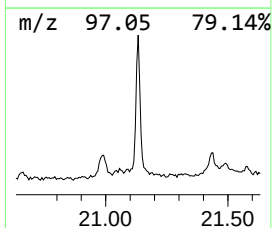
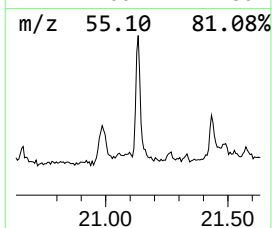
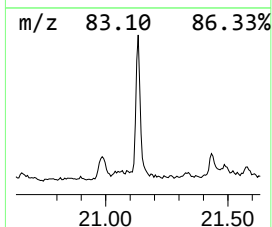
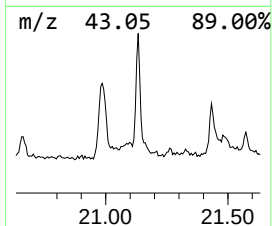
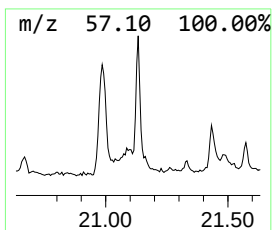
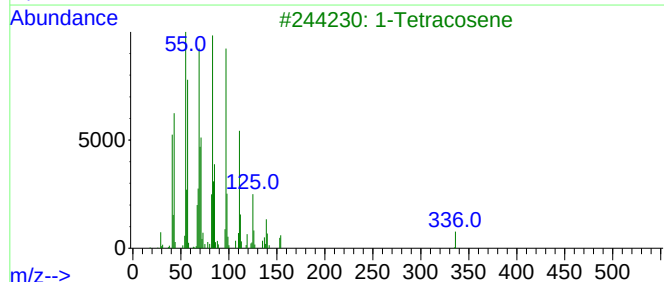
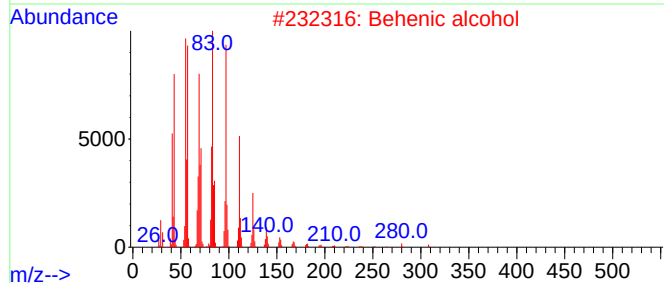
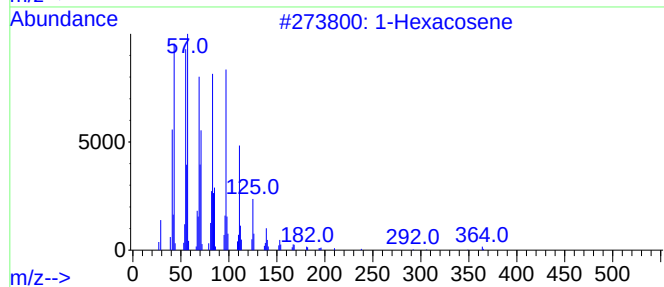
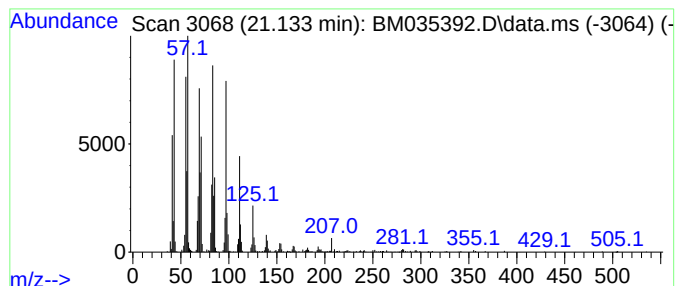
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexacosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	3.54 ng	457697	Chrysene-d12	21.415

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	95
2	Behenic alcohol		326	C22H46O	000661-19-8	94
3	1-Tetracosene		336	C24H48	010192-32-2	94
4	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
5	Pentacos-1-ene		350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
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Acq On : 03 Jun 2022 13:14
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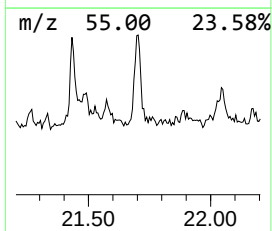
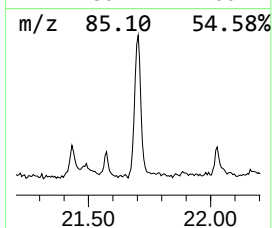
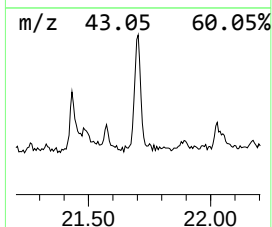
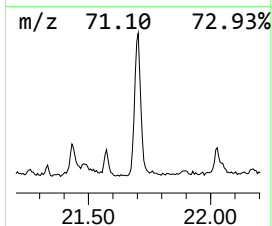
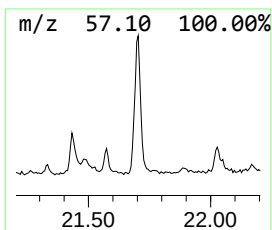
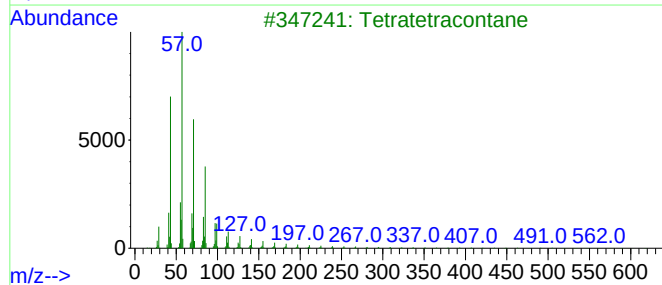
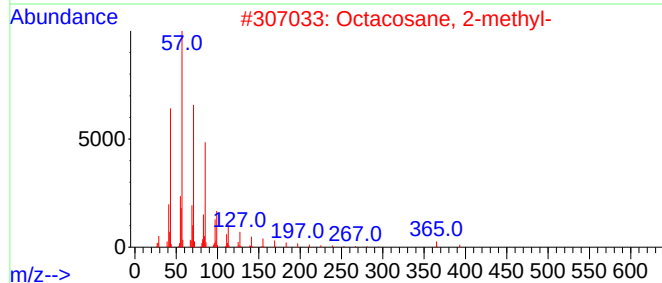
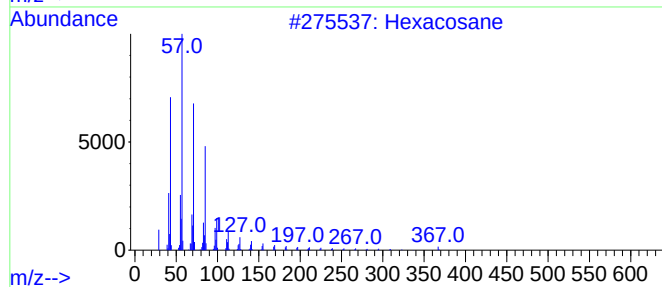
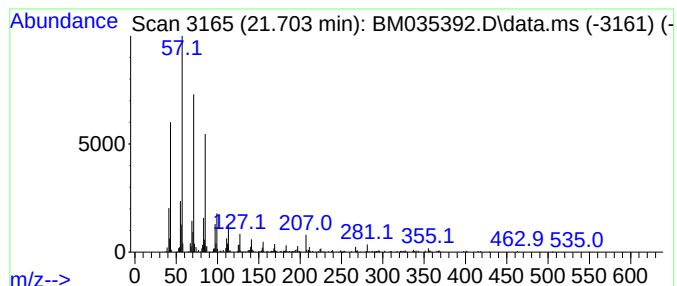
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.703	2.91 ng	376144	Chrysene-d12	21.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035392.D
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Operator : CG/JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

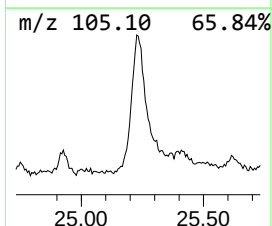
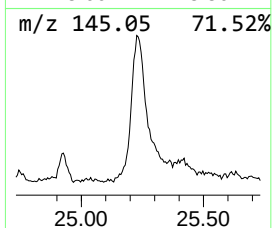
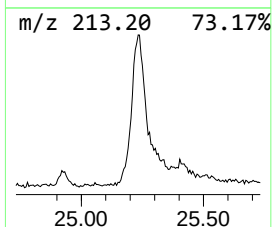
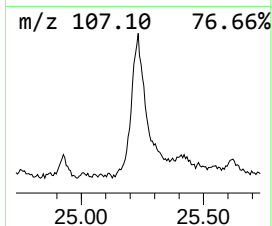
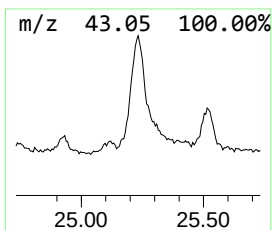
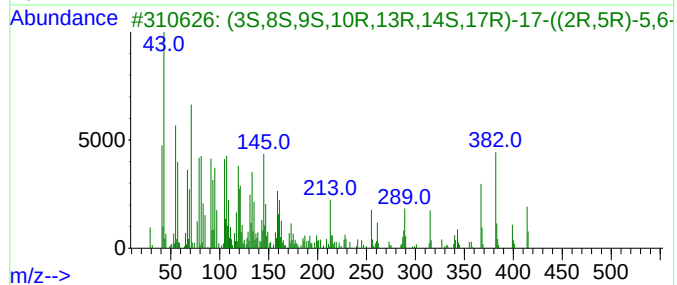
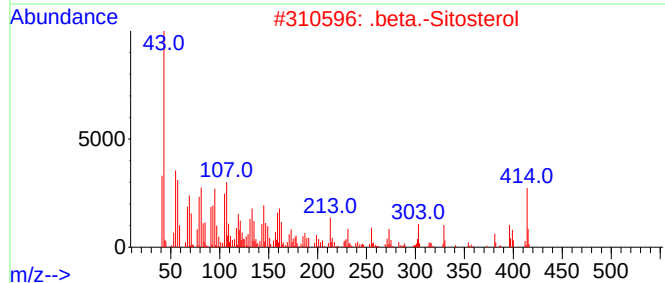
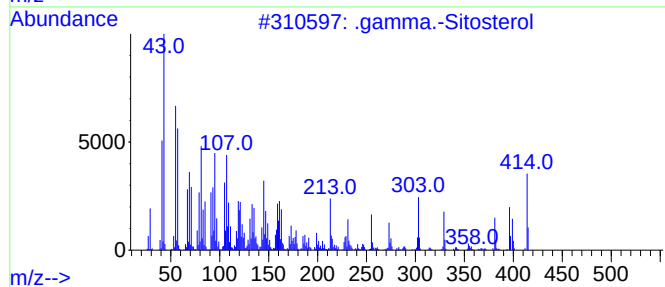
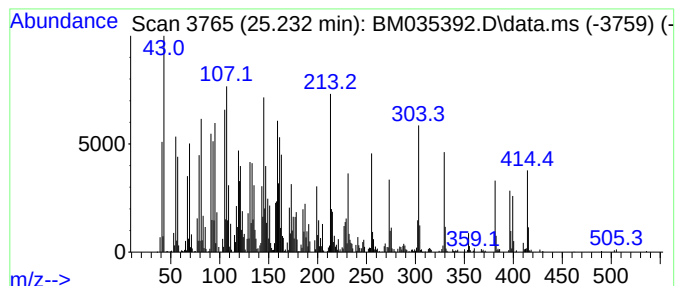
Instrument :
BNA_M
ClientSampleId :
P034-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.232	19.18 ng	2295870	Perylene-d12	23.774	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	83
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	30
4	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25
5	Campesterol	400	C28H48O	000474-62-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
 Data File : BM035392.D
 Acq On : 03 Jun 2022 13:14
 Operator : CG/JU
 Sample : N2987-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P034-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.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
(E)-4-(3-Hydrox...	16.639	3.9	ng	335170	4	17.233	1742680	20.0
n-Hexadecanoic ...	18.145	50.2	ng	4377940	4	17.233	1742680	20.0
trans-Sinapalde...	18.415	5.0	ng	432811	4	17.233	1742680	20.0
trans-Sinapyl a...	18.462	4.2	ng	367955	4	17.233	1742680	20.0
Methyl stearate	19.221	2.3	ng	201439	4	17.233	1742680	20.0
Linoelaidic acid	19.274	6.6	ng	573207	4	17.233	1742680	20.0
Tetradecyl trif...	19.297	12.7	ng	1107500	4	17.233	1742680	20.0
Octadecanoic acid	19.427	97.4	ng	12601000	5	21.415	2587250	20.0
Eicosanoic acid	20.497	2.4	ng	304955	5	21.415	2587250	20.0
Triacontane	20.986	2.3	ng	298511	5	21.415	2587250	20.0
1-Hexacosene	21.133	3.5	ng	457697	5	21.415	2587250	20.0
Hexacosane	21.703	2.9	ng	376144	5	21.415	2587250	20.0
.gamma.-Sitosterol	25.232	19.2	ng	2295870	6	23.774	2393820	20.0