

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
 Data File : BF128277.D
 Acq On : 16 May 2022 19:45
 Operator : CG\JU
 Sample : N2832-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB01

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	477	480	488	rBV	12669	16398	1.08%	0.133%
2	5.510	544	548	558	rBV	1496531	1382471	91.27%	11.235%
3	6.516	715	719	729	rBV	1525909	1351222	89.21%	10.981%
4	6.887	778	782	785	rBV	475020	412574	27.24%	3.353%
5	7.410	865	871	873	rBV5	10033	17592	1.16%	0.143%
6	7.451	873	878	881	rVV	909044	879042	58.04%	7.144%
7	7.522	885	890	893	rVB4	15402	22168	1.46%	0.180%
8	7.687	914	918	924	rVB3	16111	17741	1.17%	0.144%
9	7.798	935	937	943	rVB4	19023	20679	1.37%	0.168%
10	8.169	996	1000	1003	rBV	549340	467626	30.87%	3.800%
11	8.210	1005	1007	1010	rVB2	21057	19764	1.30%	0.161%
12	8.445	1043	1047	1052	rVB6	17705	28523	1.88%	0.232%
13	9.239	1178	1182	1186	rBV	1553473	1336435	88.23%	10.861%
14	9.310	1190	1194	1198	rVV	42605	43563	2.88%	0.354%
15	9.628	1245	1248	1254	rVB4	40153	41133	2.72%	0.334%
16	9.786	1271	1275	1280	rBV2	29403	38122	2.52%	0.310%
17	9.828	1280	1282	1287	rVB3	23256	29428	1.94%	0.239%
18	9.922	1295	1298	1302	rVB	503290	457686	30.22%	3.720%
19	10.239	1348	1352	1356	rBV4	15731	28004	1.85%	0.228%
20	10.339	1364	1369	1371	rBV2	22214	29508	1.95%	0.240%
21	10.557	1404	1406	1409	rVB	20340	17631	1.16%	0.143%
22	10.716	1429	1433	1443	rBV	1045229	881020	58.17%	7.160%
23	10.828	1447	1452	1455	rBV2	39691	55052	3.63%	0.447%
24	11.263	1523	1526	1528	rBV	26343	22866	1.51%	0.186%
25	11.292	1528	1531	1533	rVV	26159	22425	1.48%	0.182%
26	11.416	1548	1552	1554	rBV	628656	515760	34.05%	4.192%
27	11.439	1554	1556	1561	rVV	129677	107630	7.11%	0.875%
28	11.492	1562	1565	1567	rVB	25311	20738	1.37%	0.169%
29	11.645	1588	1591	1594	rBV4	16946	23589	1.56%	0.192%
30	11.692	1596	1599	1603	rVB2	21031	18084	1.19%	0.147%
31	11.927	1635	1639	1641	rBV3	44824	59438	3.92%	0.483%
32	12.033	1653	1657	1659	rBV2	33416	33749	2.23%	0.274%
33	12.098	1665	1668	1671	rBV	28233	25521	1.68%	0.207%
34	12.216	1685	1688	1690	rBV	16846	17301	1.14%	0.141%
35	12.469	1728	1731	1732	rBV	22493	18665	1.23%	0.152%
36	12.486	1732	1734	1739	rVB5	21965	28850	1.90%	0.234%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.633	1756	1759	1763	rBV	253523	212105	14.00%	1.724%
38	12.810	1787	1789	1792	rVB3	21057	17331	1.14%	0.141%
39	12.845	1792	1795	1796	rBV2	43391	45012	2.97%	0.366%
40	12.863	1796	1798	1804	rVB	245527	208581	13.77%	1.695%
41	13.004	1817	1822	1825	rBV	1622300	1514649	100.00%	12.309%
42	13.074	1831	1834	1840	rVB5	22718	36532	2.41%	0.297%
43	13.216	1856	1858	1861	rBV2	22720	22825	1.51%	0.185%
44	13.257	1863	1865	1867	rVB	29915	21354	1.41%	0.174%
45	13.416	1890	1892	1895	rBV2	23035	25961	1.71%	0.211%
46	13.910	1971	1976	1985	rVB3	113789	241423	15.94%	1.962%
47	14.063	1998	2002	2005	rBV2	613095	632095	41.73%	5.137%
48	14.086	2005	2006	2014	rVB	110330	101726	6.72%	0.827%
49	14.810	2126	2129	2133	rBV2	179317	171198	11.30%	1.391%
50	15.116	2178	2181	2184	rBV	71492	94919	6.27%	0.771%
51	15.492	2242	2245	2251	rVB	73002	93928	6.20%	0.763%
52	15.557	2252	2256	2261	rBV	287744	357094	23.58%	2.902%

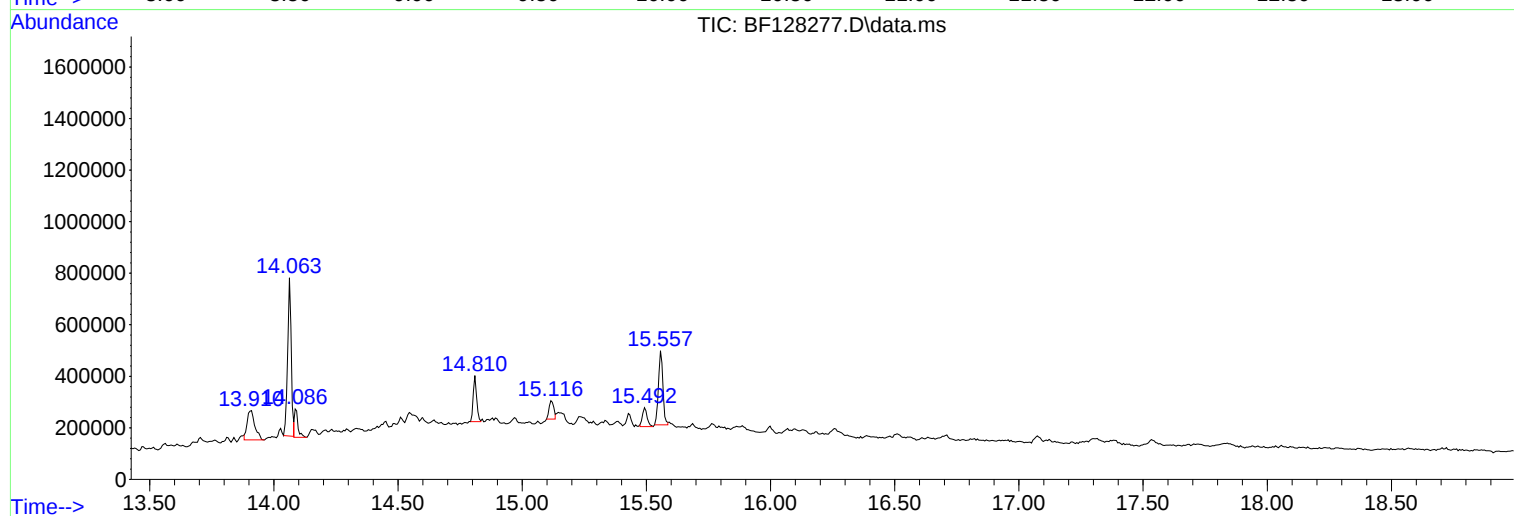
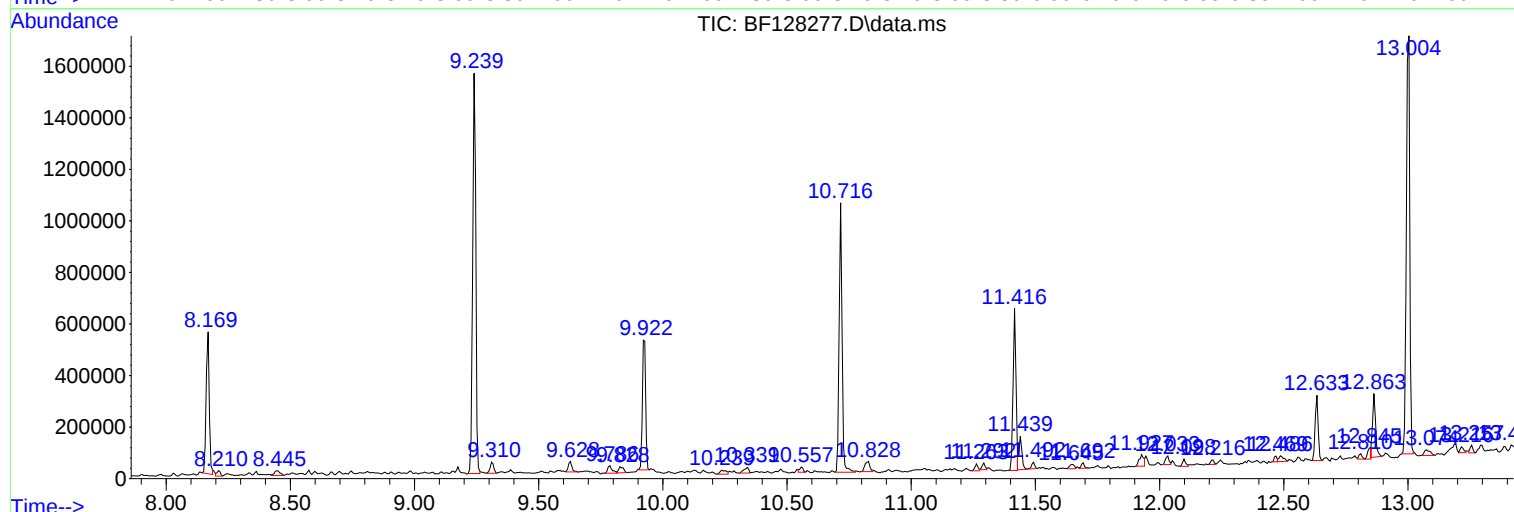
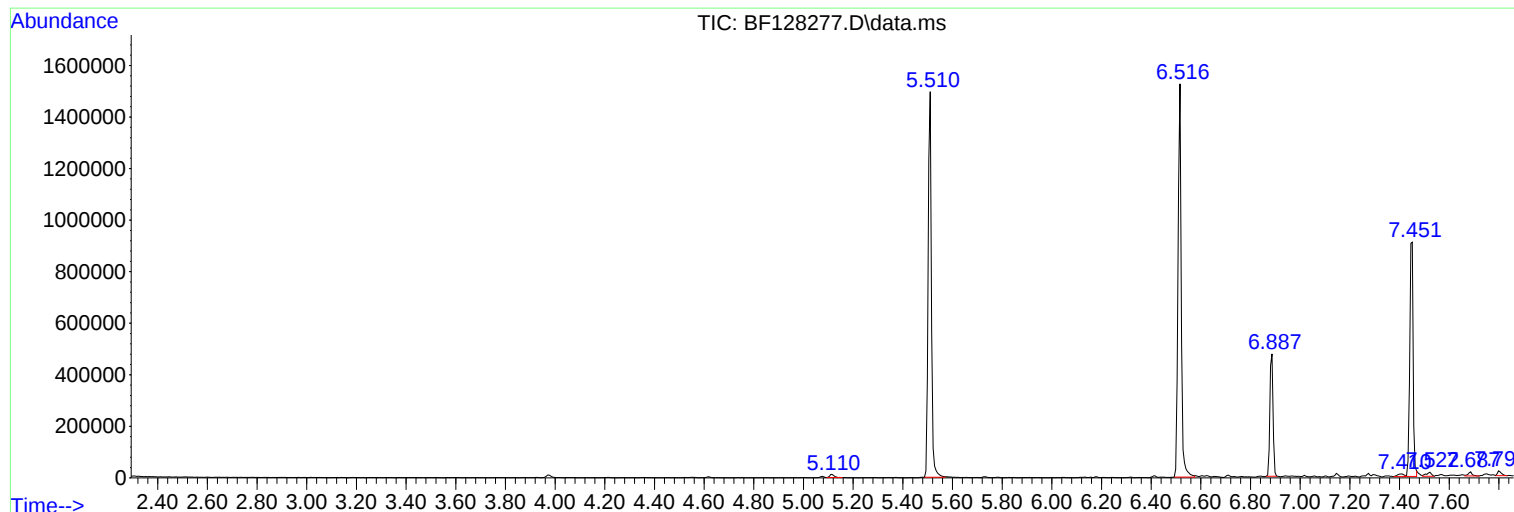
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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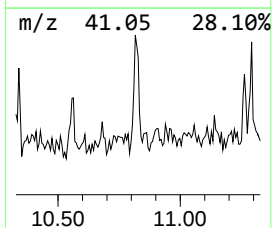
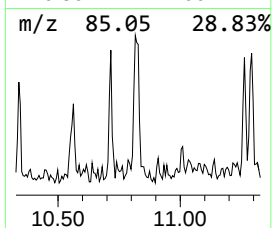
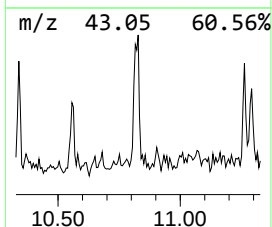
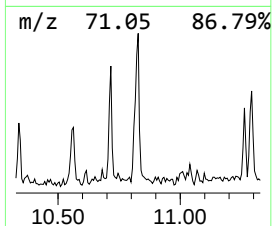
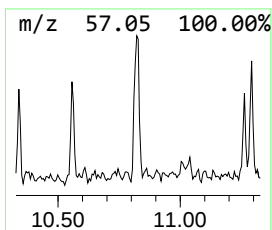
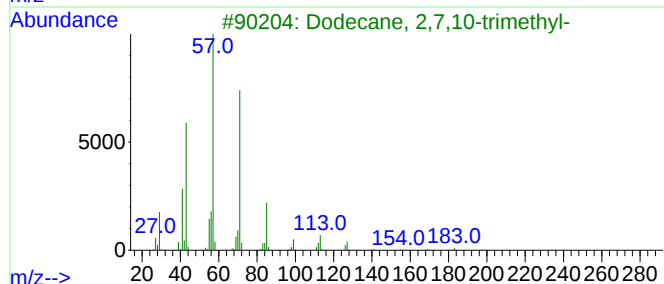
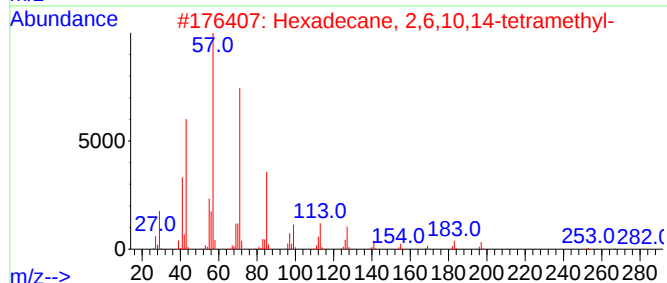
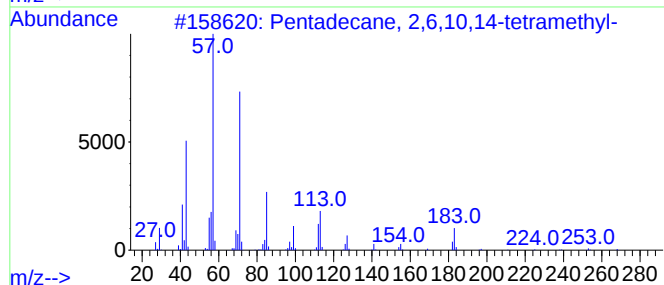
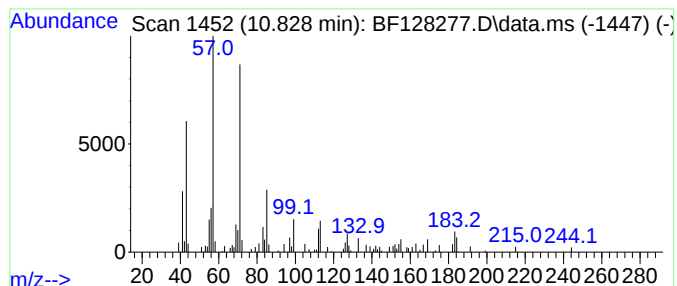
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	2.13 ng	55052	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	80
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



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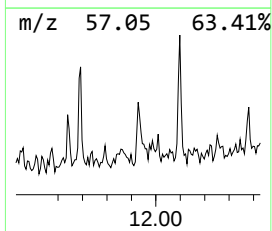
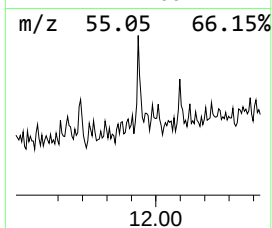
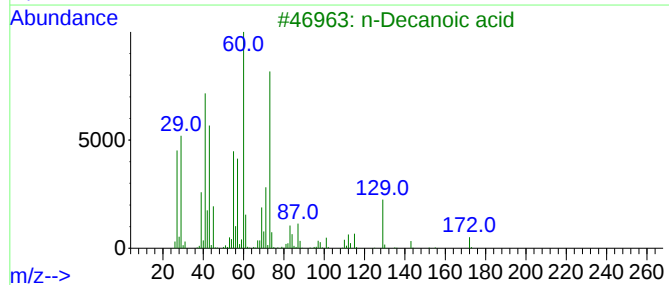
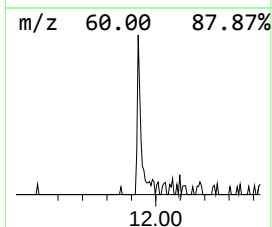
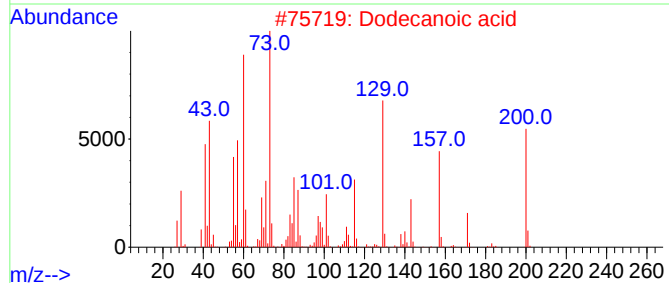
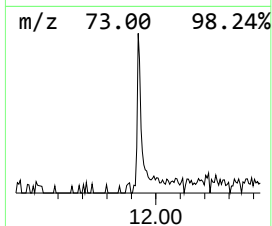
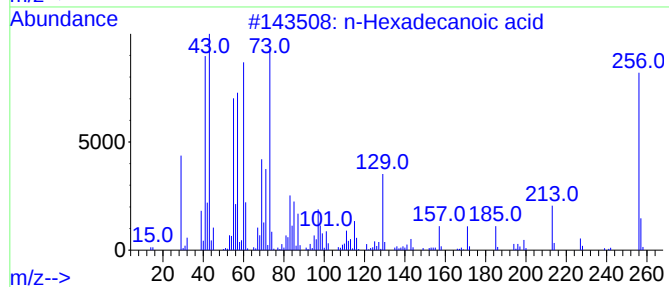
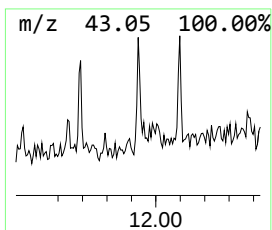
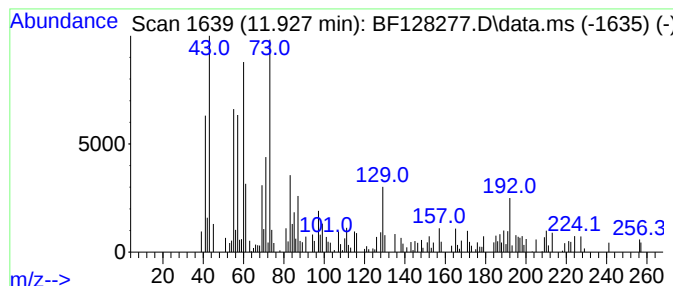
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	2.30 ng	59438	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2		Dodecanoic acid	200	C12H24O2	000143-07-7	62
3		n-Decanoic acid	172	C10H20O2	000334-48-5	58
4		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	50



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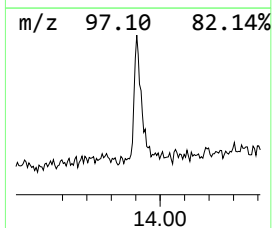
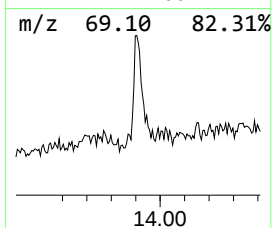
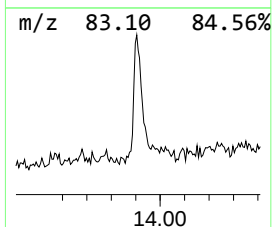
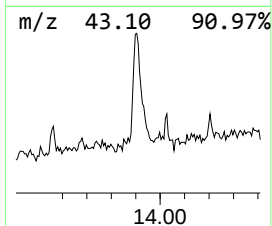
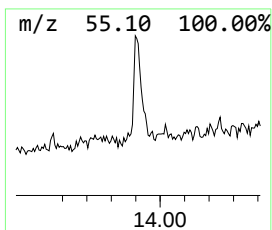
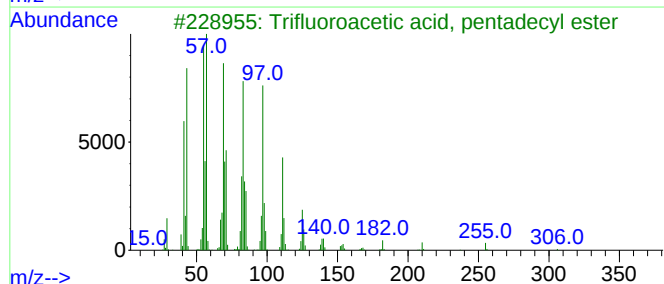
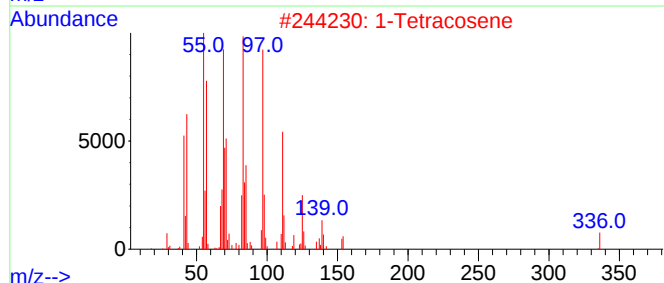
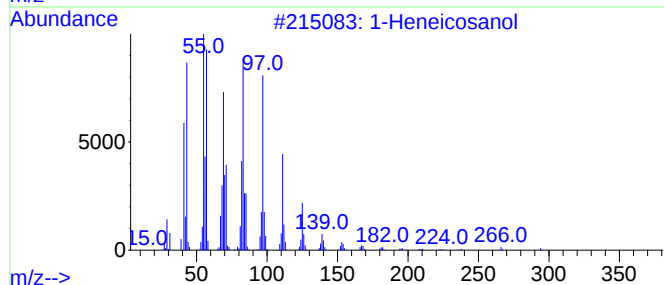
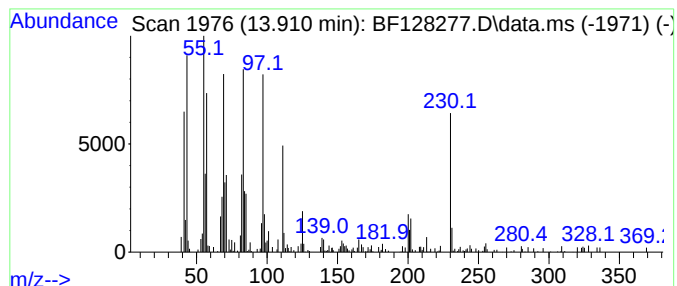
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.910	7.64 ng	241423	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Tetracosene	336	C24H48	010192-32-2	93
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
5	Cyclotetracosane	336	C24H48	000297-03-0	74



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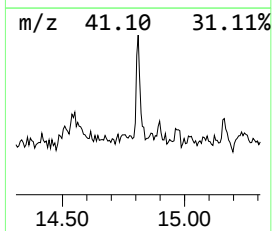
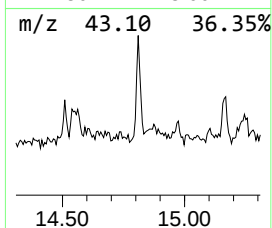
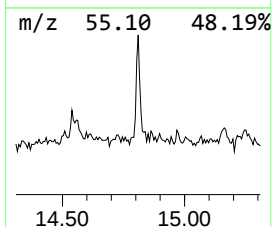
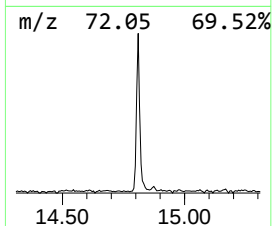
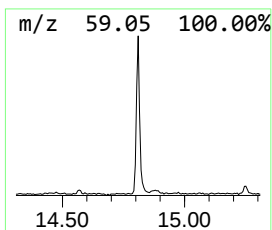
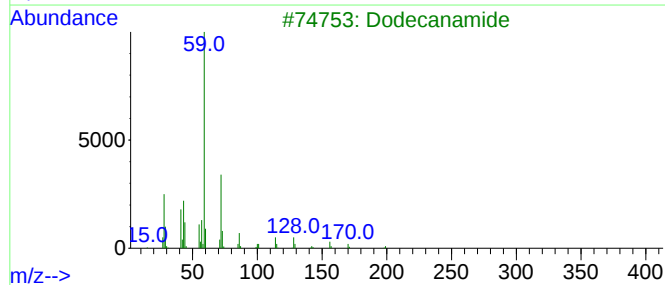
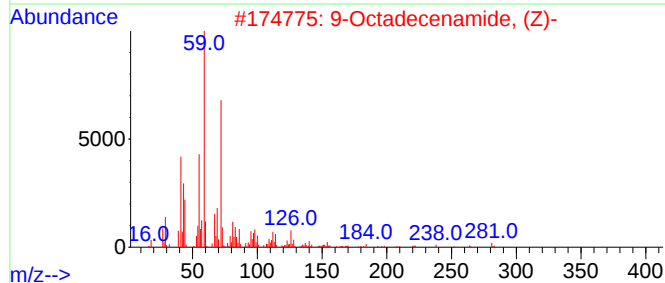
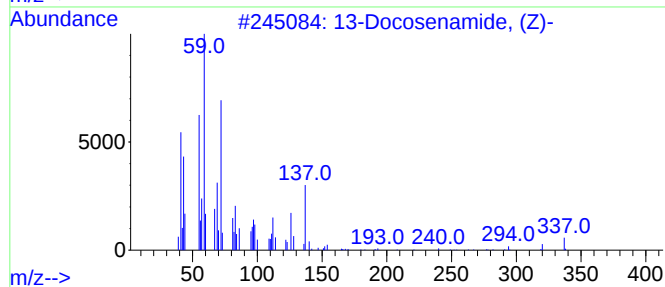
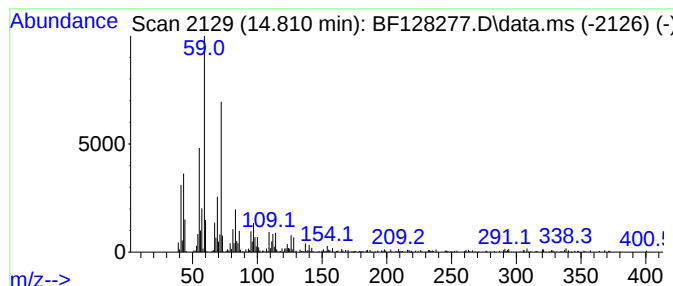
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	9.59 ng	171198	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3			Dodecanamide	199	C12H25NO	001120-16-7	47
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	43
5			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentadecane, 2,...	10.828	2.1	ng	55052	4	11.416	515760	20.0
n-Hexadecanoic ...	11.928	2.3	ng	59438	4	11.416	515760	20.0
1-Heneicosanol	13.910	7.6	ng	241423	5	14.063	632095	20.0
13-Docosenamide...	14.810	9.6	ng	171198	6	15.557	357094	20.0