

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
 Data File : BF133169.D
 Acq On : 01 May 2023 22:16
 Operator : CG\JU
 Sample : 02563-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-03-042823

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	478	482	488	rVB	54421	70143	1.55%	0.196%
2	5.340	548	553	556	rBV	4134455	3922691	86.66%	10.961%
3	6.369	723	728	731	rBV	4150606	3962466	87.54%	11.072%
4	6.728	786	789	793	rBV	1672422	1302192	28.77%	3.639%
5	7.292	880	885	888	rBV	3001417	2574651	56.88%	7.194%
6	8.016	1004	1008	1011	rBV	2033780	1773956	39.19%	4.957%
7	9.092	1187	1191	1194	rVB	5233252	4526273	100.00%	12.648%
8	9.498	1254	1260	1262	rBV3	40036	53497	1.18%	0.149%
9	9.763	1302	1305	1309	rVB	2382976	1901644	42.01%	5.314%
10	10.204	1377	1380	1383	rVB	79606	58628	1.30%	0.164%
11	10.427	1415	1418	1421	rVV	56811	53495	1.18%	0.149%
12	10.475	1423	1426	1430	rVB	593162	465031	10.27%	1.299%
13	10.551	1435	1439	1442	rBV	2720209	2236341	49.41%	6.249%
14	10.675	1458	1460	1462	rBV2	131711	143466	3.17%	0.401%
15	10.780	1476	1478	1482	rVB	56145	50436	1.11%	0.141%
16	11.127	1534	1537	1539	rBV	129017	106587	2.35%	0.298%
17	11.157	1539	1542	1546	rVB	110050	101637	2.25%	0.284%
18	11.245	1553	1557	1560	rBV	2153684	1717622	37.95%	4.800%
19	11.269	1560	1561	1564	rVV	163957	86997	1.92%	0.243%
20	11.316	1567	1569	1572	rVB2	59864	54430	1.20%	0.152%
21	11.551	1607	1609	1612	rBV	129759	94255	2.08%	0.263%
22	11.651	1623	1626	1631	rVB	498714	372945	8.24%	1.042%
23	11.786	1645	1649	1652	rBV2	567726	561393	12.40%	1.569%
24	11.957	1676	1678	1681	rBV	106775	83552	1.85%	0.233%
25	12.333	1739	1742	1744	rBV	1480445	1445130	31.93%	4.038%
26	12.357	1744	1746	1749	rVB	1129378	904089	19.97%	2.526%
27	12.451	1758	1762	1766	rBV2	274903	407881	9.01%	1.140%
28	12.569	1779	1782	1788	rBV	223522	243233	5.37%	0.680%
29	12.680	1798	1801	1804	rVB	229192	206725	4.57%	0.578%
30	12.721	1805	1808	1810	rBV	72929	56653	1.25%	0.158%
31	12.833	1823	1827	1830	rBV	3933337	3437996	75.96%	9.607%
32	13.074	1866	1868	1872	rVB2	104230	94058	2.08%	0.263%
33	13.416	1924	1926	1929	rBV2	80810	69993	1.55%	0.196%
34	13.751	1980	1983	1985	rBV3	116980	161171	3.56%	0.450%
35	13.880	2001	2005	2008	rBV	1340652	1292877	28.56%	3.613%
36	14.063	2034	2036	2039	rBV	103858	88992	1.97%	0.249%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.368	2086	2088	2090	rVB	138642	100431	2.22%	0.281%
38	15.304	2243	2247	2250	rBV	872551	1003827	22.18%	2.805%

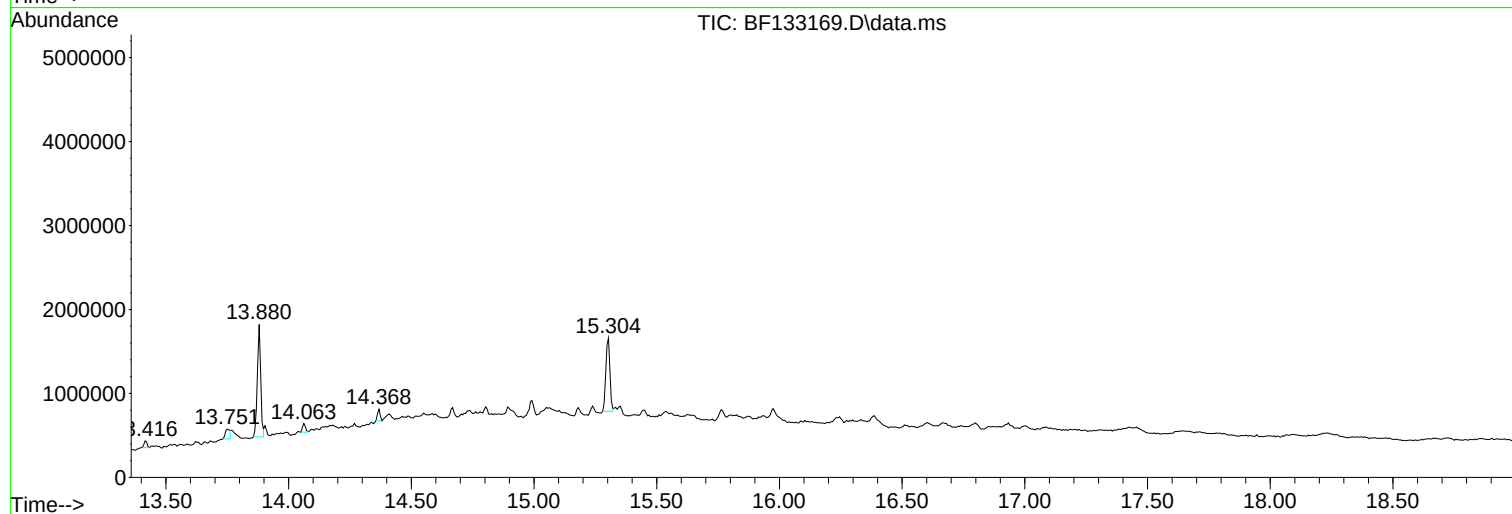
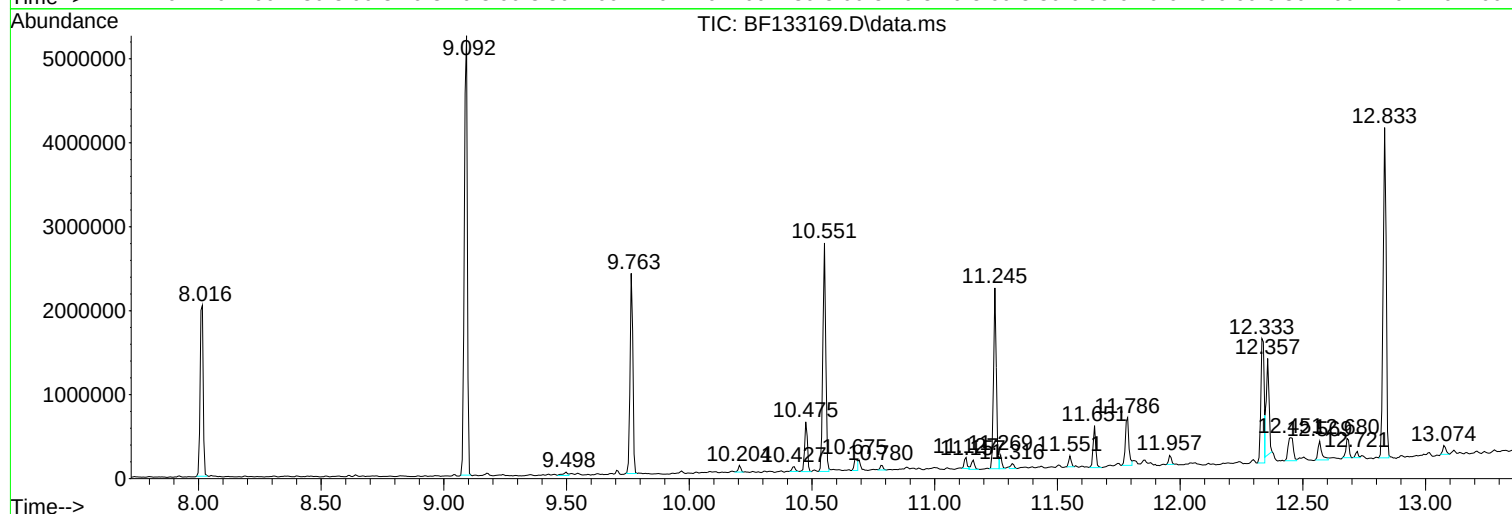
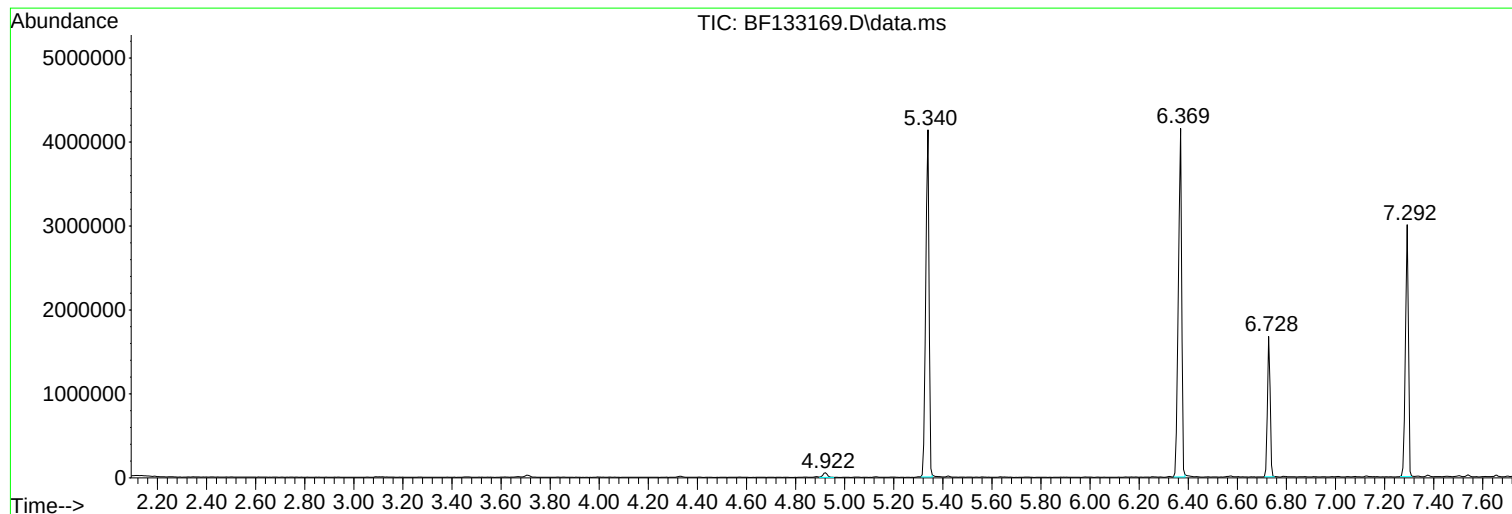
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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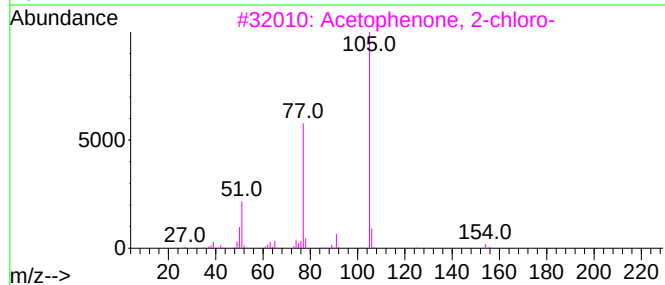
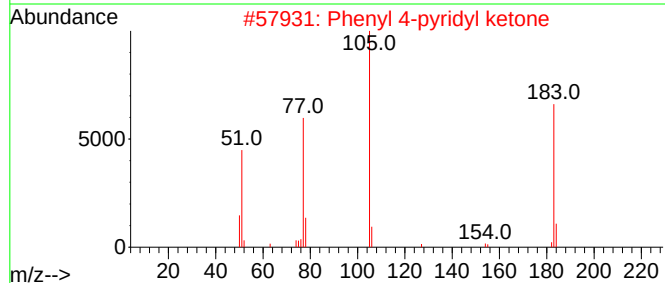
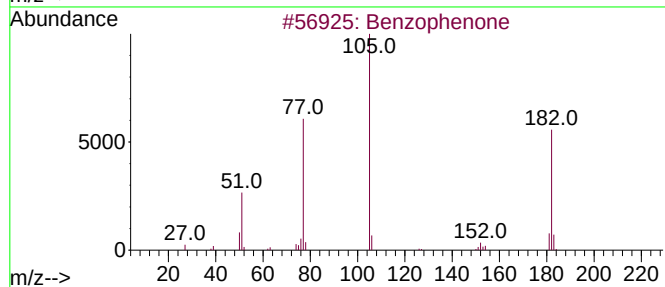
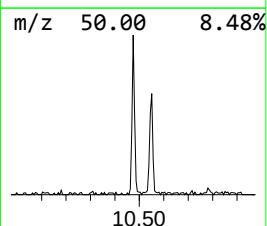
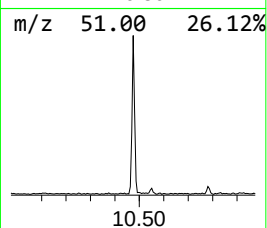
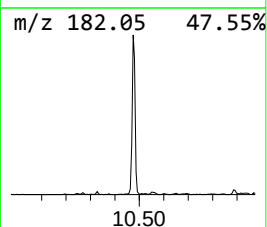
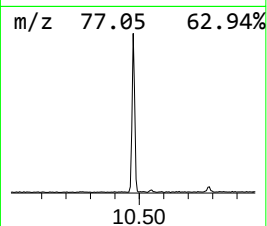
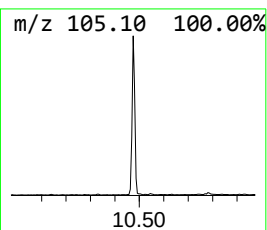
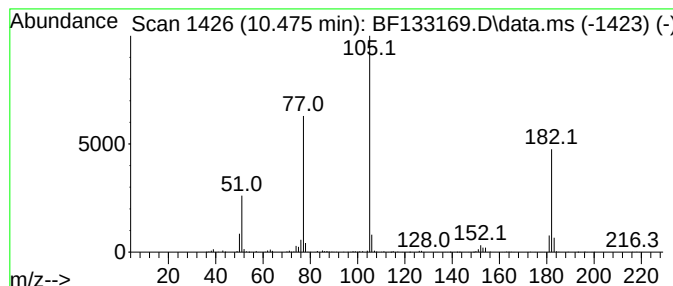
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	4.89 ng	465031	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47



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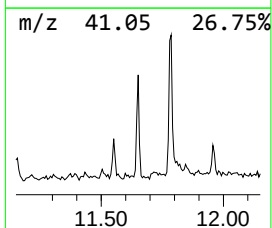
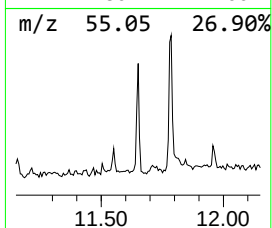
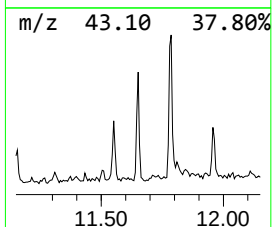
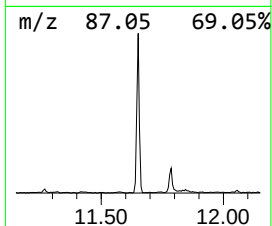
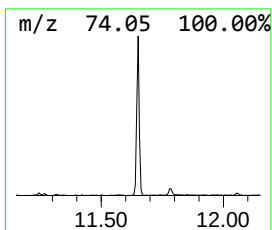
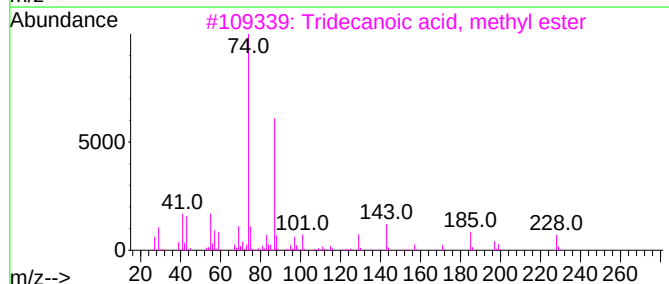
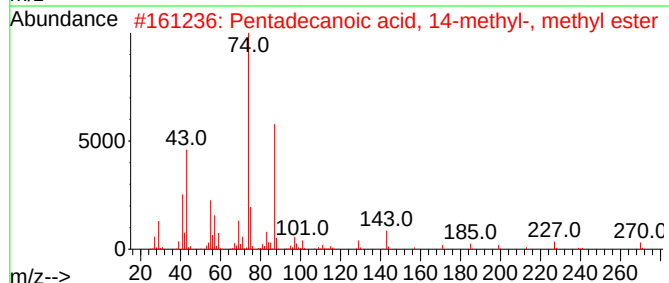
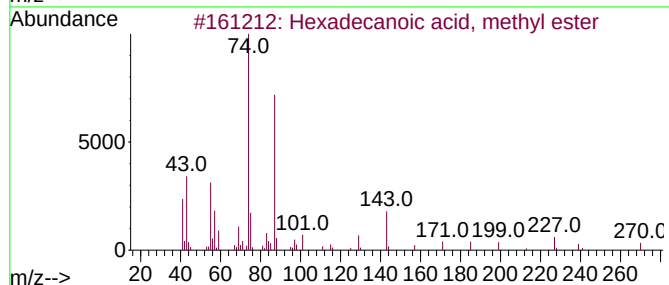
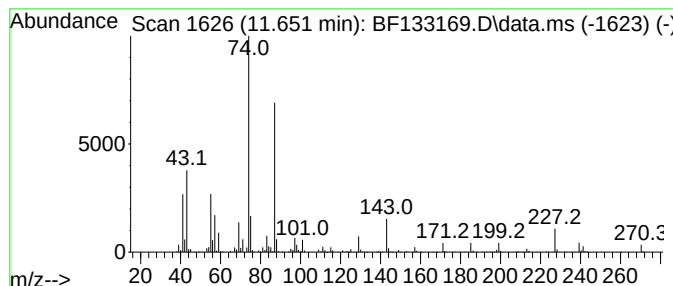
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.651	4.34 ng	372945	Phenanthrene-d10	11.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	81



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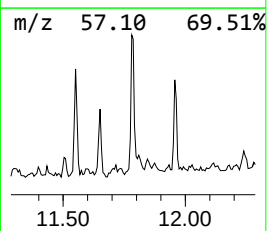
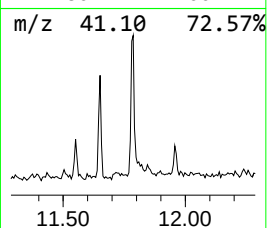
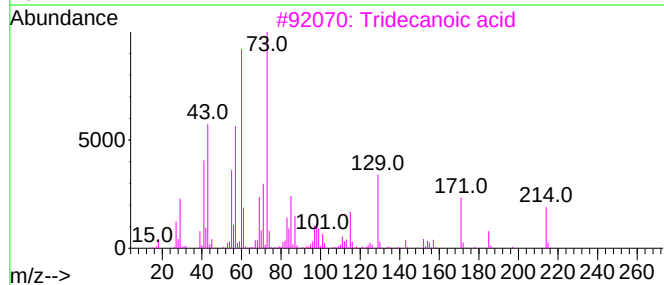
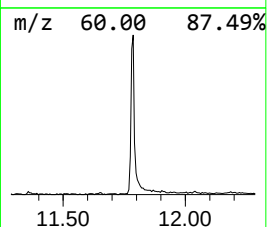
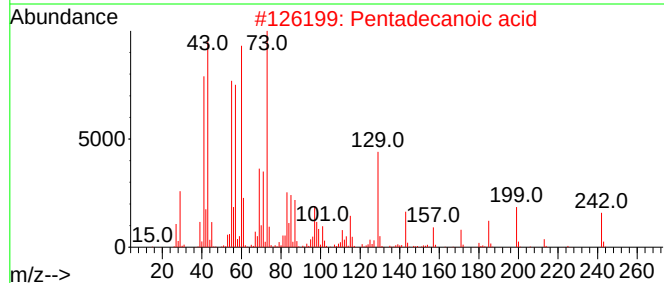
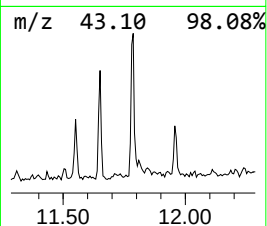
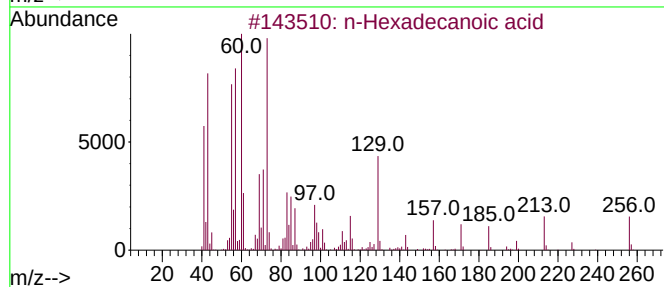
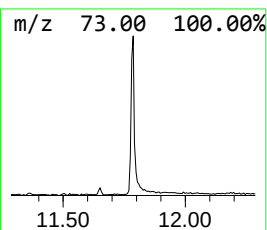
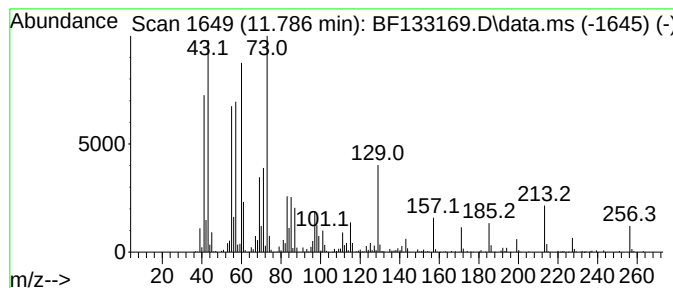
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.786	6.54 ng	561393	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	81



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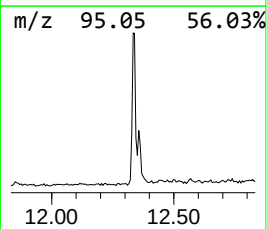
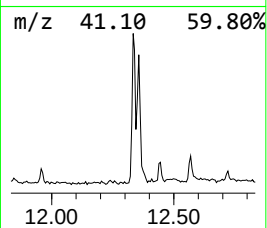
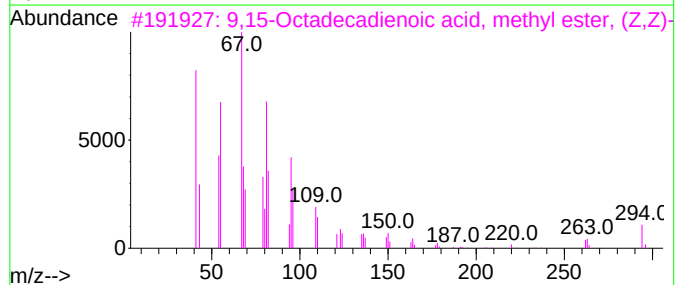
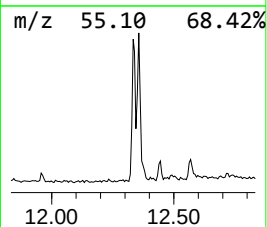
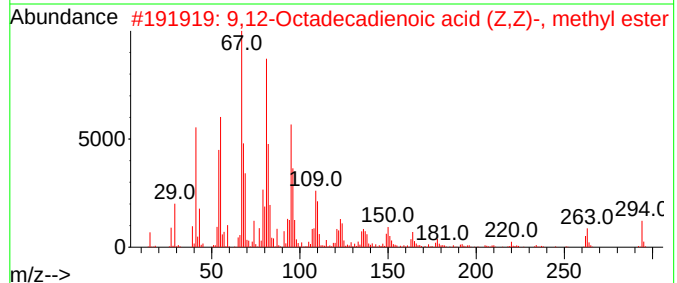
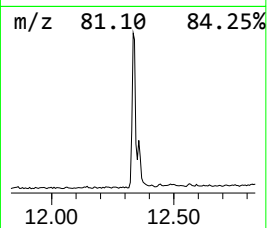
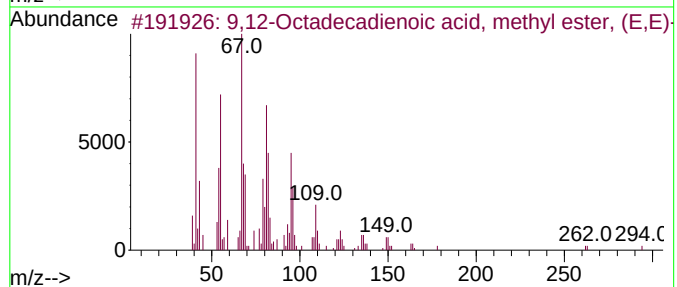
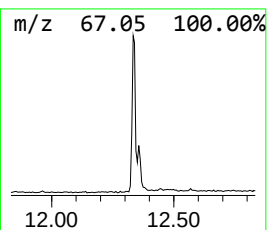
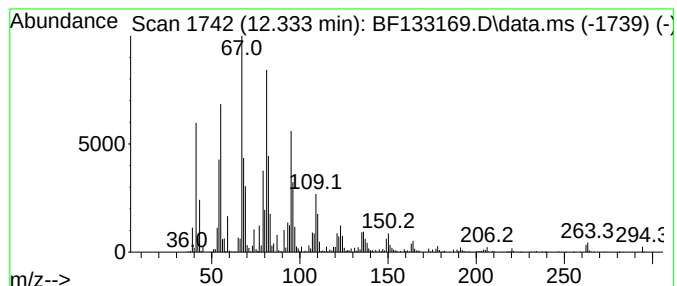
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.333	16.83 ng	1445130	Phenanthrene-d10			11.245
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	99
3	9,15-Octadecadienoic acid, methy...		294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002462-85-3	99
5	Methyl 10-trans,12-cis-octadecad...		294	C19H34O2	1000336-44-2	98



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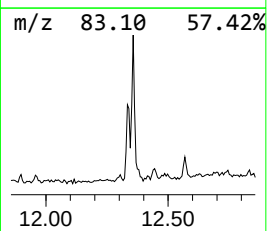
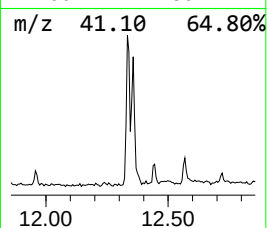
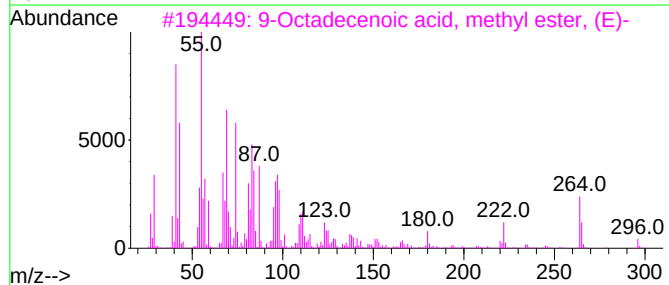
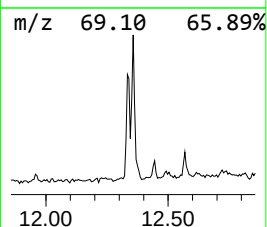
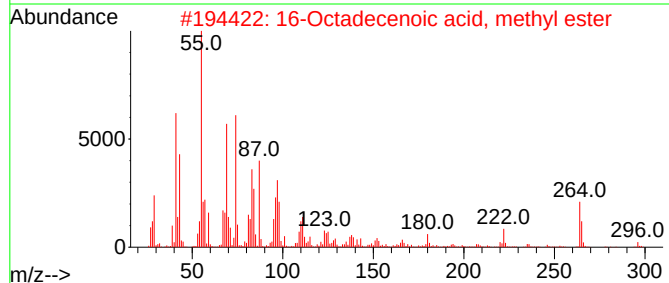
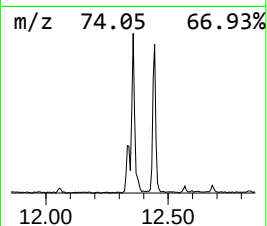
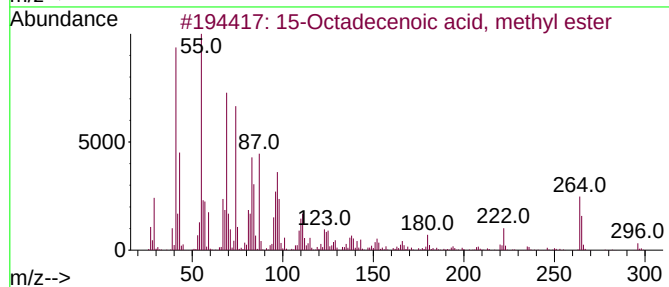
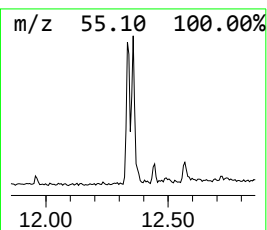
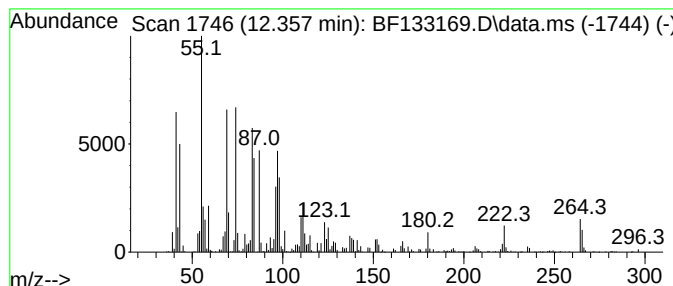
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.357	10.53 ng	904089	Phenanthrene-d10		11.245	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	99
2	16-Octadecenoic acid, methyl ester		296	C19H36O2	056554-49-5	96
3	9-Octadecenoic acid, methyl ester...		296	C19H36O2	001937-62-8	94
4	11-Octadecenoic acid, methyl est...		296	C19H36O2	001937-63-9	94
5	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133169.D
Acq On : 01 May 2023 22:16
Operator : CG\JU
Sample : 02563-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-042823

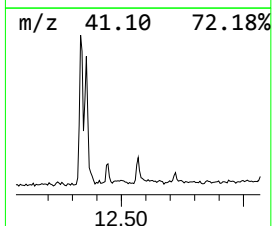
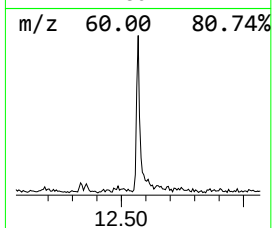
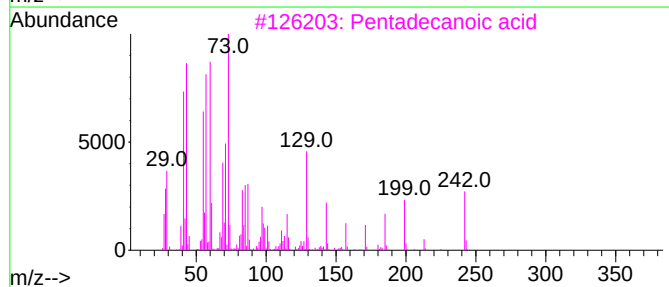
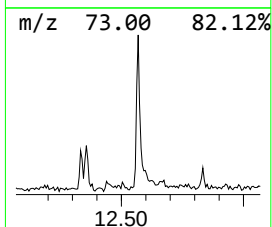
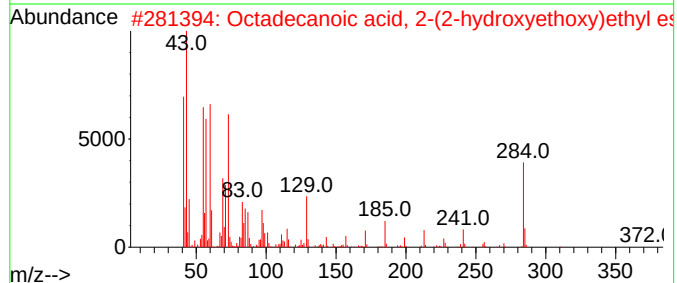
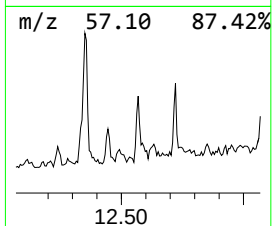
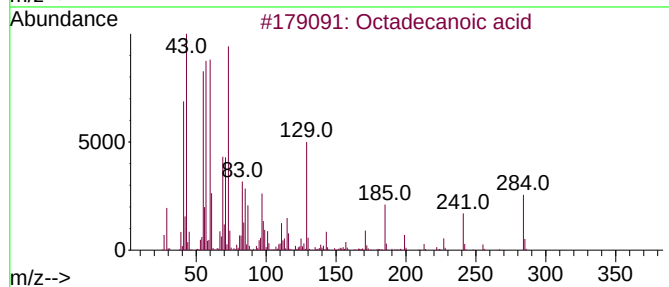
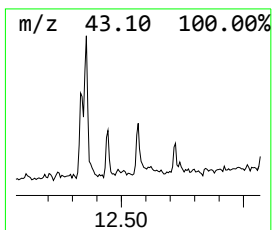
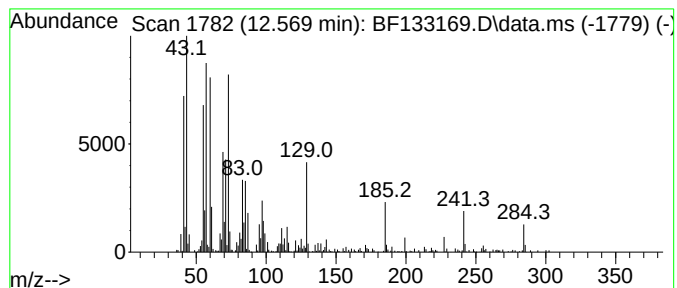
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	3.76 ng	243233	Chrysene-d12	13.880

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133169.D
Acq On : 01 May 2023 22:16
Operator : CG\JU
Sample : 02563-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-042823

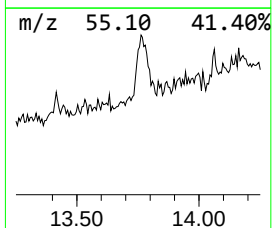
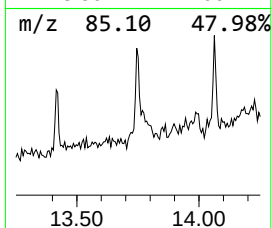
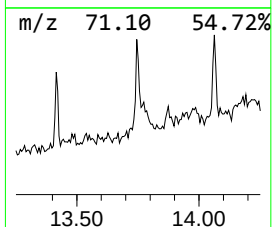
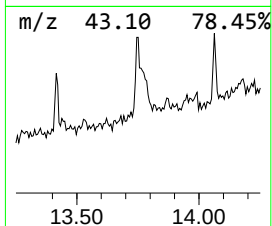
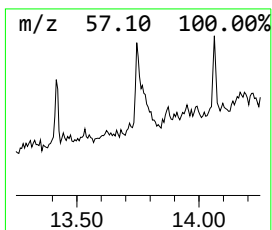
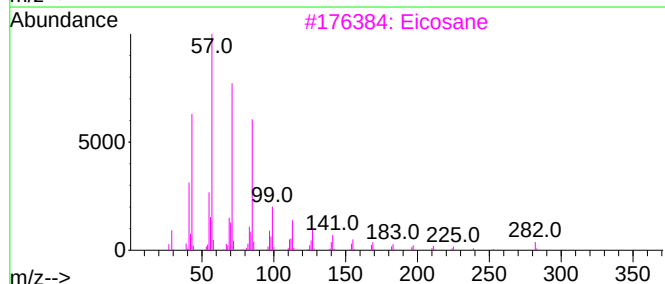
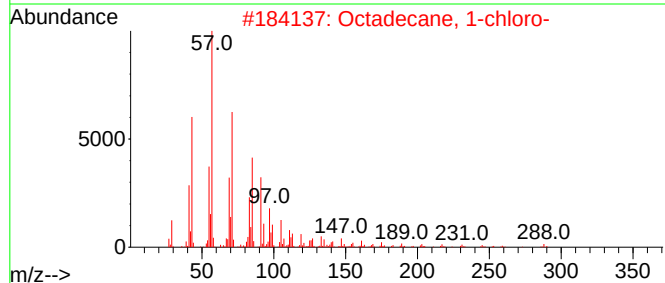
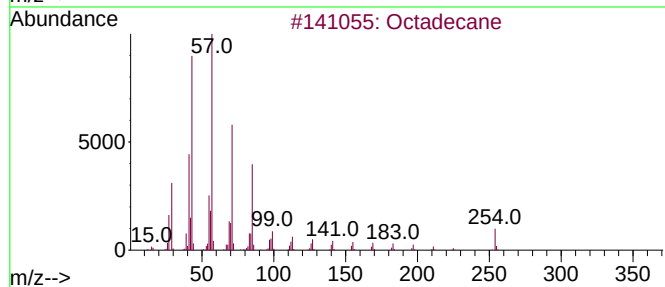
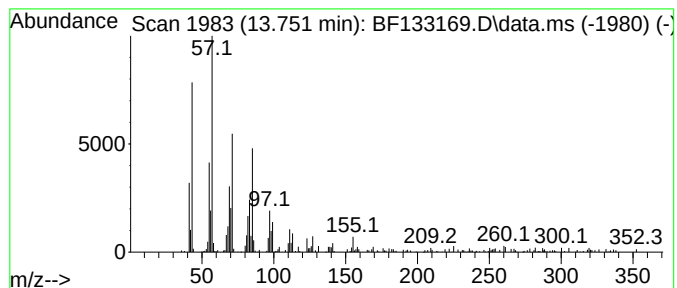
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	2.49 ng	161171	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	94
3			Eicosane	282	C20H42	000112-95-8	89
4			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	81
5			1-Heptadecene	238	C17H34	006765-39-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133169.D
Acq On : 01 May 2023 22:16
Operator : CG\JU
Sample : 02563-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-042823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.475	4.9	ng	465031	3	9.763	1901640	20.0
Hexadecanoic ac...	11.651	4.3	ng	372945	4	11.245	1717620	20.0
n-Hexadecanoic ...	11.786	6.5	ng	561393	4	11.245	1717620	20.0
9,12-Octadecadi...	12.333	16.8	ng	1445130	4	11.245	1717620	20.0
15-Octadecenoic...	12.357	10.5	ng	904089	4	11.245	1717620	20.0
Octadecanoic acid	12.569	3.8	ng	243233	5	13.880	1292880	20.0
Octadecane	13.751	2.5	ng	161171	5	13.880	1292880	20.0