

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
 Data File : BF096969.D
 Acq On : 22 Jul 2017 4:39
 Operator : SJ/JU
 Sample : I4274-01
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 M-COMB-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.163	351	370	371	rBV2	32208	139491	3.62%	0.265%
2	4.704	459	462	463	rBV	112577	120030	3.12%	0.228%
3	4.722	463	465	476	rVB	319486	365307	9.48%	0.694%
4	4.934	478	501	505	rBV2	97784	451901	11.73%	0.859%
5	5.104	515	530	533	rBV2	118850	344494	8.94%	0.655%
6	5.157	537	539	549	rVB	296434	286799	7.44%	0.545%
7	5.493	567	596	599	rBV2	161958	859930	22.32%	1.634%
8	6.210	714	718	723	rBV2	215154	377305	9.79%	0.717%
9	6.322	735	737	744	rVB	466276	437343	11.35%	0.831%
10	6.551	773	776	780	rBV	700052	639655	16.60%	1.215%
11	6.710	799	803	810	rVV	1300989	1180318	30.64%	2.243%
12	6.981	842	849	859	rVB2	755136	935208	24.27%	1.777%
13	7.116	867	872	876	rBV	930795	869037	22.56%	1.651%
14	7.181	880	883	886	rVV	247902	197146	5.12%	0.375%
15	7.304	901	904	911	rBV	227052	262338	6.81%	0.498%
16	7.657	953	964	967	rBV3	334255	719937	18.69%	1.368%
17	7.757	977	981	985	rBV	403232	375882	9.76%	0.714%
18	7.840	991	995	997	rBV	906616	859361	22.31%	1.633%
19	7.863	997	999	1003	rVB3	138665	181038	4.70%	0.344%
20	7.975	1014	1018	1020	rBV	196414	179317	4.65%	0.341%
21	8.004	1020	1023	1033	rVB	407886	493559	12.81%	0.938%
22	8.139	1040	1046	1048	rBV	212684	273971	7.11%	0.521%
23	8.163	1048	1050	1056	rVV3	97067	130600	3.39%	0.248%
24	8.434	1094	1096	1101	rVV3	118906	173879	4.51%	0.330%
25	8.481	1101	1104	1108	rVB	781338	642321	16.67%	1.220%
26	8.798	1154	1158	1161	rVV	404231	457636	11.88%	0.869%
27	8.916	1173	1178	1181	rVV	1689154	1513676	39.29%	2.876%
28	9.022	1191	1196	1202	rVB2	130444	151994	3.95%	0.289%
29	9.204	1223	1227	1233	rVB4	89232	126978	3.30%	0.241%
30	9.310	1241	1245	1248	rBV	322769	256858	6.67%	0.488%
31	9.410	1258	1262	1269	rBV	788485	707883	18.37%	1.345%
32	9.581	1287	1291	1295	rVV	1374261	1245946	32.34%	2.367%
33	9.645	1299	1302	1310	rVV	176448	309949	8.05%	0.589%
34	9.845	1327	1336	1339	rBV	757087	1089109	28.27%	2.069%

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35	9.922	1346	1349	1352	rBV	256890	206654	5.36%	0.393%
36	10.010	1361	1364	1366	rBV	282091	220775	5.73%	0.419%
37	10.304	1410	1414	1417	rVV	206759	196912	5.11%	0.374%
38	10.369	1421	1425	1428	rBV	274205	255548	6.63%	0.486%
39	10.410	1428	1432	1435	rVV	632327	628318	16.31%	1.194%
40	10.445	1435	1438	1441	rVV2	87021	104513	2.71%	0.199%
41	10.480	1441	1444	1446	rVV3	103735	121647	3.16%	0.231%
42	10.504	1446	1448	1451	rVV	168723	184436	4.79%	0.350%
43	10.533	1451	1453	1458	rVV	665895	668449	17.35%	1.270%
44	10.598	1458	1464	1468	rVV	453410	498170	12.93%	0.946%
45	10.769	1489	1493	1496	rVV	455498	462887	12.01%	0.879%
46	10.869	1507	1510	1515	rVV	684532	604181	15.68%	1.148%
47	10.951	1521	1524	1527	rVB	114437	95965	2.49%	0.182%
48	11.057	1535	1542	1549	rBV	888746	908902	23.59%	1.727%
49	11.245	1571	1574	1579	rVV	668845	586983	15.24%	1.115%
50	11.304	1581	1584	1591	rVV2	582996	640858	16.63%	1.218%
51	11.410	1600	1602	1606	rVV	190578	192998	5.01%	0.367%
52	11.480	1611	1614	1620	rVB2	223553	204148	5.30%	0.388%
53	11.645	1632	1642	1654	rBV	2221902	3852643	100.00%	7.320%
54	11.769	1660	1663	1673	rVB	252104	289139	7.50%	0.549%
55	11.892	1681	1684	1691	rVB	356677	328402	8.52%	0.624%
56	12.027	1702	1707	1717	rBV7	62011	170637	4.43%	0.324%
57	12.122	1720	1723	1727	rVB	322943	280253	7.27%	0.532%
58	12.169	1727	1731	1734	rBV	209373	189051	4.91%	0.359%
59	12.333	1752	1759	1761	rBV2	549600	872278	22.64%	1.657%
60	12.422	1768	1774	1782	rVB	1238211	1480362	38.42%	2.813%
61	12.551	1792	1796	1802	rVB	218172	214015	5.56%	0.407%
62	12.639	1808	1811	1814	rVV	1026346	1013819	26.31%	1.926%
63	12.669	1814	1816	1826	rVB	170472	198182	5.14%	0.377%
64	12.798	1835	1838	1842	rVB	266118	234981	6.10%	0.446%
65	12.839	1842	1845	1848	rBV	253442	237386	6.16%	0.451%
66	12.910	1854	1857	1864	rVB3	292943	340676	8.84%	0.647%
67	13.151	1895	1898	1903	rVB2	188923	191507	4.97%	0.364%
68	13.486	1953	1955	1958	rVV	144306	147613	3.83%	0.280%
69	13.521	1958	1961	1964	rVV	510087	491158	12.75%	0.933%
70	13.557	1964	1967	1971	rVB2	185808	220398	5.72%	0.419%
71	13.598	1971	1974	1977	rBV	98926	98179	2.55%	0.187%

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72	13.686	1985	1989	1991	rBV	748944	668844	17.36%	1.271%
73	13.710	1991	1993	2001	rVB	247198	232837	6.04%	0.442%
74	13.780	2003	2005	2008	rBV	115874	120452	3.13%	0.229%
75	13.816	2008	2011	2015	rVB2	272892	266595	6.92%	0.507%
76	14.027	2044	2047	2052	rVB	140452	146244	3.80%	0.278%
77	14.180	2070	2073	2077	rBV2	108229	120431	3.13%	0.229%
78	14.333	2095	2099	2102	rBV	525026	492691	12.79%	0.936%
79	14.380	2105	2107	2113	rVB	241494	242760	6.30%	0.461%
80	14.533	2130	2133	2137	rVV	870656	896698	23.27%	1.704%
81	14.627	2146	2149	2154	rVV2	213281	282557	7.33%	0.537%
82	14.674	2154	2157	2160	rVB	133807	138895	3.61%	0.264%
83	14.839	2181	2185	2188	rBV2	75494	100416	2.61%	0.191%
84	14.951	2200	2204	2207	rVV	366099	480710	12.48%	0.913%
85	14.992	2207	2211	2216	rVV	560503	674317	17.50%	1.281%
86	15.051	2216	2221	2226	rVB	525111	600236	15.58%	1.140%
87	15.345	2267	2271	2274	rBV2	173174	217398	5.64%	0.413%
88	15.574	2307	2310	2317	rVB3	77445	148536	3.86%	0.282%
89	15.663	2318	2325	2337	rBV4	1172910	3585164	93.06%	6.811%
90	15.757	2337	2341	2345	rVB	259593	400408	10.39%	0.761%
91	15.821	2345	2352	2359	rBV	1579434	3151770	81.81%	5.988%
92	16.139	2401	2406	2416	rVV2	235606	582403	15.12%	1.107%
93	16.221	2416	2420	2427	rVB3	106692	204389	5.31%	0.388%
94	16.327	2434	2438	2447	rVB8	90000	179893	4.67%	0.342%
95	16.445	2455	2458	2471	rVB7	96750	247369	6.42%	0.470%
96	16.604	2479	2485	2491	rBV2	180923	402286	10.44%	0.764%
97	16.674	2491	2497	2509	rVV2	315750	971932	25.23%	1.847%
98	16.804	2510	2519	2531	rVB8	308909	1095212	28.43%	2.081%
99	17.309	2598	2605	2619	rVB3	146170	446526	11.59%	0.848%
100	18.068	2725	2734	2749	rBV3	155507	546804	14.19%	1.039%

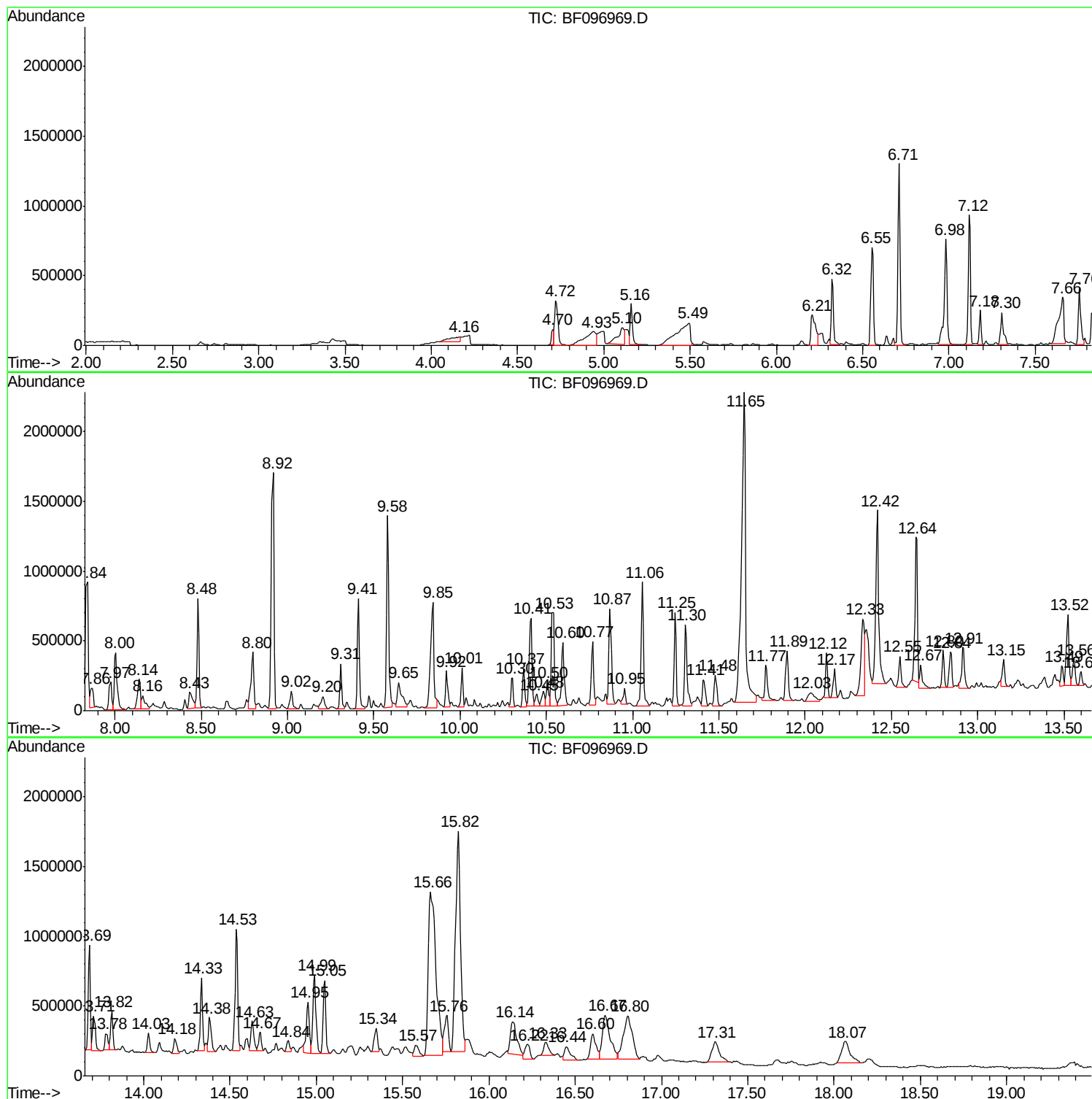
Sum of corrected areas: 52633992

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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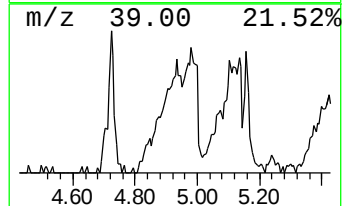
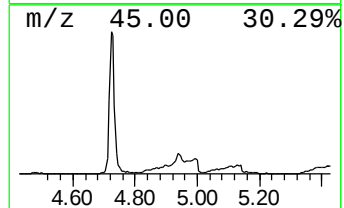
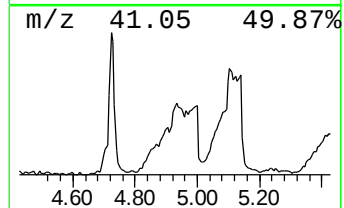
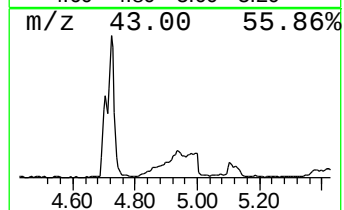
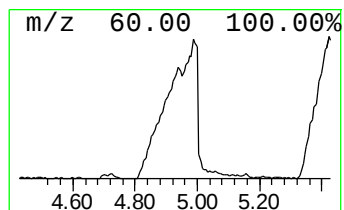
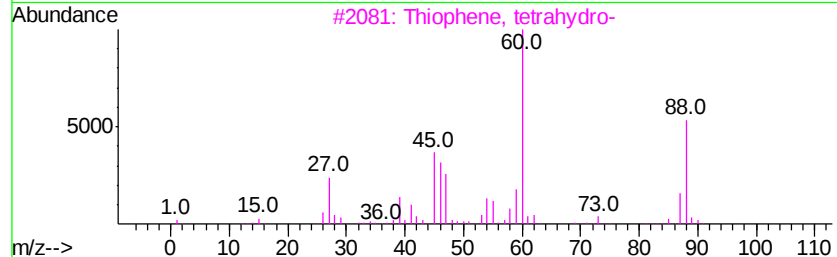
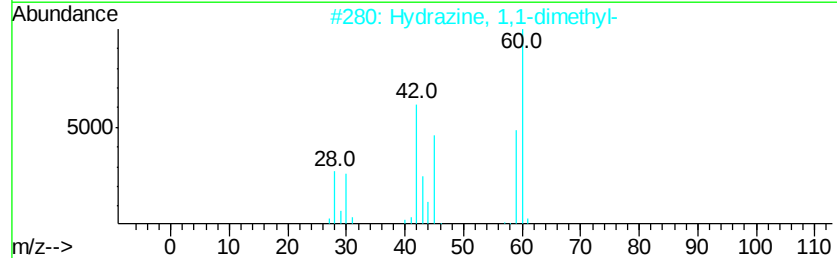
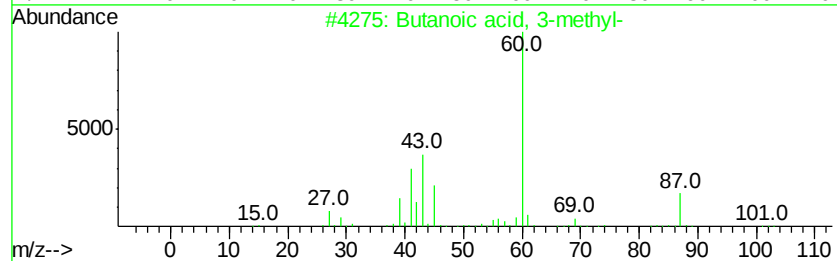
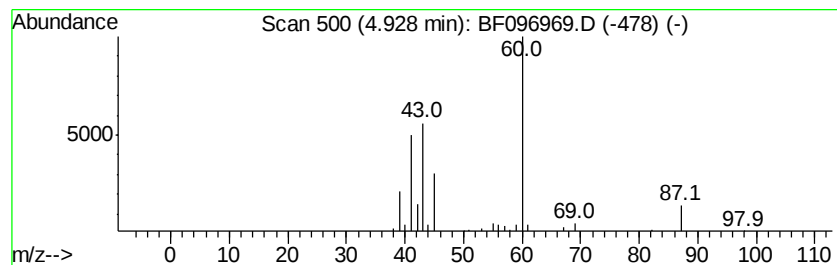
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	14.13 ng	451901	1,4-Dichlorobenzene-d4	6.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	59
3			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	40
4			Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	16
5			3-Hexanone, 5-hydroxy-2-methyl-	130	C7H14O2	059357-07-2	16



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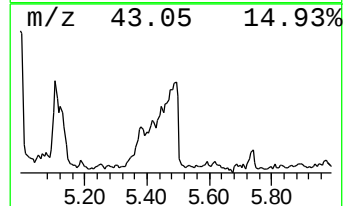
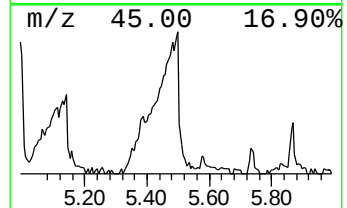
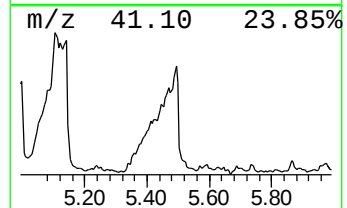
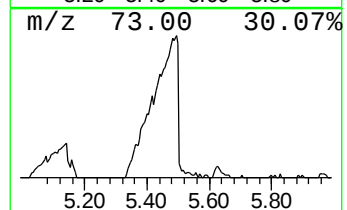
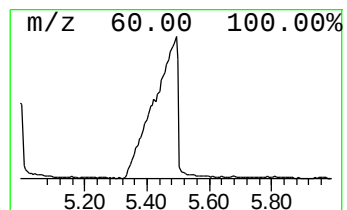
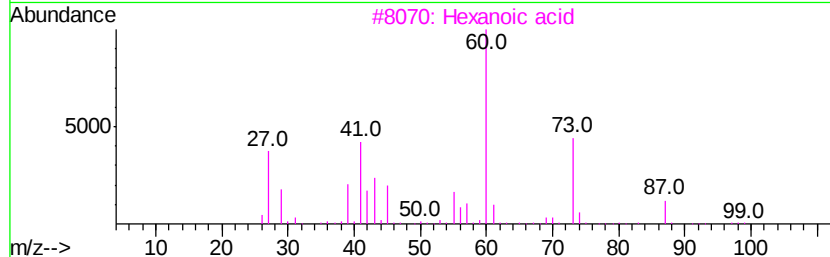
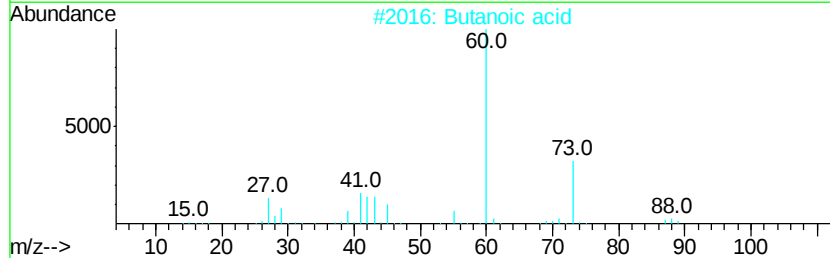
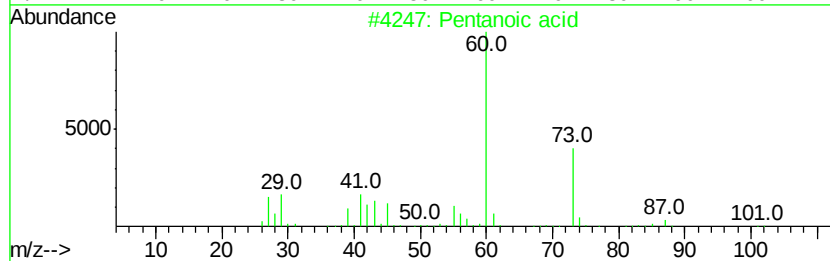
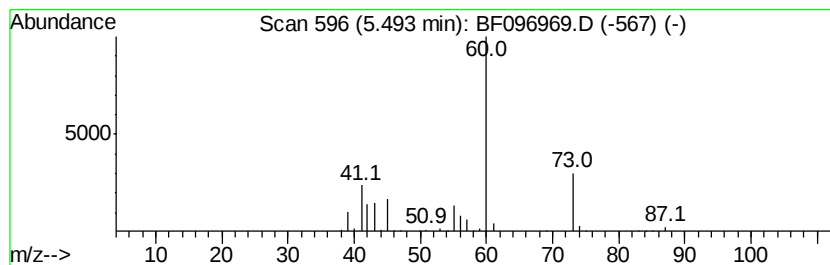
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	26.89 ng	859930	1,4-Dichlorobenzene-d4	6.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	83
2			Butanoic acid	88	C4H8O2	000107-92-6	78
3			Hexanoic acid	116	C6H12O2	000142-62-1	64
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40
5			.beta.-Methyl xyloside	164	C6H12O5	1000130-04-0	40



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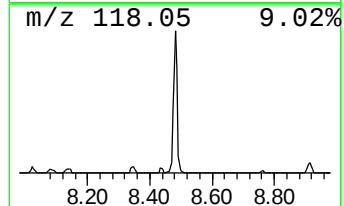
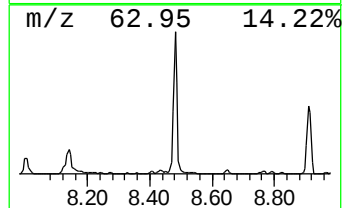
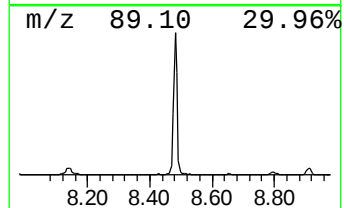
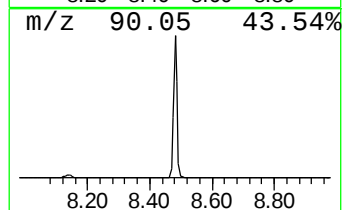
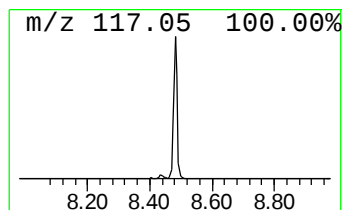
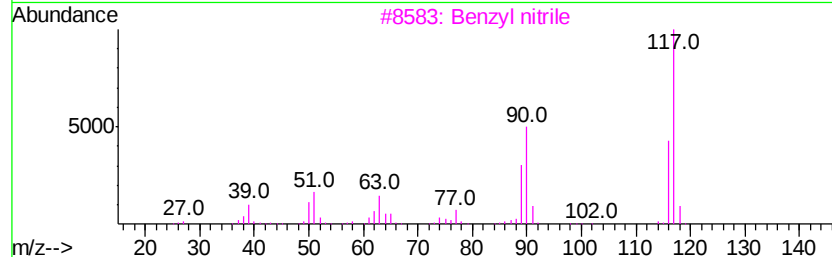
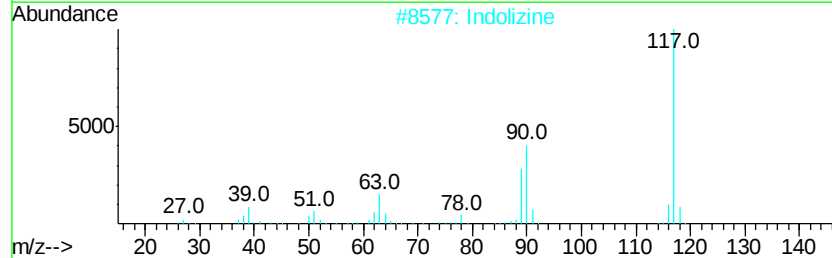
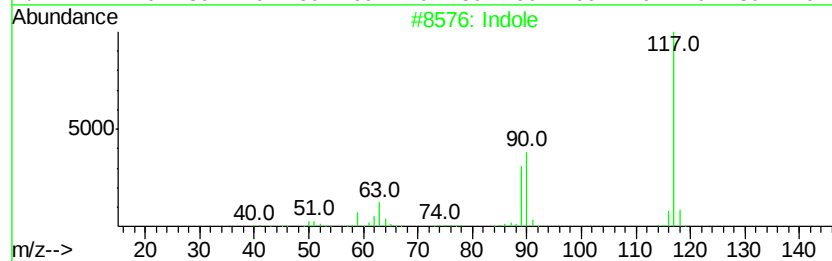
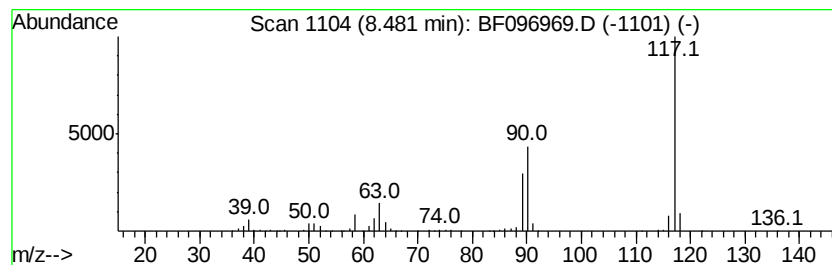
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Peak Number 3 Indole Concentration Rank 15

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8.48	14.95 ng	642321	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indole	117	C8H7N	000120-72-9	97
2		Indolizine	117	C8H7N	000274-40-8	94
3		Benzyl nitrile	117	C8H7N	000140-29-4	91
4		Benzene, 1-isocvano-2-methyl-	117	C8H7N	010468-64-1	87
5		Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	86



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Operator : SJ/JU
Sample : I4274-01
Misc :
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Instrument :
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ClientSampleId :
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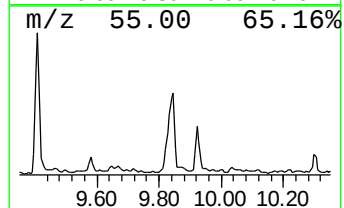
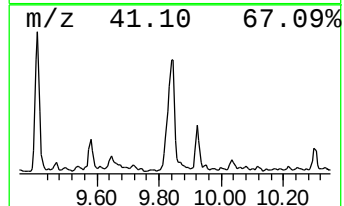
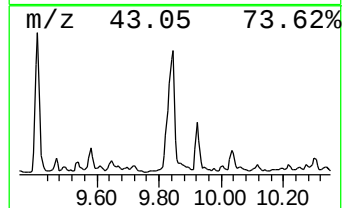
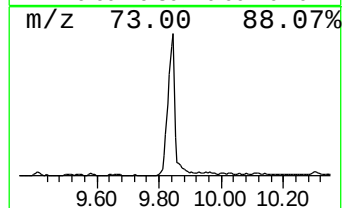
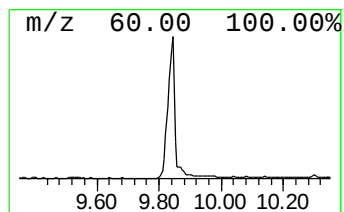
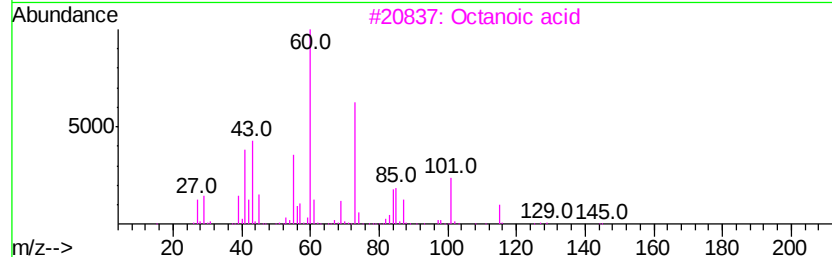
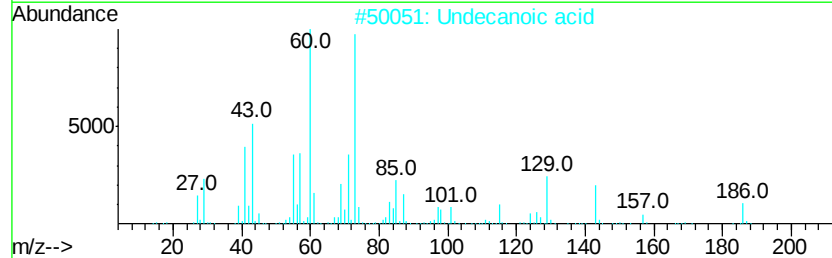
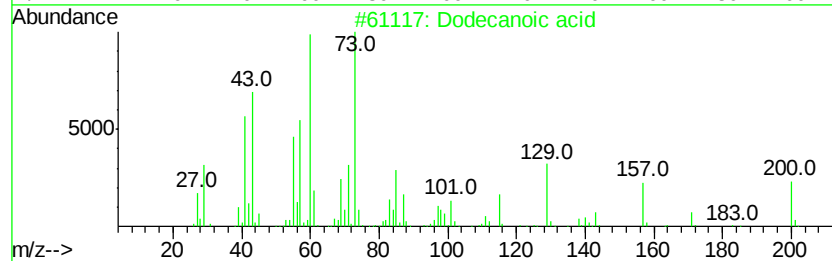
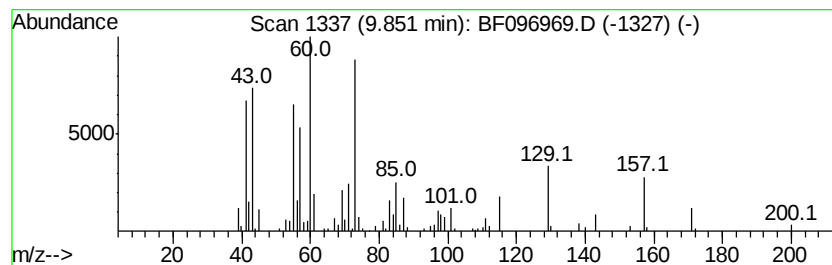
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	17.48 ng	1089110	Acenaphthene-d10	9.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2		Undecanoic acid	186	C11H22O2	000112-37-8	80
3		Octanoic acid	144	C8H16O2	000124-07-2	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Hexanoic acid	116	C6H12O2	000142-62-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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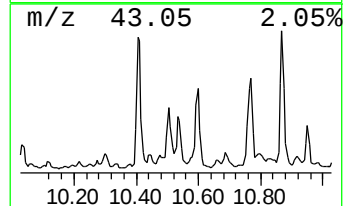
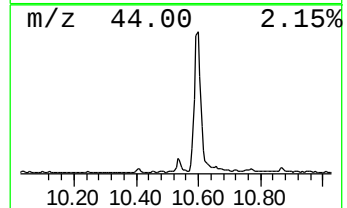
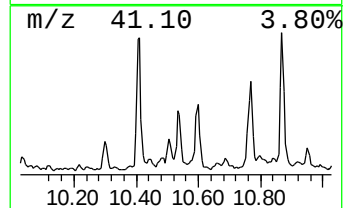
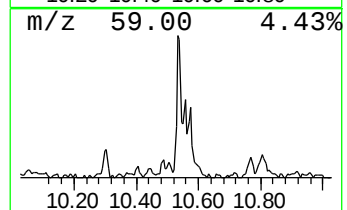
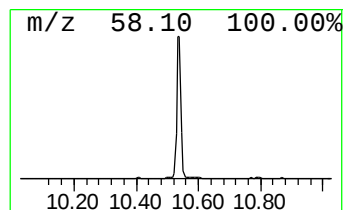
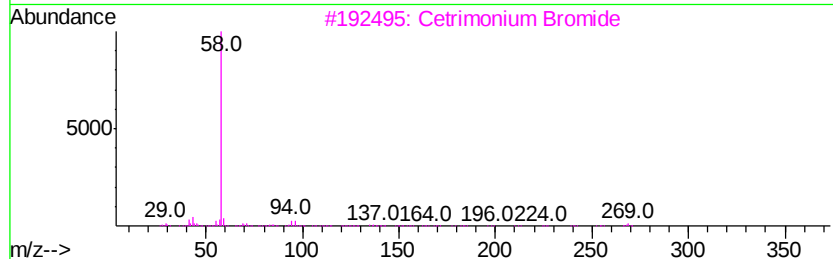
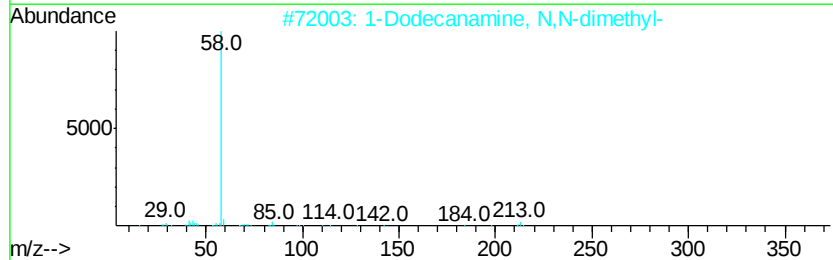
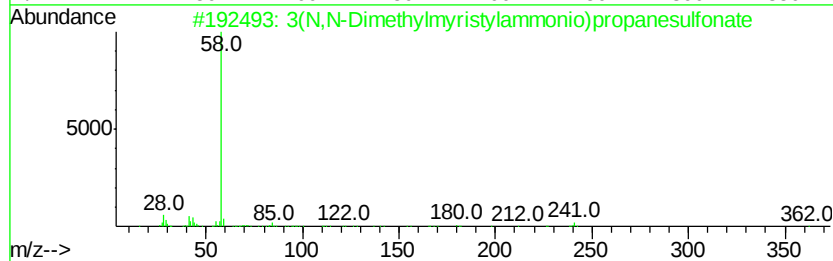
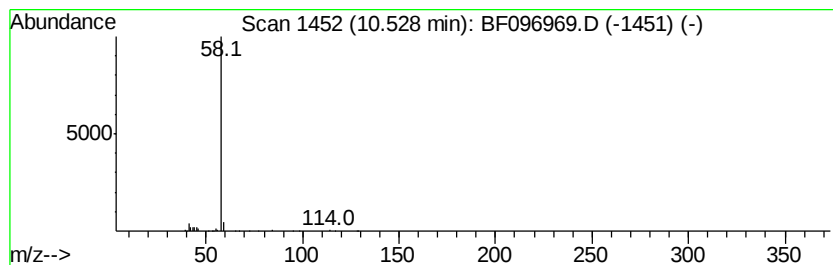
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3(N,N-Dimethylmyristylammon... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	14.71 ng	668449	Phenanthrene-d10	11.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3(N,N-Dimethylmyristylammonio)pr...	363	C19H41N03S	014933-09-6	78
2		1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78
3		Cetrimonium Bromide	363	C19H42BrN	000057-09-0	78
4		1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	78
5		Dimantine	297	C20H43N	000124-28-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
Acq On : 22 Jul 2017 4:39
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Misc :
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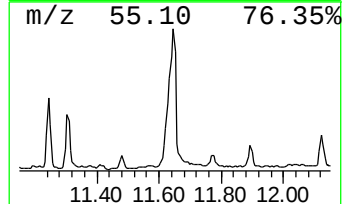
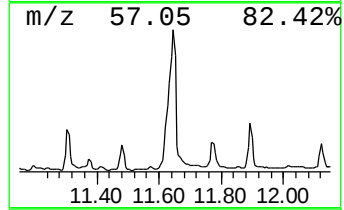
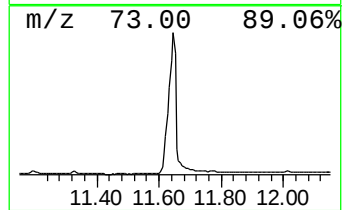
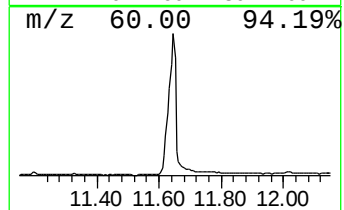
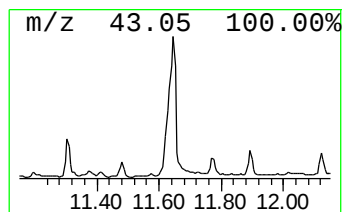
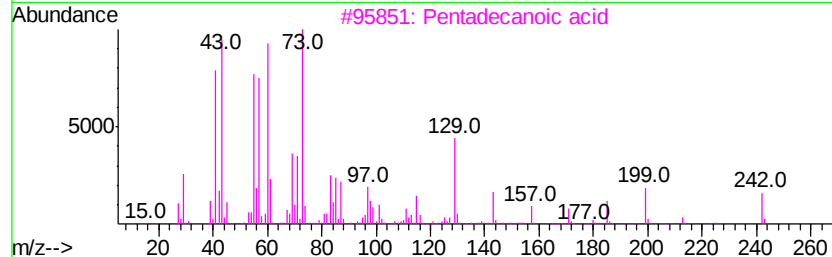
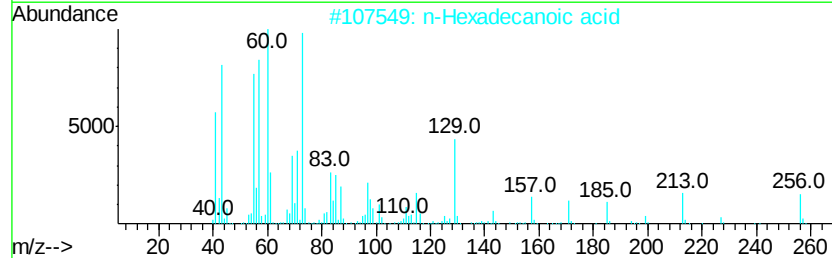
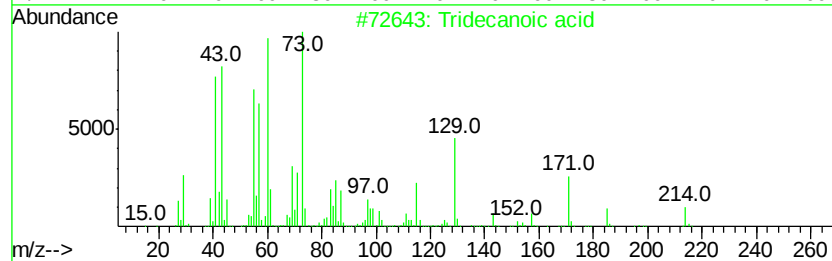
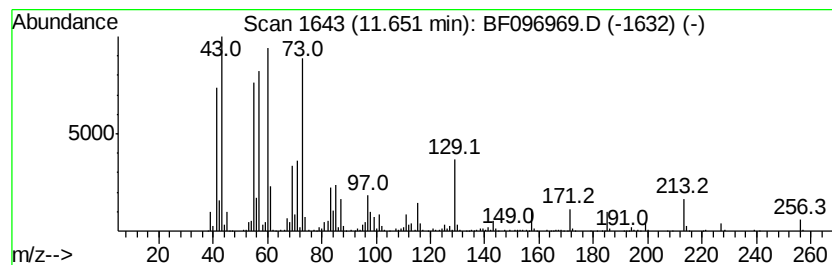
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	84.78 ng	3852640	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
Acq On : 22 Jul 2017 4:39
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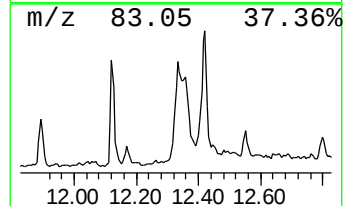
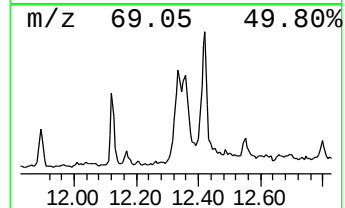
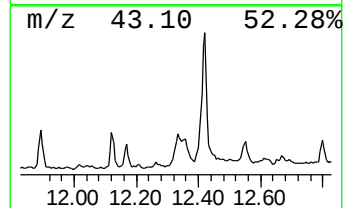
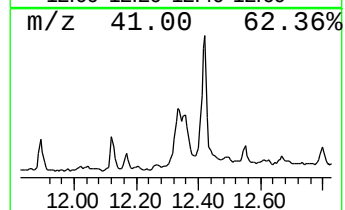
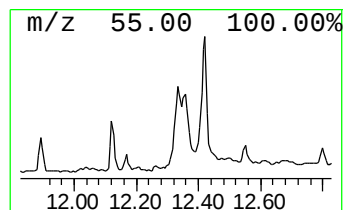
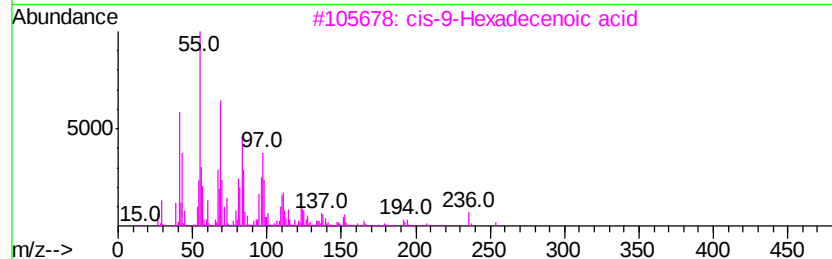
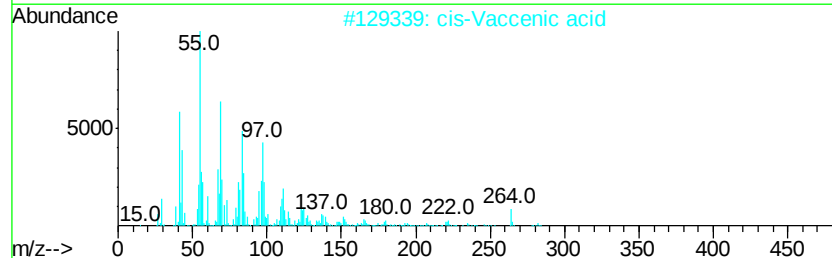
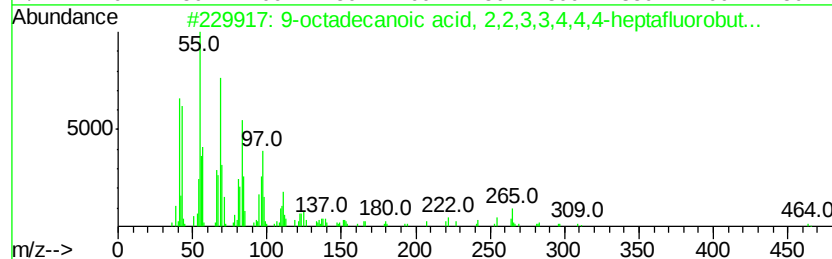
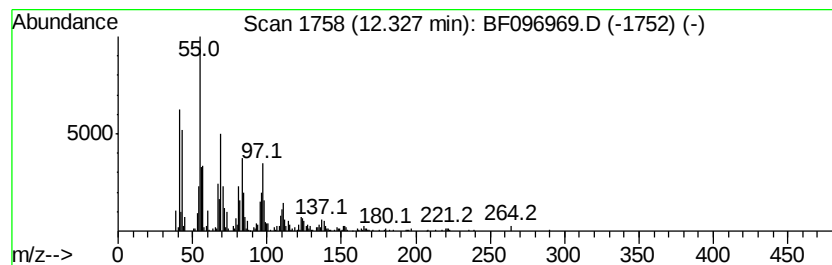
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-octadecanoic acid, 2,2,3,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	19.19 ng	872278	Phenanthrene-d10	11.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90
2		cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
3		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	90
4		9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	87
5		9-Hexadecenoic acid	254	C16H30O2	002091-29-4	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
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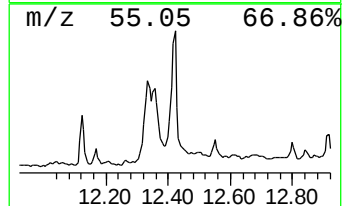
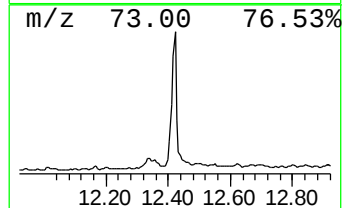
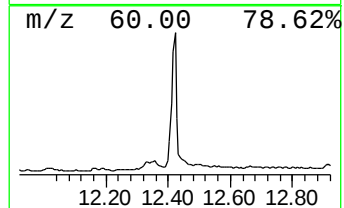
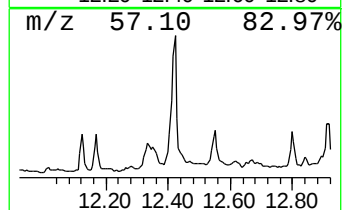
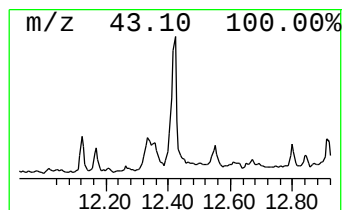
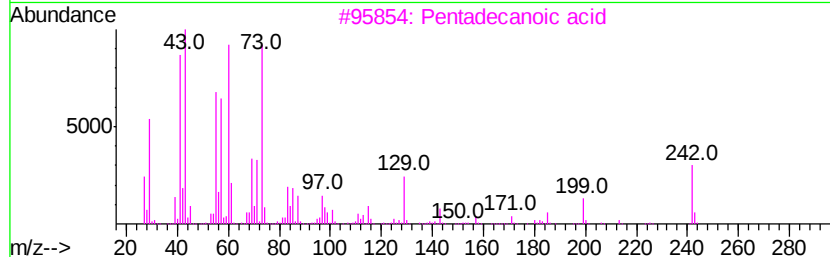
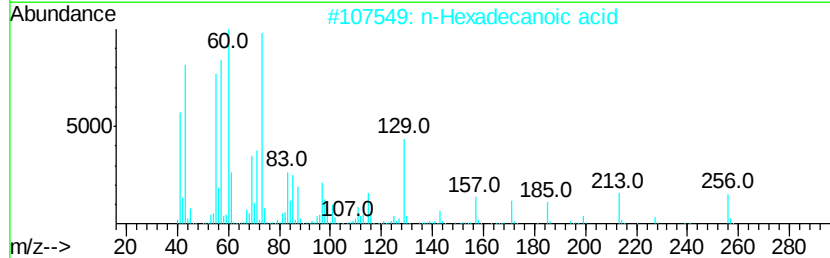
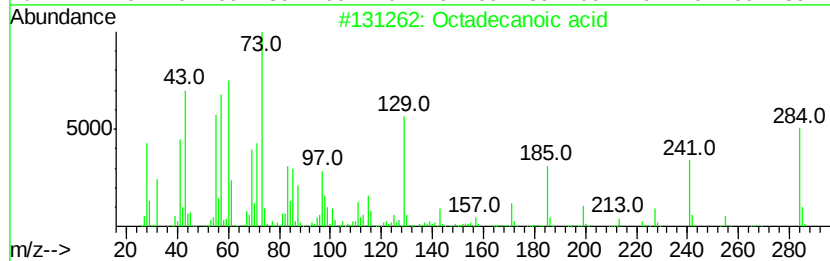
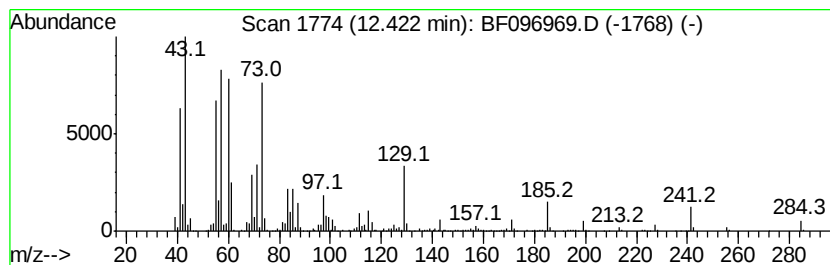
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	44.27 ng	1480360	Chrysene-d12	13.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Undecanoic acid	186	C11H22O2	000112-37-8	70



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ClientSampleId :
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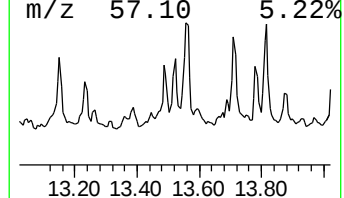
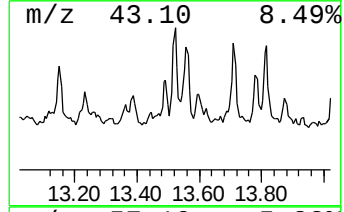
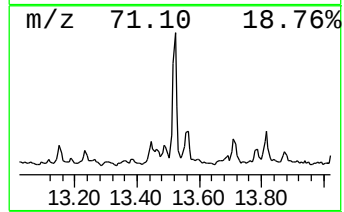
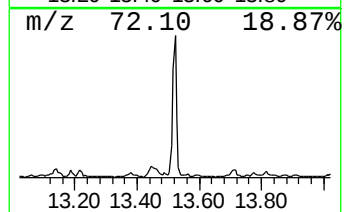
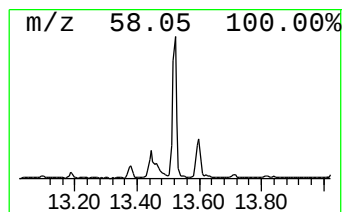
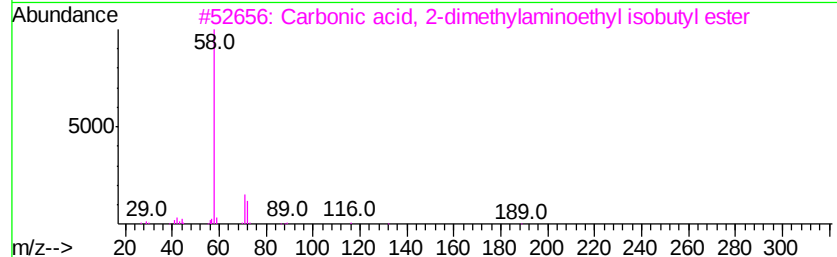
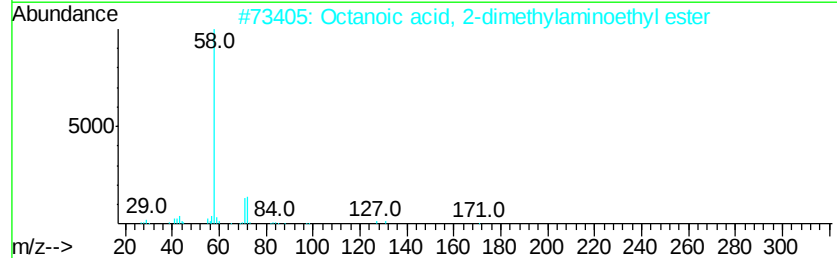
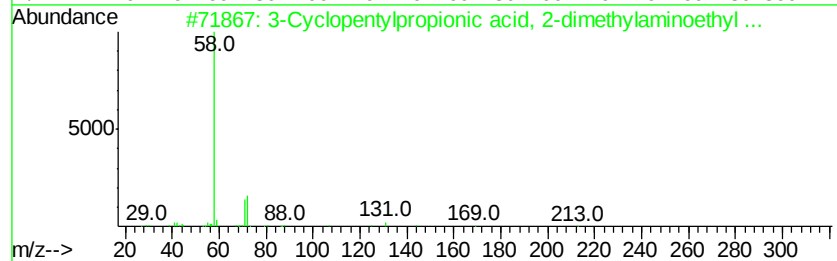
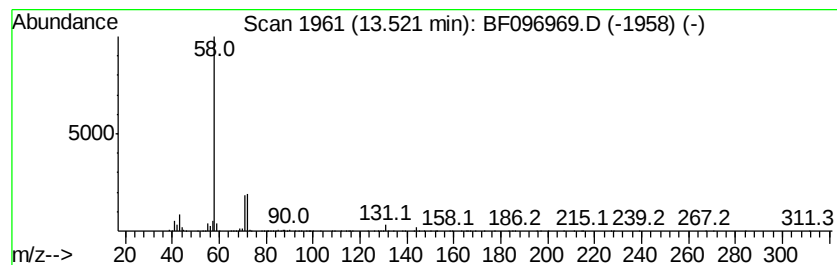
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 3-Cyclopentylpropionic acid... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	14.69 ng	491158	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Cyclopentylpropionic acid, 2-d...	213	C12H23NO2	1000331-24-3	78
2		Octanoic acid, 2-dimethylaminoet...	215	C12H25NO2	1000330-94-6	78
3		Carbonic acid, 2-dimethylaminoet...	189	C9H19NO3	1000331-40-0	72
4		Phenylacetic acid, 2-dimethylami...	207	C12H17NO2	1000331-13-5	64
5		Fumaric acid, 2-dimethylaminoeth...	411	C24H45NO4	1000331-65-4	64



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ALS Vial : 32 Sample Multiplier: 1

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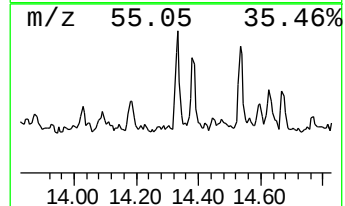
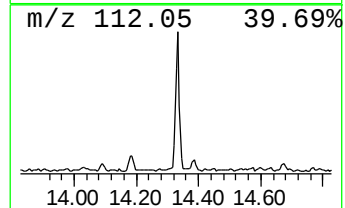
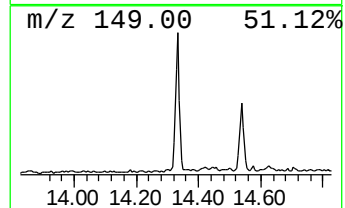
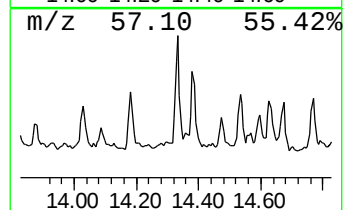
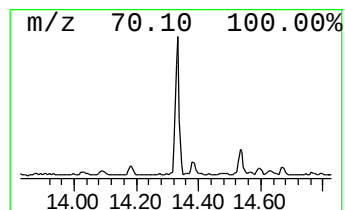
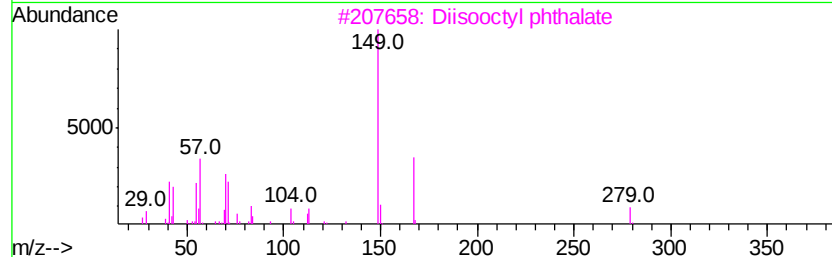
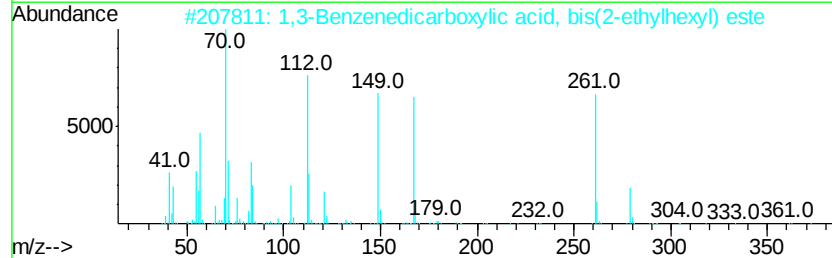
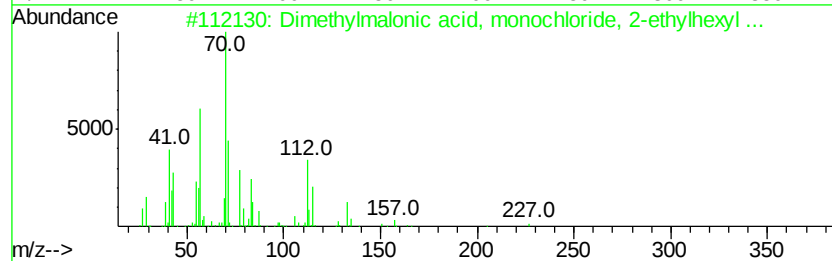
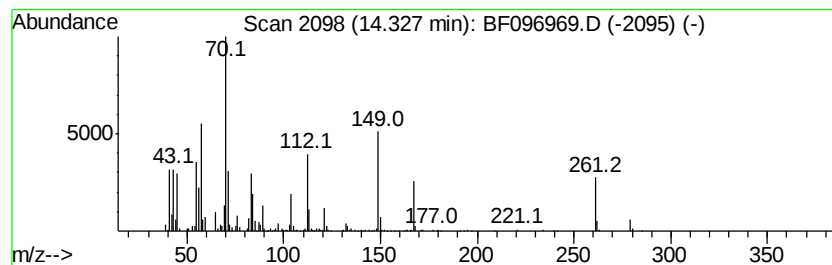
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.33 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	14.73 ng	492691	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	38
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	35
3		Diisooctyl phthalate	390	C24H38O4	000131-20-4	22
4		1-Methoxy-2,3-cis-dimethylazirid...	101	C5H11NO	061593-25-7	14
5		Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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Acq On : 22 Jul 2017 4:39
Operator : SJ/JU
Sample : I4274-01
Misc :
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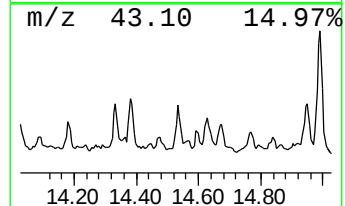
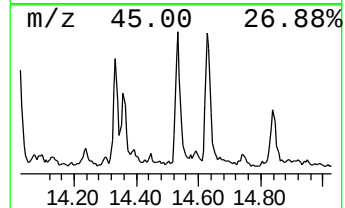
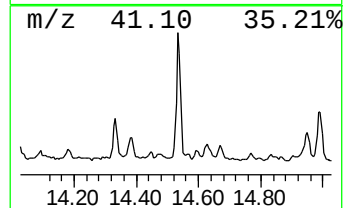
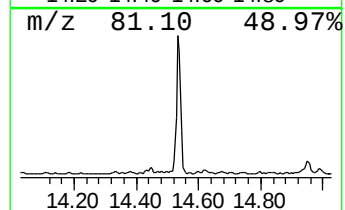
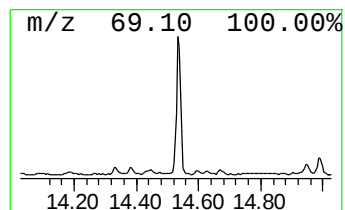
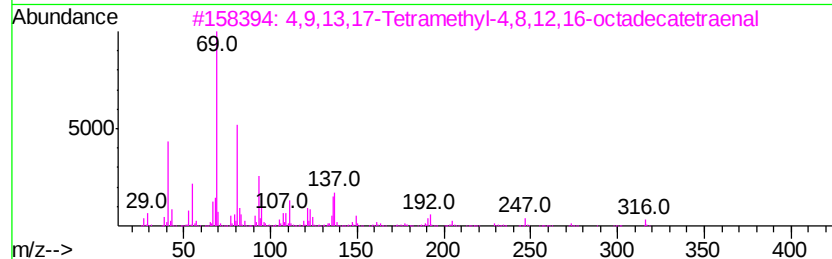
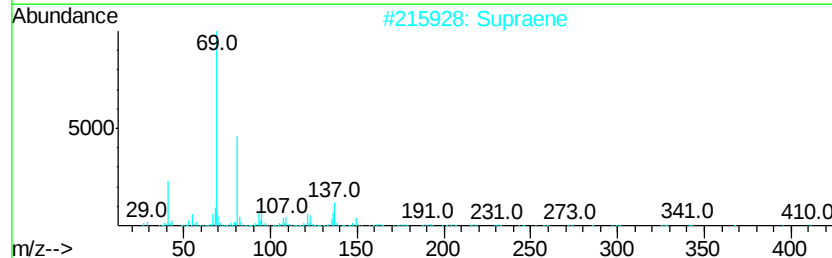
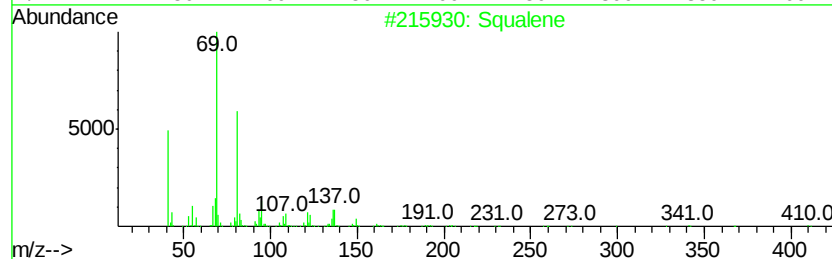
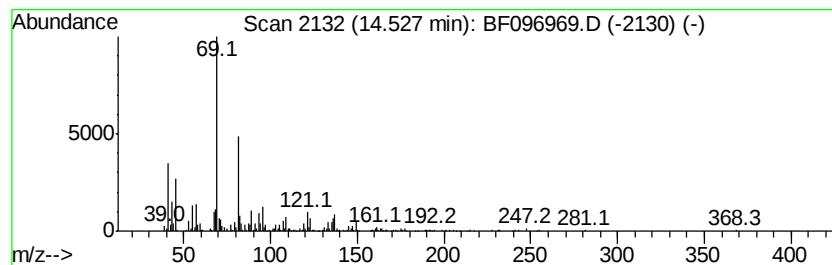
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	29.88 ng	896698	Perylene-d12	15.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	83
4	Farnesol isomer a	222 C15H26O	1000108-92-4	64
5	2,6,10,14-Hexadecatetraenoic aci...	332 C22H36O2	024035-35-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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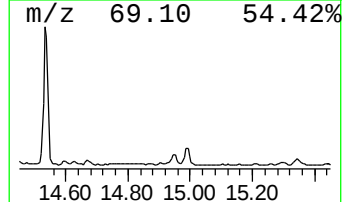
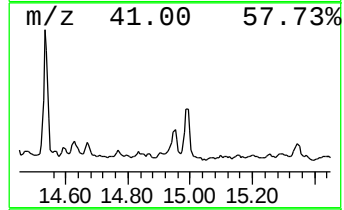
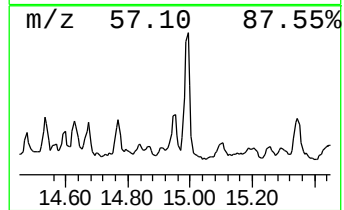
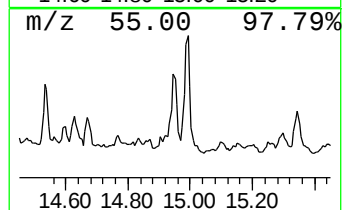
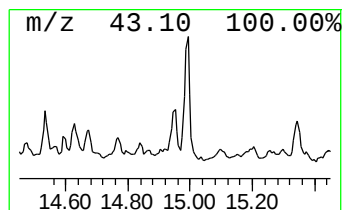
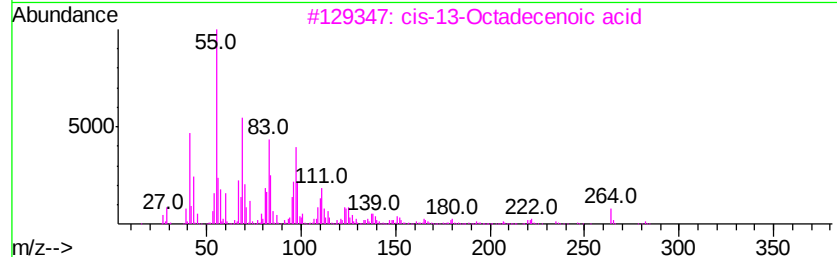
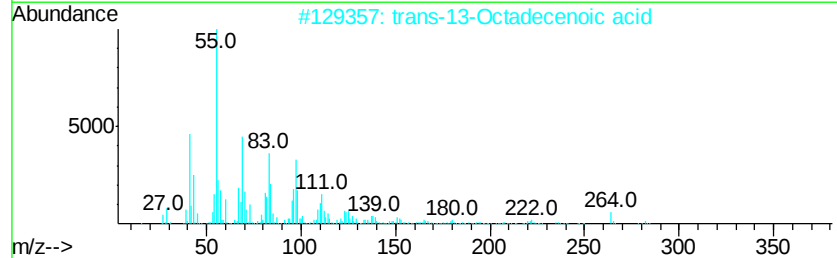
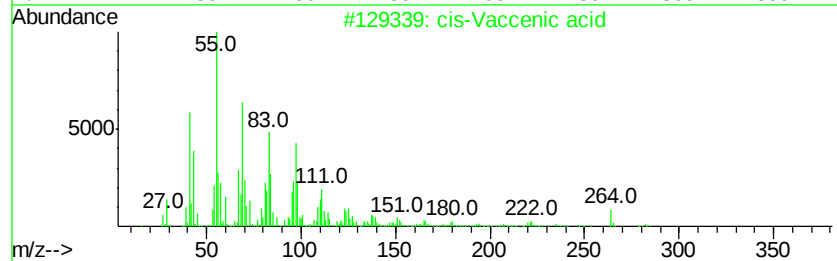
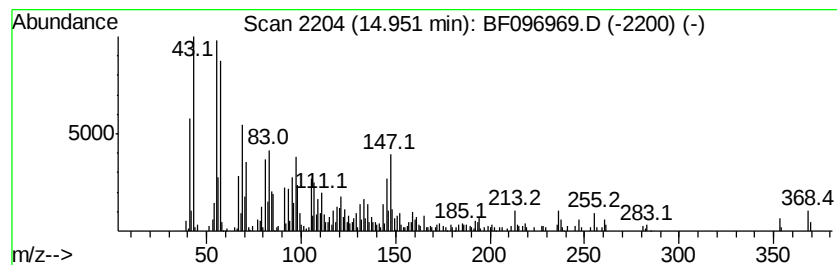
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown14.95 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	16.02 ng	480710	Perylene-d12	15.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	42
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	42
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	42
4			Behenic alcohol	326	C22H46O	000661-19-8	38
5			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
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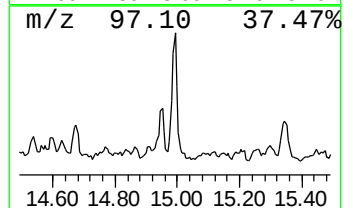
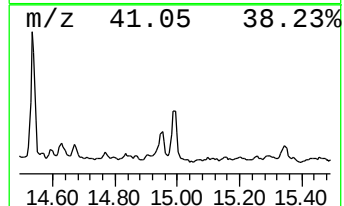
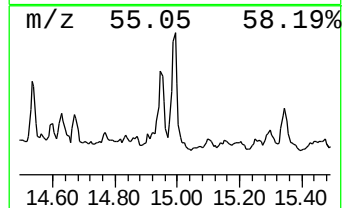
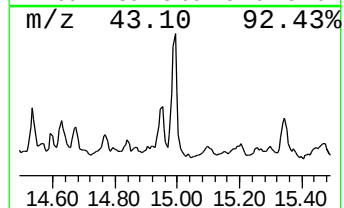
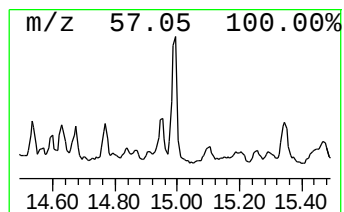
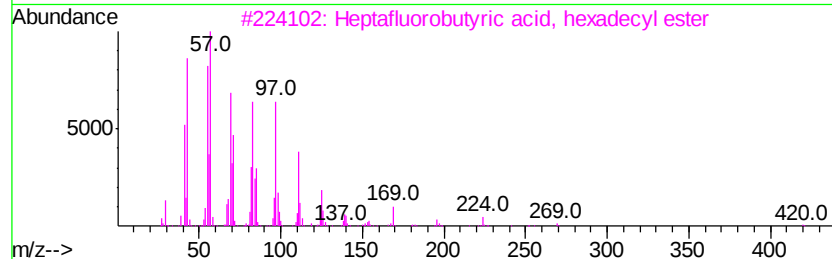
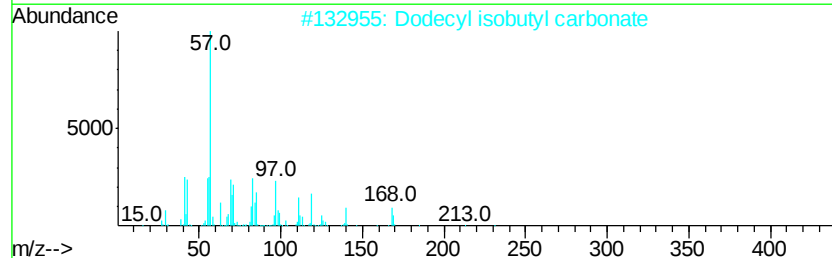
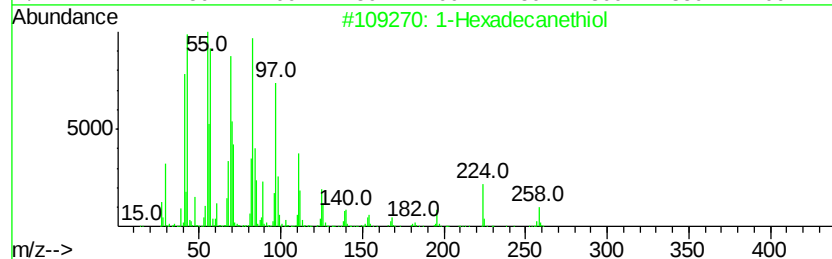
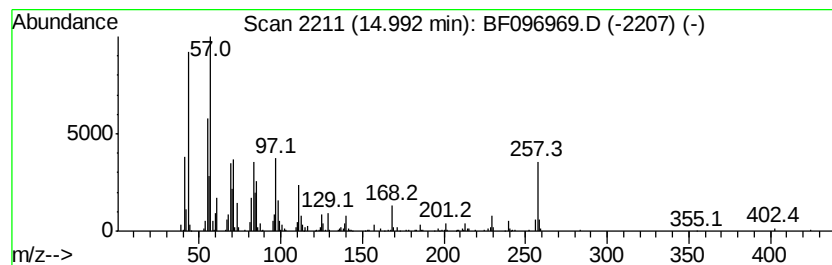
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-Hexadecanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.99	22.47 ng	674317	Perylene-d12	15.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanethiol	258	C16H34S	002917-26-2	64
2		Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	58
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	55
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	53
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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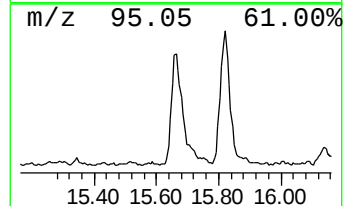
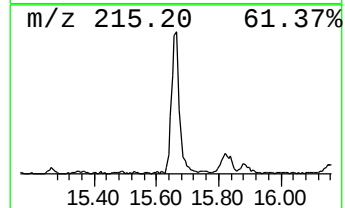
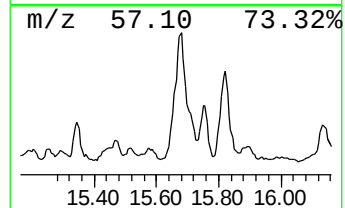
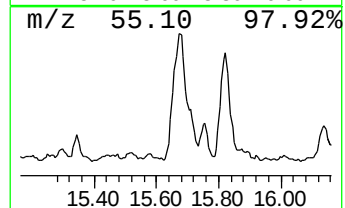
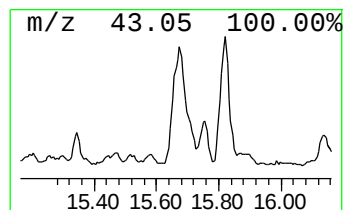
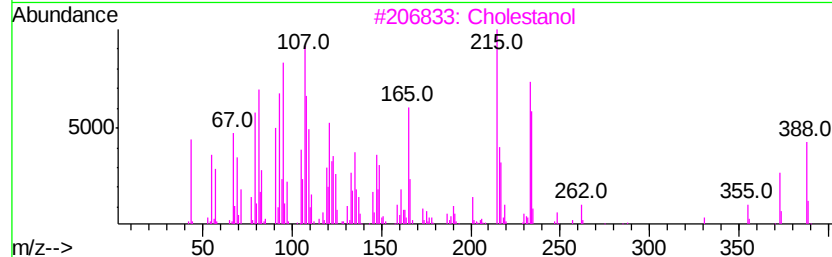
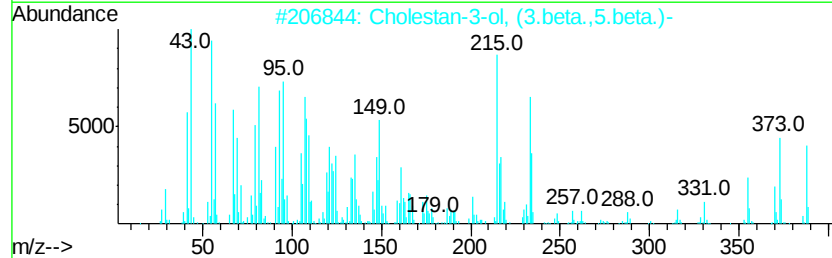
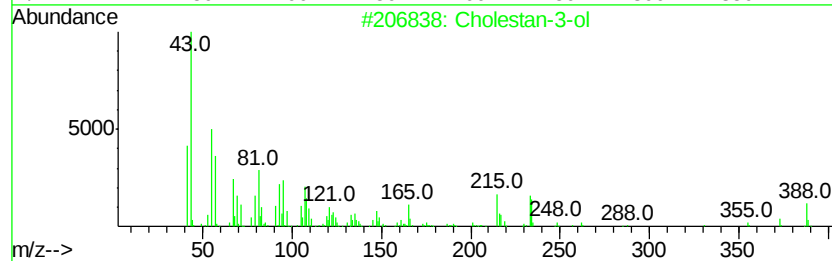
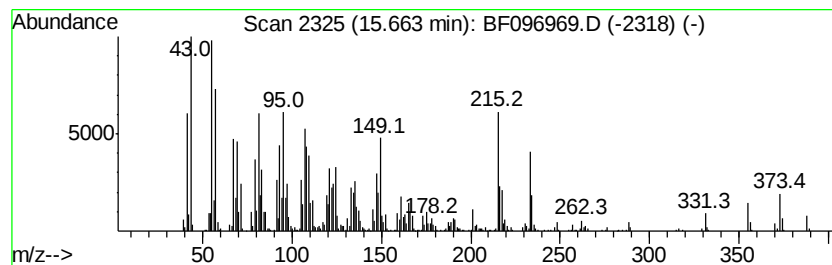
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Cholestan-3-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	119.46 ng	3585160	Perylene-d12	15.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholestan-3-ol	388	C27H48O	027409-41-2	93
2		Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	83
3		Cholestanol	388	C27H48O	000080-97-7	59
4		Epicholestanol	388	C27H48O	000516-95-0	47
5		2,3-Dichlorothiophene-5-sulfonyl...	250	C4HCl3O2S2	126714-85-0	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
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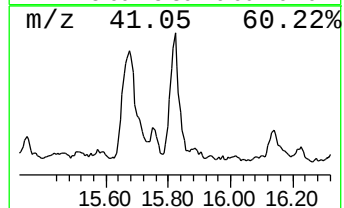
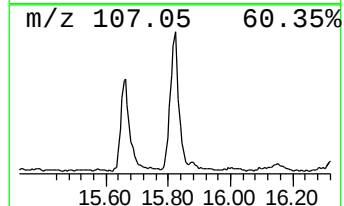
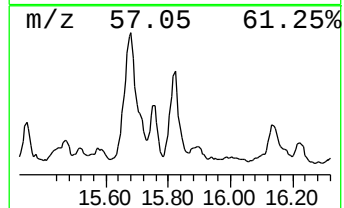
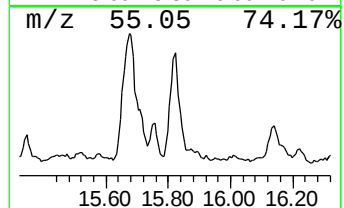
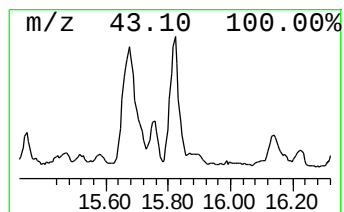
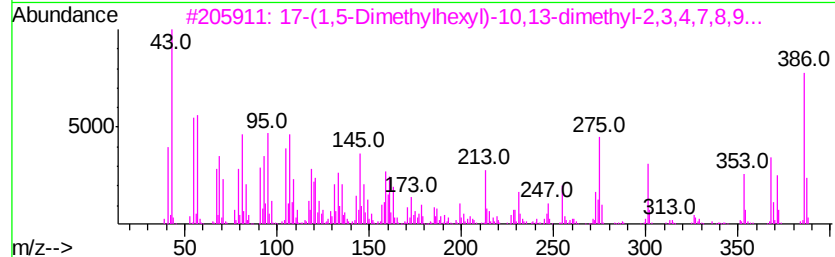
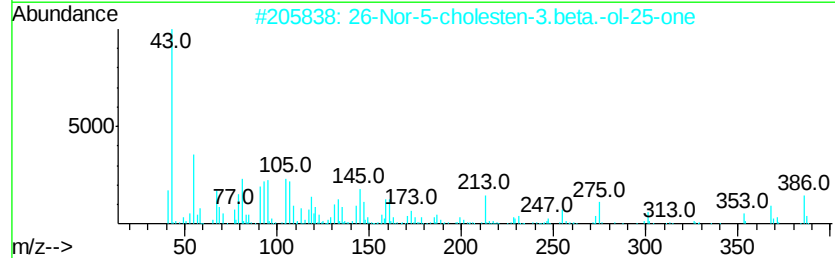
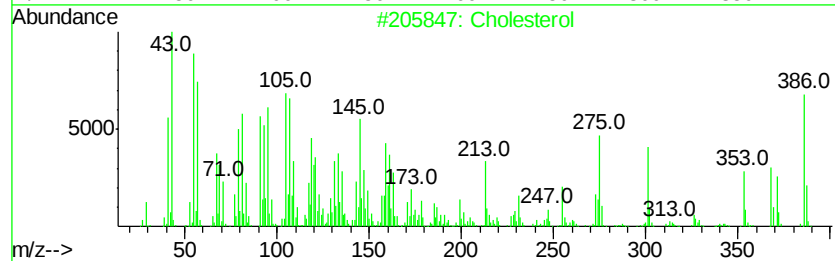
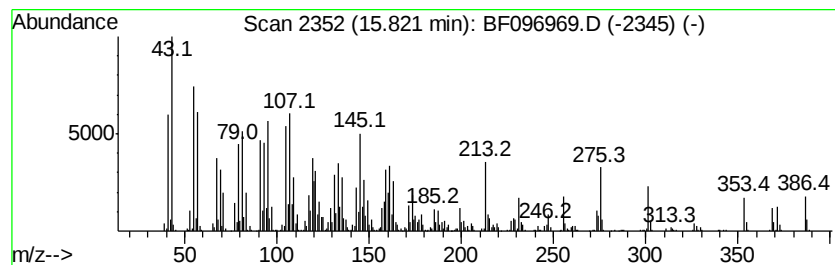
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Cholesterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.82	105.02 ng	3151770	Perylene-d12	15.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	96
4	Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	60
5	Cholestan-3-one	386	C27H46O	015600-08-5	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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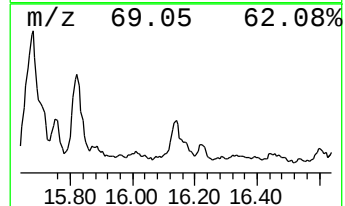
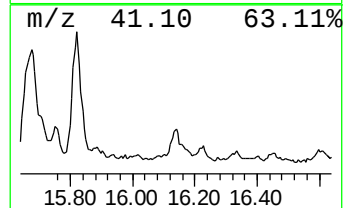
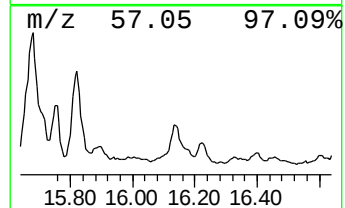
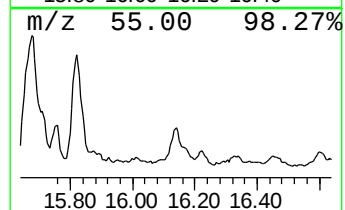
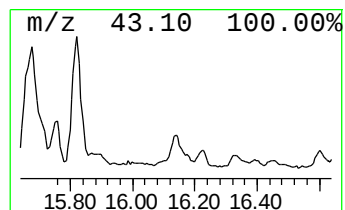
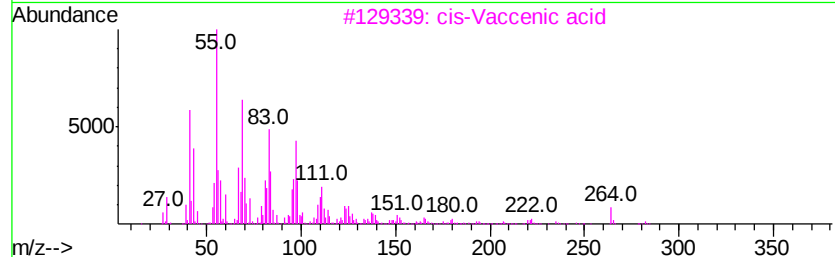
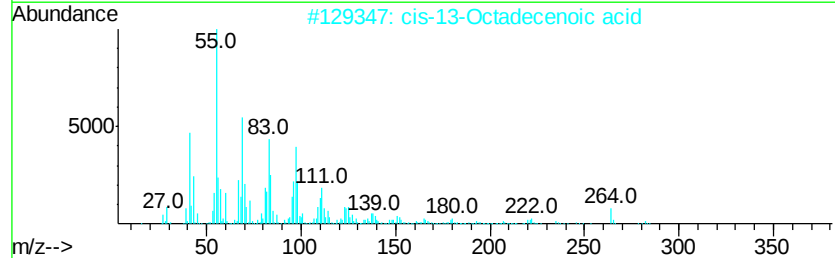
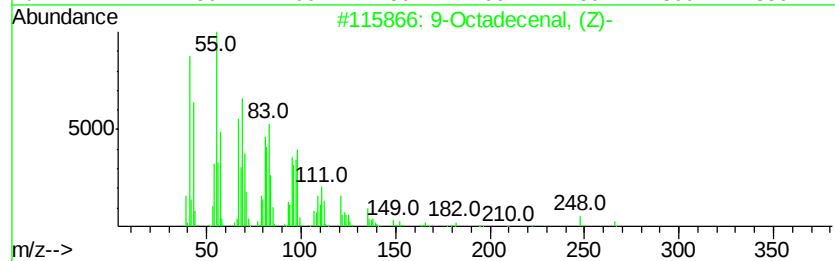
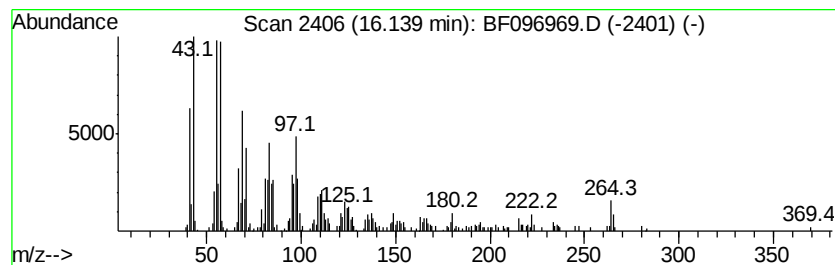
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 9-Octadecenal, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	19.41 ng	582403	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenal, (Z)-	266	C18H34O	002423-10-1	83
2		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	83
3		cis-Vaccenic acid	282	C18H34O2	000506-17-2	81
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	78
5		Oleic Acid	282	C18H34O2	000112-80-1	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096969.D
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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
M-COMB-3

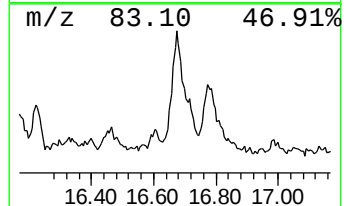
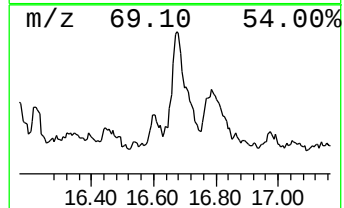
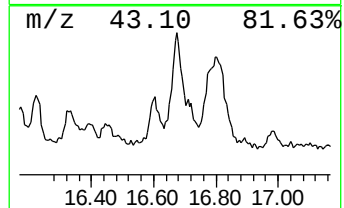
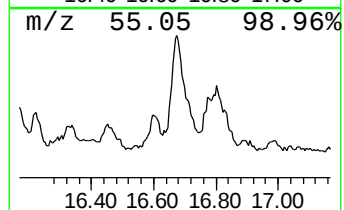
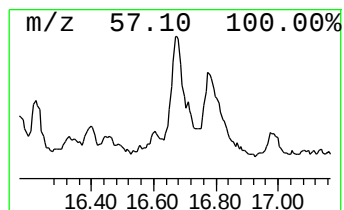
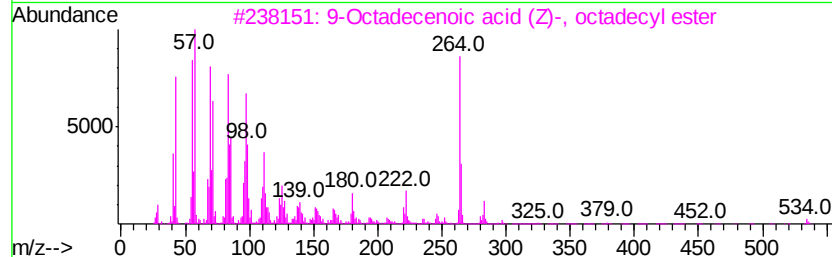
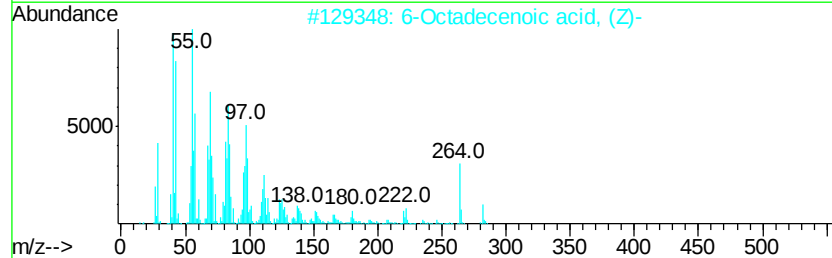
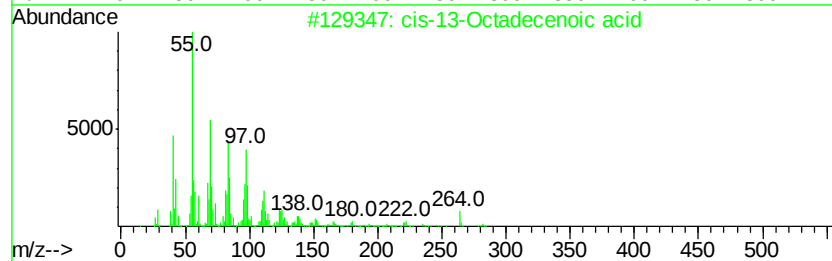
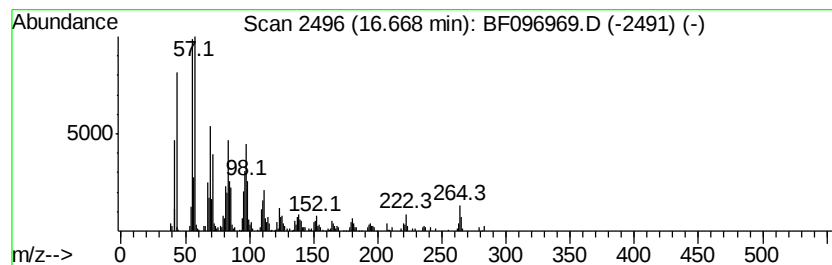
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 cis-13-Octadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	32.39 ng	971932	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87
2		6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	80
3		9-Octadecenoic acid (Z)-, octade...	535	C36H70O2	017673-49-3	68
4		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	62
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
Acq On : 22 Jul 2017 4:39
Operator : SJ/JU
Sample : I4274-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

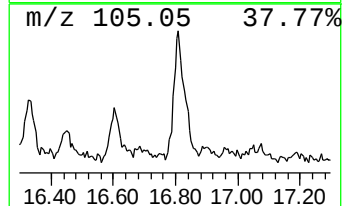
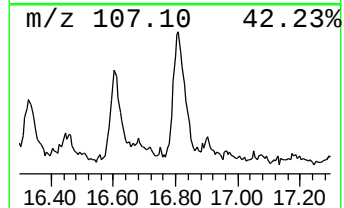
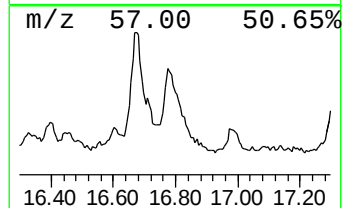
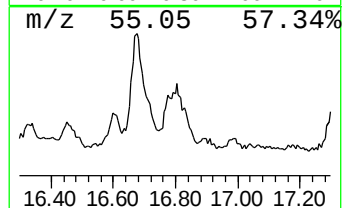
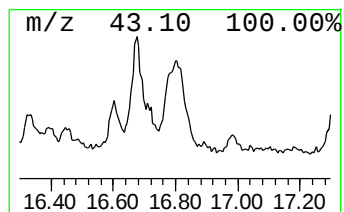
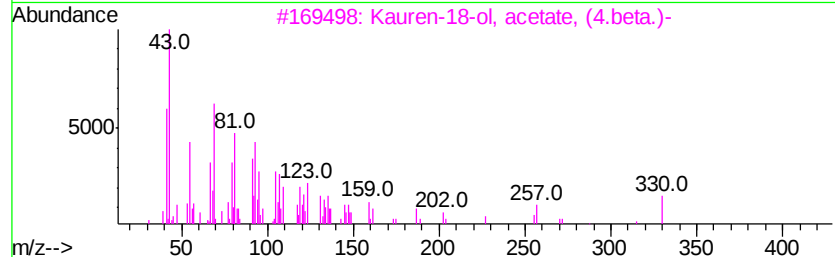
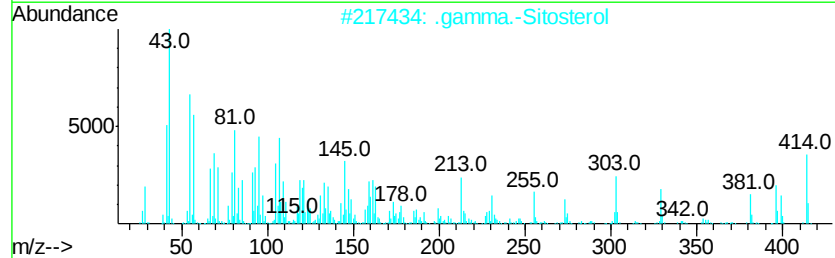
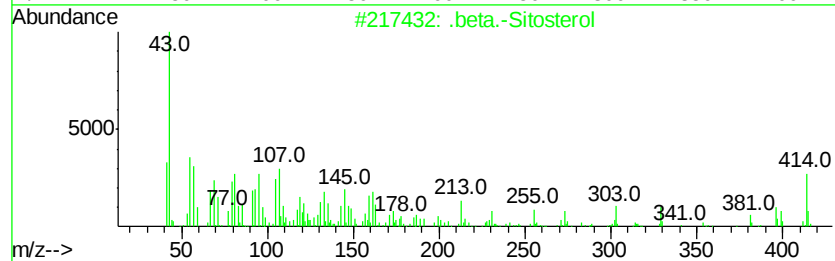
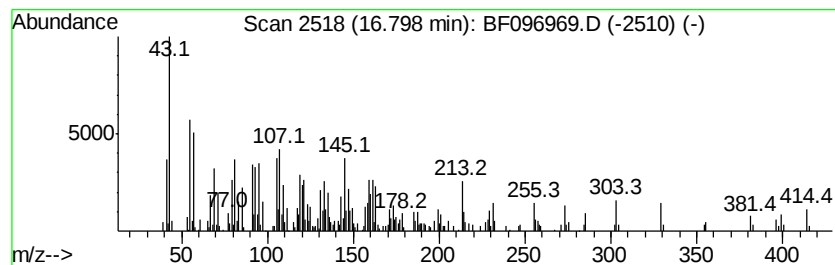
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ClientSampleId :
M-COMB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.80	36.49 ng	1095210	Perylene-d12	15.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	96
3	Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	37
4	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	25
5	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	23



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
Acq On : 22 Jul 2017 4:39
Operator : SJ/JU
Sample : I4274-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
M-COMB-3

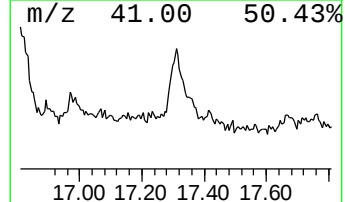
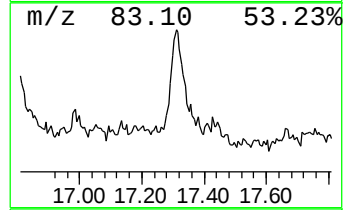
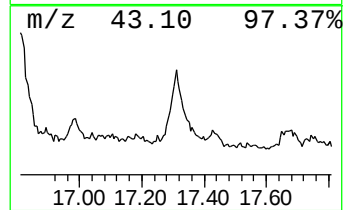
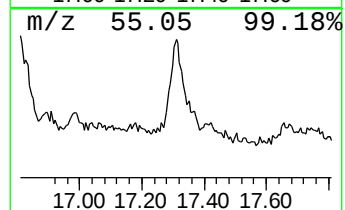
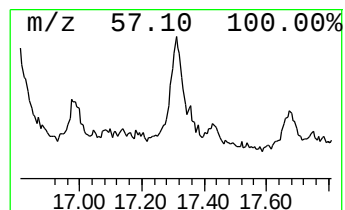
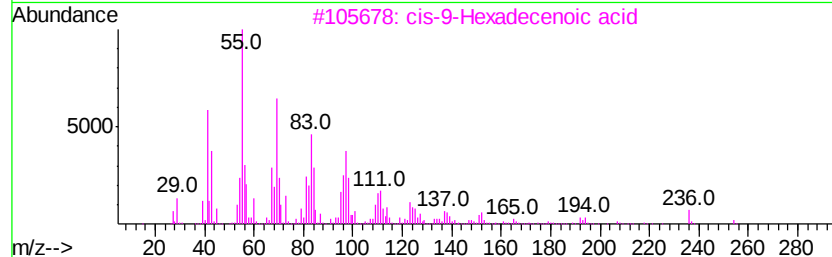
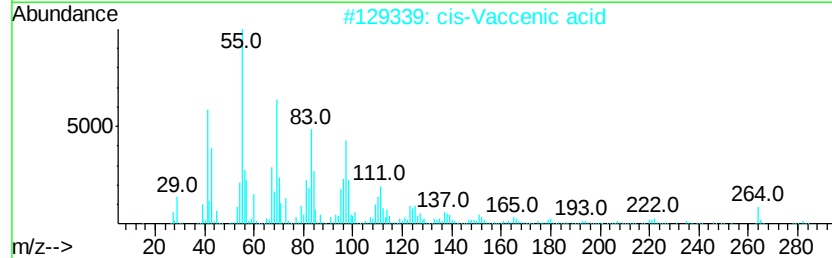
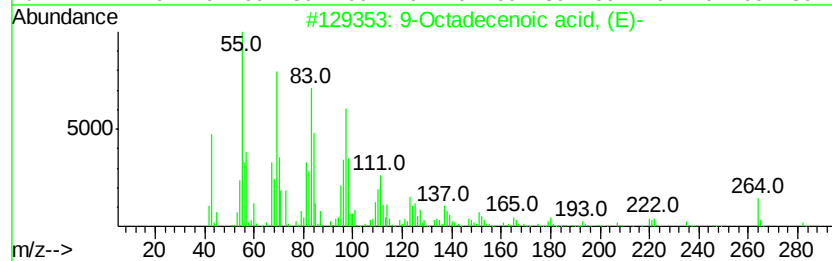
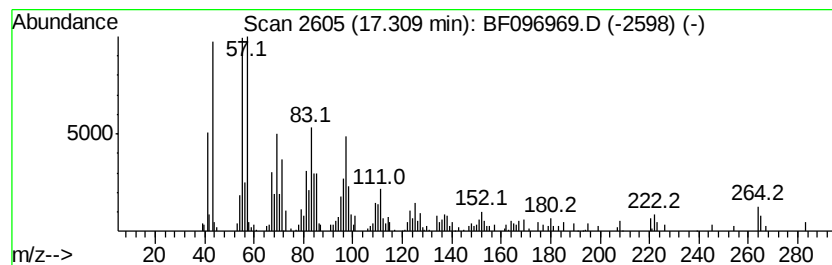
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 9-Octadecenoic acid, (E)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	14.88 ng	446526	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93
2		cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
3		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	90
4		Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	87
5		Oleic Acid	282	C18H34O2	000112-80-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096969.D
Acq On : 22 Jul 2017 4:39
Operator : SJ/JU
Sample : I4274-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
M-COMB-3

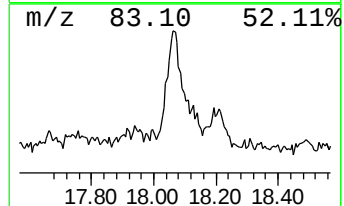
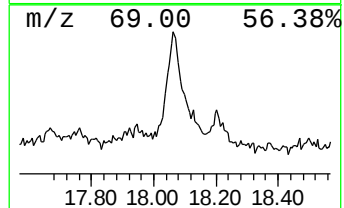
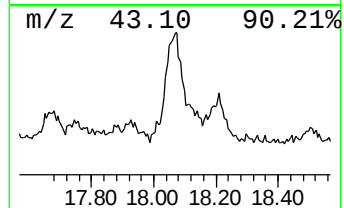
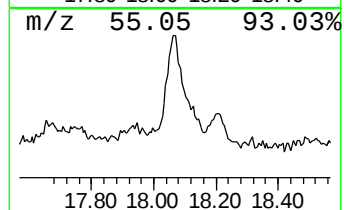
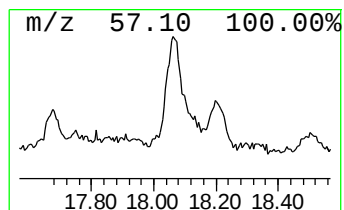
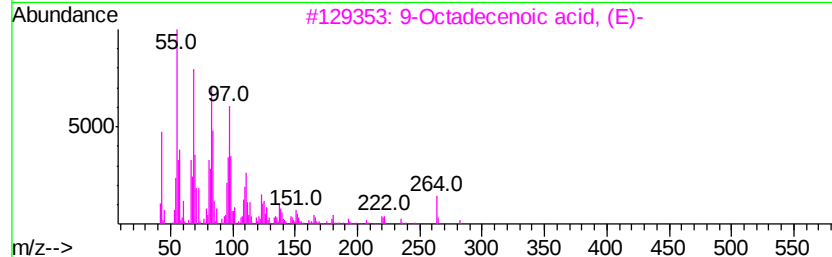
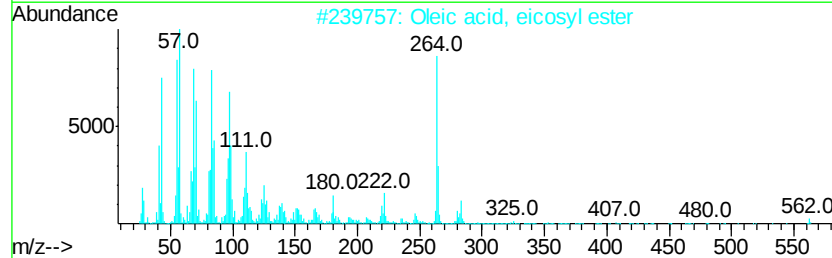
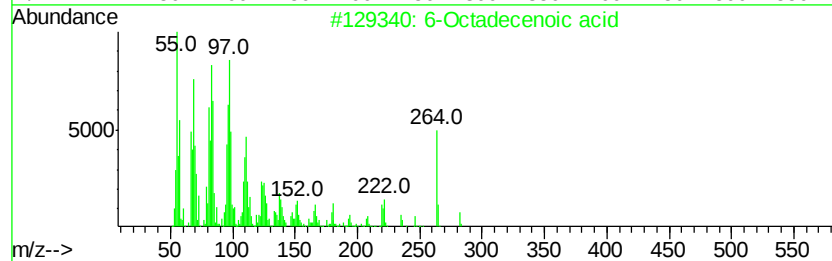
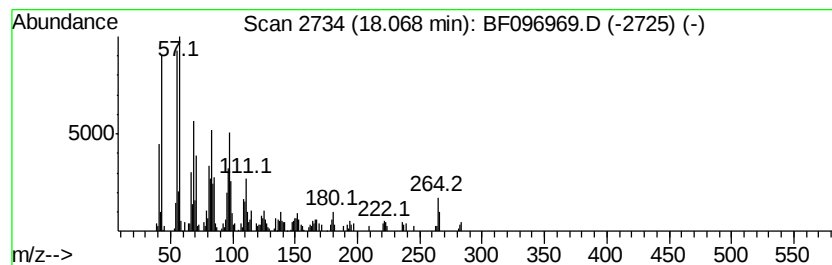
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 6-Octadecenoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	18.22 ng	546804	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	92
2		Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	90
3		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	89
4		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	89
5		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	89



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
 Data File : BF096969.D
 Acq On : 22 Jul 2017 4:39
 Operator : SJ/JU
 Sample : I4274-01
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, 3-...	4.93	14.1 ng		451901	1	6.55	639655	20.0
Pentanoic acid	5.49	26.9 ng		859930	1	6.55	639655	20.0
Indole	8.48	14.9 ng		642321	2	7.84	859361	20.0
Dodecanoic acid	9.85	17.5 ng		1089110	3	9.58	1245950	20.0
3(N,N-Dimethylmyr...	10.53	14.7 ng		668449	4	11.06	908902	20.0
Tridecanoic acid	11.65	84.8 ng		3852640	4	11.06	908902	20.0
9-octadecanoic ac...	12.33	19.2 ng		872278	4	11.06	908902	20.0
Octadecanoic acid	12.42	44.3 ng		1480360	5	13.69	668844	20.0
3-Cyclopentylprop...	13.52	14.7 ng		491158	5	13.69	668844	20.0
unknown14.33	14.33	14.7 ng		492691	5	13.69	668844	20.0
Squalene	14.53	29.9 ng		896698	6	15.05	600236	20.0
unknown14.95	14.95	16.0 ng		480710	6	15.05	600236	20.0
1-Hexadecanethiol	14.99	22.5 ng		674317	6	15.05	600236	20.0
Cholestan-3-ol	15.66	119.5 ng		3585160	6	15.05	600236	20.0
Cholesterol	15.82	105.0 ng		3151770	6	15.05	600236	20.0
9-Octadecenal, (Z)-	16.14	19.4 ng		582403	6	15.05	600236	20.0
cis-13-Octadeceno...	16.67	32.4 ng		971932	6	15.05	600236	20.0
.beta.-Sitosterol	16.80	36.5 ng		1095210	6	15.05	600236	20.0
9-Octadecenoic ac...	17.31	14.9 ng		446526	6	15.05	600236	20.0
6-Octadecenoic acid	18.07	18.2 ng		546804	6	15.05	600236	20.0