

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
 Data File : BF132274.D
 Acq On : 01 Feb 2023 22:42
 Operator : CG\JU
 Sample : 01345-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-346

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132274.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.307	415	420	429	rVB	916366	1084664	35.30%	4.334%
2	5.690	480	485	489	rBV	2769321	2740931	89.20%	10.952%
3	6.678	648	653	657	rVB	2495007	2658173	86.51%	10.621%
4	7.066	716	719	723	rVB	1013711	868557	28.27%	3.471%
5	7.601	805	810	811	rBV	49620	43550	1.42%	0.174%
6	7.631	811	815	818	rVB	2067279	1743057	56.73%	6.965%
7	7.860	852	854	861	rVB4	35491	45233	1.47%	0.181%
8	8.089	890	893	895	rVB	45459	38935	1.27%	0.156%
9	8.213	908	914	918	rVB2	38938	45205	1.47%	0.181%
10	8.354	935	938	941	rBV	1386552	1092164	35.54%	4.364%
11	9.431	1117	1121	1124	rBV	3912087	3072683	100.00%	12.278%
12	9.501	1130	1133	1137	rBV3	36364	48411	1.58%	0.193%
13	9.825	1185	1188	1190	rBV2	50364	42789	1.39%	0.171%
14	10.119	1235	1238	1241	rVB	1463979	1145200	37.27%	4.576%
15	10.530	1305	1308	1311	rVB3	36463	39298	1.28%	0.157%
16	10.754	1342	1346	1349	rBV2	47614	52761	1.72%	0.211%
17	10.830	1357	1359	1362	rVB	89175	71414	2.32%	0.285%
18	10.913	1369	1373	1376	rBV	2105499	1795808	58.44%	7.176%
19	11.013	1387	1390	1391	rBV2	76278	74452	2.42%	0.297%
20	11.460	1464	1466	1469	rBV	46379	40965	1.33%	0.164%
21	11.495	1469	1472	1474	rBV	50994	47204	1.54%	0.189%
22	11.619	1489	1493	1495	rBV	1200297	1009551	32.86%	4.034%
23	11.642	1495	1497	1500	rVB	308296	233274	7.59%	0.932%
24	11.695	1503	1506	1508	rVB	66728	58961	1.92%	0.236%
25	11.842	1528	1531	1537	rBV	43917	55320	1.80%	0.221%
26	12.124	1575	1579	1582	rBV2	418935	390307	12.70%	1.560%
27	12.148	1582	1583	1588	rVB2	73747	55619	1.81%	0.222%
28	12.236	1594	1598	1600	rBV2	81972	83773	2.73%	0.335%
29	12.419	1626	1629	1631	rBV	47653	39899	1.30%	0.159%
30	12.566	1651	1654	1656	rVB2	68541	51879	1.69%	0.207%
31	12.842	1697	1701	1704	rBV	564521	499194	16.25%	1.995%
32	12.877	1704	1707	1709	rVB2	109499	84024	2.73%	0.336%
33	12.913	1710	1713	1719	rBV2	133845	149456	4.86%	0.597%
34	13.071	1734	1740	1746	rBV	607800	640587	20.85%	2.560%
35	13.207	1760	1763	1767	rVB	2427137	2265395	73.73%	9.052%
36	13.348	1785	1787	1790	rBV	62725	57287	1.86%	0.229%

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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-BF013123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.401	1793	1796	1798	rVB	80794	71678	2.33%	0.286%
38	13.466	1805	1807	1810	rVB	55802	46994	1.53%	0.188%
39	14.107	1913	1916	1926	rVB2	184892	342901	11.16%	1.370%
40	14.277	1941	1945	1948	rBV2	961604	1058139	34.44%	4.228%
41	14.301	1948	1949	1956	rVB	225614	192478	6.26%	0.769%
42	15.389	2131	2134	2137	rBV	133339	168599	5.49%	0.674%
43	15.865	2211	2215	2224	rVB	456452	679890	22.13%	2.717%

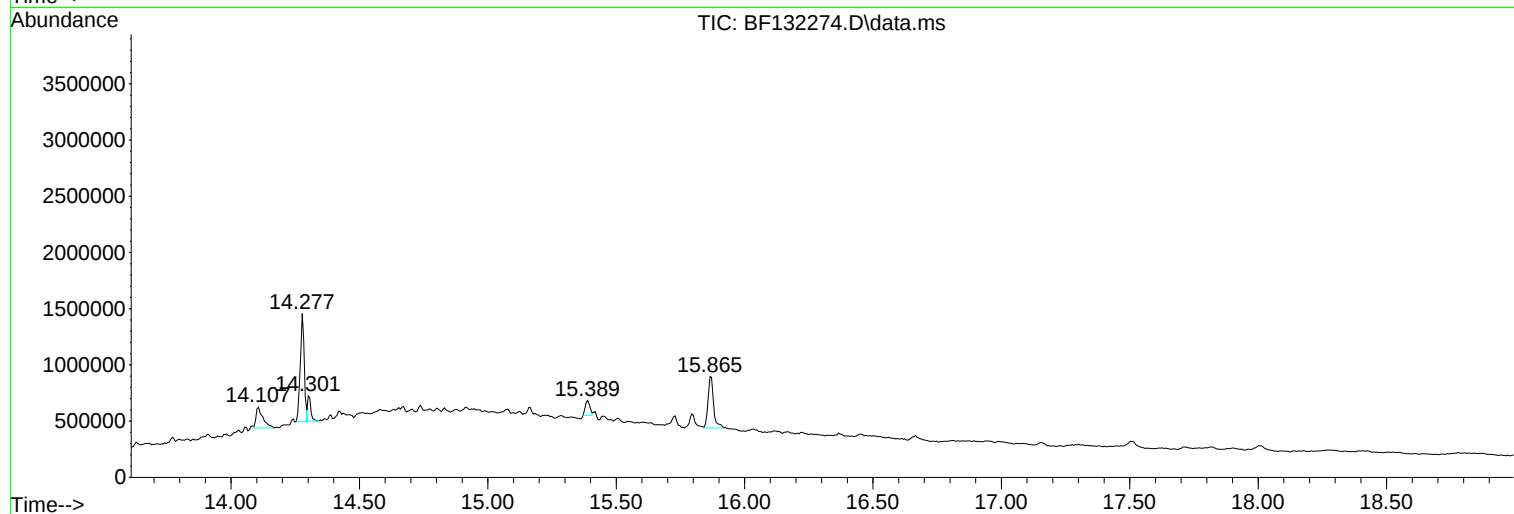
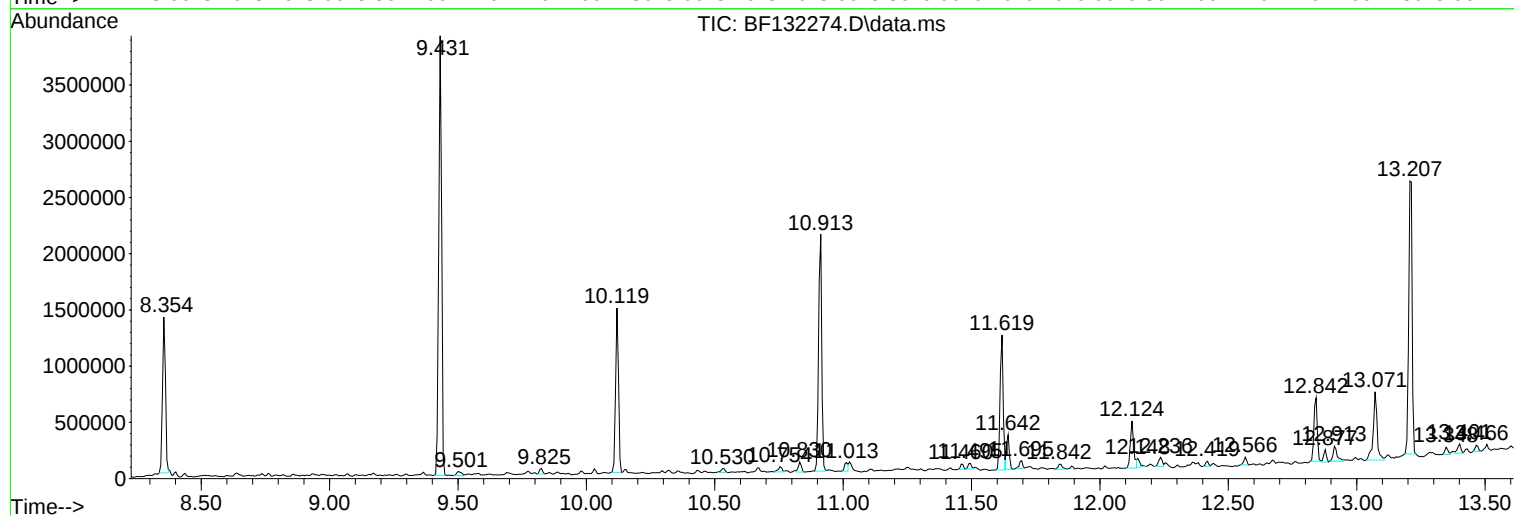
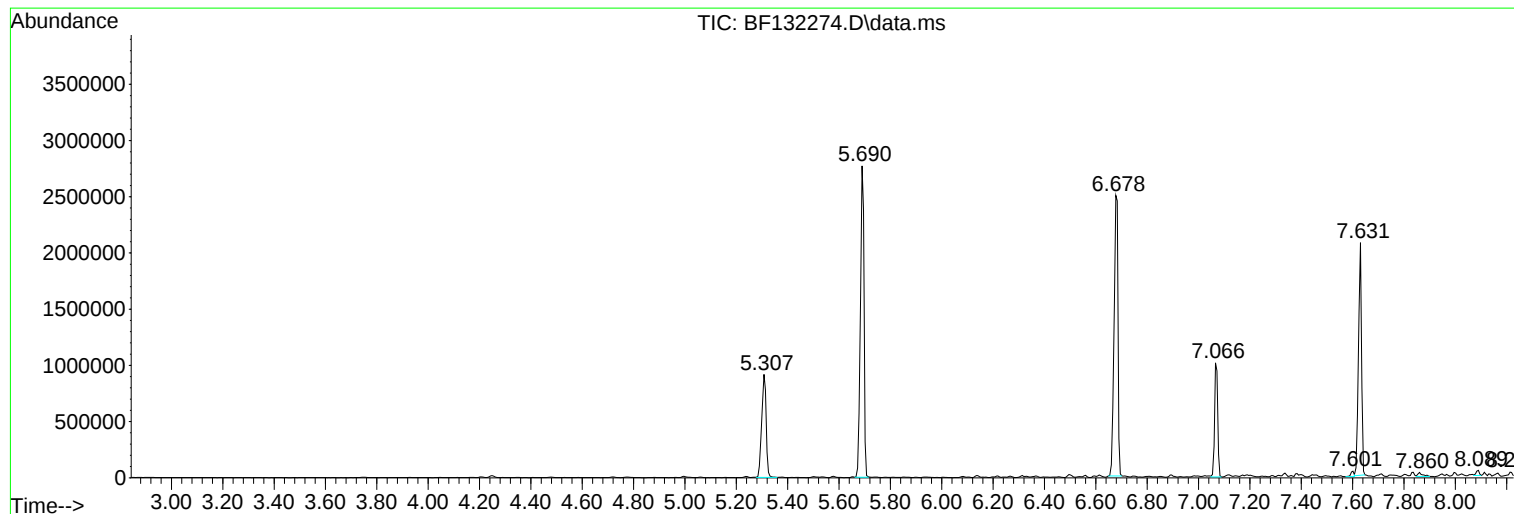
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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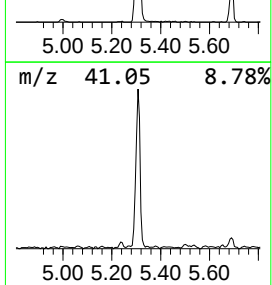
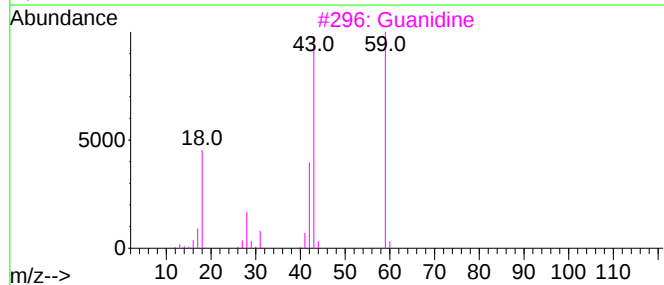
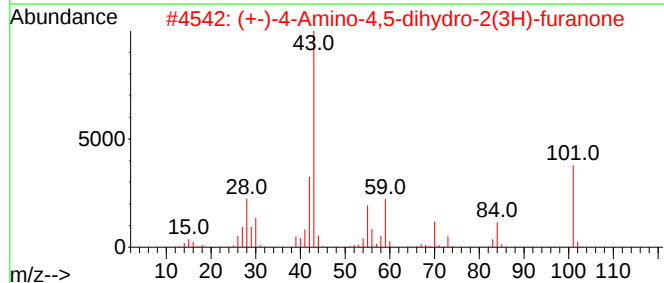
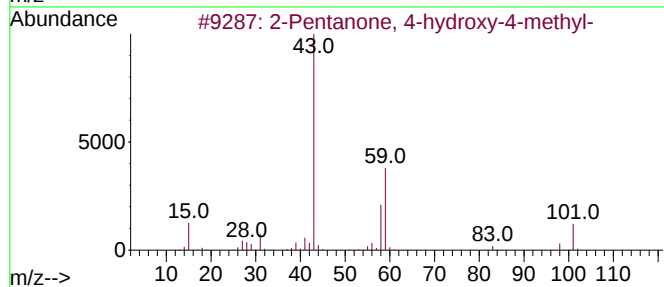
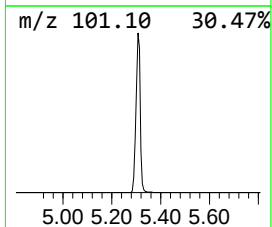
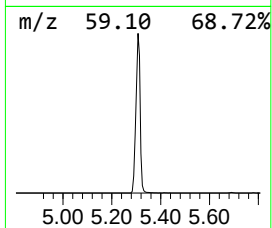
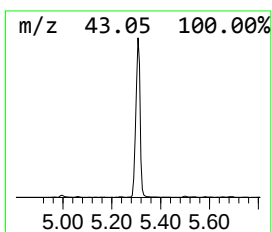
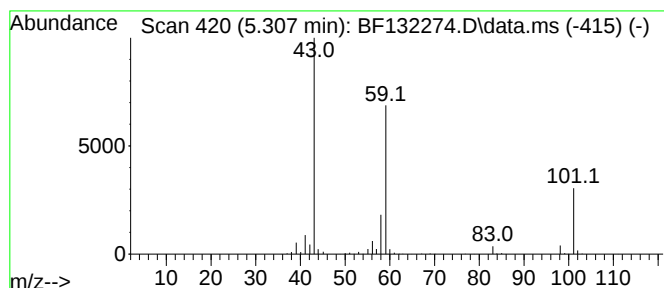
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	24.98 ng	1084660	1,4-Dichlorobenzene-d4	7.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17



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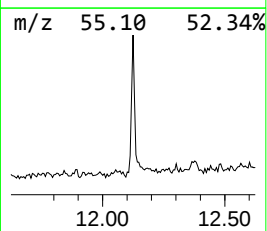
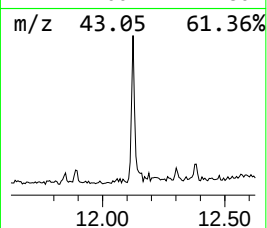
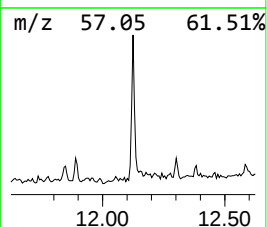
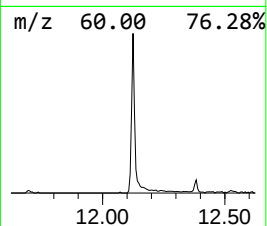
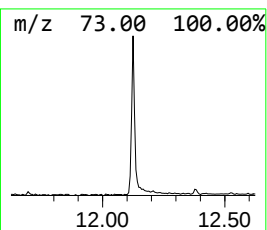
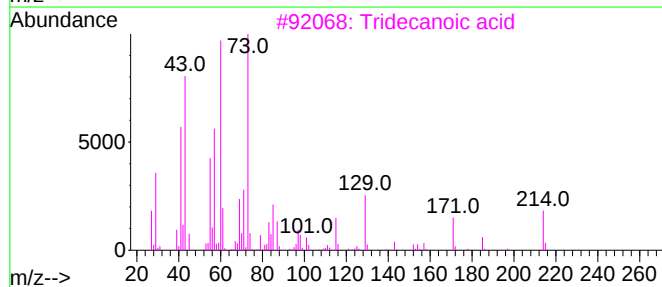
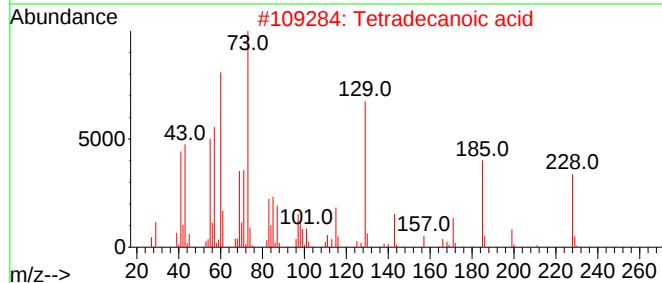
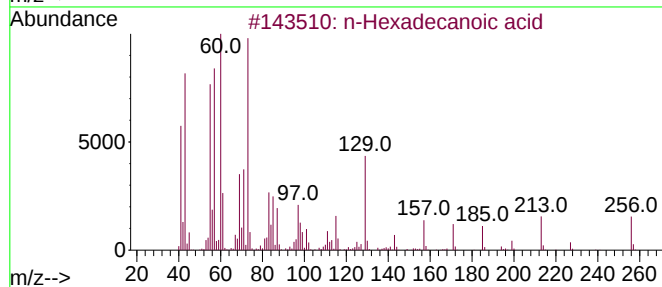
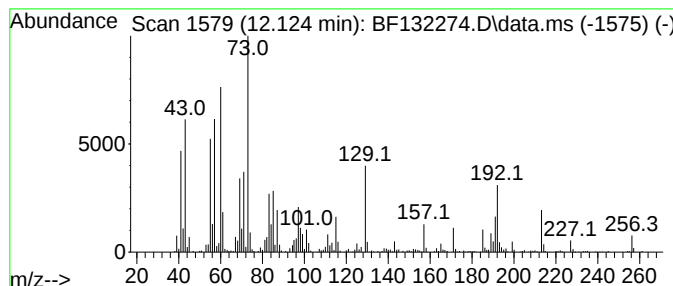
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	7.73 ng	390307	Phenanthrene-d10	11.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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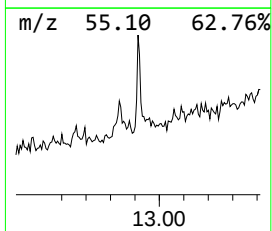
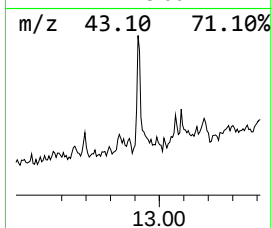
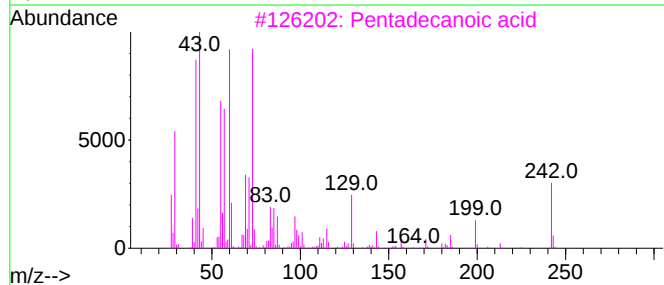
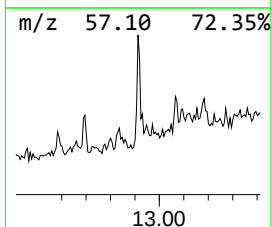
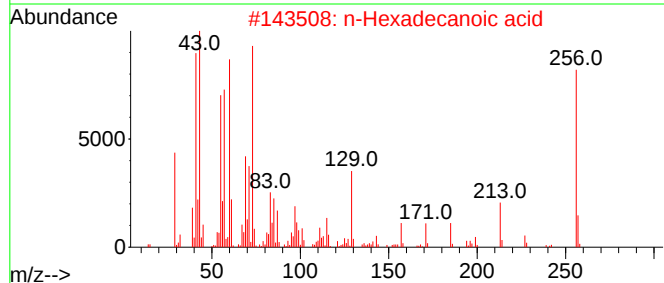
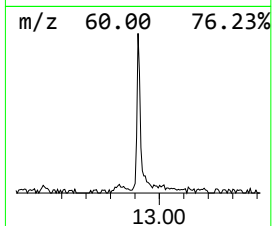
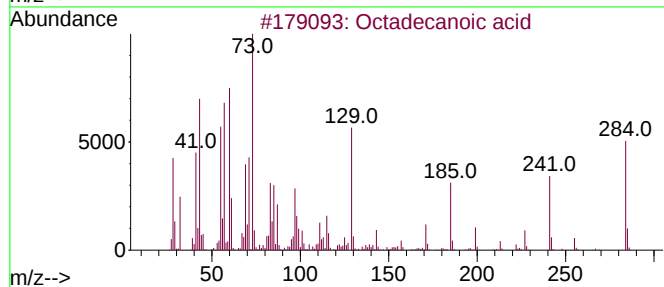
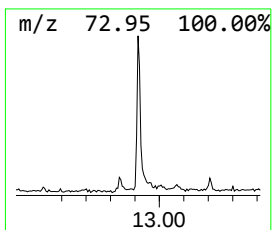
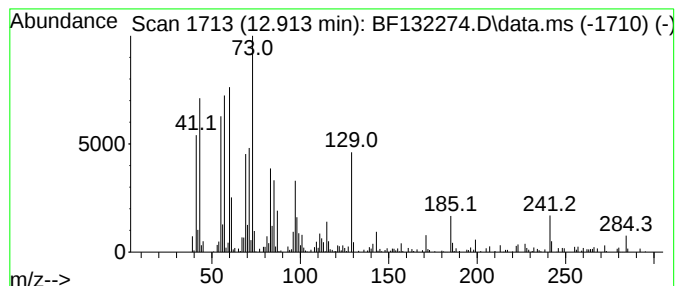
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.913	2.96 ng	149456	Phenanthrene-d10	11.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Nonadecane	268	C19H40	000629-92-5	56



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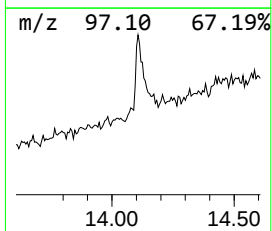
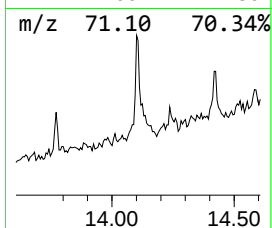
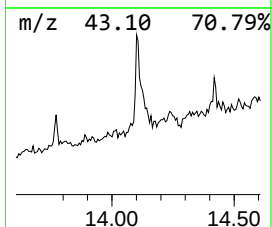
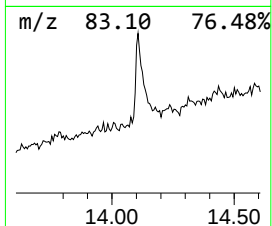
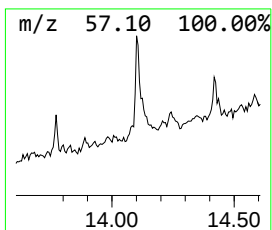
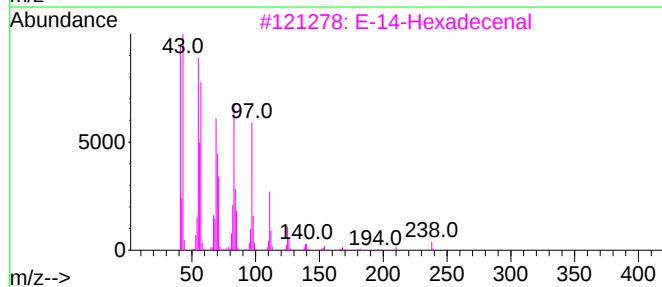
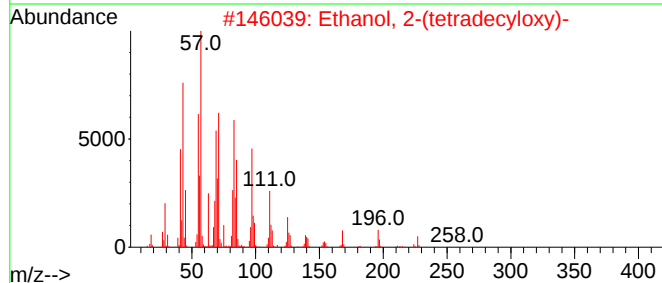
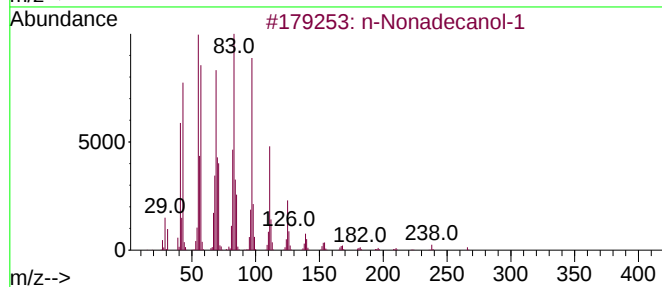
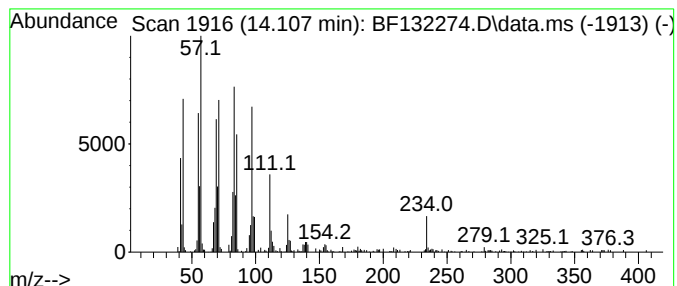
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.107	6.48 ng	342901	Chrysene-d12	14.277	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	E-14-Hexadecenal	238	C16H30O	330207-53-9	90
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86



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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-...	5.307	25.0	ng	1084660	1	7.072	868557	20.0
n-Hexadecanoic ...	12.124	7.7	ng	390307	4	11.619	1009550	20.0
Octadecanoic acid	12.913	3.0	ng	149456	4	11.619	1009550	20.0
n-Nonadecanol-1	14.107	6.5	ng	342901	5	14.277	1058140	20.0