

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081023\
 Data File : BF134716.D
 Acq On : 10 Aug 2023 18:59
 Operator : CG\JU
 Sample : 03954-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-17

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: BF134716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	497	501	510	rVB	82186	98270	3.34%	0.402%
2	5.434	564	569	572	rBV	2806325	2667727	90.79%	10.918%
3	6.434	734	739	742	rBV	2670379	2689647	91.53%	11.007%
4	6.634	769	773	778	rBV	59914	62011	2.11%	0.254%
5	6.798	798	801	805	rBV	1412294	1111514	37.83%	4.549%
6	7.357	892	896	899	rBV	1842257	1654683	56.31%	6.772%
7	8.075	1015	1018	1021	rBV	1654826	1420220	48.33%	5.812%
8	8.098	1021	1022	1027	rVB	108226	65147	2.22%	0.267%
9	8.792	1136	1140	1144	rVB	38048	34174	1.16%	0.140%
10	9.151	1197	1201	1212	rBV	3033366	2938449	100.00%	12.026%
11	9.275	1218	1222	1225	rVB	82935	79585	2.71%	0.326%
12	9.428	1242	1248	1256	rBV4	31975	42811	1.46%	0.175%
13	9.692	1290	1293	1299	rBV	48565	40726	1.39%	0.167%
14	9.833	1313	1317	1321	rBV	1712550	1451745	49.41%	5.941%
15	10.039	1348	1352	1356	rBV	46504	48723	1.66%	0.199%
16	10.380	1407	1410	1414	rBV	55721	49892	1.70%	0.204%
17	10.622	1447	1451	1462	rBV	1871586	1672009	56.90%	6.843%
18	11.216	1550	1552	1558	rVB	36732	35311	1.20%	0.145%
19	11.322	1566	1570	1572	rBV	1506165	1300331	44.25%	5.322%
20	11.345	1572	1574	1578	rVV	465898	359560	12.24%	1.471%
21	11.392	1578	1582	1586	rVB	87544	95707	3.26%	0.392%
22	11.557	1605	1610	1612	rBV2	26299	31518	1.07%	0.129%
23	11.722	1635	1638	1644	rVB2	27990	33265	1.13%	0.136%
24	11.857	1657	1661	1666	rBV2	363539	322860	10.99%	1.321%
25	11.933	1671	1674	1677	rBV2	45577	42212	1.44%	0.173%
26	12.122	1703	1706	1709	rBV	31748	31859	1.08%	0.130%
27	12.433	1753	1759	1761	rVB4	28971	37191	1.27%	0.152%
28	12.533	1773	1776	1780	rBV	315297	292524	9.96%	1.197%
29	12.645	1790	1795	1800	rBV2	85920	117643	4.00%	0.481%
30	12.763	1809	1815	1819	rBV	280854	291884	9.93%	1.195%
31	12.916	1837	1841	1844	rBV	2807476	2383275	81.11%	9.754%
32	13.157	1879	1882	1886	rVB2	27255	30500	1.04%	0.125%
33	13.198	1886	1889	1893	rBV2	29870	30805	1.05%	0.126%
34	13.821	1992	1995	2003	rVB2	218529	239094	8.14%	0.978%
35	13.968	2015	2020	2023	rBV	1196636	1143475	38.91%	4.680%
36	13.992	2023	2024	2031	rVV	122922	108354	3.69%	0.443%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.074	2035	2038	2041	rVB2	41665	42935	1.46%	0.176%
38	14.145	2048	2050	2054	rBV2	37054	37665	1.28%	0.154%
39	14.457	2100	2103	2105	rBV3	60698	66754	2.27%	0.273%
40	14.745	2148	2152	2154	rBV	84379	107426	3.66%	0.440%
41	14.839	2165	2168	2172	rBV3	57959	63861	2.17%	0.261%
42	15.010	2194	2197	2209	rVB	76896	153837	5.24%	0.630%
43	15.374	2256	2259	2263	rBV	64352	78040	2.66%	0.319%
44	15.439	2266	2270	2275	rBV	649408	829722	28.24%	3.396%

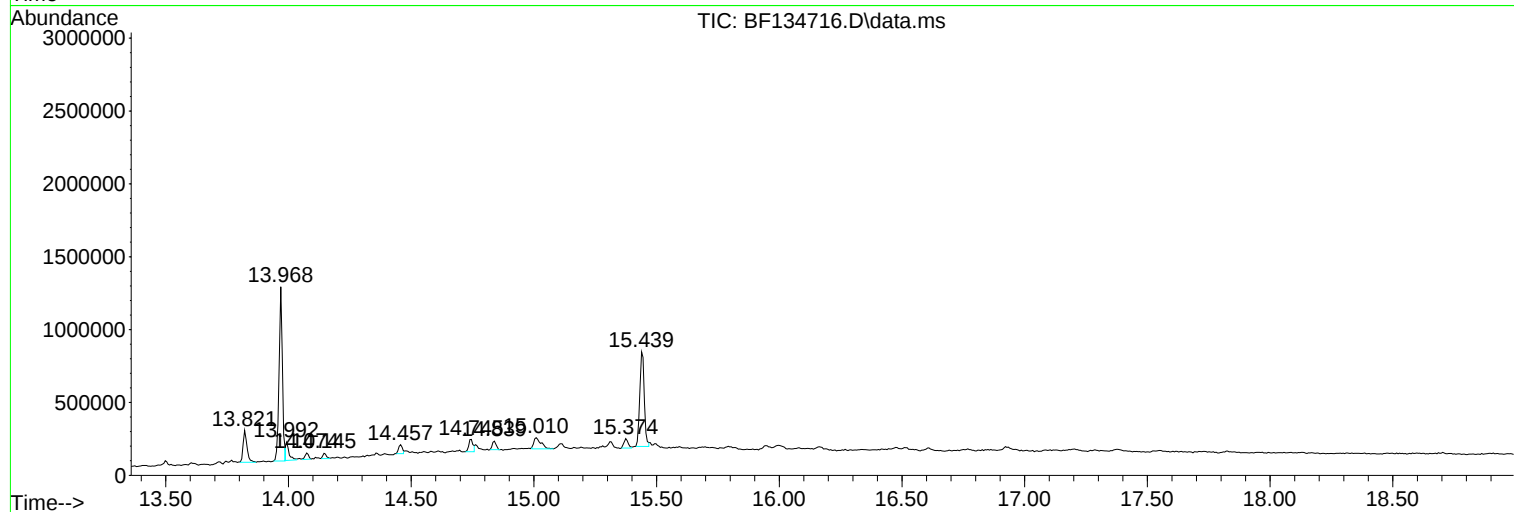
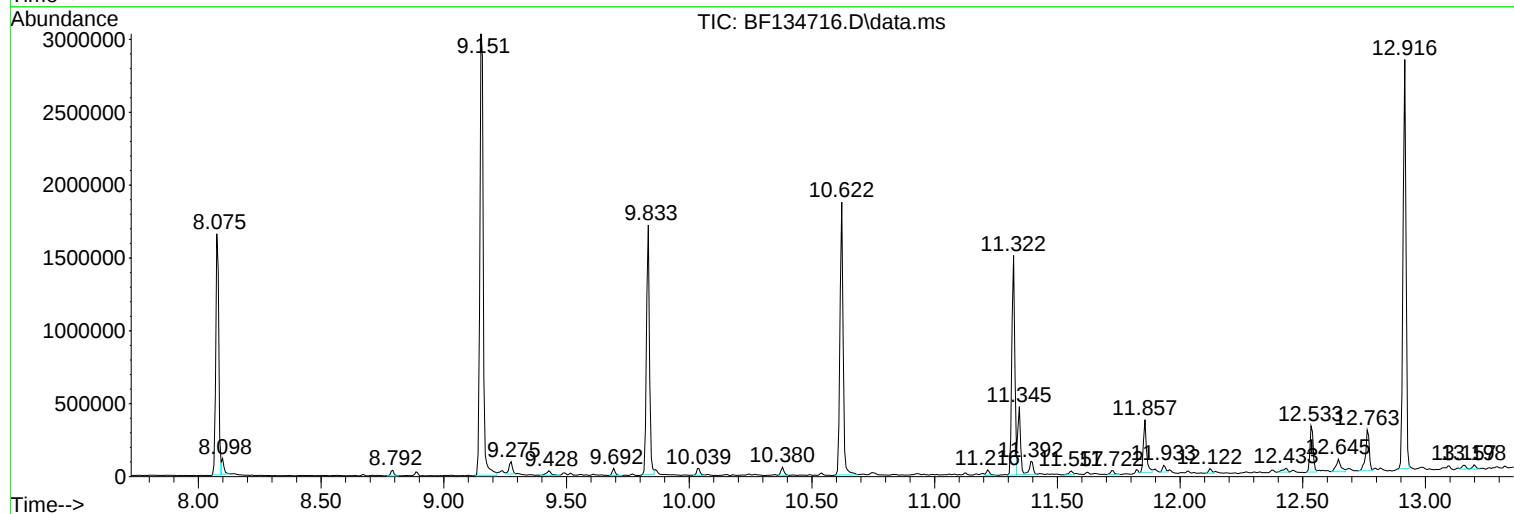
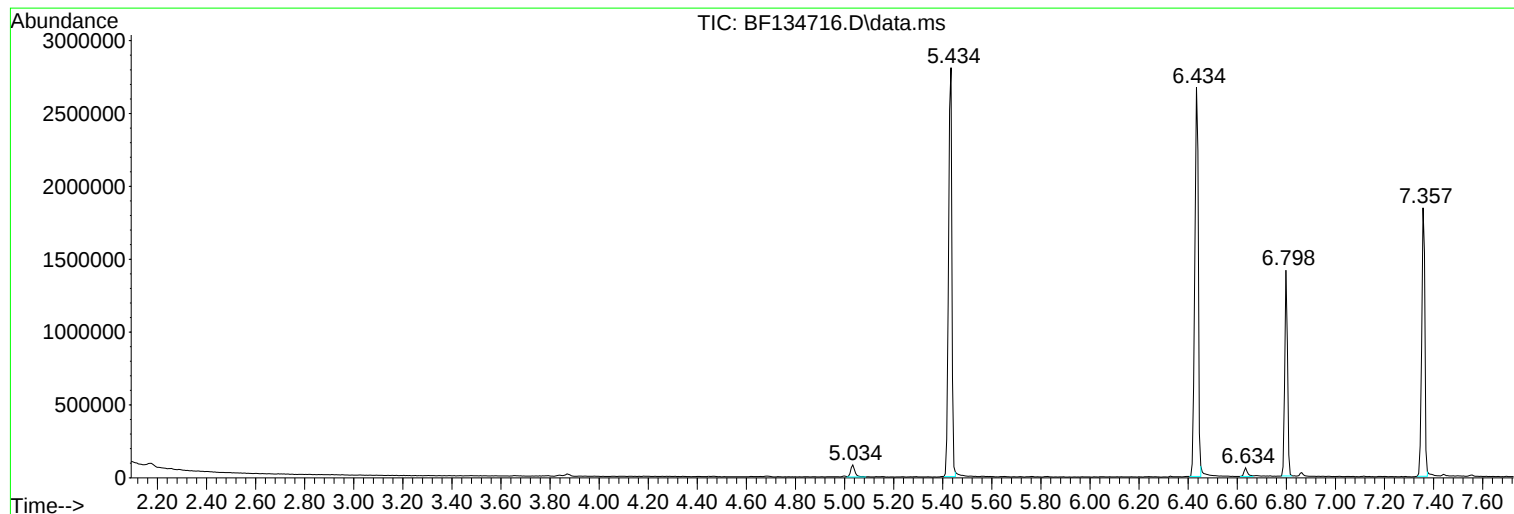
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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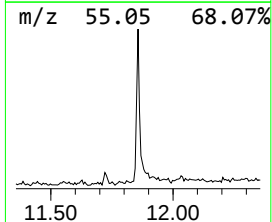
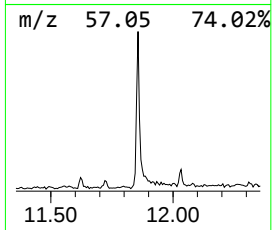
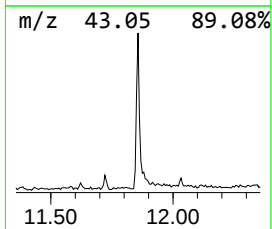
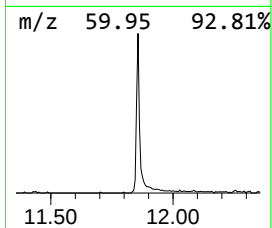
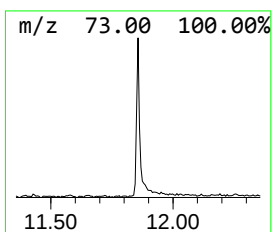
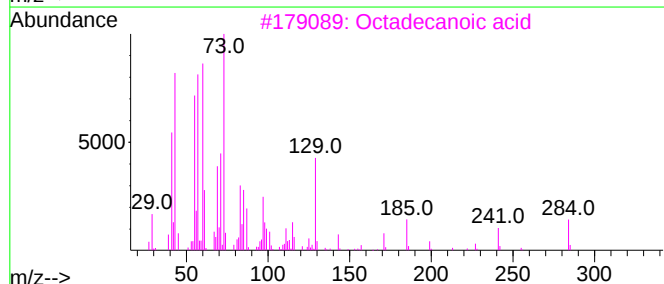
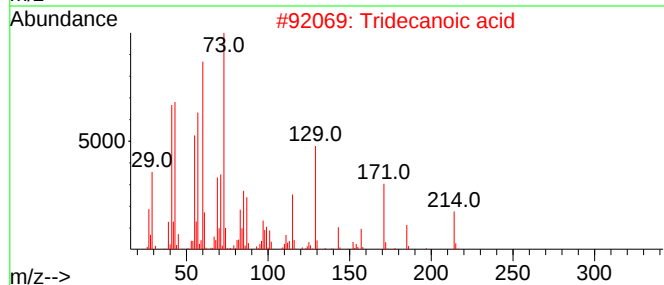
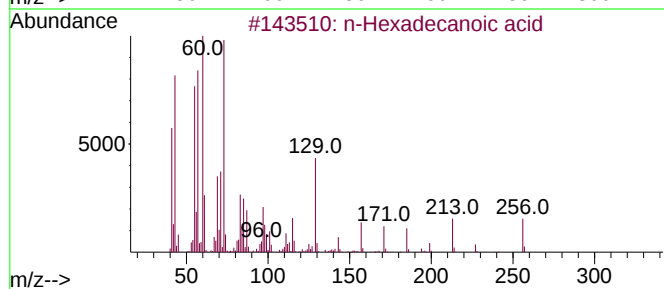
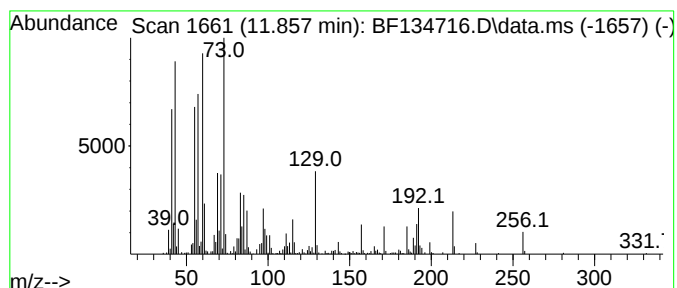
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.97 ng	322860	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	96
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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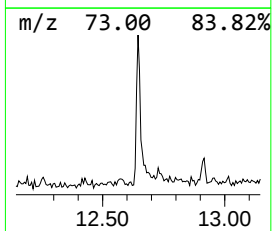
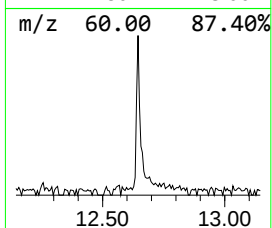
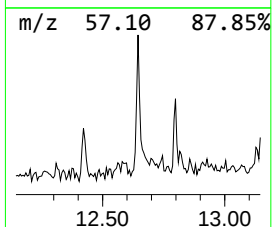
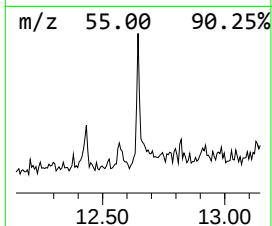
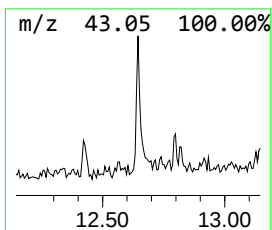
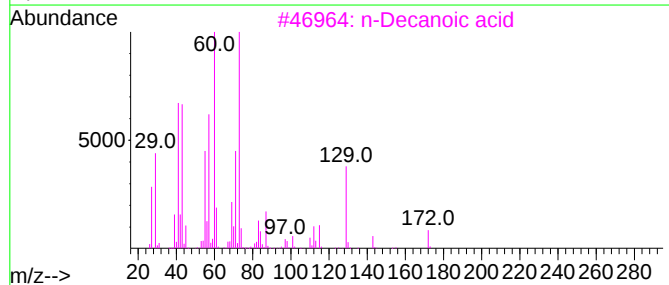
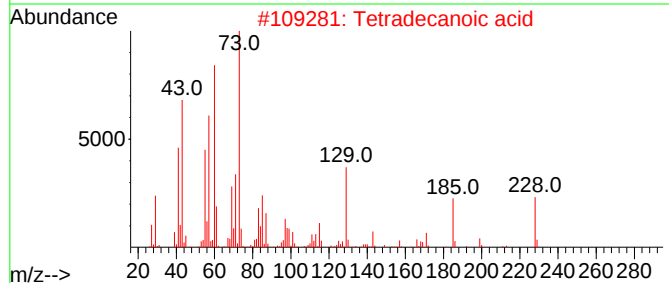
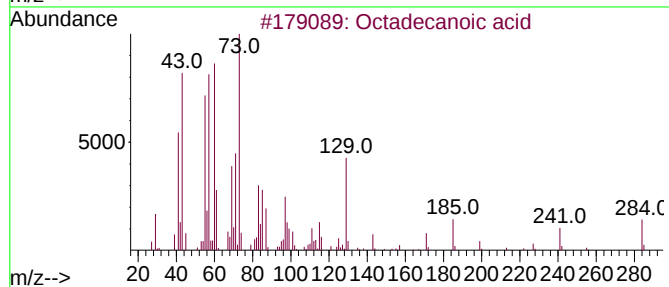
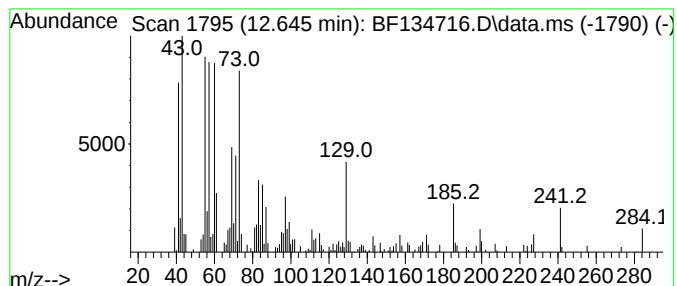
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.06 ng	117643	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			n-Decanoic acid	172	C10H20O2	000334-48-5	62
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			Hexadecane	226	C16H34	000544-76-3	25



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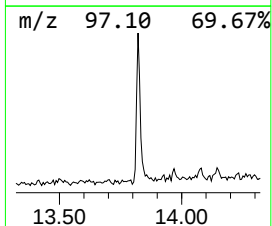
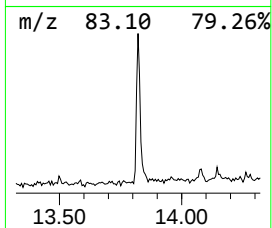
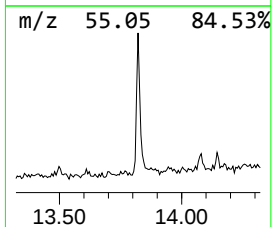
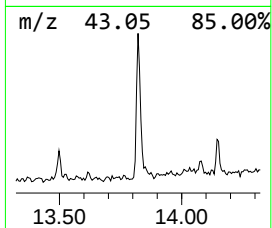
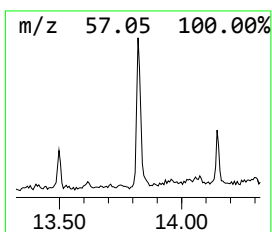
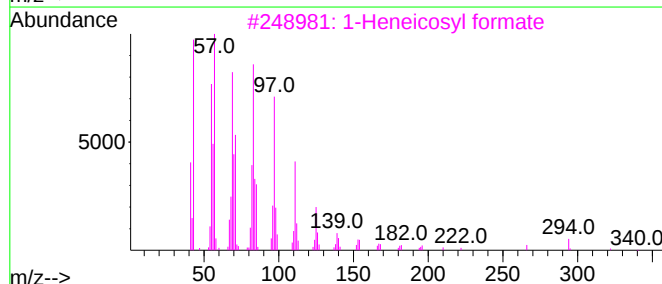
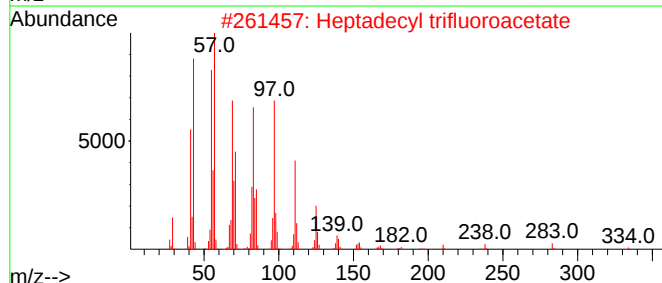
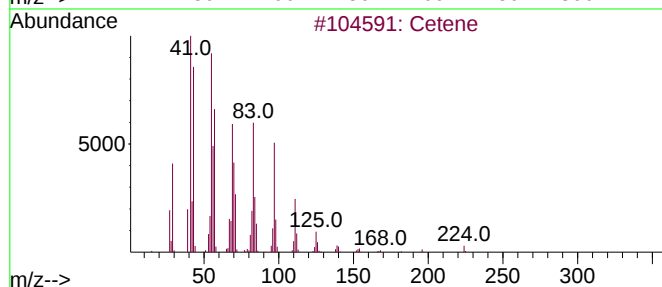
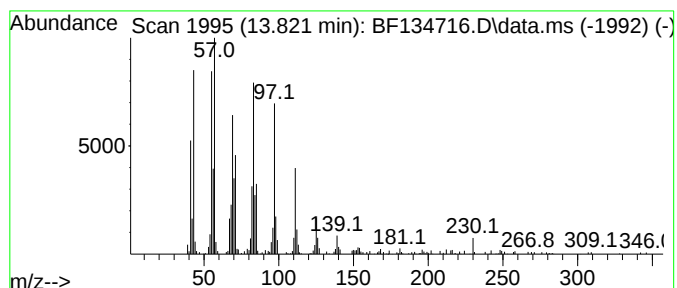
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	4.18 ng	239094	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	95
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			1-Tricosene	322	C23H46	018835-32-0	91



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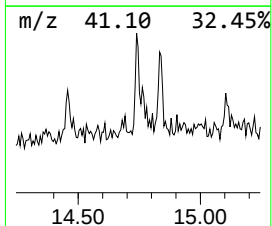
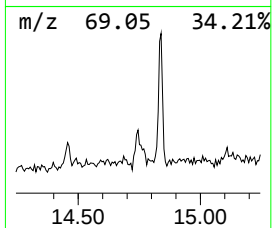
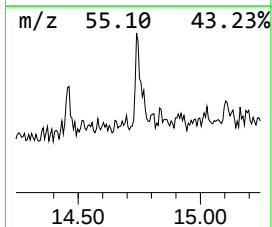
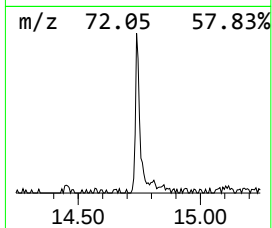
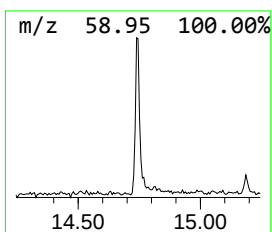
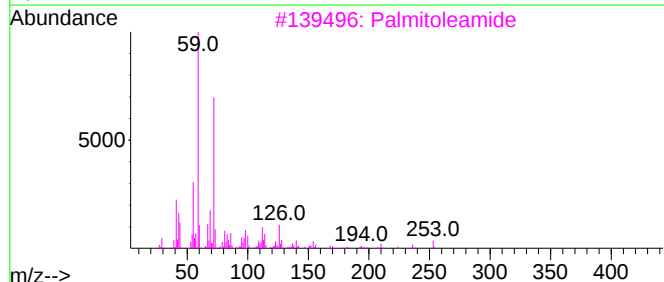
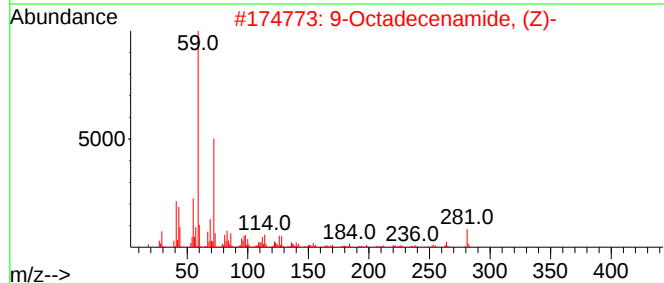
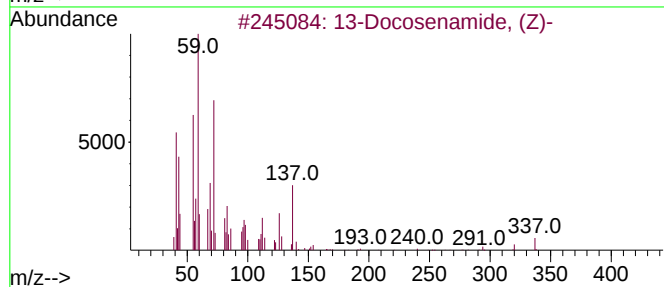
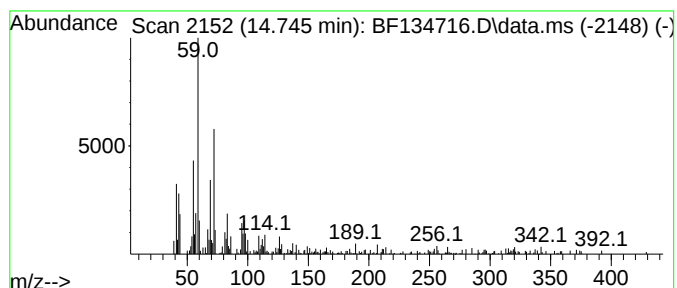
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.59 ng	107426	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3			Palmitoleamide	253	C16H31NO	106010-22-4	72
4			Nonadecanamide	297	C19H39NO	058185-32-3	59
5			Octadecanamide	283	C18H37NO	000124-26-5	50



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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
n-Hexadecanoic ...	11.857	5.0	ng	322860	4	11.322	1300330	20.0
Octadecanoic acid	12.645	2.1	ng	117643	5	13.969	1143480	20.0
Cetene	13.821	4.2	ng	239094	5	13.969	1143480	20.0
13-Docosenamide...	14.745	2.6	ng	107426	6	15.439	829722	20.0