

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135849.D
 Acq On : 18 Oct 2023 16:07
 Operator : CG\JU
 Sample : 04767-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-1

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	485	488	503	rBV	115623	169564	5.44%	0.868%
2	5.375	556	559	583	rBV	987583	1403489	45.06%	7.184%
3	6.392	729	732	749	rBV	681522	1018268	32.69%	5.212%
4	6.739	787	791	803	rBV	564860	540756	17.36%	2.768%
5	7.169	857	864	867	rBV	213975	338434	10.86%	1.732%
6	7.198	867	869	884	rVV3	42413	96344	3.09%	0.493%
7	7.310	884	888	899	rVV	2021564	1779596	57.13%	9.109%
8	7.792	966	970	977	rBV	47602	72041	2.31%	0.369%
9	8.016	1005	1008	1021	rBV	933894	808743	25.96%	4.140%
10	8.245	1044	1047	1049	rBV	38678	41379	1.33%	0.212%
11	8.275	1049	1052	1063	rVB	49519	76801	2.47%	0.393%
12	8.392	1069	1072	1080	rBV3	39962	57976	1.86%	0.297%
13	9.098	1188	1192	1195	rBV	3488518	2905092	93.26%	14.870%
14	9.216	1207	1212	1219	rBV	71746	78048	2.51%	0.400%
15	9.275	1219	1222	1234	rVB	28796	53653	1.72%	0.275%
16	9.775	1303	1307	1312	rBV	967214	791975	25.42%	4.054%
17	9.986	1340	1343	1348	rBV2	40008	59261	1.90%	0.303%
18	10.333	1399	1402	1408	rVB2	34316	35848	1.15%	0.183%
19	10.575	1439	1443	1460	rBV	2150247	2115538	67.92%	10.829%
20	11.092	1528	1531	1535	rBV	80146	74429	2.39%	0.381%
21	11.274	1558	1562	1564	rBV	1070350	919163	29.51%	4.705%
22	11.298	1564	1566	1571	rVV	353340	290835	9.34%	1.489%
23	11.351	1571	1575	1580	rVB2	55494	69700	2.24%	0.357%
24	11.522	1600	1604	1610	rBV	60100	68069	2.19%	0.348%
25	11.657	1624	1627	1630	rVB3	37369	34929	1.12%	0.179%
26	11.810	1650	1653	1660	rBV3	226849	280662	9.01%	1.437%
27	11.892	1664	1667	1670	rBV	47342	42595	1.37%	0.218%
28	12.439	1755	1760	1766	rVB	35197	44545	1.43%	0.228%
29	12.498	1766	1770	1772	rBV	302733	279598	8.98%	1.431%
30	12.516	1772	1773	1781	rVV	106437	126714	4.07%	0.649%
31	12.598	1784	1787	1794	rVV2	130631	153308	4.92%	0.785%
32	12.727	1804	1809	1816	rVB	216412	218100	7.00%	1.116%
33	12.874	1829	1834	1837	rBV	3106882	3114946	100.00%	15.944%
34	13.263	1897	1900	1912	rBV2	159832	355626	11.42%	1.820%
35	13.939	2011	2015	2019	rBV	544071	536162	17.21%	2.744%
36	14.692	2139	2143	2150	rBV4	32453	47150	1.51%	0.241%

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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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.415	2262	2266	2276	rBV	297767	436972	14.03%	2.237%
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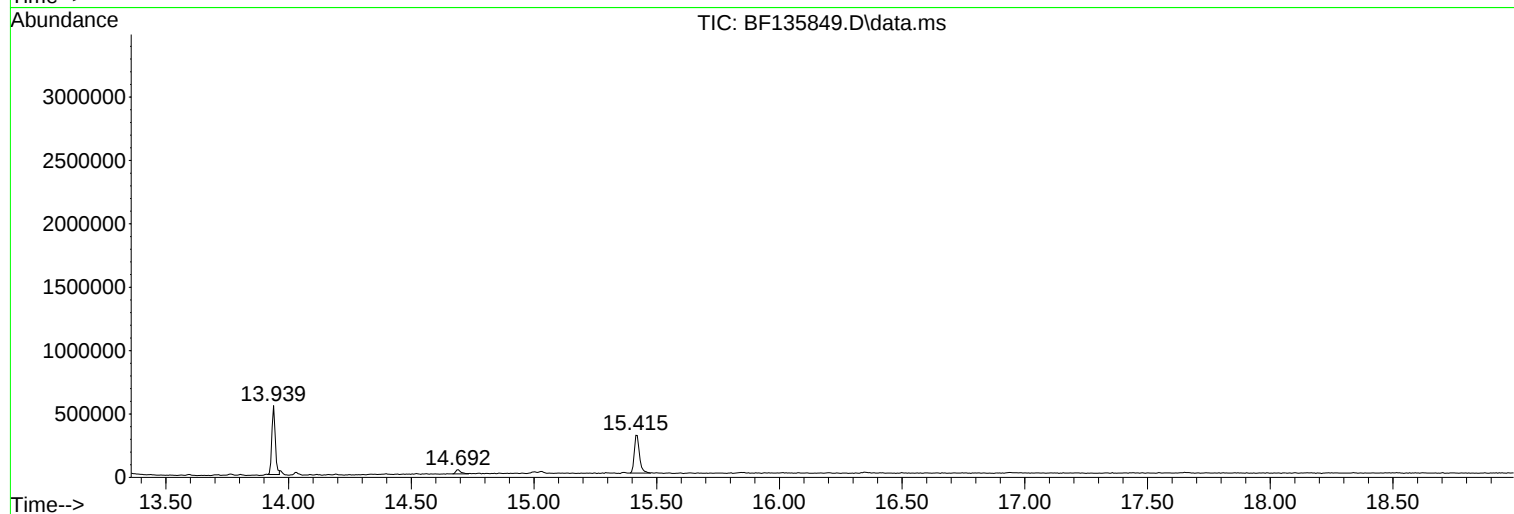
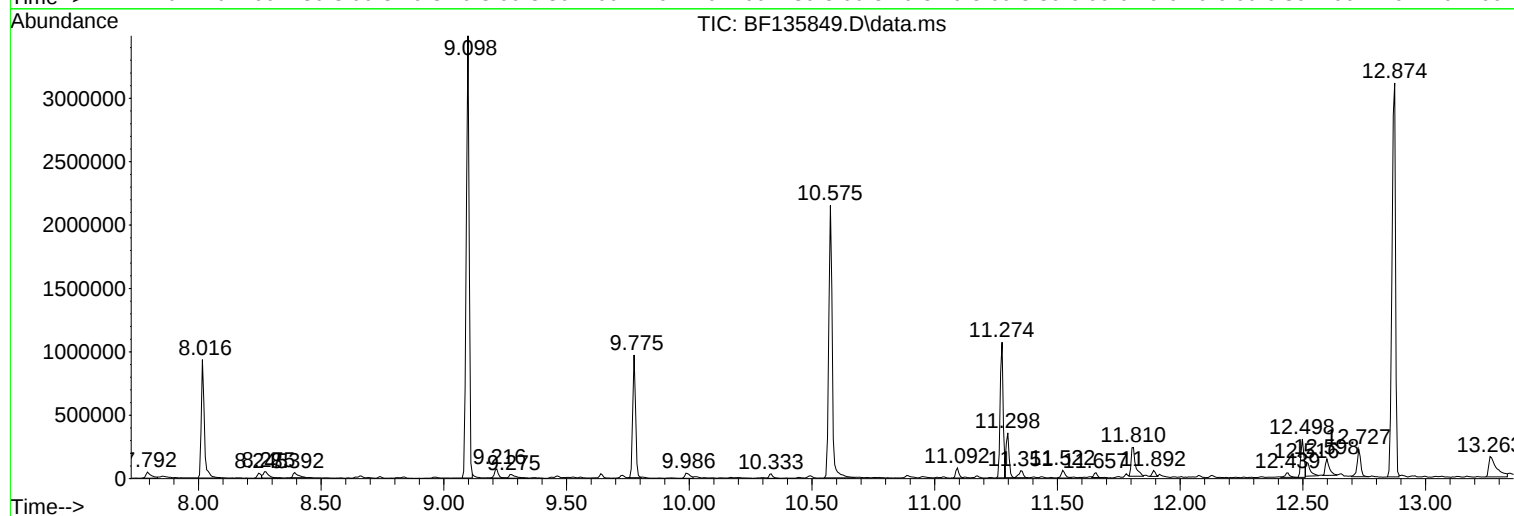
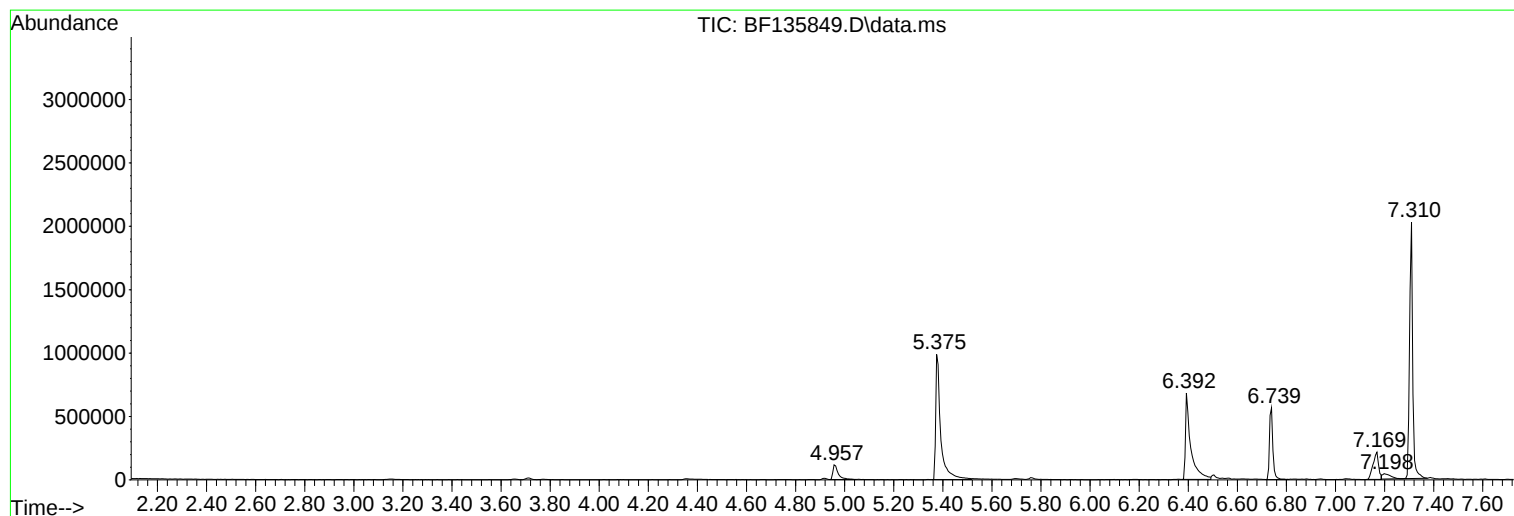
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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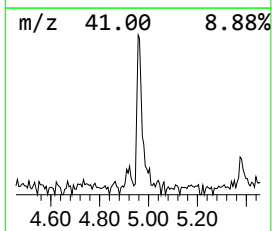
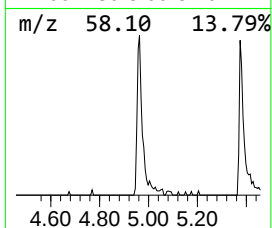
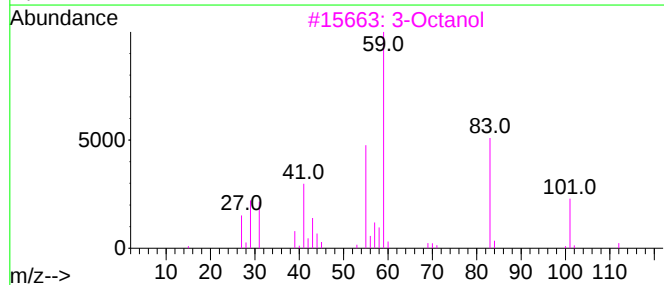
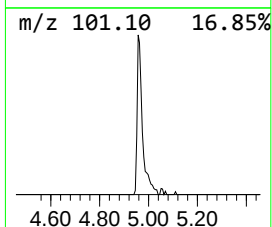
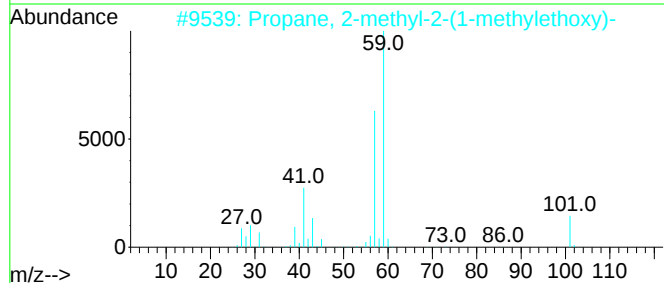
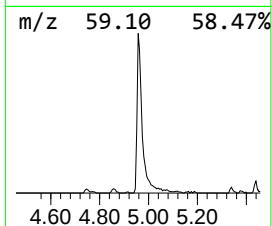
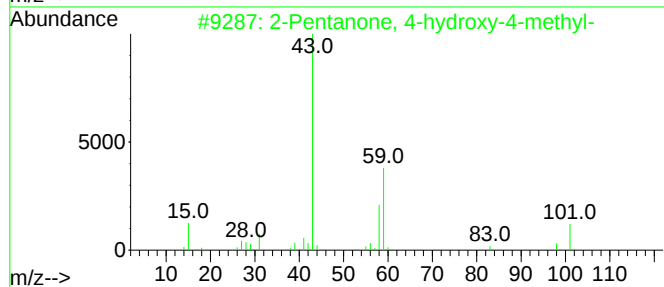
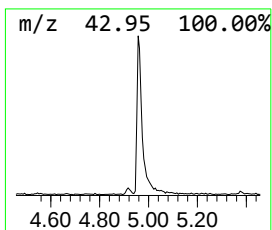
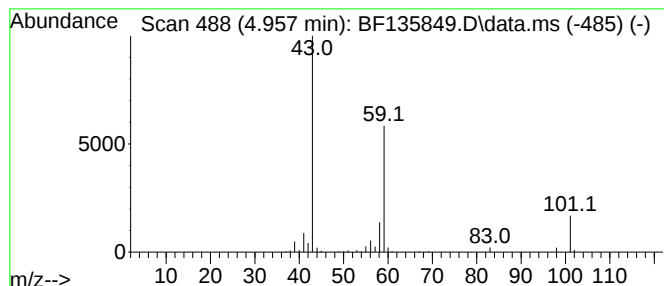
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	6.27 ng	169564	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	3-Octanol	130	C8H18O	000589-98-0	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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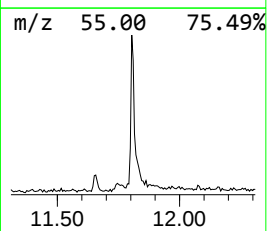
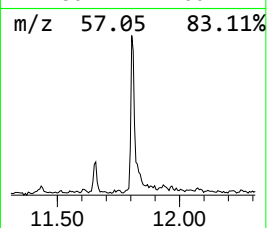
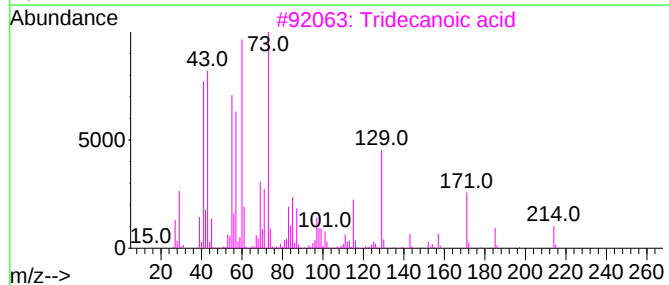
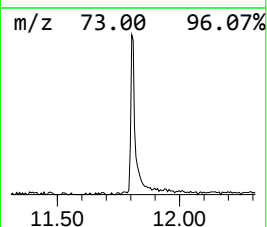
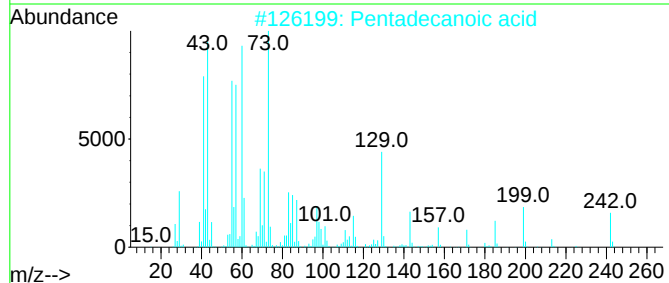
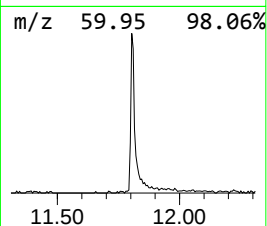
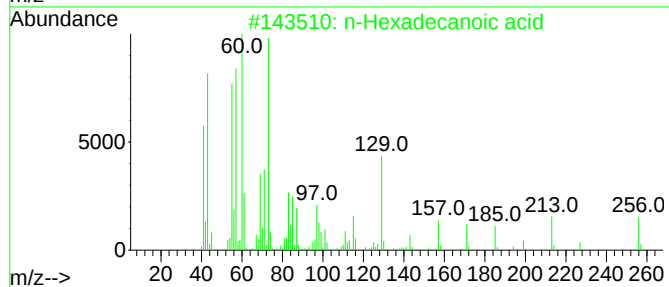
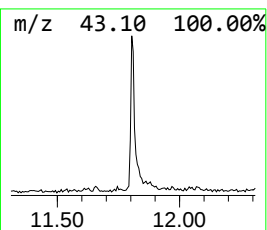
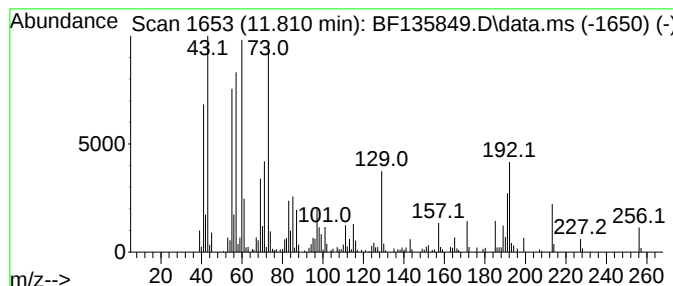
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	6.11 ng	280662	Phenanthrene-d10	11.275

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	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	78
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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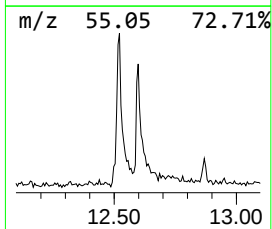
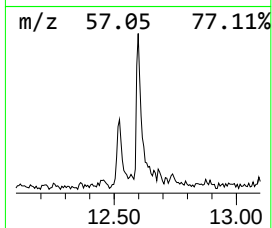
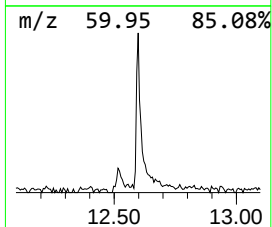
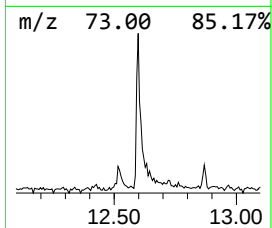
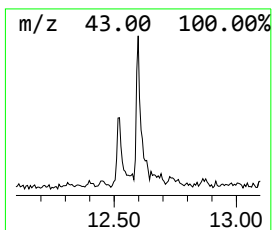
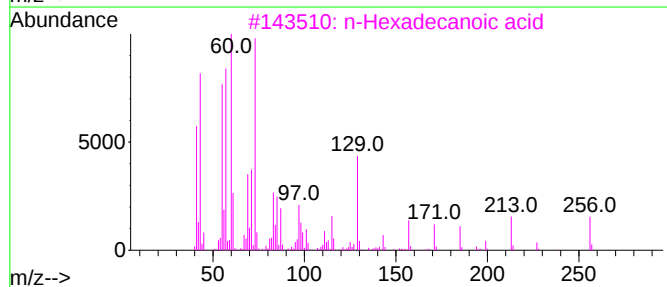
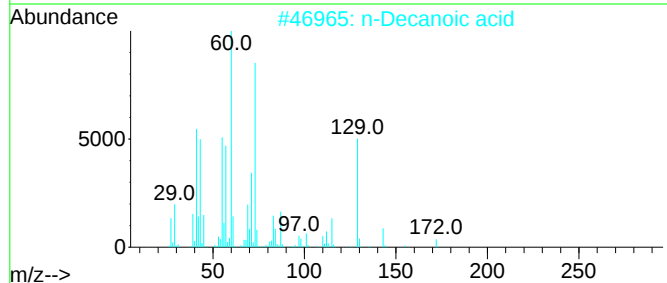
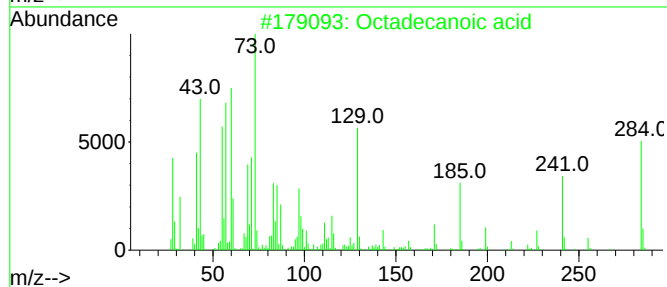
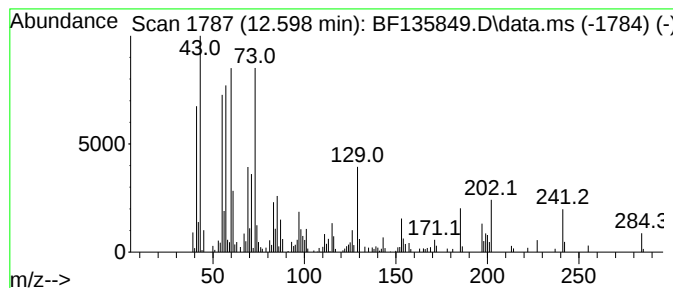
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	3.34 ng	153308	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			n-Decanoic acid	172	C10H20O2	000334-48-5	78
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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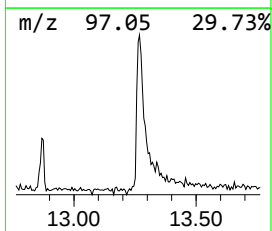
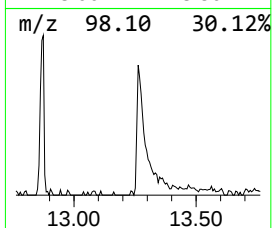
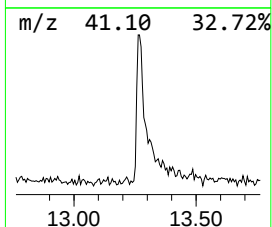
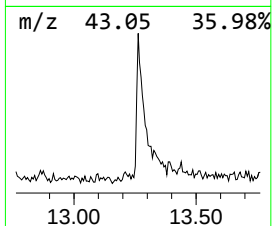
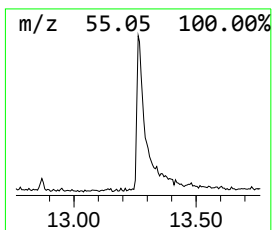
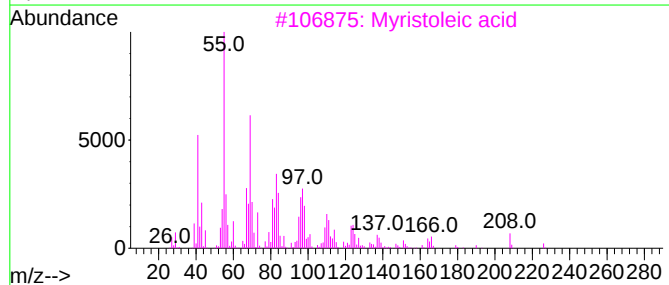
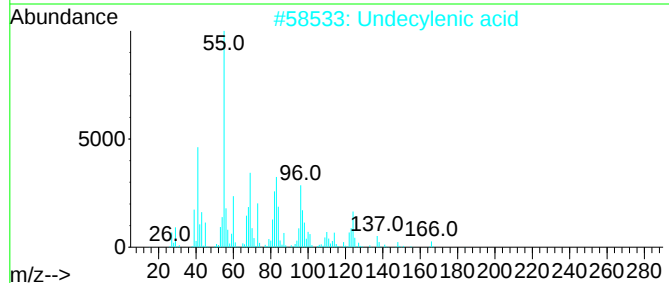
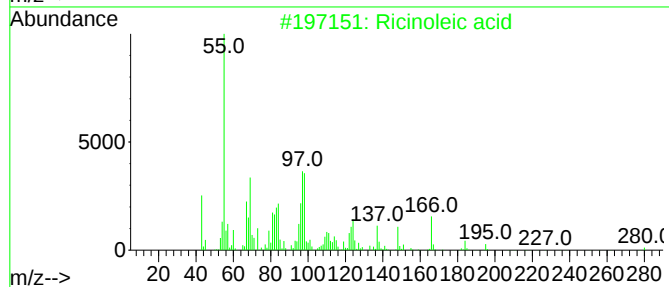
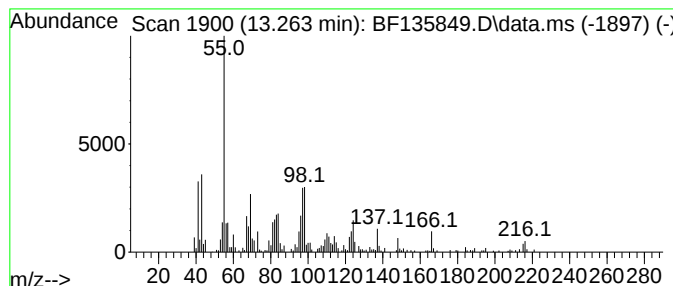
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ricinoleic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	13.27 ng	355626	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ricinoleic acid	298	C18H34O3	000141-22-0	91
2			Undecylenic acid	184	C11H20O2	000112-38-9	47
3			Myristoleic acid	226	C14H26O2	000544-64-9	46
4			9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	43
5			Oct-3-enoic acid, undec-2-en-1-y...	294	C19H34O2	1000406-95-3	35



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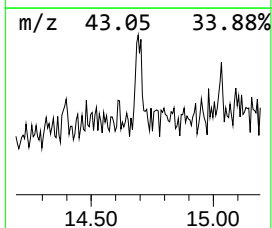
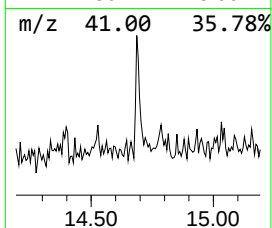
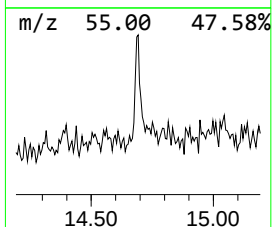
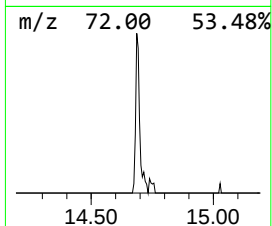
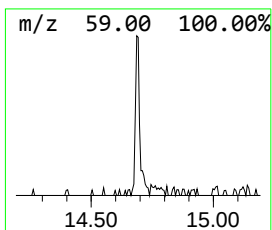
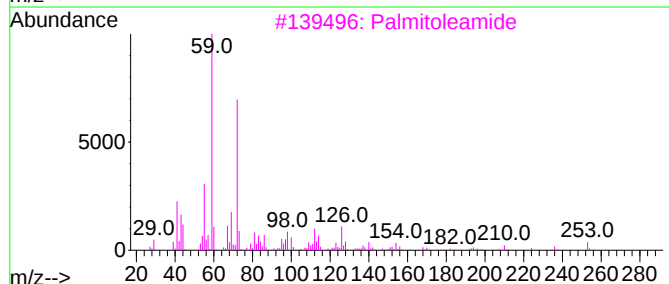
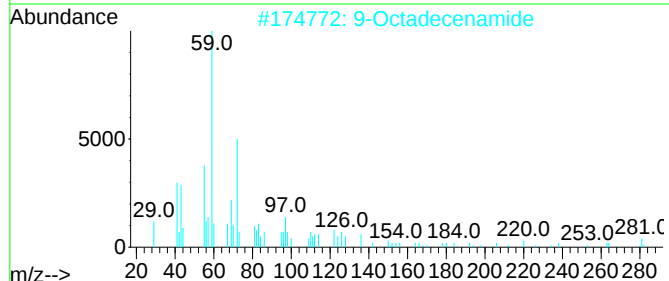
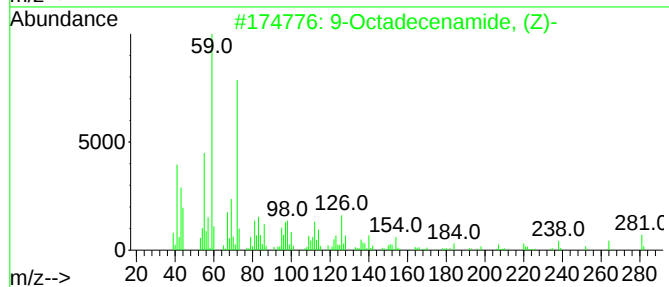
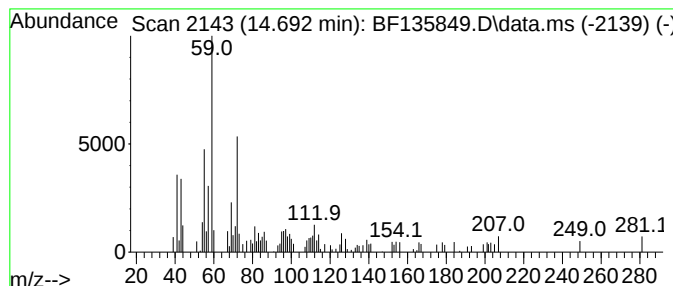
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.692	2.16 ng	47150	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	9-Octadecenamide	281	C18H35NO	003322-62-1	74
3	Palmitoleamide	253	C16H31NO	106010-22-4	72
4	Tetradecanamide	227	C14H29NO	000638-58-4	64
5	Dodecanamide	199	C12H25NO	001120-16-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135849.D
Acq On : 18 Oct 2023 16:07
Operator : CG\JU
Sample : 04767-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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
2-Pentanone, 4-...	4.957	6.3	ng	169564	1	6.739	540756	20.0
n-Hexadecanoic ...	11.810	6.1	ng	280662	4	11.275	919163	20.0
Octadecanoic acid	12.598	3.3	ng	153308	4	11.275	919163	20.0
Ricinoleic acid	13.263	13.3	ng	355626	5	13.939	536162	20.0
9-Octadecenamid...	14.692	2.2	ng	47150	6	15.421	436972	20.0