

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
 Data File : BF140634.D
 Acq On : 26 Nov 2024 11:52
 Operator : RC/JU
 Sample : P4960-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW2

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140634.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	34	rVB	627266	1035120	42.95%	5.719%
2	5.099	506	511	520	rVB	20341	31700	1.32%	0.175%
3	5.504	574	580	597	rBV	1391388	1908683	79.20%	10.546%
4	6.510	744	751	769	rBV	1422465	1986161	82.41%	10.974%
5	6.869	807	812	819	rBV	420273	510357	21.18%	2.820%
6	7.434	902	908	917	rBV	936638	1269368	52.67%	7.013%
7	7.681	943	950	957	rBV	25090	35119	1.46%	0.194%
8	8.151	1024	1030	1044	rBV	511442	662087	27.47%	3.658%
9	9.222	1206	1212	1223	rBV	1851439	2409982	100.00%	13.315%
10	9.904	1323	1328	1339	rBV	591646	757701	31.44%	4.186%
11	10.622	1444	1450	1455	rBV	266134	354420	14.71%	1.958%
12	10.698	1458	1463	1477	rVB	1143173	1483706	61.57%	8.198%
13	10.928	1498	1502	1507	rVB	25983	32361	1.34%	0.179%
14	11.057	1517	1524	1533	rBV7	18227	59860	2.48%	0.331%
15	11.398	1576	1582	1589	rBV	598103	778005	32.28%	4.299%
16	11.916	1664	1670	1691	rBV	301646	542555	22.51%	2.998%
17	12.075	1692	1697	1700	rBV2	38259	71016	2.95%	0.392%
18	12.569	1775	1781	1786	rBV	33037	67215	2.79%	0.371%
19	12.616	1786	1789	1798	rVV8	13542	32976	1.37%	0.182%
20	12.704	1799	1804	1816	rVV	78677	145845	6.05%	0.806%
21	12.980	1846	1851	1870	rBV	1608336	2092179	86.81%	11.559%
22	13.392	1915	1921	1928	rBV	39266	76411	3.17%	0.422%
23	13.522	1936	1943	1955	rVB	160379	335085	13.90%	1.851%
24	13.880	1999	2004	2017	rBV	65748	142746	5.92%	0.789%
25	14.045	2023	2032	2040	rVB	331481	524309	21.76%	2.897%
26	14.545	2113	2117	2123	rVB	36768	64594	2.68%	0.357%
27	15.057	2199	2204	2209	rBV2	19593	36316	1.51%	0.201%
28	15.533	2279	2285	2294	rBV	297808	545006	22.61%	3.011%
29	16.710	2479	2485	2502	rVB	31032	108550	4.50%	0.600%

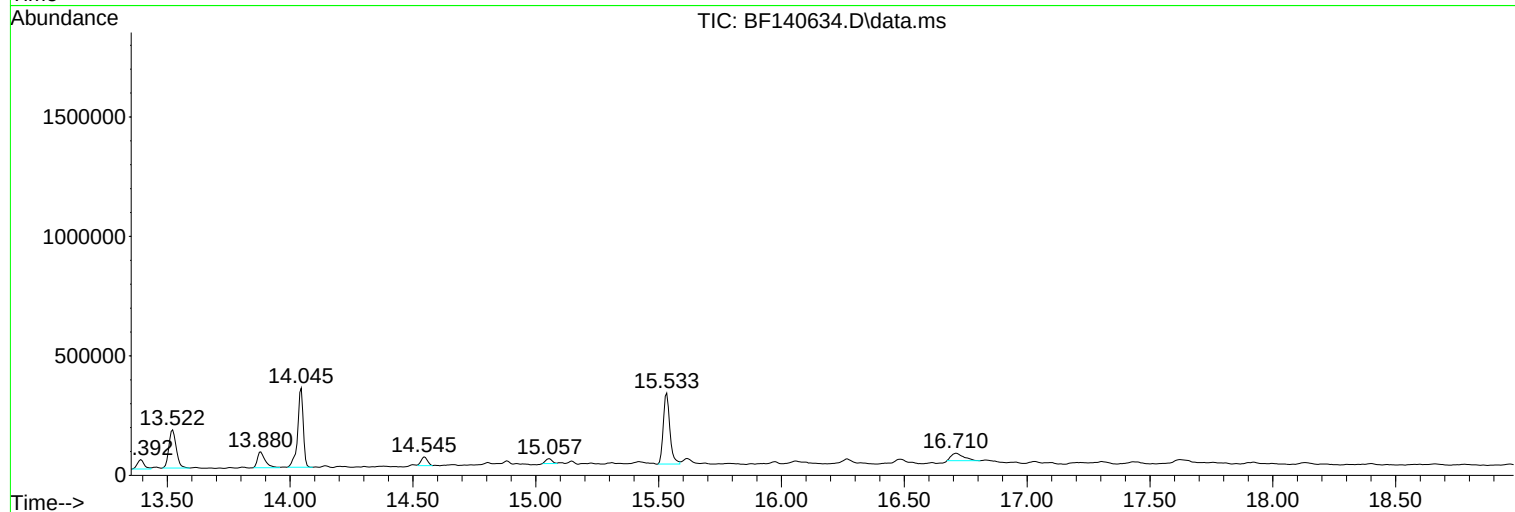
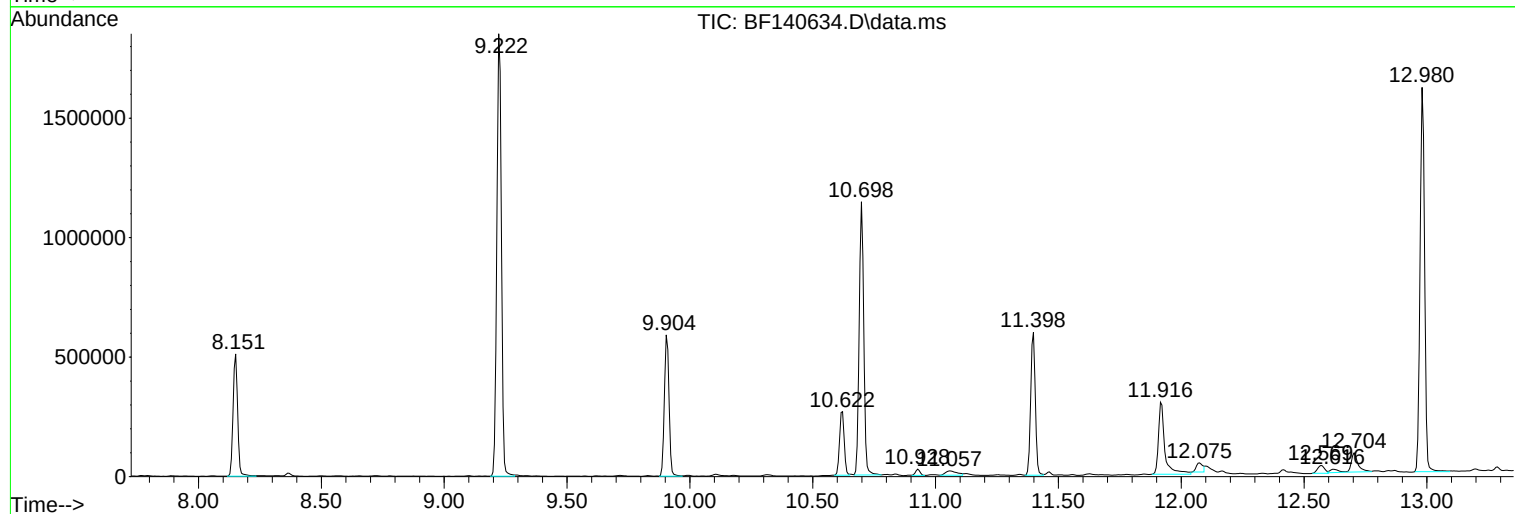
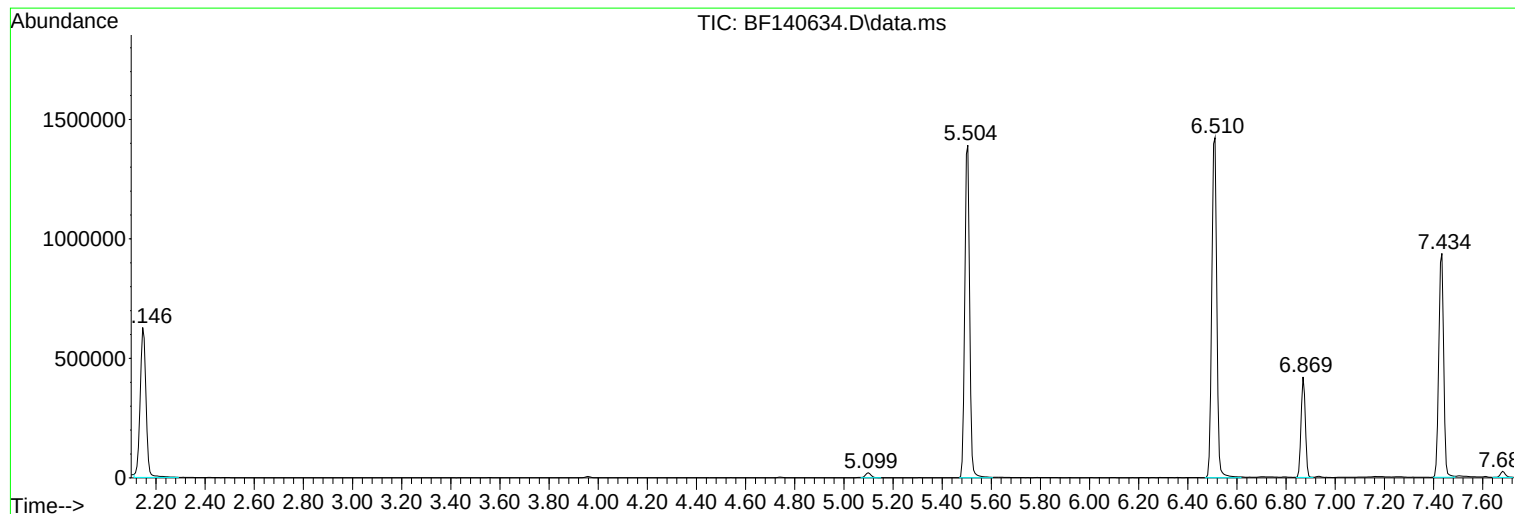
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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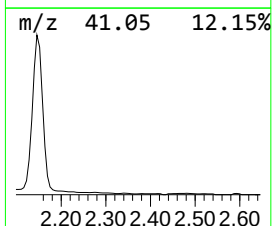
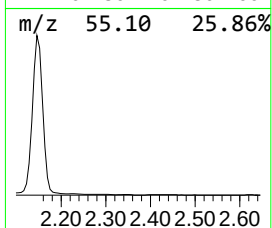
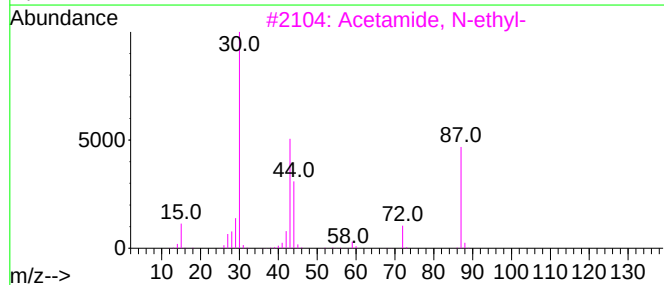
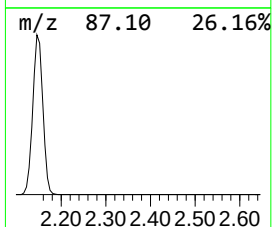
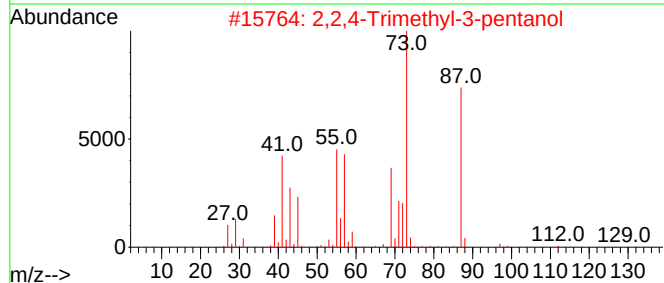
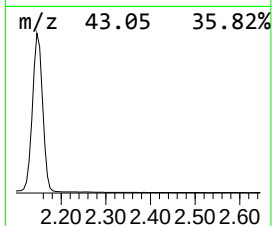
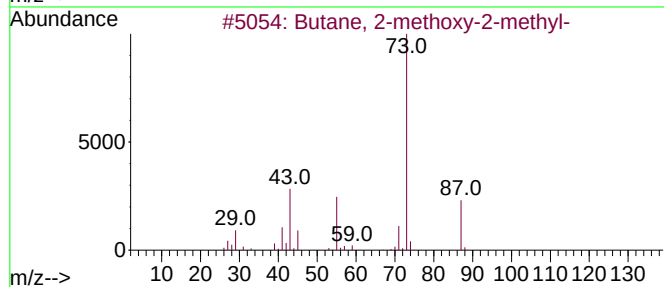
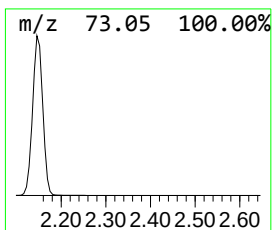
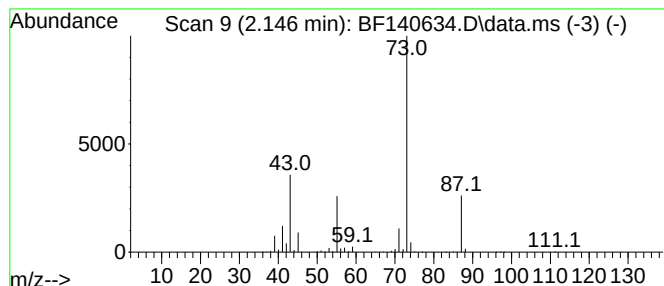
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	40.56 ng	1035120	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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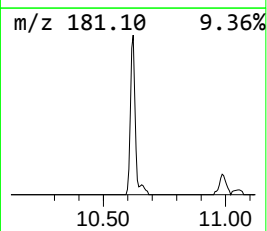
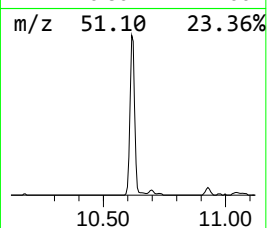
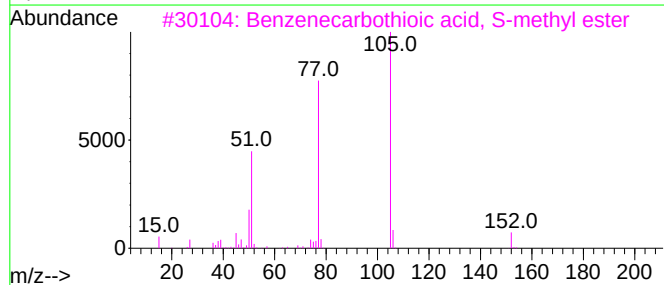
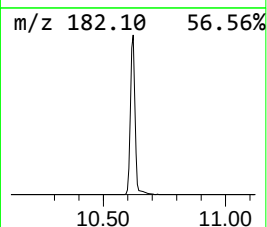
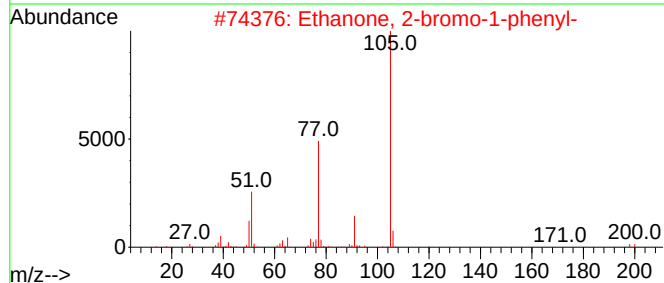
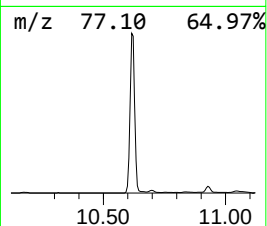
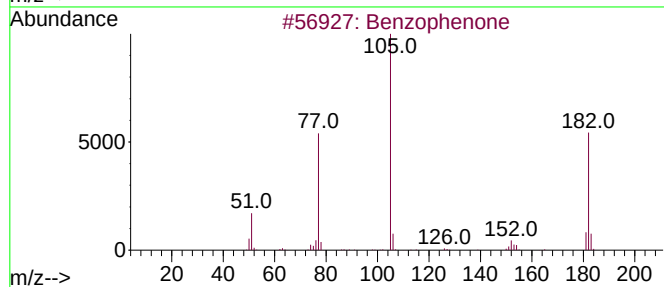
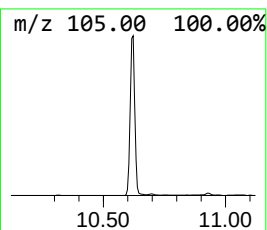
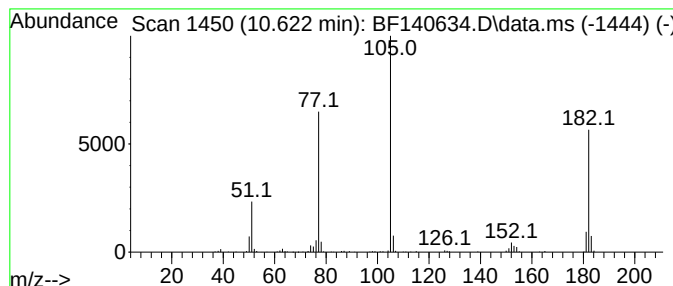
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	9.36 ng	354420	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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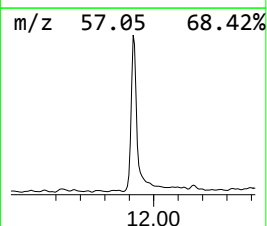
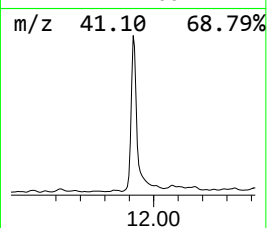
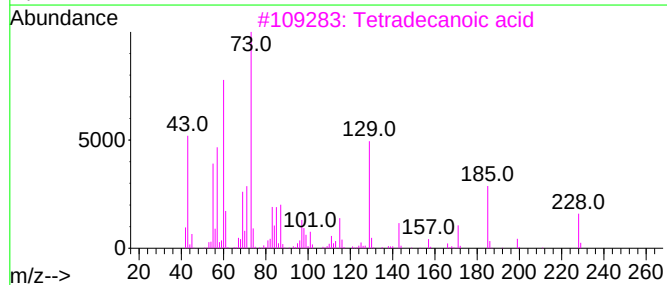
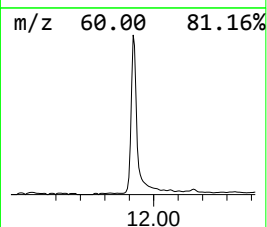
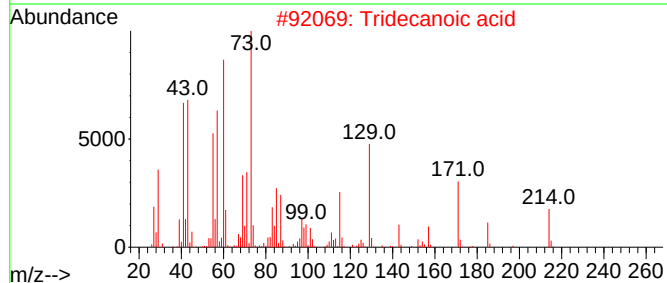
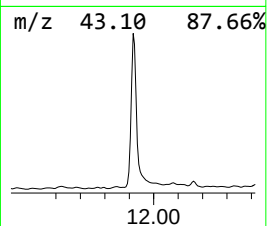
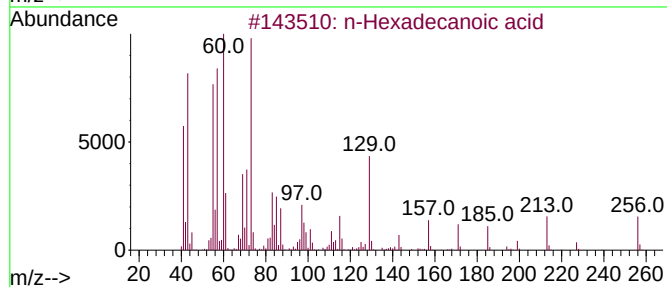
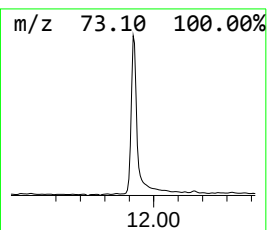
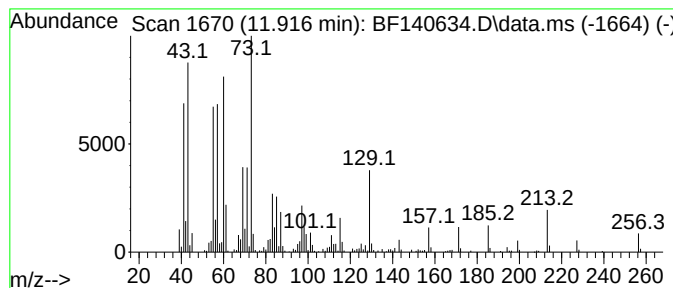
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	13.95 ng	542555	Phenanthrene-d10	11.398

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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ALS Vial : 7 Sample Multiplier: 1

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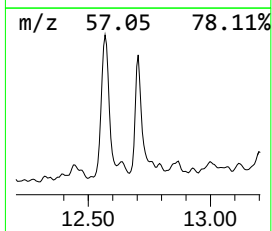
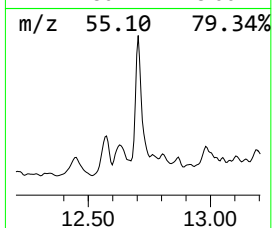
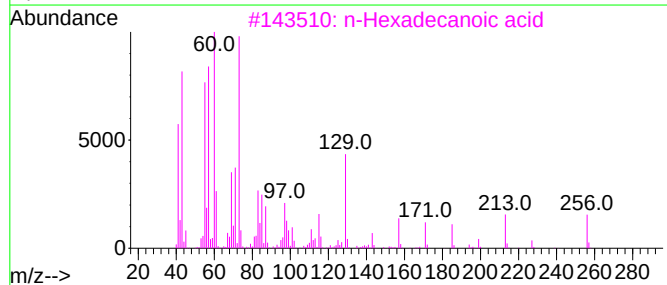
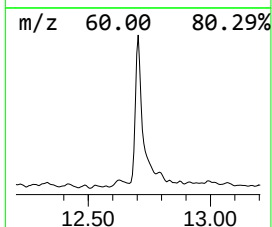
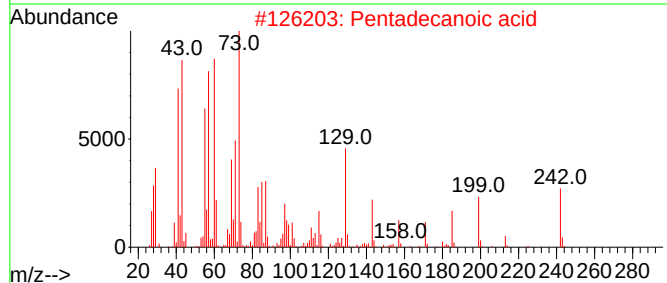
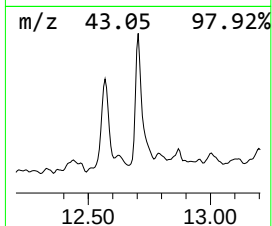
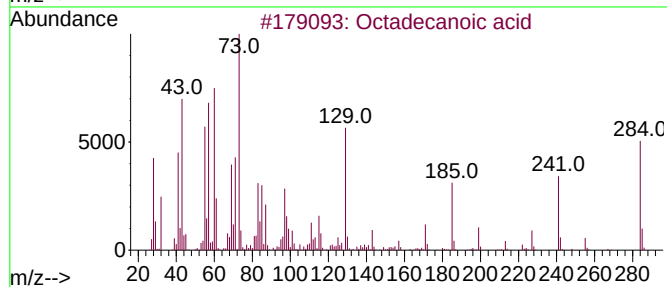
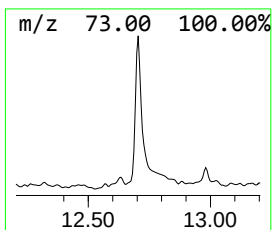
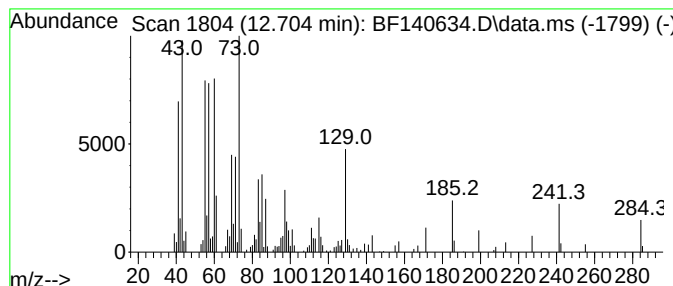
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.75 ng	145845	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	55



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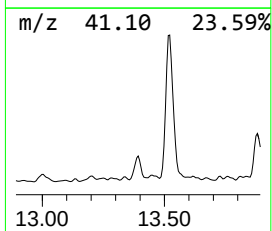
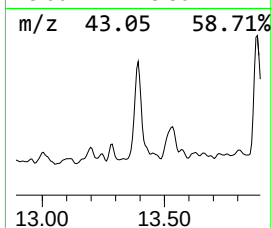
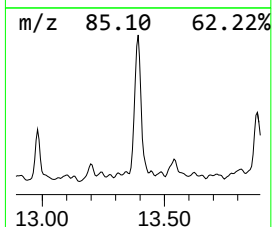
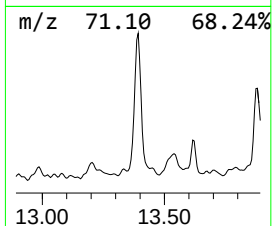
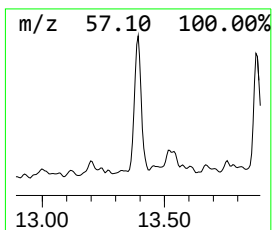
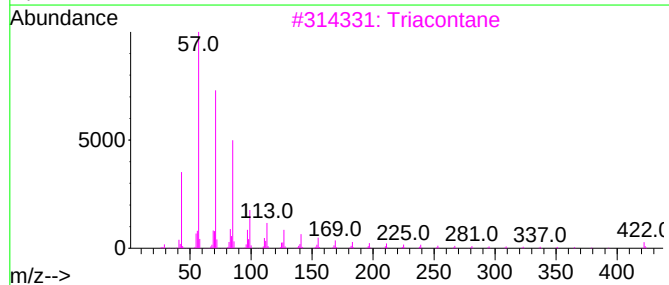
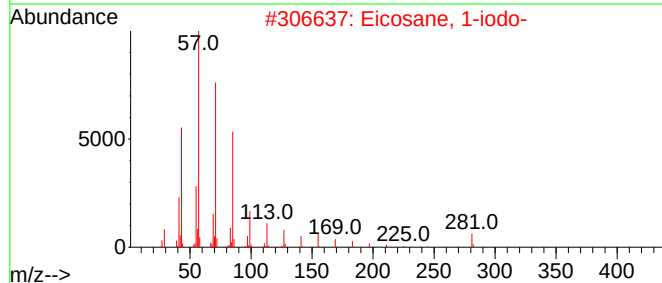
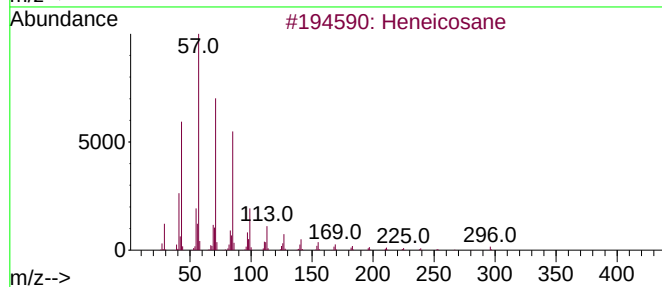
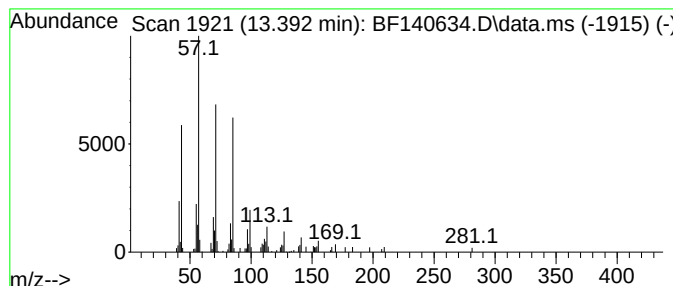
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.392	2.91 ng	76411	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	90



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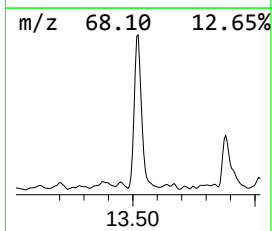
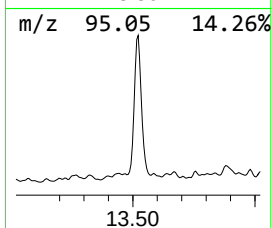
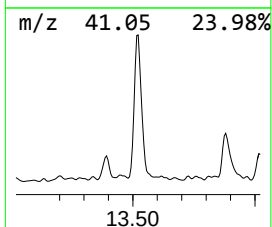
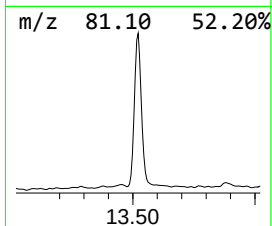
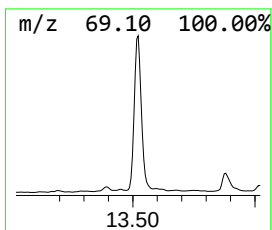
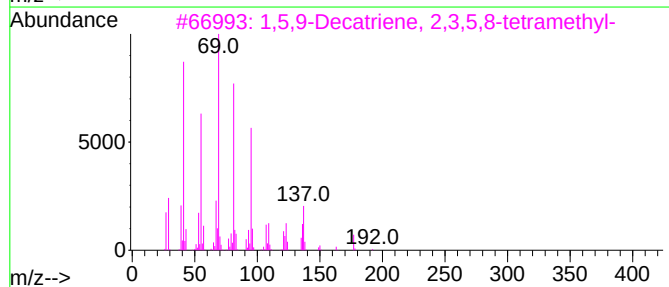
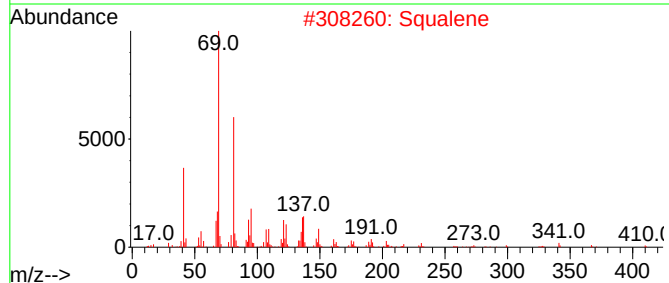
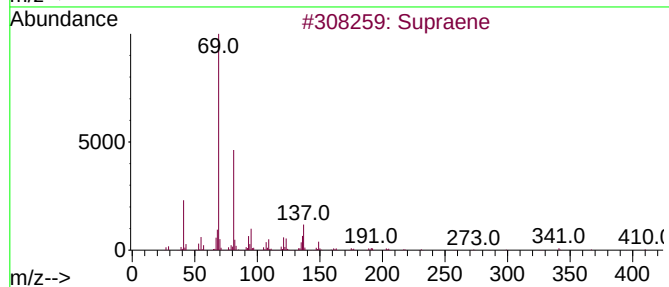
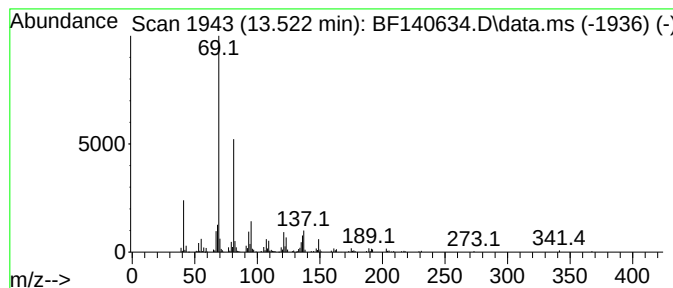
Instrument :
BNA_F
ClientSampleId :
SW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.522	12.78 ng	335085	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
4	(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140634.D
Acq On : 26 Nov 2024 11:52
Operator : RC/JU
Sample : P4960-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

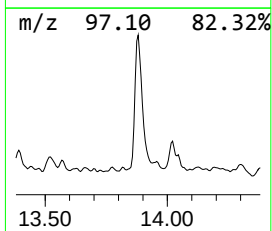
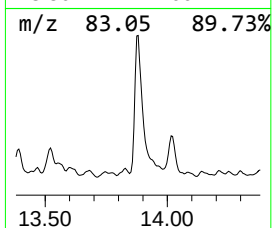
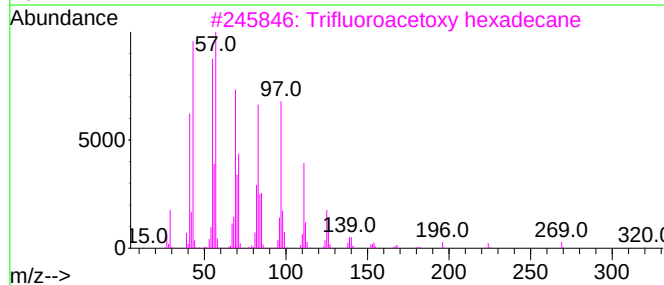
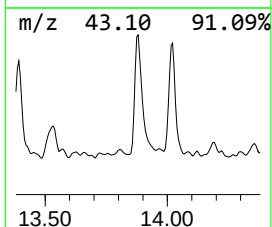
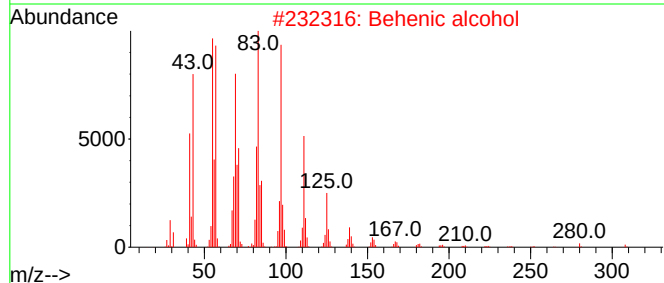
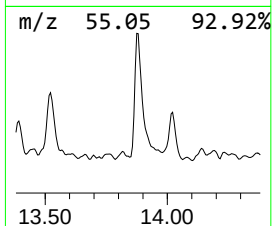
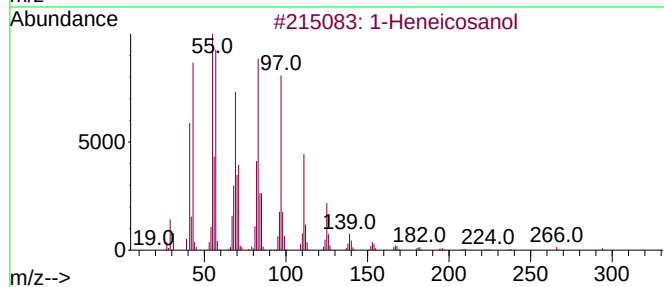
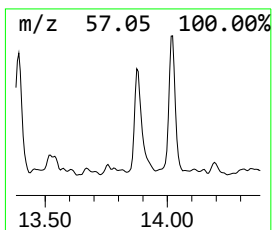
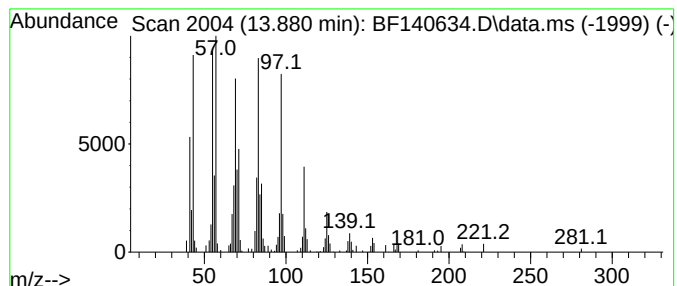
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.45 ng	142746	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4			1-Hexacosene	364	C26H52	018835-33-1	95
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140634.D
Acq On : 26 Nov 2024 11:52
Operator : RC/JU
Sample : P4960-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

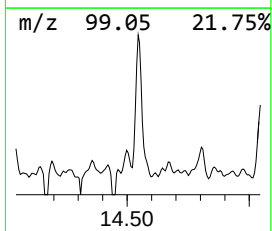
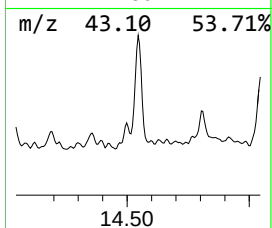
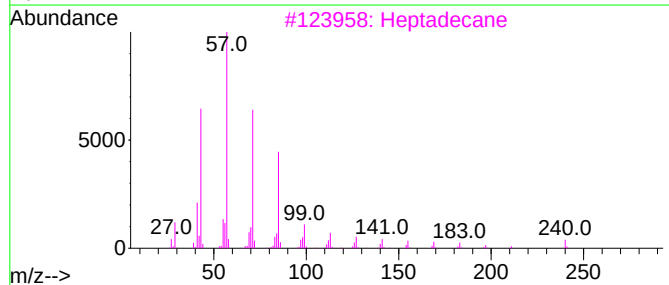
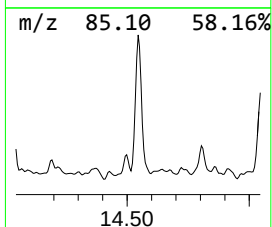
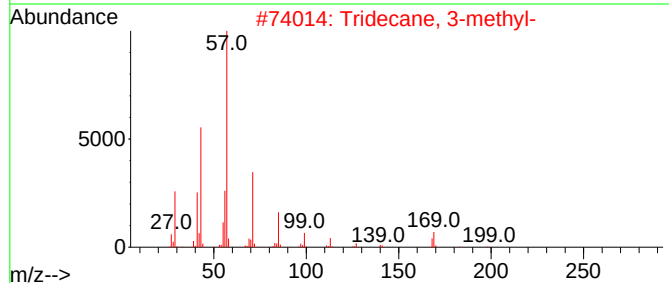
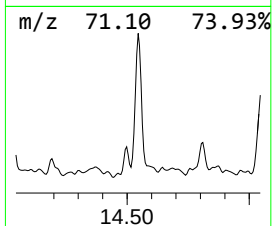
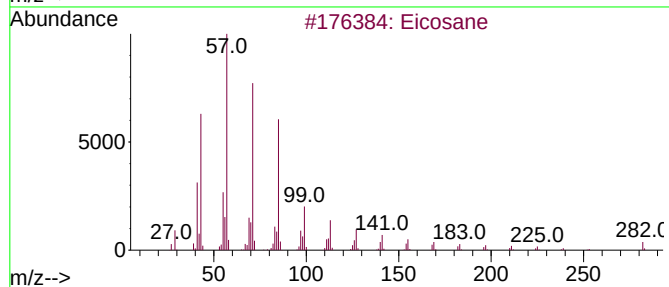
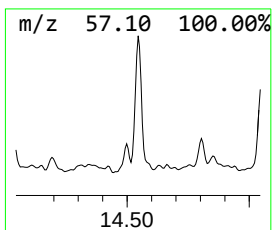
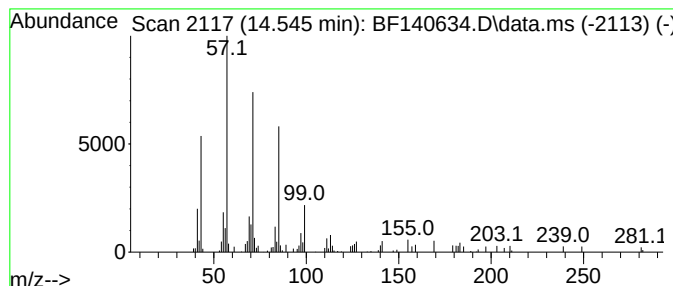
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	2.46 ng	64594	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	86
2			Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
3			Heptadecane	240	C17H36	000629-78-7	80
4			Heneicosane	296	C21H44	000629-94-7	80
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140634.D
Acq On : 26 Nov 2024 11:52
Operator : RC/JU
Sample : P4960-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

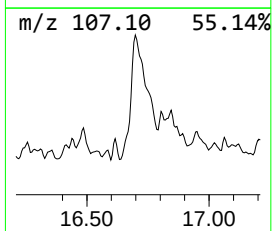
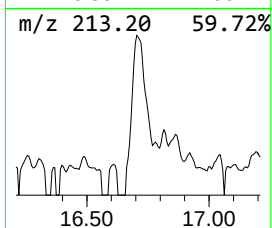
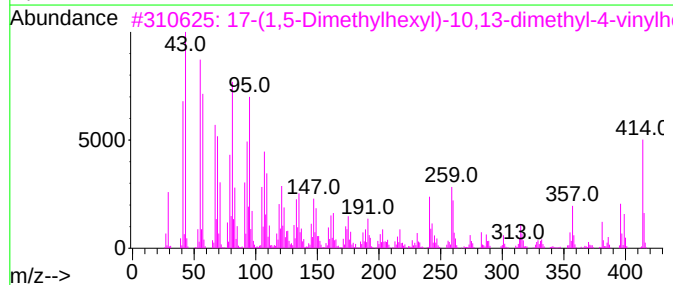
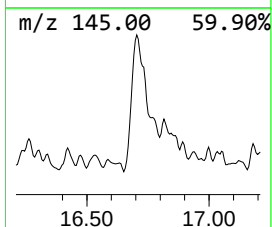
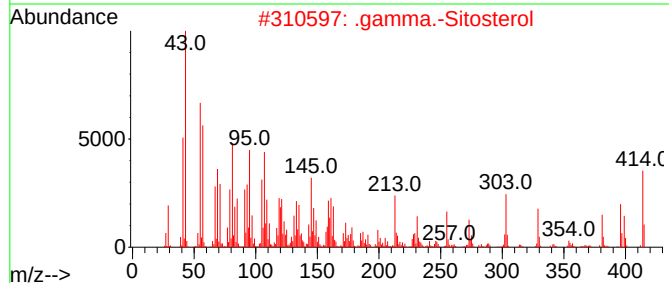
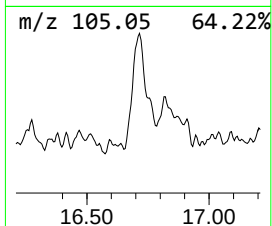
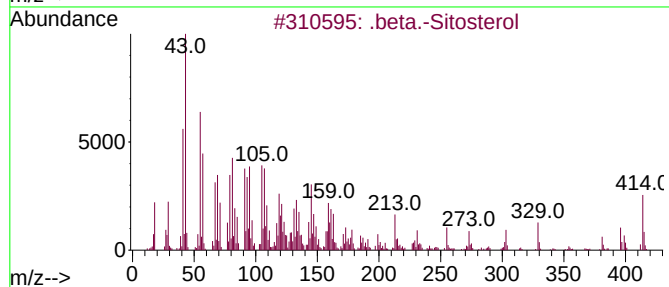
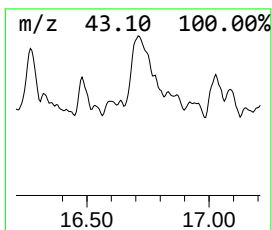
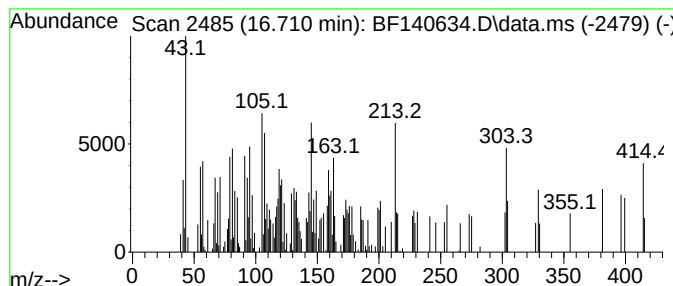
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	3.98 ng	108550	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	93
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
3			17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	56
4			(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	10
5			Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140634.D
Acq On : 26 Nov 2024 11:52
Operator : RC/JU
Sample : P4960-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	40.6	ng	1035120	1	6.869	510357	20.0
Benzophenone	10.622	9.4	ng	354420	3	9.904	757701	20.0
n-Hexadecanoic ...	11.916	13.9	ng	542555	4	11.398	778005	20.0
Octadecanoic acid	12.704	3.8	ng	145845	4	11.398	778005	20.0
Heneicosane	13.392	2.9	ng	76411	5	14.045	524309	20.0
Supraene	13.522	12.8	ng	335085	5	14.045	524309	20.0
1-Heneicosanol	13.880	5.5	ng	142746	5	14.045	524309	20.0
Eicosane	14.545	2.5	ng	64594	5	14.045	524309	20.0
.beta.-Sitosterol	16.709	4.0	ng	108550	6	15.533	545006	20.0