

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
 Data File : BF134646.D
 Acq On : 07 Aug 2023 10:52
 Operator : CG\JU
 Sample : 03891-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	13	18	29	rBV	69984	100944	2.50%	0.234%
2	3.322	203	210	219	rBV3	17503	41326	1.02%	0.096%
3	5.040	498	502	510	rVB	111623	137944	3.41%	0.319%
4	5.428	563	568	571	rBV	3895013	4040138	99.94%	9.349%
5	6.434	733	739	742	rBV	3714313	4042386	100.00%	9.355%
6	6.628	768	772	777	rBV	169836	155977	3.86%	0.361%
7	6.798	797	801	804	rBV	2788790	2231551	55.20%	5.164%
8	7.357	891	896	899	rBV	2713252	2560466	63.34%	5.925%
9	7.439	906	910	913	rBV	125217	105603	2.61%	0.244%
10	8.075	1013	1018	1022	rBV	3270411	2960988	73.25%	6.852%
11	9.151	1196	1201	1205	rBV	4345729	4005049	99.08%	9.268%
12	9.269	1218	1221	1225	rBV	109511	97470	2.41%	0.226%
13	9.833	1311	1317	1320	rBV	3773880	3153128	78.00%	7.297%
14	10.622	1446	1451	1457	rBV	3134073	2789704	69.01%	6.456%
15	11.039	1519	1522	1526	rBV	84720	64783	1.60%	0.150%
16	11.321	1566	1570	1573	rBV	3738624	3189159	78.89%	7.380%
17	11.392	1576	1582	1585	rVB3	72211	75980	1.88%	0.176%
18	11.721	1633	1638	1642	rBV2	58499	87051	2.15%	0.201%
19	11.857	1657	1661	1670	rBV	385796	392158	9.70%	0.908%
20	11.933	1671	1674	1683	rVB2	58409	67892	1.68%	0.157%
21	12.433	1756	1759	1762	rVB2	62784	59258	1.47%	0.137%
22	12.533	1772	1776	1779	rBV	163608	140550	3.48%	0.325%
23	12.645	1792	1795	1805	rBV4	35179	46573	1.15%	0.108%
24	12.739	1808	1811	1813	rBV	350029	298370	7.38%	0.690%
25	12.763	1813	1815	1818	rVB	120722	103796	2.57%	0.240%
26	12.915	1836	1841	1844	rBV	4231558	3702726	91.60%	8.569%
27	13.404	1919	1924	1925	rBV	1347810	1188319	29.40%	2.750%
28	13.421	1925	1927	1934	rVV	1469392	1399096	34.61%	3.238%
29	13.480	1934	1937	1946	rVB	238602	284500	7.04%	0.658%
30	13.821	1991	1995	2003	rBV	357164	374830	9.27%	0.867%
31	13.968	2015	2020	2023	rBV	2518371	2265361	56.04%	5.242%
32	14.457	2101	2103	2112	rVB5	34523	60913	1.51%	0.141%
33	14.751	2148	2153	2165	rBV	373786	695058	17.19%	1.608%
34	15.004	2193	2196	2199	rBV	36931	50439	1.25%	0.117%
35	15.368	2255	2258	2263	rVB	37367	42584	1.05%	0.099%
36	15.439	2264	2270	2277	rBV	1719576	2200926	54.45%	5.093%

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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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

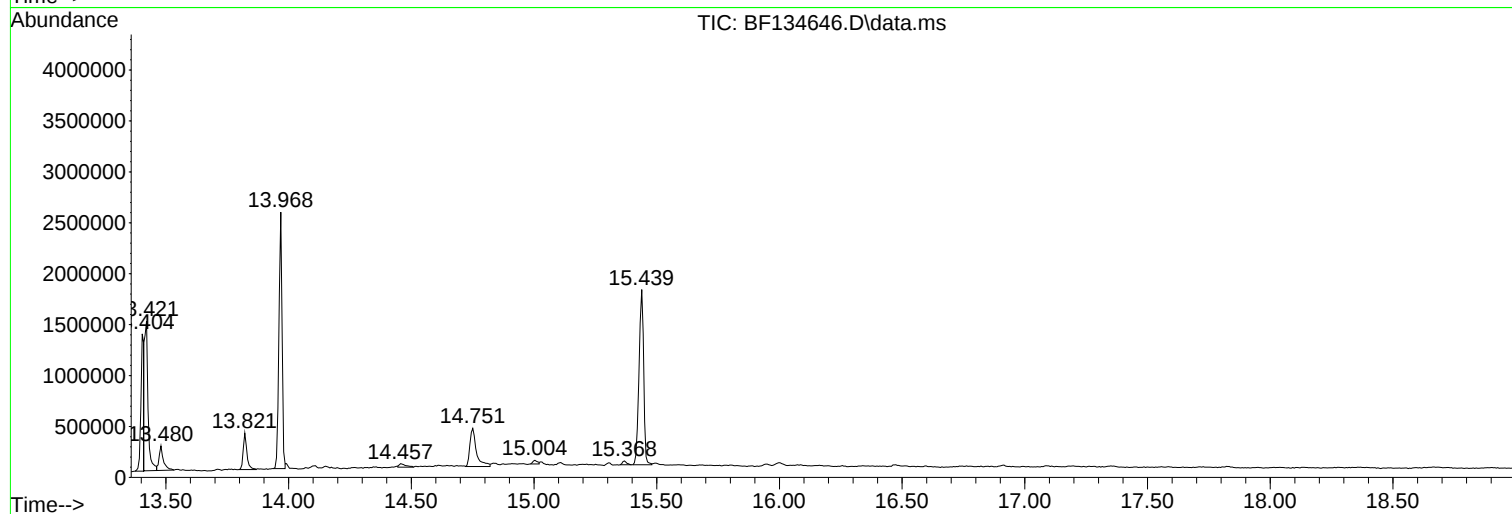
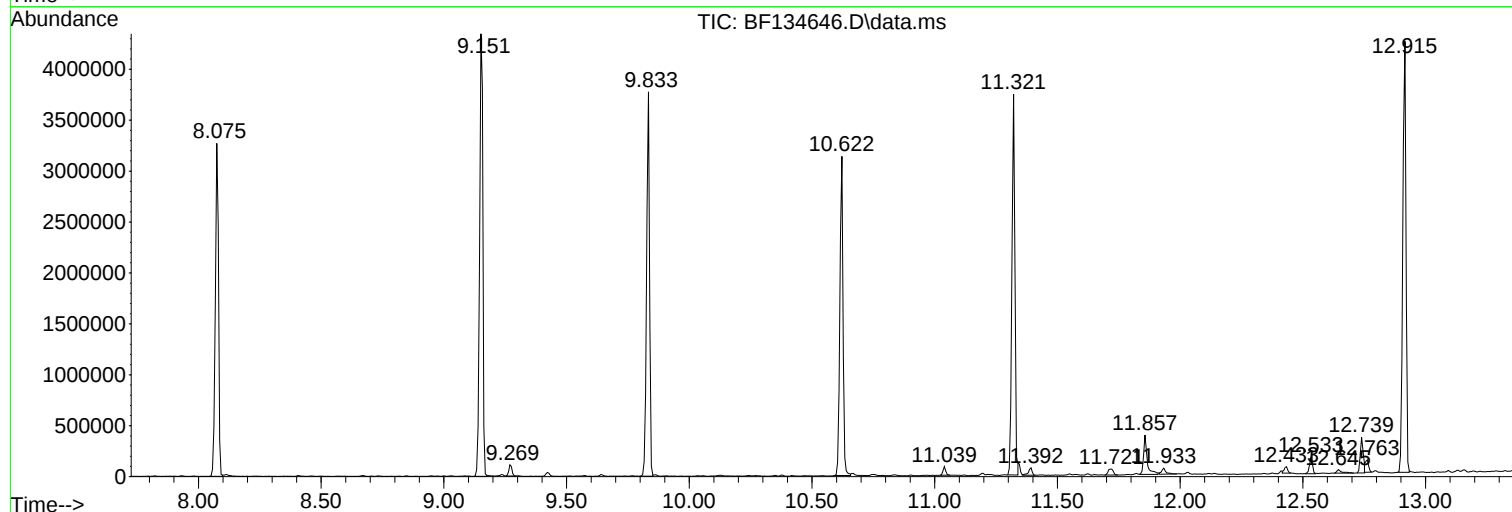
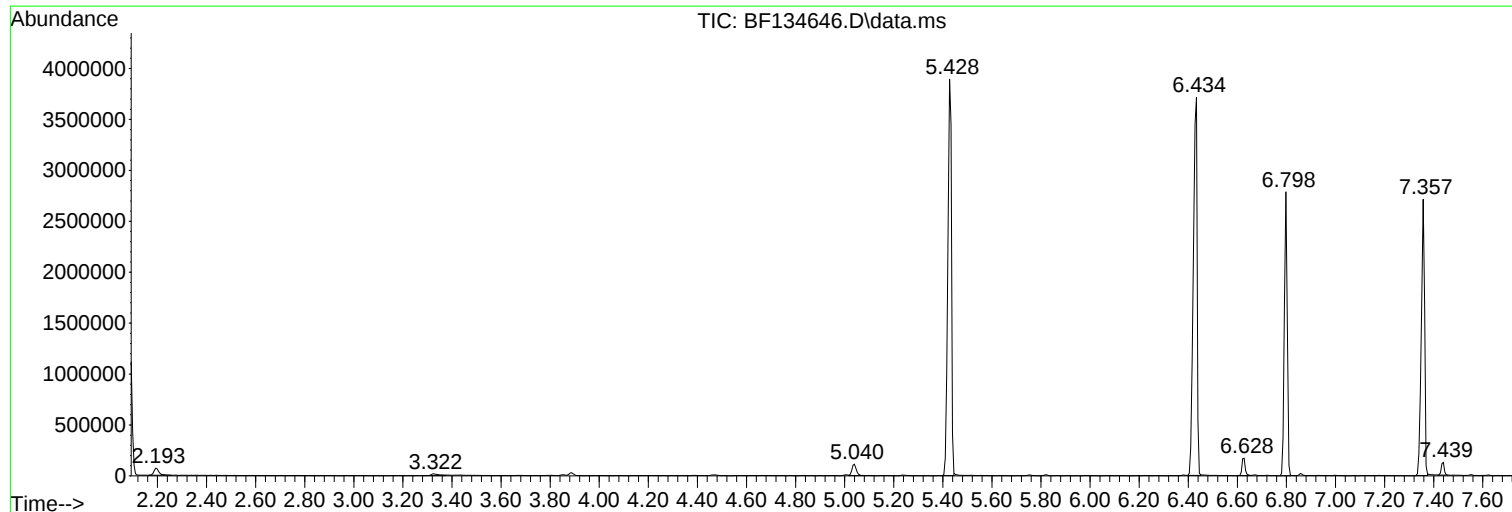
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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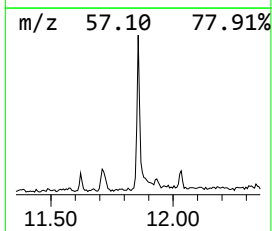
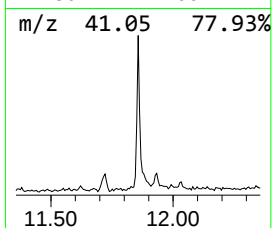
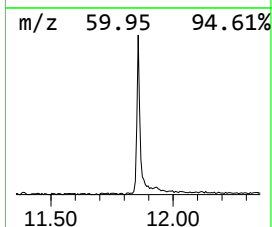
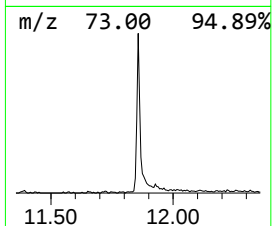
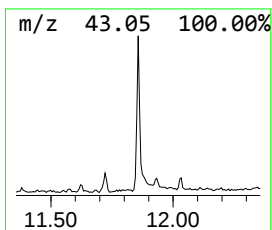
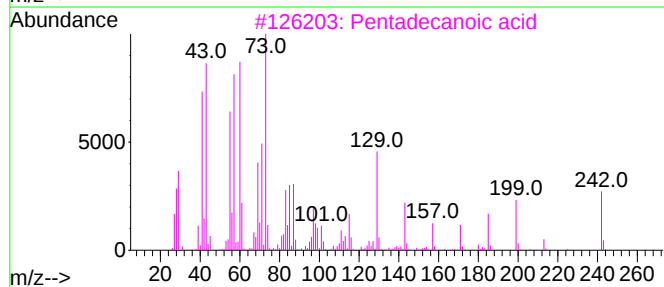
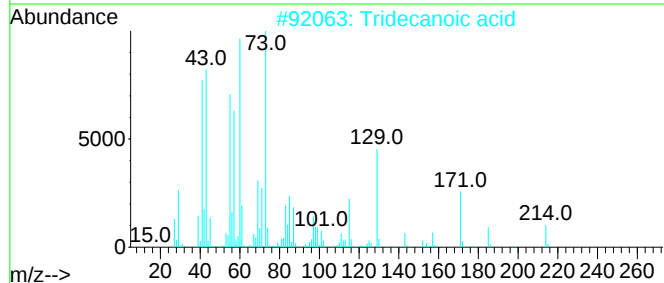
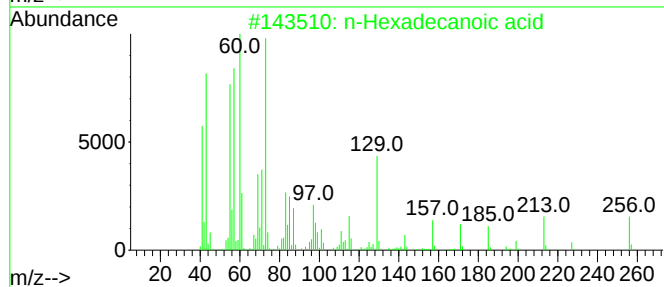
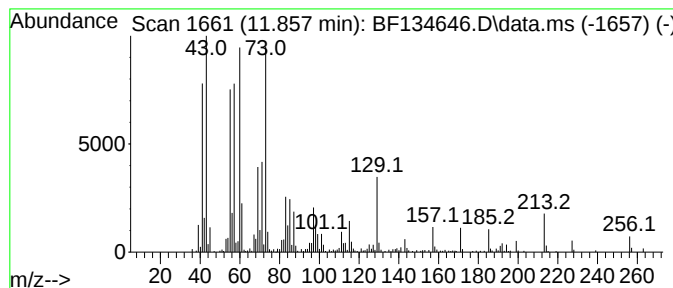
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.46 ng	392158	Phenanthrene-d10	11.322

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	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83



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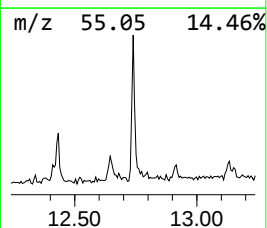
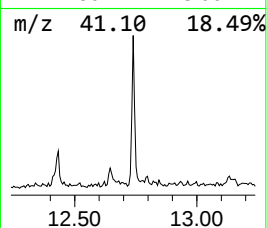
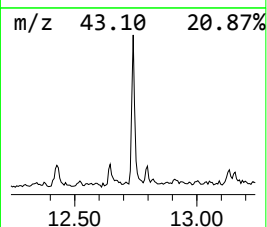
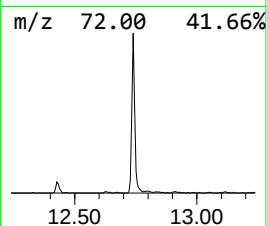
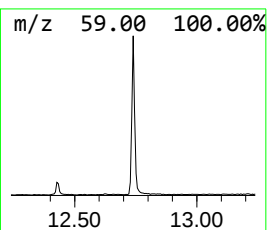
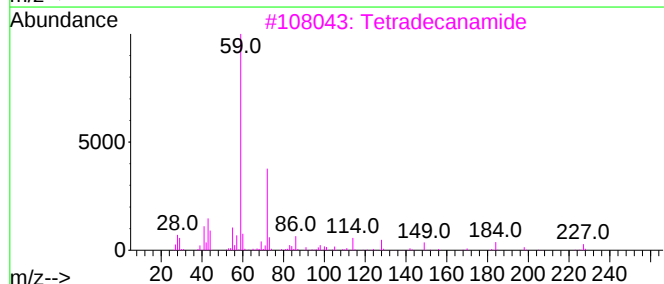
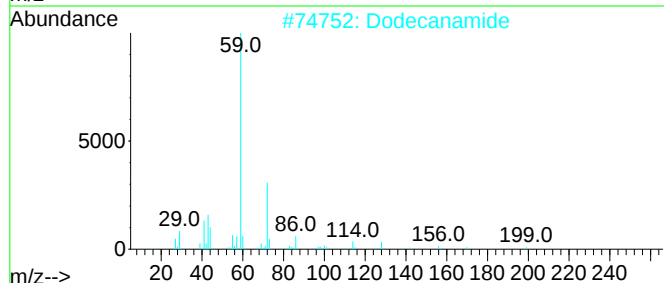
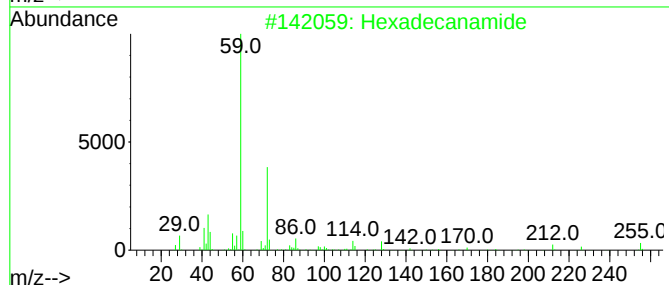
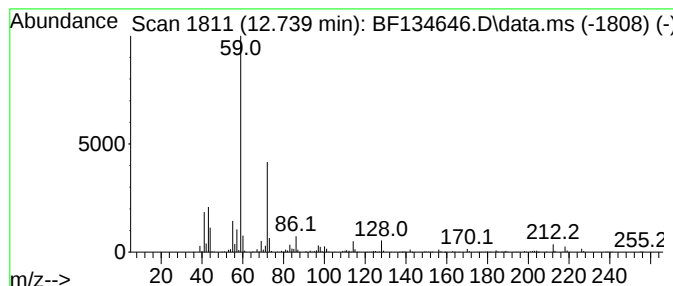
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.63 ng	298370	Chrysene-d12	13.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanamide	255	C16H33NO	000629-54-9	91
2		Dodecanamide	199	C12H25NO	001120-16-7	86
3		Tetradecanamide	227	C14H29NO	000638-58-4	86
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
5		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64



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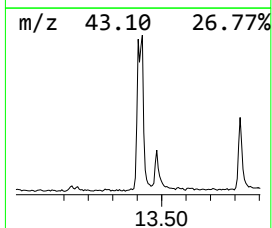
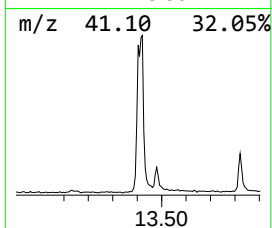
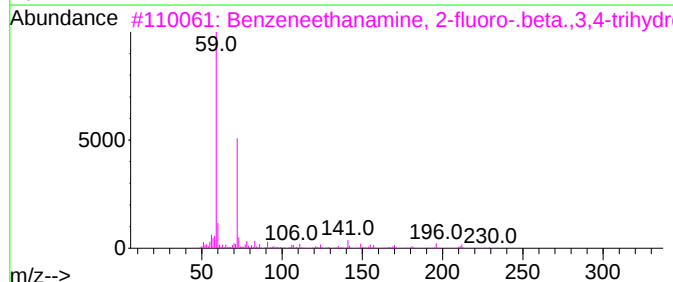
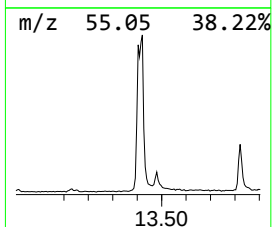
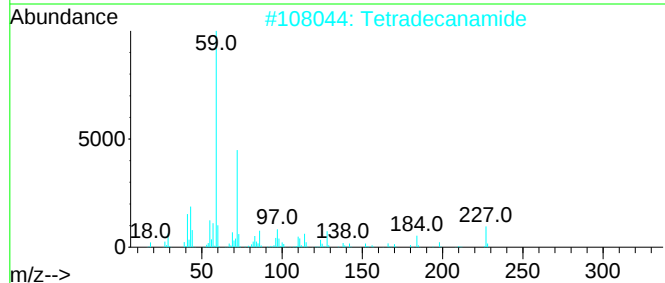
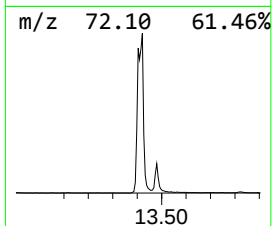
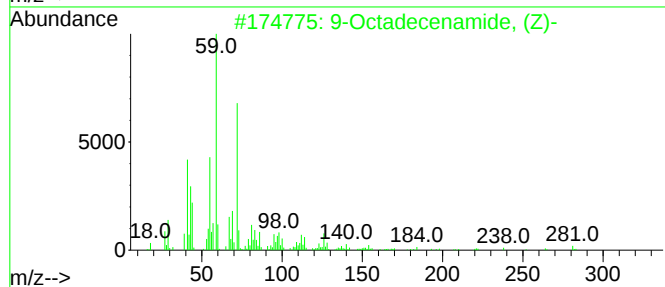
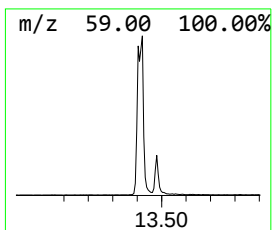
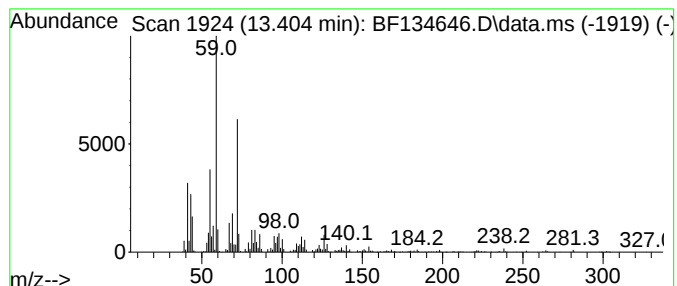
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.404	10.49 ng	1188320	Chrysene-d12	13.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2		Tetradecanamide	227	C14H29NO	000638-58-4	72
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Octanamide	143	C8H17NO	000629-01-6	59
5		Nonanamide	157	C9H19NO	001120-07-6	59



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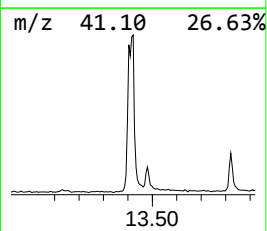
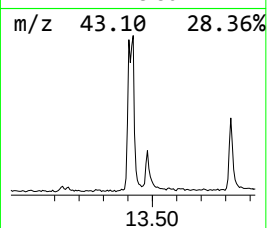
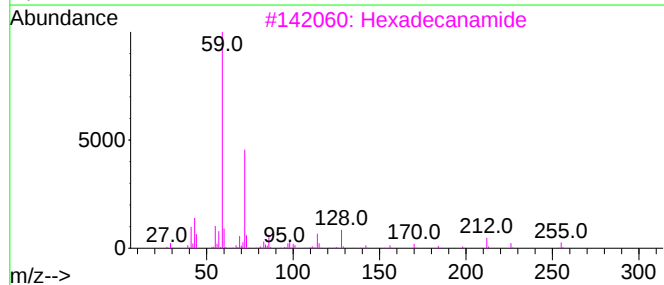
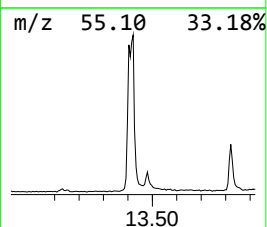
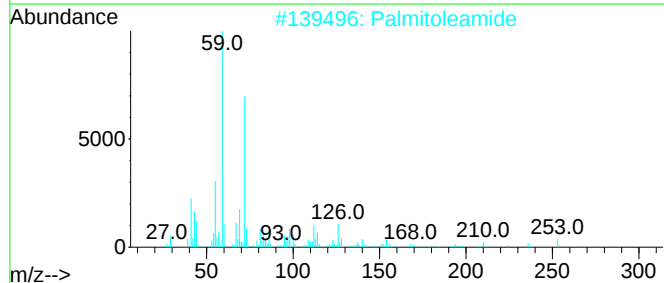
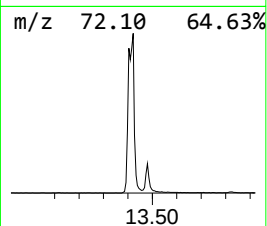
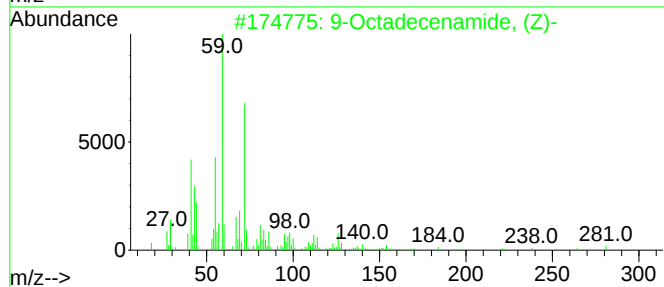
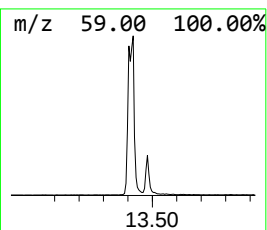
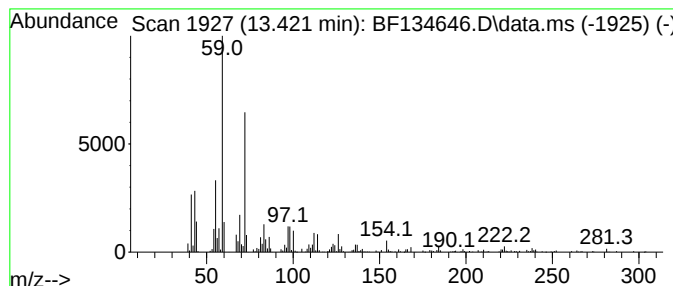
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Palmitoleamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	12.35 ng	1399100	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	93
2	Palmitoleamide			253	C16H31NO	106010-22-4	78
3	Hexadecanamide			255	C16H33NO	000629-54-9	72
4	Dodecanamide			199	C12H25NO	001120-16-7	64
5	Benzeneethanamine, 2-fluoro-.bet...			229	C11H16FN03	061338-98-5	64



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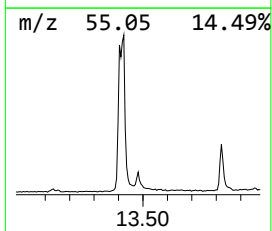
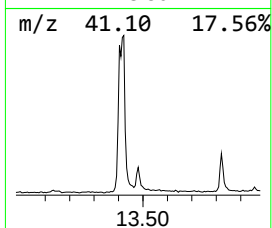
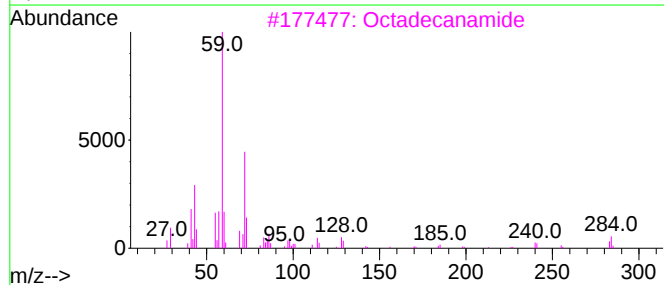
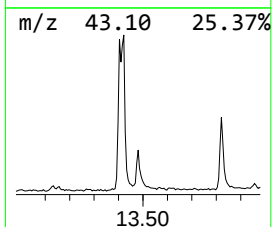
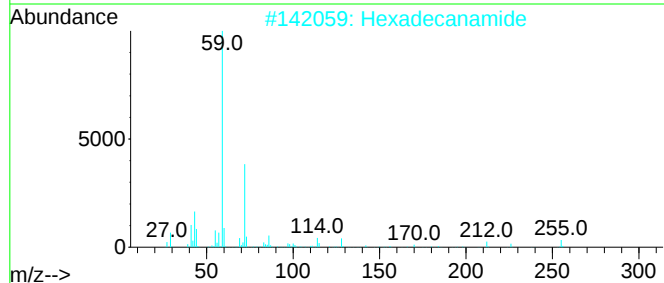
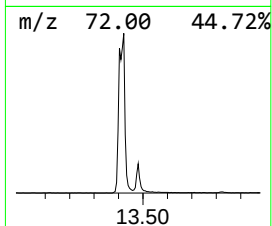
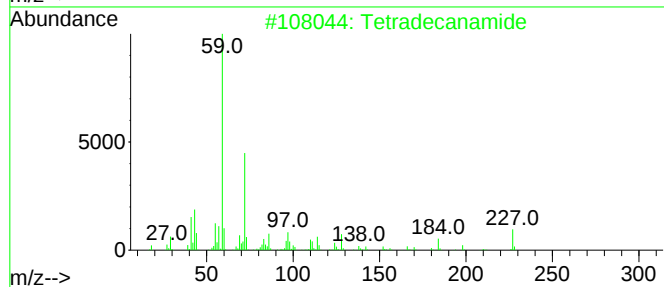
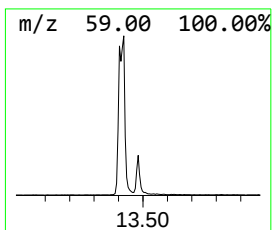
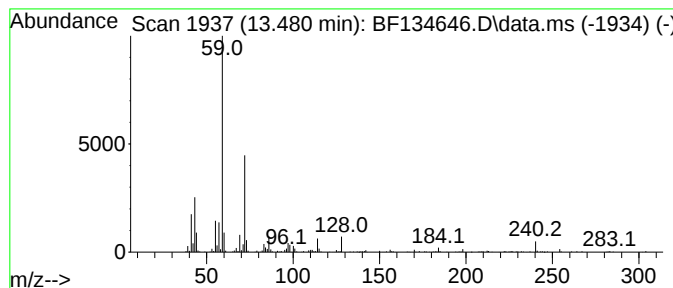
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetradecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.480	2.51 ng	284500	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	87
2			Hexadecanamide	255	C16H33NO	000629-54-9	86
3			Octadecanamide	283	C18H37NO	000124-26-5	78
4			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
5			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64



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Data File : BF134646.D
Acq On : 07 Aug 2023 10:52
Operator : CG\JU
Sample : 03891-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

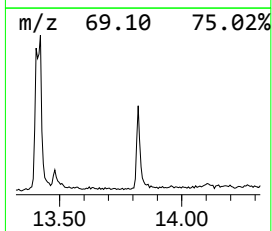
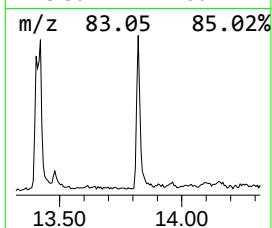
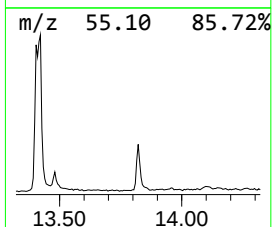
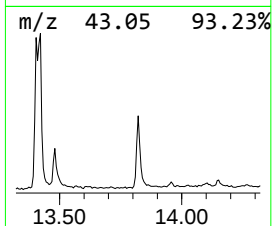
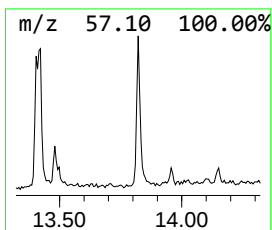
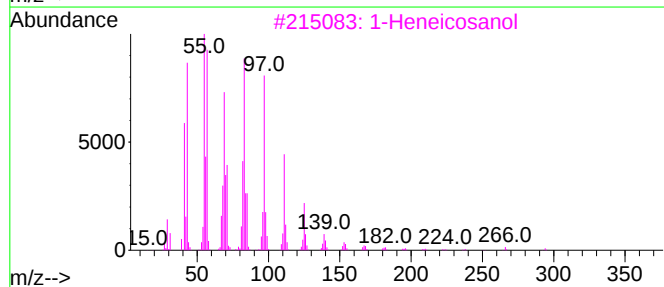
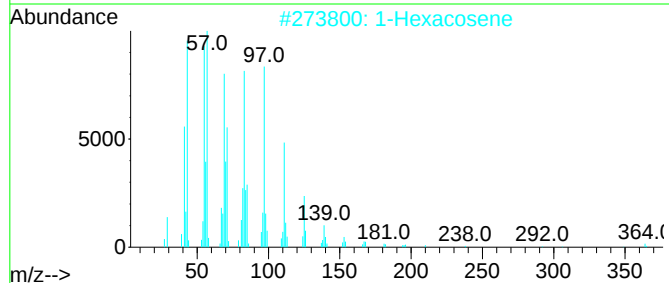
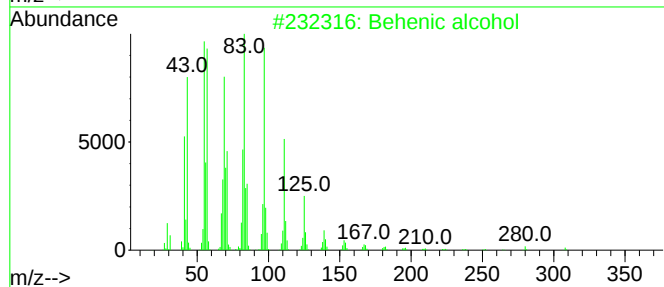
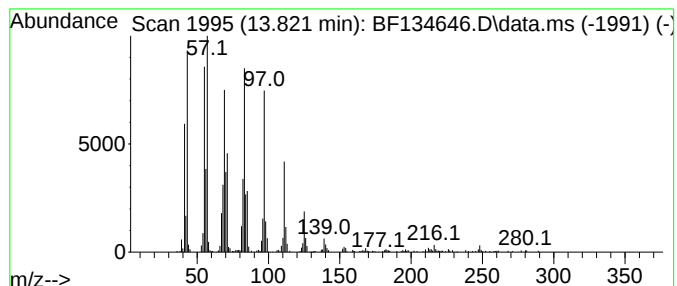
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	3.31 ng	374830	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
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Sample : 03891-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

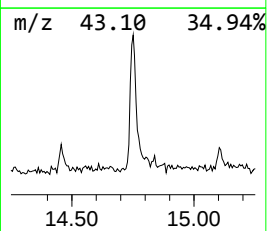
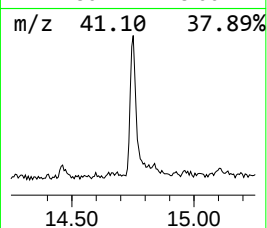
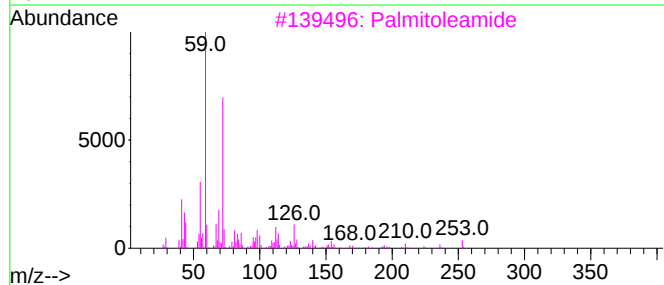
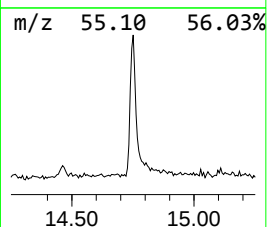
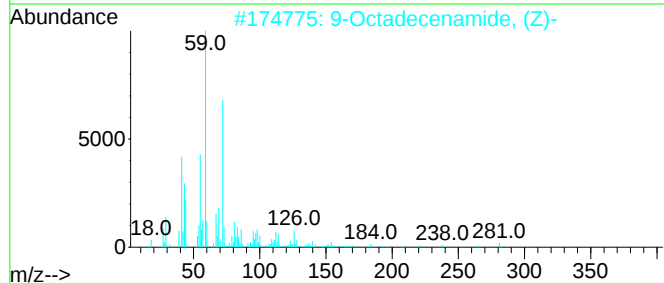
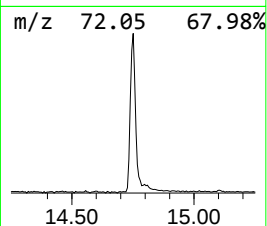
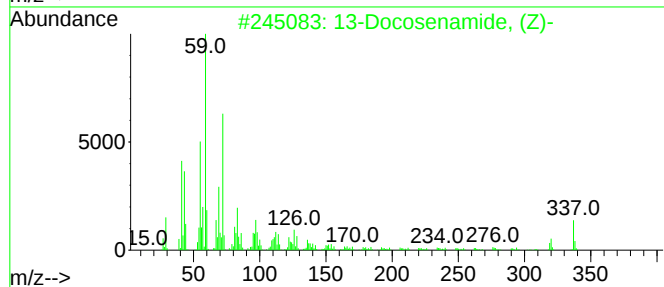
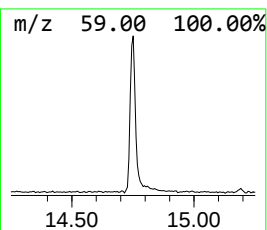
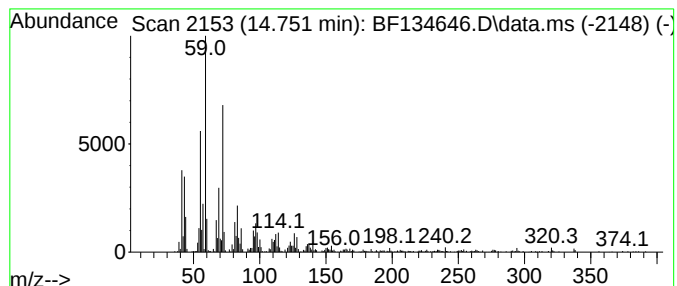
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	6.32 ng	695058	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3			Palmitoleamide	253	C16H31NO	106010-22-4	86
4			Octadecanamide	283	C18H37NO	000124-26-5	64
5			Tetradecanamide	227	C14H29NO	000638-58-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
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Operator : CG\JU
Sample : 03891-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
n-Hexadecanoic ...	11.857	2.5	ng	392158	4	11.322	3189160	20.0
Hexadecanamide	12.739	2.6	ng	298370	5	13.968	2265360	20.0
9-Octadecenamid...	13.404	10.5	ng	1188320	5	13.968	2265360	20.0
Palmitoleamide	13.421	12.4	ng	1399100	5	13.968	2265360	20.0
Tetradecanamide	13.480	2.5	ng	284500	5	13.968	2265360	20.0
Behenic alcohol	13.821	3.3	ng	374830	5	13.968	2265360	20.0
13-Docosenamide...	14.751	6.3	ng	695058	6	15.439	2200930	20.0