

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
 Data File : BF134098.D
 Acq On : 06 Jul 2023 15:00
 Operator : CG\JU
 Sample : 03021-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-303-20230601

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_F\Methods\8270-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	29	rVB	1893403	2724167	73.82%	11.781%
2	5.075	505	508	518	rBV	110170	131728	3.57%	0.570%
3	5.475	572	576	585	rBV	1359688	1274661	34.54%	5.512%
4	6.475	742	746	758	rBV	905028	775492	21.02%	3.354%
5	6.845	805	809	815	rBV	831672	683484	18.52%	2.956%
6	7.410	900	905	908	rBV	2268239	2064352	55.94%	8.927%
7	8.122	1023	1026	1030	rBV	1089229	866316	23.48%	3.746%
8	9.204	1206	1210	1213	rBV	4395428	3690153	100.00%	15.958%
9	9.880	1322	1325	1329	rBV	1147471	945003	25.61%	4.087%
10	10.598	1444	1447	1450	rBV	68497	54325	1.47%	0.235%
11	10.680	1456	1461	1464	rBV	2366874	2365522	64.10%	10.230%
12	11.374	1576	1579	1584	rBV	1048492	938197	25.42%	4.057%
13	11.598	1614	1617	1620	rBV	38088	44717	1.21%	0.193%
14	11.686	1627	1632	1635	rBV2	53345	79126	2.14%	0.342%
15	11.904	1664	1669	1680	rVB3	208737	285169	7.73%	1.233%
16	12.380	1744	1750	1759	rVB4	45877	137646	3.73%	0.595%
17	12.698	1799	1804	1809	rBV2	75506	111736	3.03%	0.483%
18	12.974	1847	1851	1854	rBV	3234389	2874987	77.91%	12.433%
19	13.321	1904	1910	1918	rVB2	75098	140542	3.81%	0.608%
20	13.445	1924	1931	1940	rVB	326386	585061	15.85%	2.530%
21	13.904	2004	2009	2018	rVB	60598	116506	3.16%	0.504%
22	13.992	2019	2024	2028	rVV	79879	147543	4.00%	0.638%
23	14.033	2028	2031	2038	rVB	588119	554873	15.04%	2.400%
24	14.533	2108	2116	2125	rBV2	86745	156168	4.23%	0.675%
25	15.068	2201	2207	2217	rBV2	71270	159325	4.32%	0.689%
26	15.174	2221	2225	2240	rVB10	34877	118341	3.21%	0.512%
27	15.539	2282	2287	2300	rVV	487700	679611	18.42%	2.939%
28	15.662	2303	2308	2316	rVB3	44885	87141	2.36%	0.377%
29	16.351	2419	2425	2430	rBV4	36586	74905	2.03%	0.324%
30	16.804	2495	2502	2515	rBV4	38154	150163	4.07%	0.649%
31	17.421	2600	2607	2616	rVB9	34855	106909	2.90%	0.462%

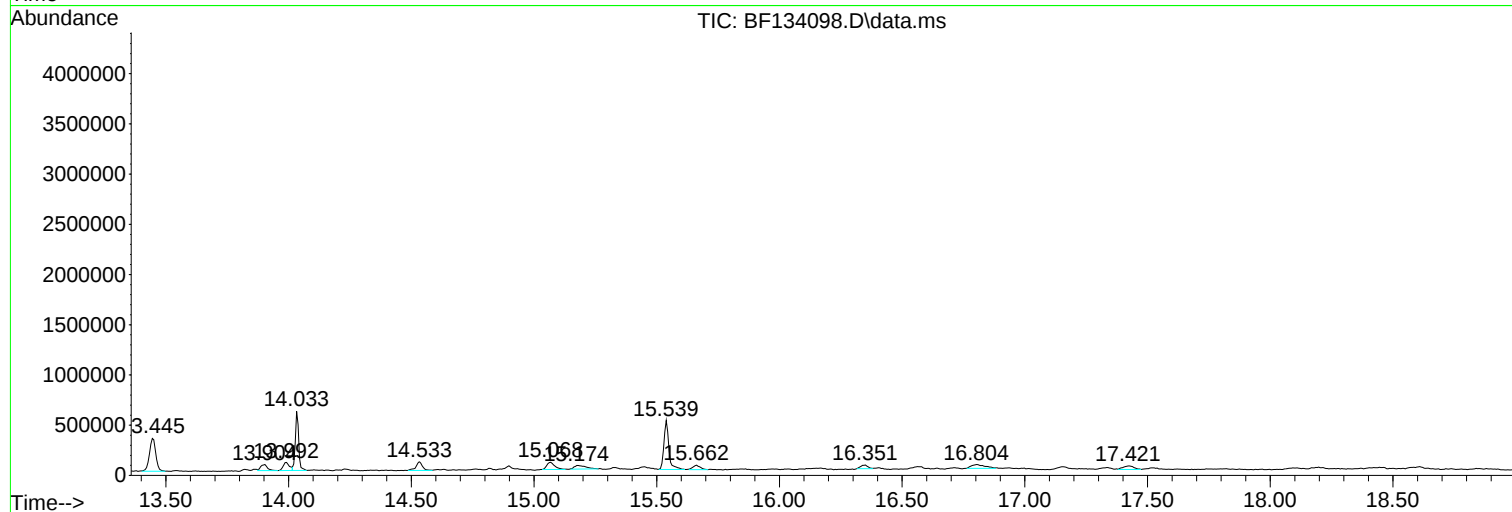
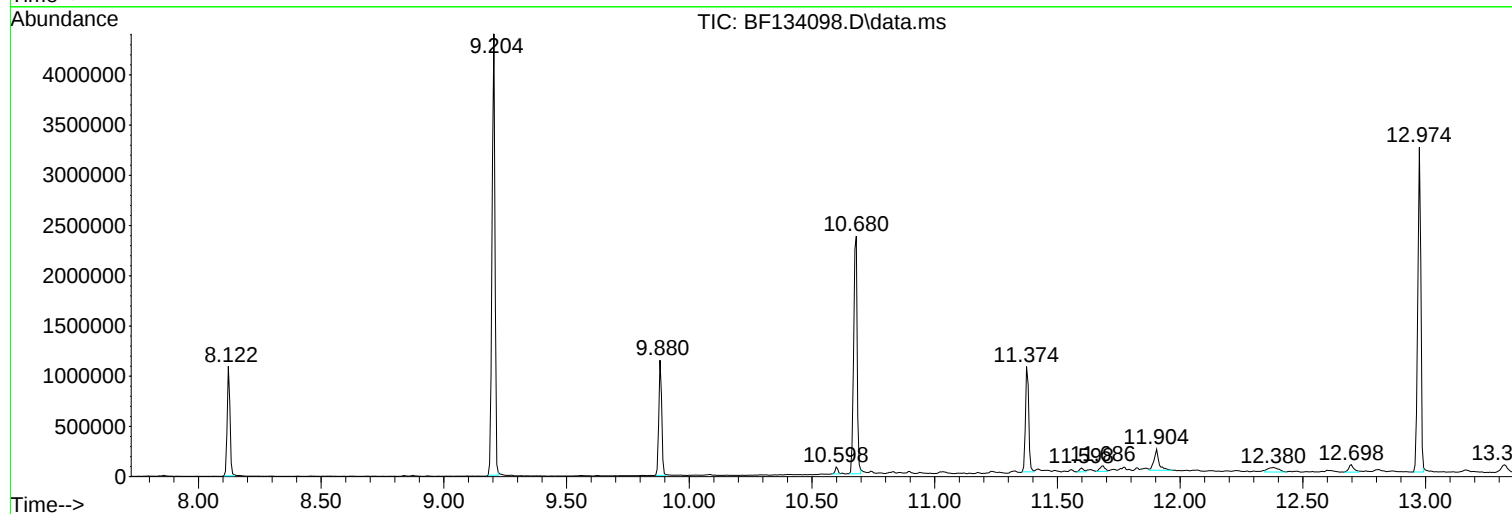
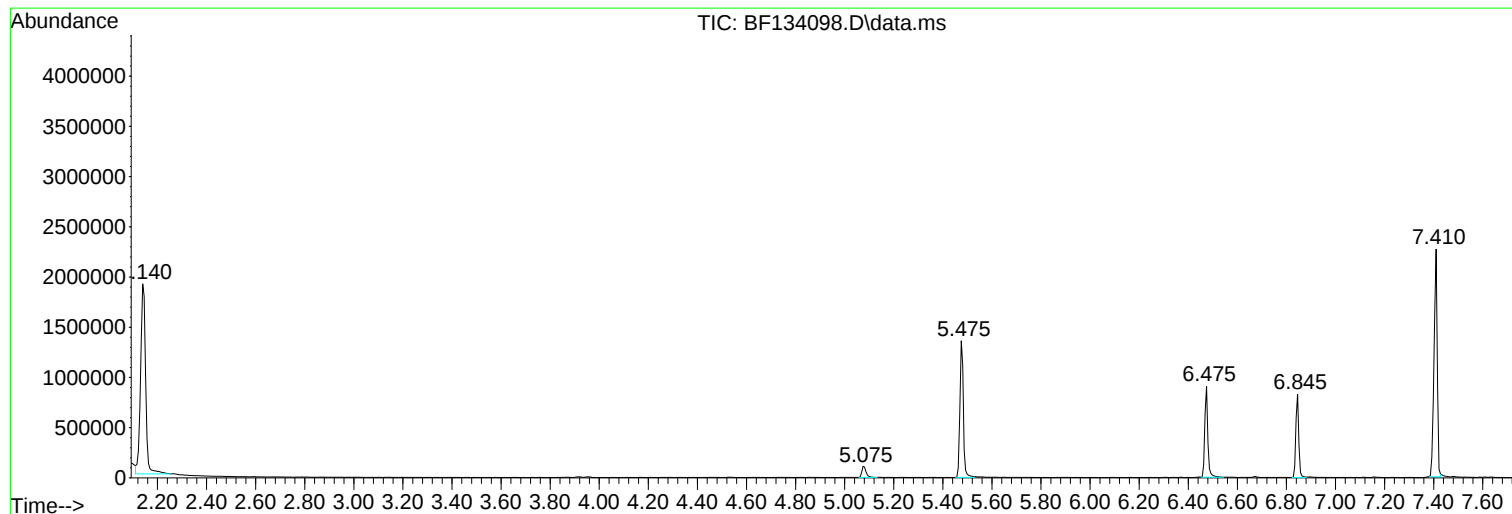
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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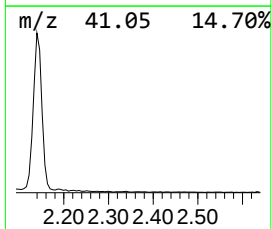
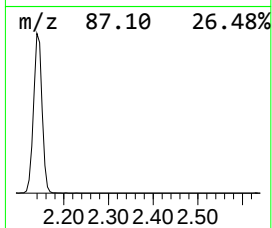
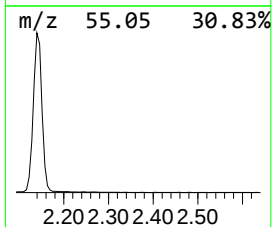
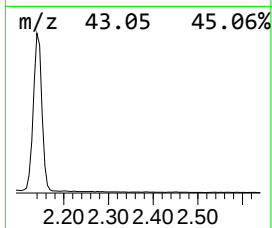
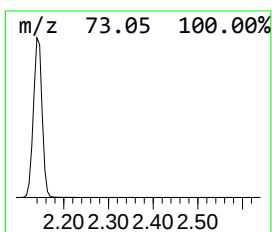
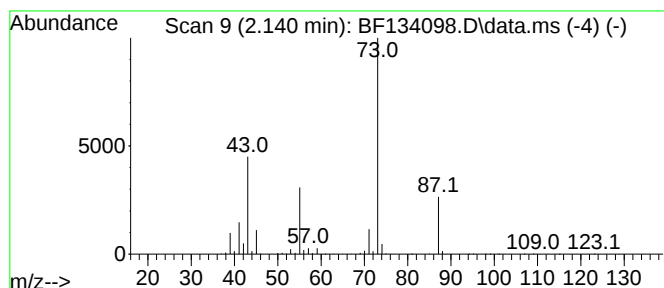
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	79.71 ng	2724170	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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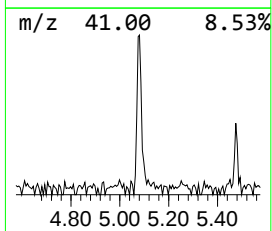
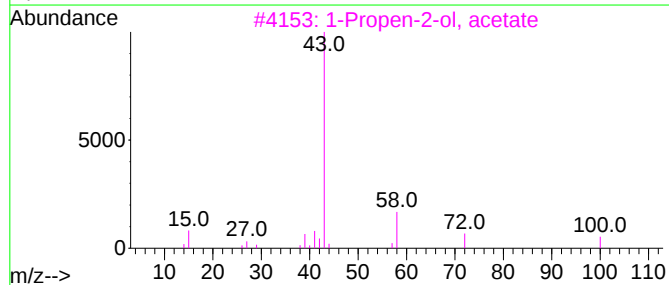
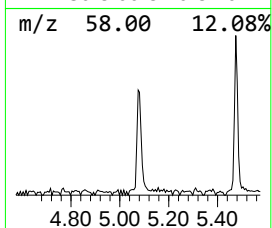
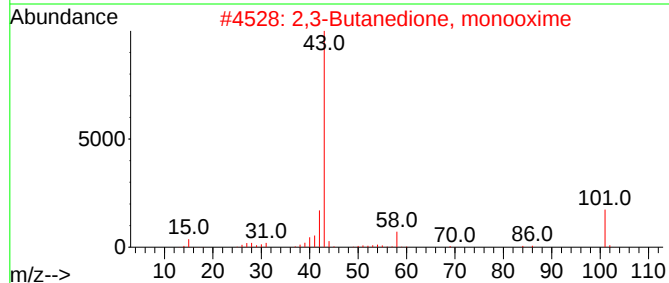
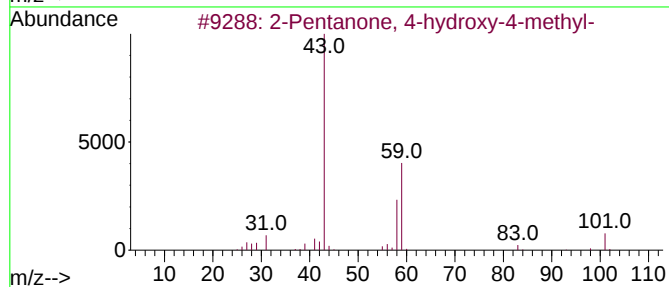
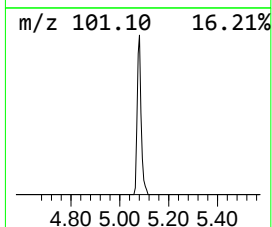
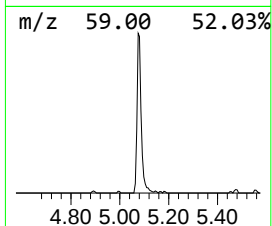
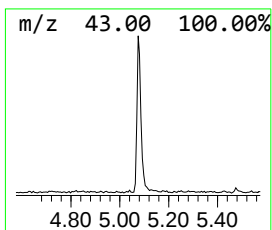
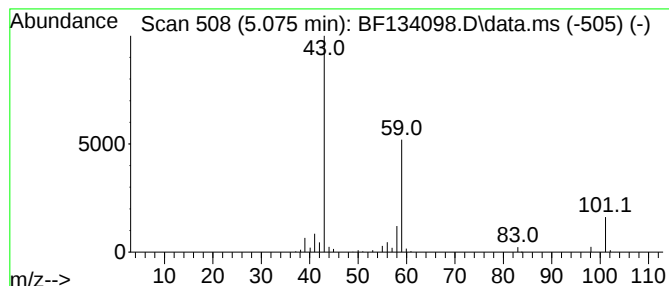
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.85 ng	131728	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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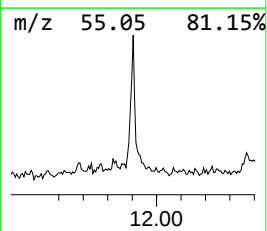
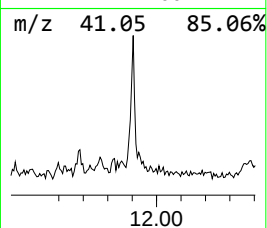
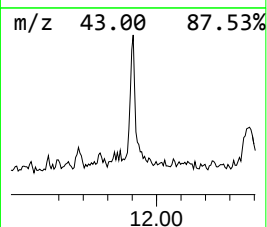
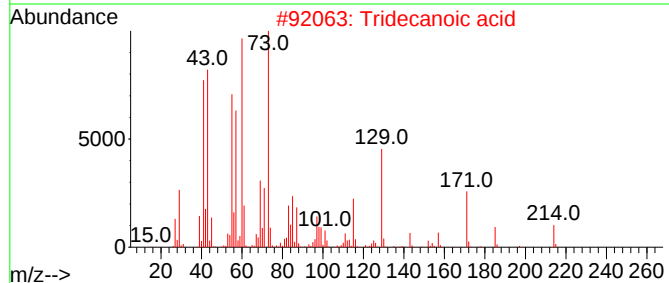
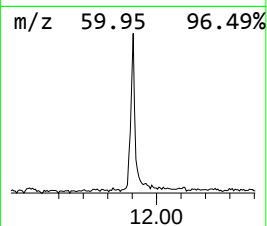
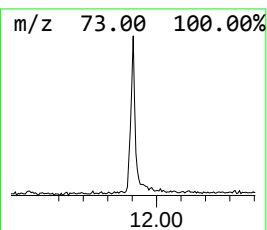
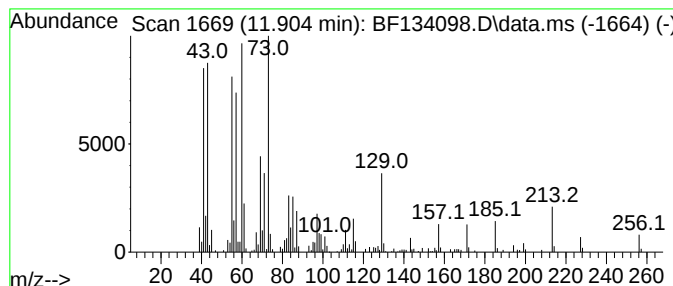
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	6.08 ng	285169	Phenanthrene-d10	11.374

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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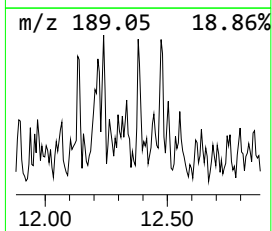
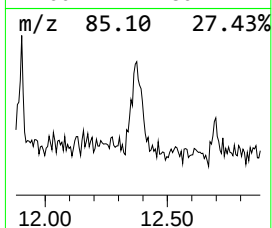
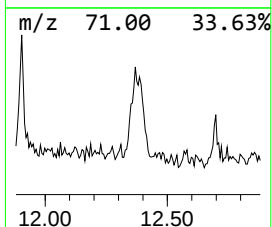
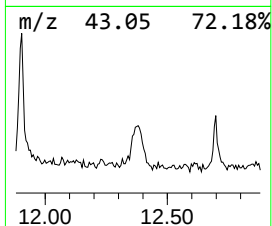
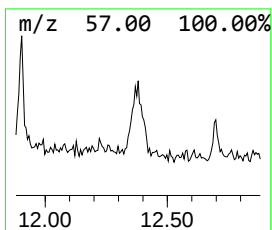
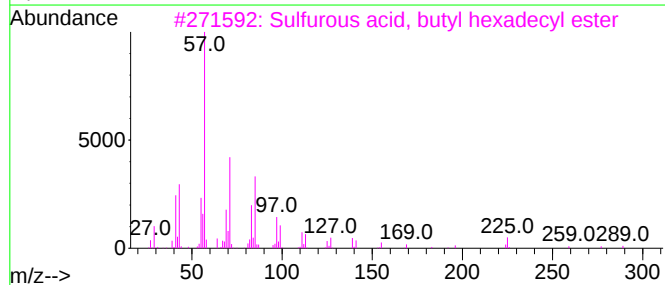
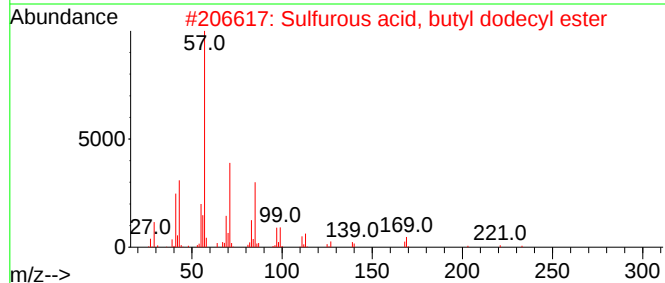
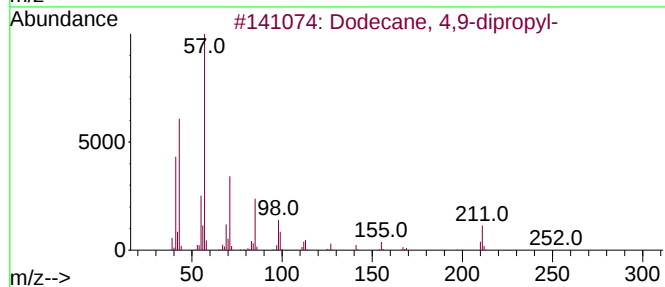
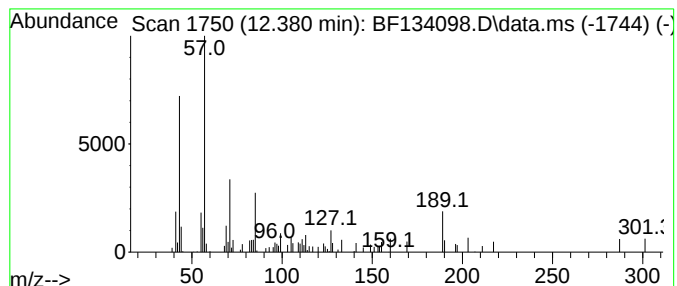
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Peak Number 4 unknown12.380 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	2.93 ng	137646	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	47
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	47
3			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	47
4			Pentadecane, 2-methyl-	226	C16H34	001560-93-6	46
5			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	43



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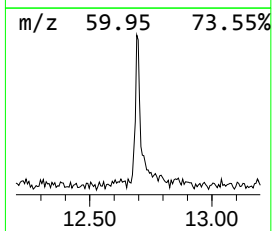
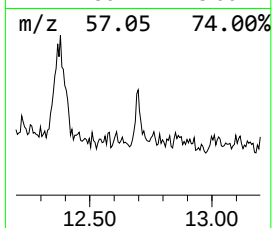
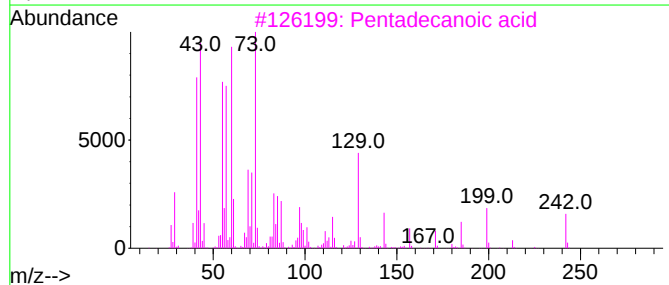
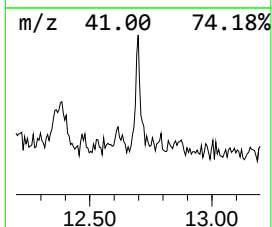
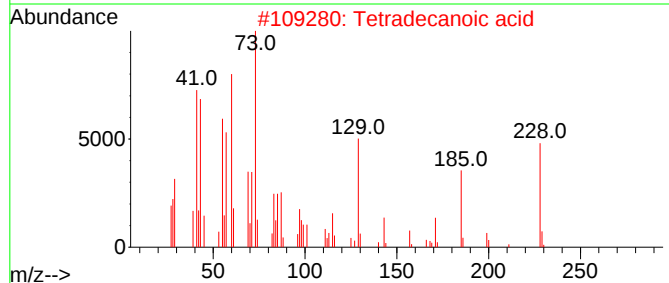
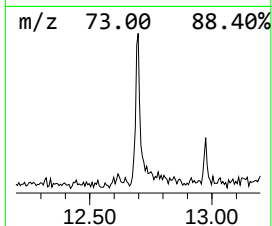
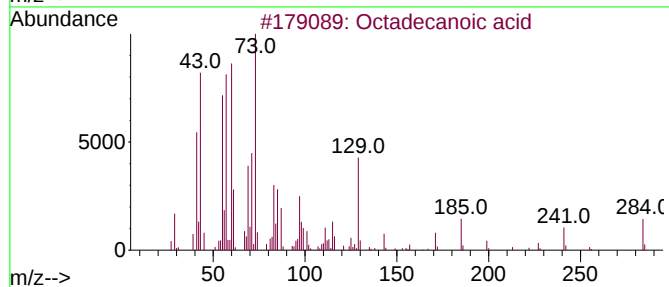
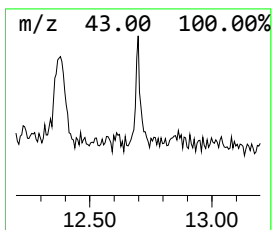
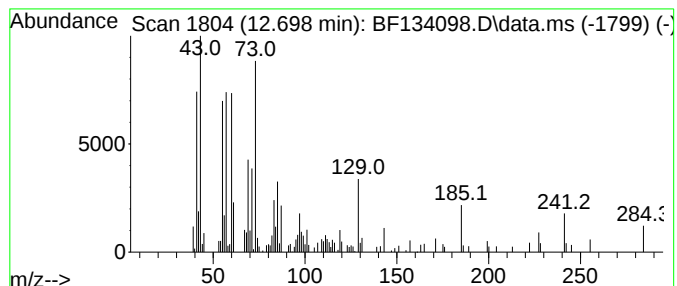
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.38 ng	111736	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58



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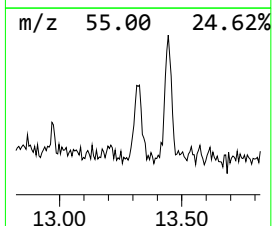
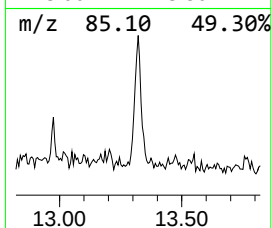
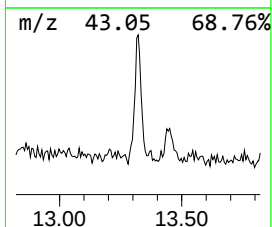
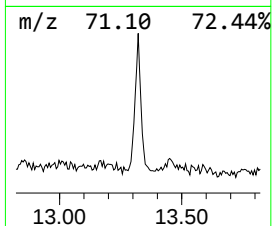
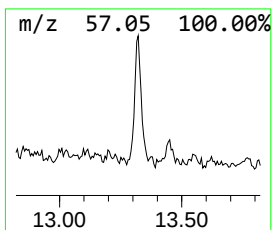
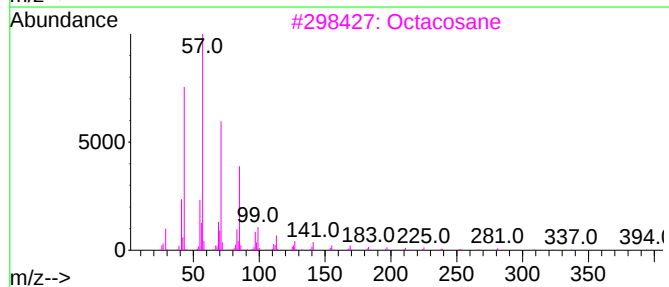
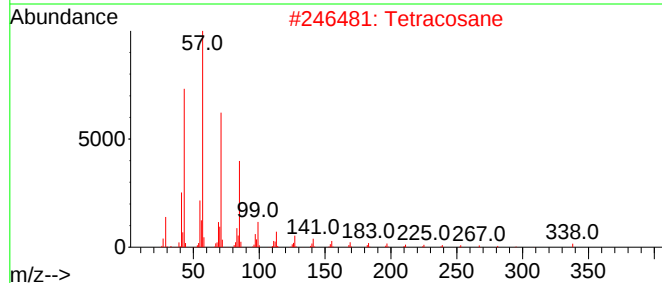
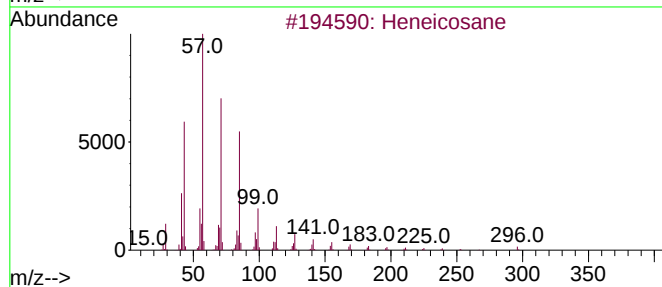
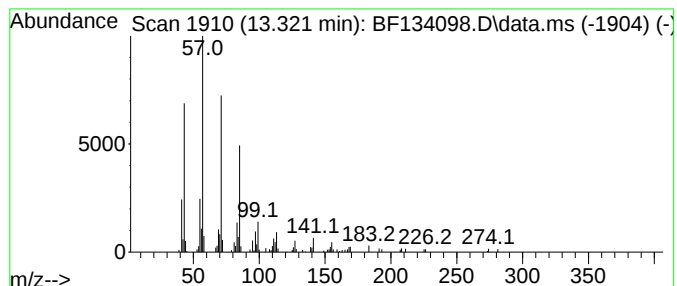
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.321	5.07 ng	140542	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	90
2		Tetracosane	338	C24H50	000646-31-1	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	86
5		2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20230601

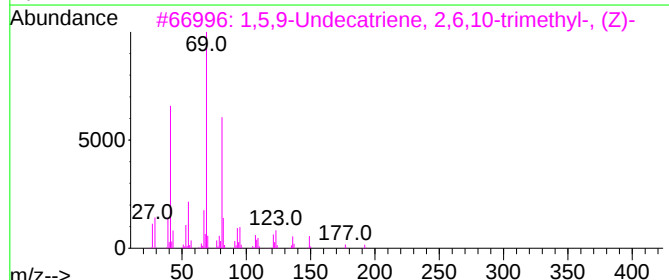
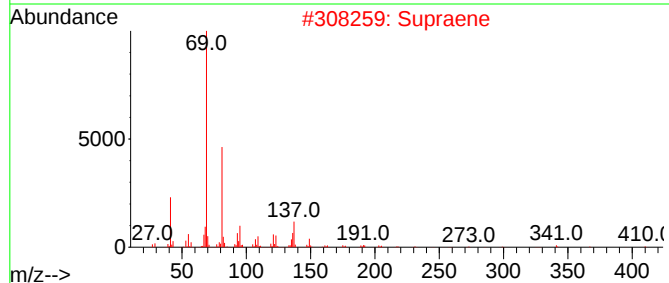
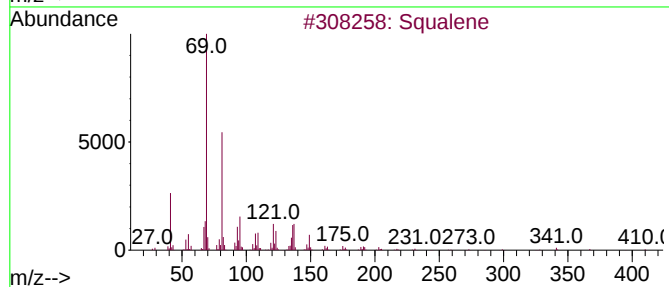
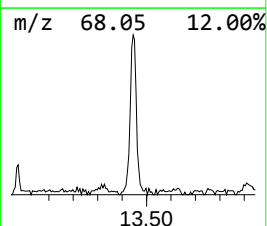
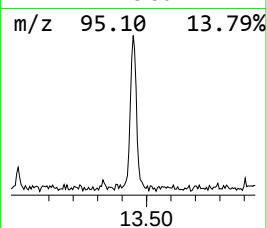
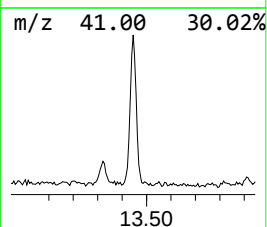
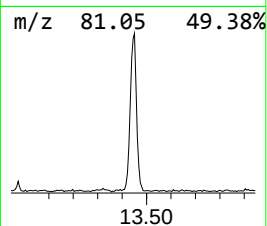
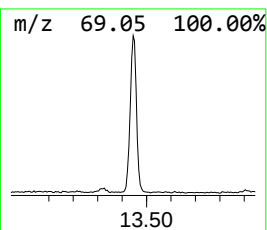
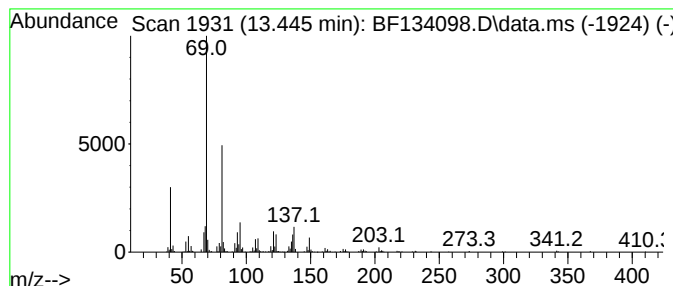
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	21.09 ng	585061	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5			3,7-Dimethyl-1-phenylsulfonfyl-2,...	278	C16H22O2S	1000432-27-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
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Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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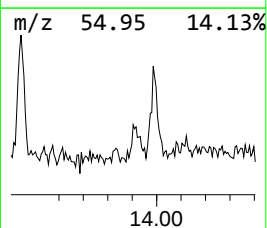
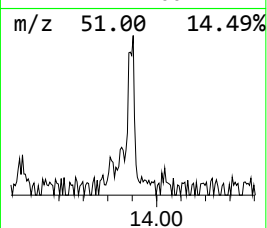
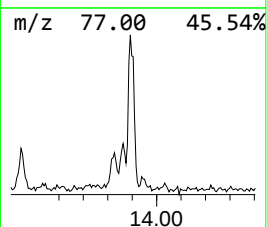
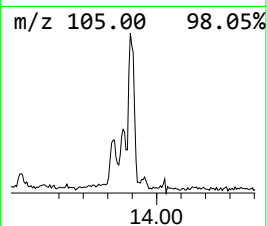
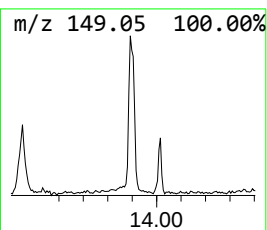
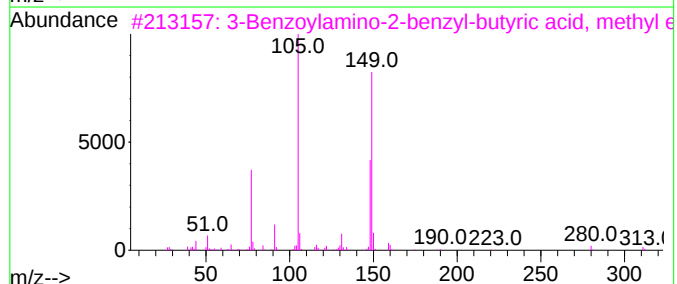
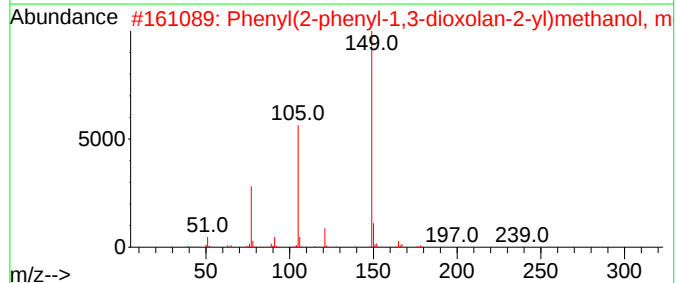
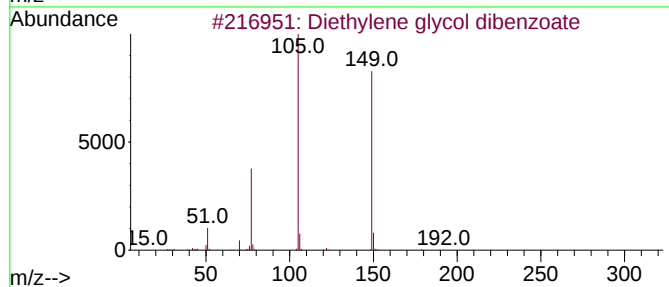
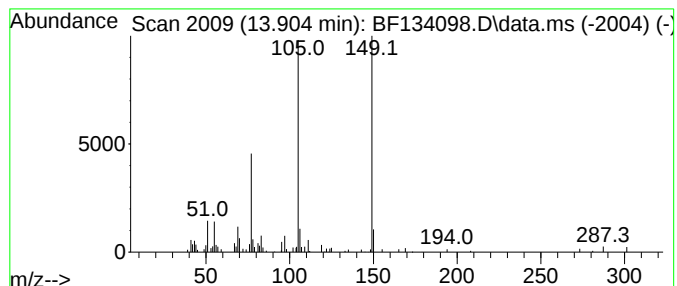
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.20 ng	116506	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol, methyl ester	270	C17H18O3	1000507-07-6	78
3			3-Benzoylamino-2-benzyl-butyric acid, methyl ester	311	C19H21NO3	1000193-12-7	78
4			Benzene, 1-isocyanato-3-methoxy-	149	C8H7NO2	018908-07-1	46
5			Phthalic acid, 2-cyclohexylethyl ester	402	C25H38O4	1000309-06-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
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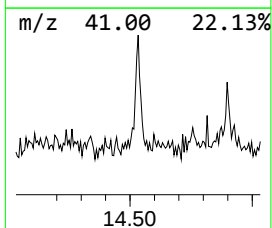
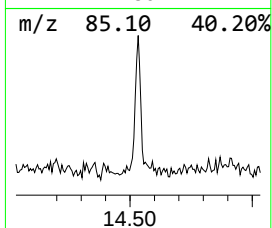
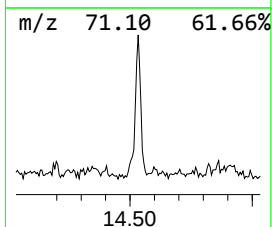
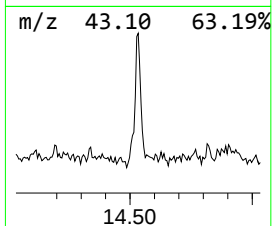
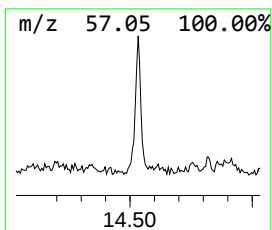
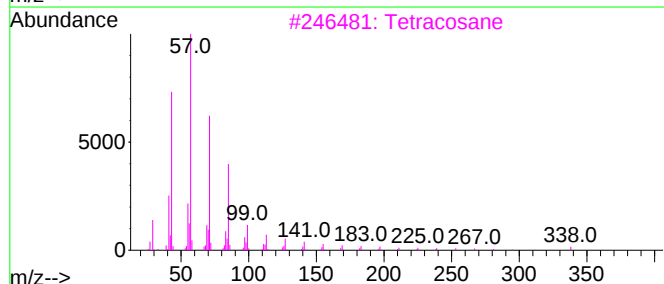
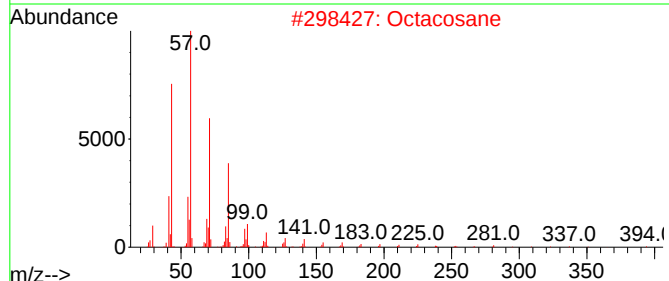
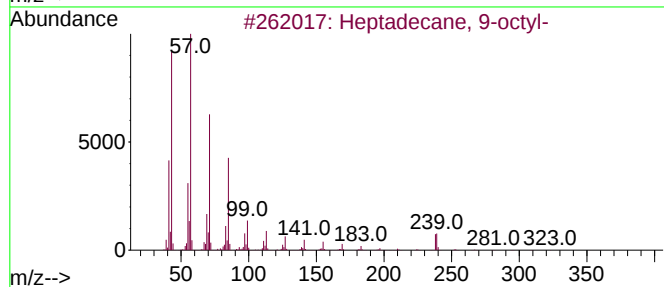
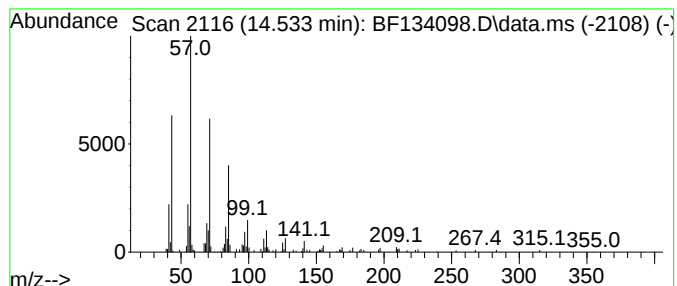
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	5.63 ng	156168	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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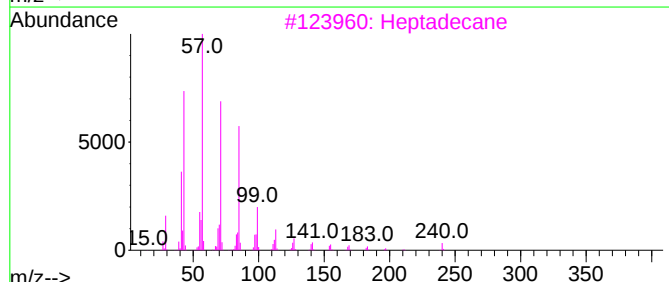
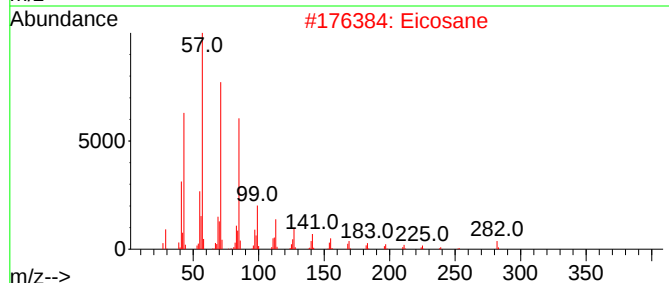
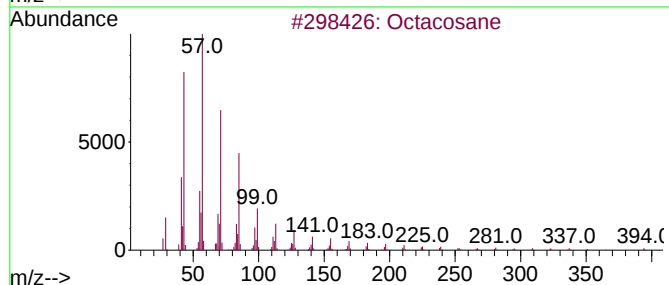
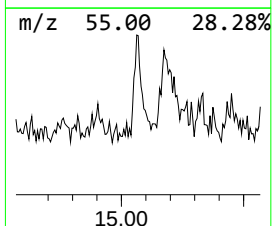
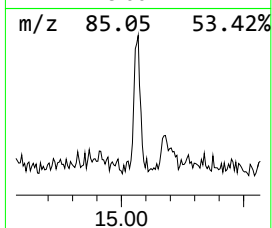
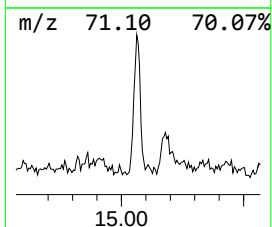
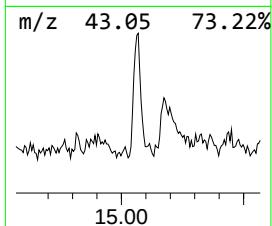
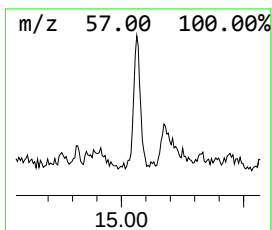
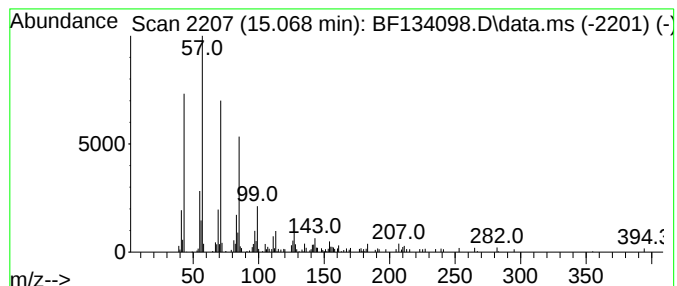
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.068	4.69 ng	159325	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
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Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-303-20230601

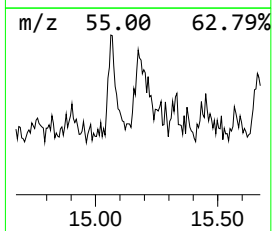
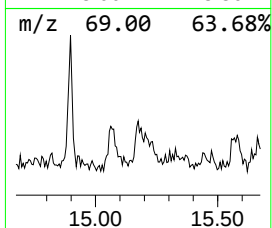
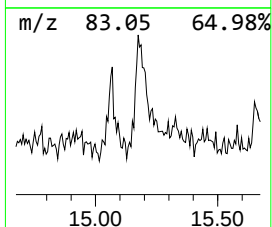
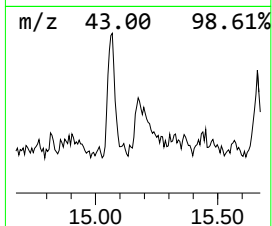
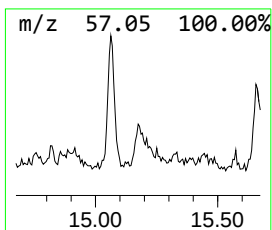
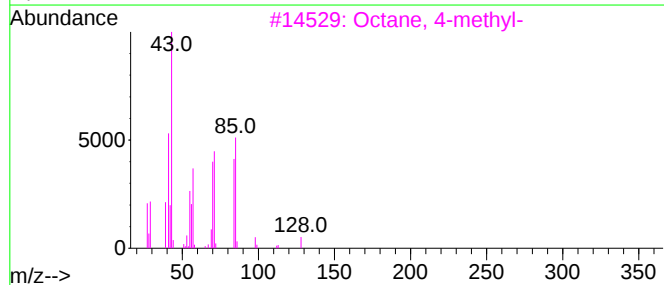
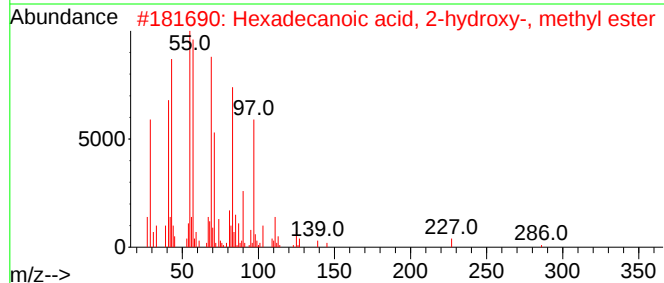
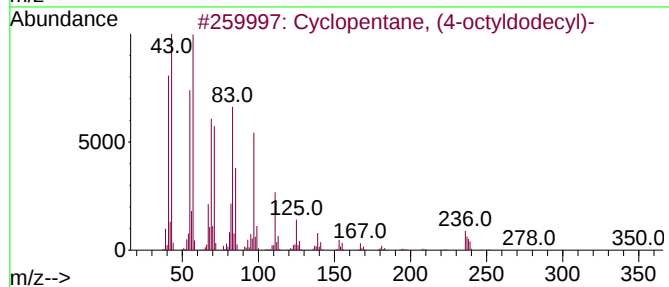
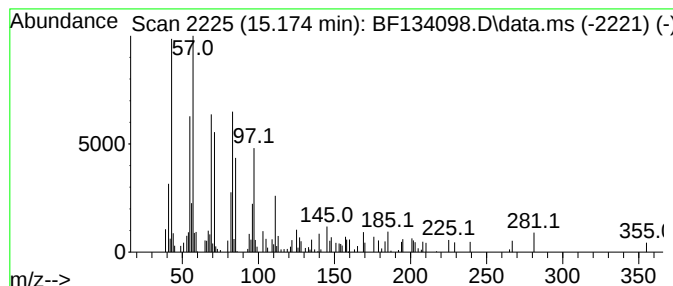
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentane, (4-octyldodec... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.48 ng	118341	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	58
2		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	38
3		Octane, 4-methyl-	128	C9H20	002216-34-4	25
4		Tridecane	184	C13H28	000629-50-5	22
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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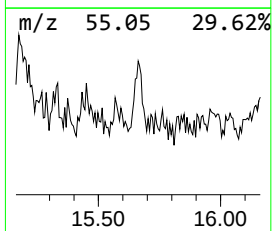
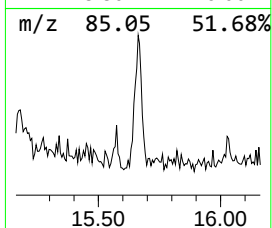
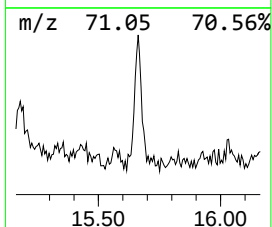
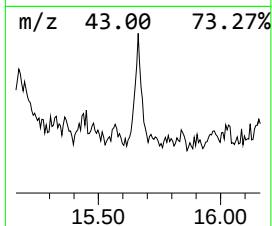
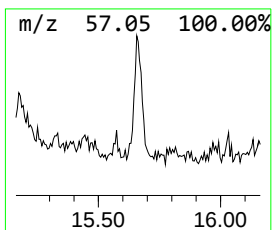
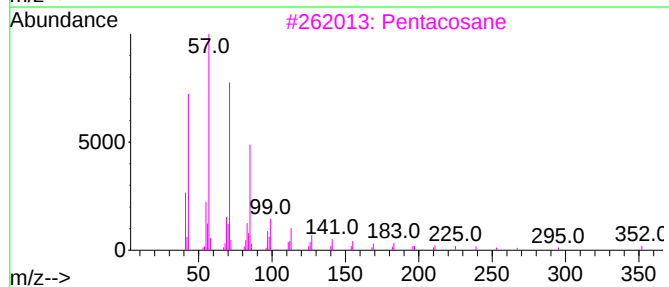
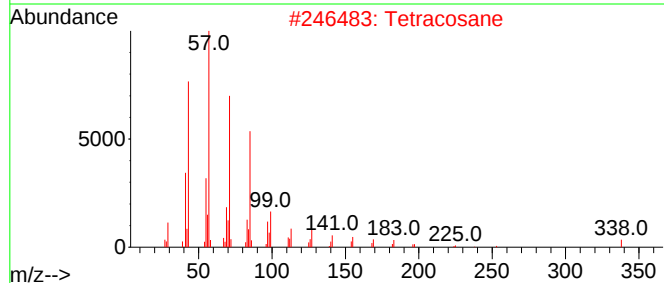
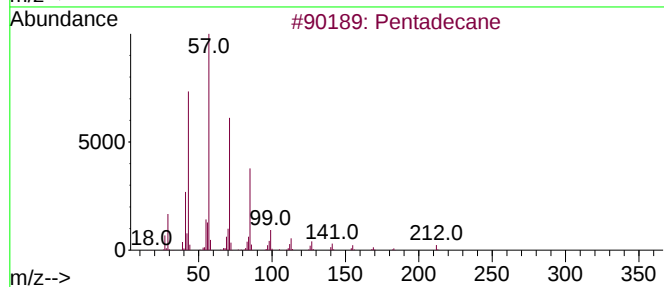
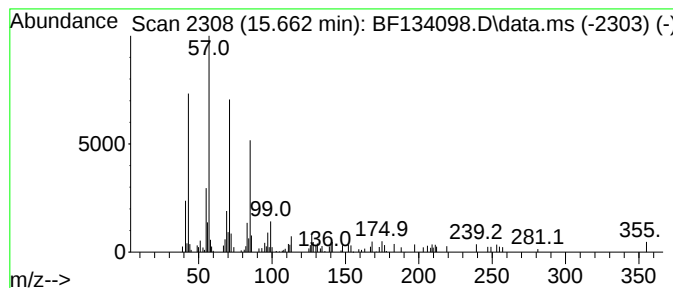
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.662	2.56 ng	87141	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane	212	C15H32	000629-62-9	90
2		Tetracosane	338	C24H50	000646-31-1	81
3		Pentacosane	352	C25H52	000629-99-2	74
4		Octacosane	394	C28H58	000630-02-4	74
5		Hexacosane	366	C26H54	000630-01-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-303-20230601

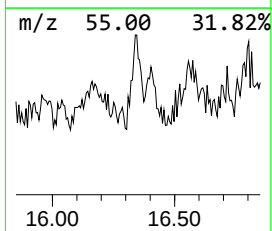
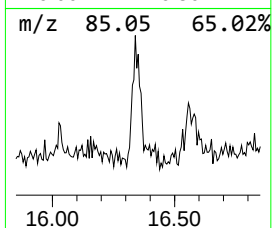
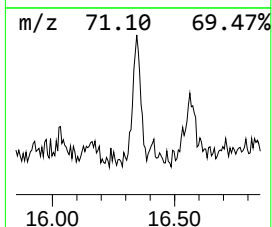
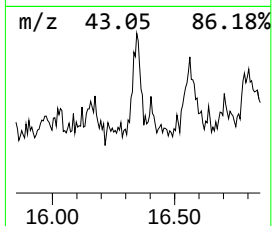
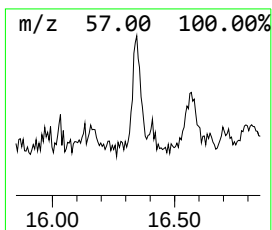
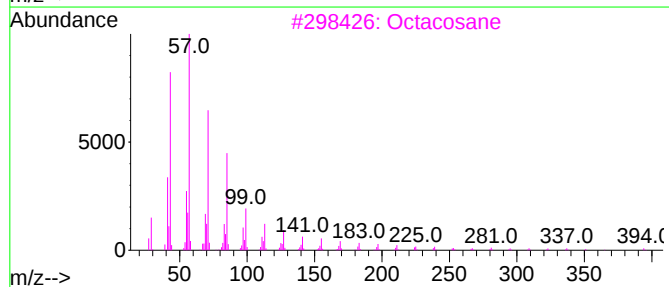
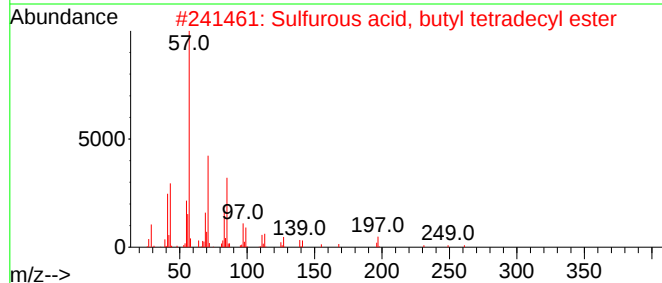
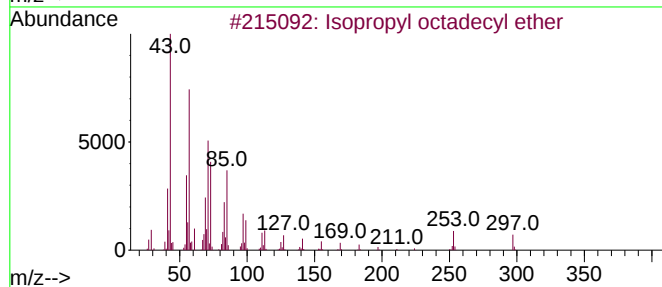
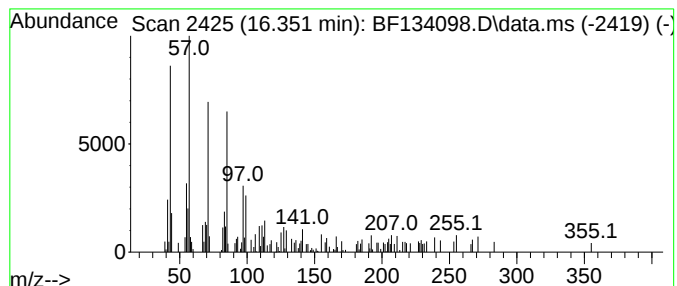
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Isopropyl octadecyl ether Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.351	2.20 ng	74905	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl octadecyl ether	312	C21H44O	1000406-34-2	72
2			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	72
3			Octacosane	394	C28H58	000630-02-4	68
4			4-Methylheneicosane	310	C22H46	025117-29-7	64
5			Heneicosane	296	C21H44	000629-94-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20230601

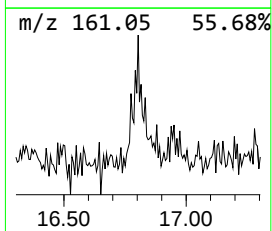
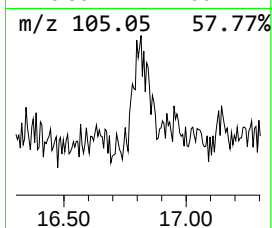
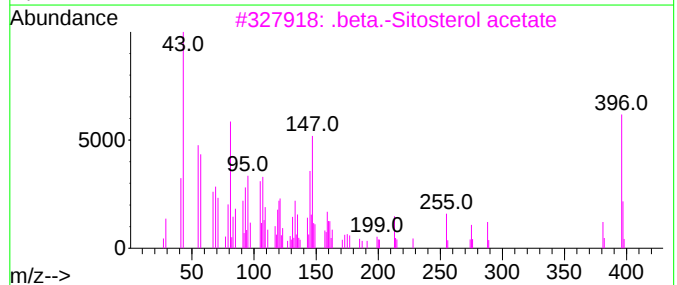
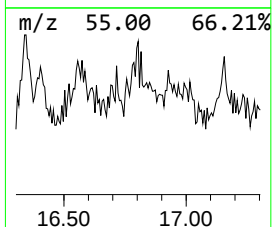
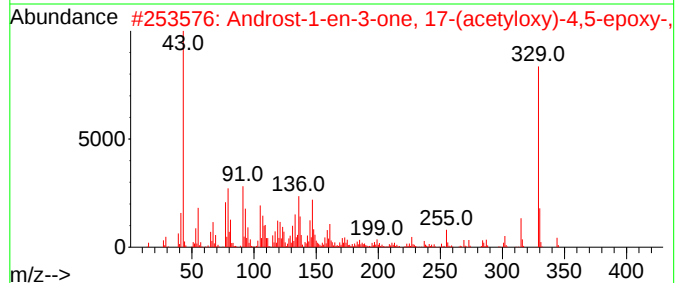
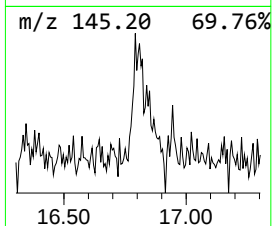
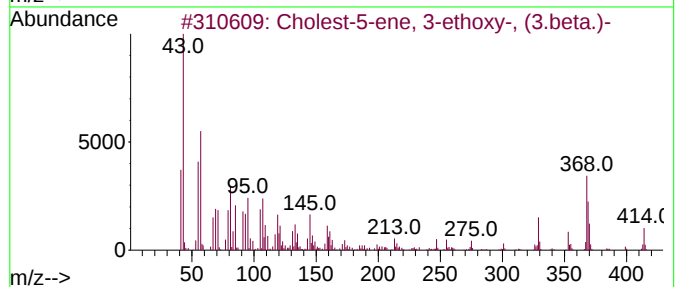
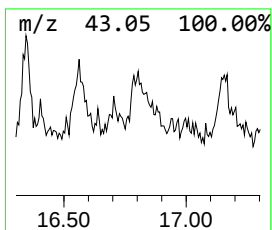
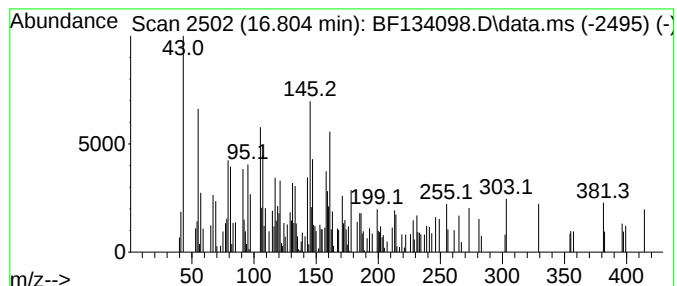
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.804 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.804	4.42 ng	150163	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	38
2			Androst-1-en-3-one, 17-(acetylox...	344	C21H28O4	013731-42-5	16
3			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	16
4			1-Methylcholest-1,3,5(10)-trien-...	382	C27H42O	017605-79-7	15
5			Norflurazon	303	C12H9ClF3N3O	027314-13-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134098.D
Acq On : 06 Jul 2023 15:00
Operator : CG\JU
Sample : 03021-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20230601

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.140	79.7	ng	2724170	1	6.845	683484	20.0
2-Pentanone, 4-...	5.075	3.9	ng	131728	1	6.845	683484	20.0
n-Hexadecanoic ...	11.904	6.1	ng	285169	4	11.374	938197	20.0
unknown12.380	12.380	2.9	ng	137646	4	11.374	938197	20.0
Octadecanoic acid	12.698	2.4	ng	111736	4	11.374	938197	20.0
Heneicosane	13.321	5.1	ng	140542	5	14.033	554873	20.0
Squalene	13.445	21.1	ng	585061	5	14.033	554873	20.0
Diethylene glyc...	13.904	4.2	ng	116506	5	14.033	554873	20.0
Heptadecane, 9-...	14.533	5.6	ng	156168	5	14.033	554873	20.0
Octacosane	15.068	4.7	ng	159325	6	15.539	679611	20.0
Cyclopentane, (...)	15.174	3.5	ng	118341	6	15.539	679611	20.0
Pentadecane	15.662	2.6	ng	87141	6	15.539	679611	20.0
Isopropyl octad...	16.351	2.2	ng	74905	6	15.539	679611	20.0
unknown16.804	16.804	4.4	ng	150163	6	15.539	679611	20.0