

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
 Data File : BF096346.D
 Acq On : 30 Jun 2017 19:51
 Operator : SJ/MA
 Sample : I3959-01 5X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-062717-A

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-BF062717.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	4.940	481	485	492	rVB	128518	129189	9.39%	0.685%
2	5.363	553	557	561	rVB	1025296	873206	63.44%	4.632%
3	6.381	726	730	735	rBV	1036765	884543	64.27%	4.692%
4	6.522	750	754	758	rBV	998414	874621	63.55%	4.639%
5	6.757	790	794	798	rBV	1043394	917950	66.69%	4.869%
6	6.822	803	805	809	rBV3	10652	14747	1.07%	0.078%
7	6.916	817	821	824	rVV	752940	624391	45.37%	3.312%
8	6.945	824	826	830	rVB3	16837	16617	1.21%	0.088%
9	7.039	840	842	846	rVB3	15189	16417	1.19%	0.087%
10	7.163	860	863	865	rBV	20044	16660	1.21%	0.088%
11	7.310	881	888	892	rBV	592202	554888	40.32%	2.943%
12	7.369	896	898	901	rVV2	27488	26445	1.92%	0.140%
13	7.404	901	904	910	rVB5	36664	50185	3.65%	0.266%
14	7.575	930	933	936	rVB	29274	26731	1.94%	0.142%
15	7.669	941	949	950	rBV6	14727	29939	2.18%	0.159%
16	7.692	950	953	956	rVB4	29391	34433	2.50%	0.183%
17	7.734	956	960	963	rBV4	30127	33461	2.43%	0.177%
18	7.816	971	974	979	rVB6	17100	25224	1.83%	0.134%
19	7.875	979	984	988	rBV8	19070	29842	2.17%	0.158%
20	7.922	988	992	993	rBV	19560	19412	1.41%	0.103%
21	8.039	1008	1012	1018	rBV	1400243	1376351	100.00%	7.301%
22	8.116	1023	1025	1027	rVB	35270	27812	2.02%	0.148%
23	8.222	1037	1043	1045	rBV5	18522	28228	2.05%	0.150%
24	8.257	1046	1049	1052	rVV2	37527	34928	2.54%	0.185%
25	8.339	1056	1063	1066	rBV6	41689	68245	4.96%	0.362%
26	8.398	1071	1073	1075	rBV3	26156	20546	1.49%	0.109%
27	8.433	1075	1079	1083	rVB7	22627	32600	2.37%	0.173%
28	8.481	1083	1087	1091	rBV2	97002	127875	9.29%	0.678%
29	8.551	1096	1099	1103	rBV5	21280	25116	1.82%	0.133%
30	8.592	1103	1106	1111	rBV4	32129	44751	3.25%	0.237%
31	8.645	1112	1115	1120	rBV4	38083	55178	4.01%	0.293%
32	8.751	1129	1133	1135	rVB3	61768	81233	5.90%	0.431%
33	8.798	1138	1141	1144	rBV4	21256	32066	2.33%	0.170%
34	8.851	1144	1150	1154	rVV6	47915	69472	5.05%	0.369%

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35	8.933	1161	1164	1165	rBV2	32415	28429	2.07%	0.151%
36	9.081	1186	1189	1191	rVB	106928	94705	6.88%	0.502%
37	9.116	1191	1195	1198	rBV	1055690	832200	60.46%	4.414%
38	9.163	1201	1203	1205	rBV2	13992	15098	1.10%	0.080%
39	9.210	1207	1211	1215	rBV4	72628	92863	6.75%	0.493%
40	9.257	1215	1219	1224	rBV7	28453	53287	3.87%	0.283%
41	9.316	1227	1229	1234	rVB4	25490	35433	2.57%	0.188%
42	9.375	1237	1239	1246	rBV5	41102	63438	4.61%	0.336%
43	9.457	1250	1253	1255	rVV	58463	58666	4.26%	0.311%
44	9.480	1255	1257	1259	rVV2	49643	39390	2.86%	0.209%
45	9.510	1259	1262	1264	rVV	175245	150859	10.96%	0.800%
46	9.533	1264	1266	1268	rVB2	91006	68171	4.95%	0.362%
47	9.569	1270	1272	1274	rVB3	25035	18861	1.37%	0.100%
48	9.716	1295	1297	1299	rVB	47035	39205	2.85%	0.208%
49	9.739	1299	1301	1305	rBV	45011	38343	2.79%	0.203%
50	9.792	1305	1310	1314	rBV	1258037	1193267	86.70%	6.329%
51	9.828	1314	1316	1319	rVB	129923	99790	7.25%	0.529%
52	9.904	1326	1329	1333	rVB4	28013	40979	2.98%	0.217%
53	9.998	1342	1345	1348	rVB	101220	85646	6.22%	0.454%
54	10.033	1349	1351	1354	rVB	27809	24298	1.77%	0.129%
55	10.069	1354	1357	1362	rBV3	35948	47216	3.43%	0.250%
56	10.116	1362	1365	1367	rVV3	21001	20168	1.47%	0.107%
57	10.139	1367	1369	1372	rVB3	22226	16920	1.23%	0.090%
58	10.204	1378	1380	1384	rVV5	18320	21175	1.54%	0.112%
59	10.239	1384	1386	1388	rVB	40665	27172	1.97%	0.144%
60	10.339	1400	1403	1405	rBV	124929	93418	6.79%	0.496%
61	10.404	1412	1414	1416	rVB3	21985	14346	1.04%	0.076%
62	10.457	1420	1423	1428	rVV2	35718	47310	3.44%	0.251%
63	10.498	1428	1430	1435	rVB5	23737	29027	2.11%	0.154%
64	10.575	1439	1443	1447	rBV	504763	424834	30.87%	2.253%
65	10.710	1463	1466	1467	rBV	46234	38721	2.81%	0.205%
66	10.886	1493	1496	1498	rBV3	19392	18856	1.37%	0.100%
67	11.010	1512	1517	1519	rBV6	19899	28424	2.07%	0.151%
68	11.169	1540	1544	1546	rBV2	37562	46377	3.37%	0.246%
69	11.274	1558	1562	1564	rBV	1011403	880762	63.99%	4.672%
70	11.298	1564	1566	1569	rVB	568971	426187	30.96%	2.261%
71	11.345	1569	1574	1577	rVB	162209	145434	10.57%	0.771%

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72	11.380	1577	1580	1584	rBV4	23673	37944	2.76%	0.201%
73	11.498	1597	1600	1604	rBV	39536	34979	2.54%	0.186%
74	11.680	1627	1631	1636	rBV	410544	334894	24.33%	1.776%
75	11.774	1644	1647	1649	rBV	52265	51863	3.77%	0.275%
76	11.804	1649	1652	1657	rVV	155702	149679	10.88%	0.794%
77	11.845	1657	1659	1662	rVV3	28252	29488	2.14%	0.156%
78	11.886	1663	1666	1668	rVV	136166	126714	9.21%	0.672%
79	11.910	1668	1670	1673	rVB	36742	28207	2.05%	0.150%
80	12.069	1694	1697	1699	rBV	35015	36651	2.66%	0.194%
81	12.321	1738	1740	1743	rBV2	35072	36992	2.69%	0.196%
82	12.363	1743	1747	1749	rBV	1360424	1239182	90.03%	6.573%
83	12.386	1749	1751	1754	rVB	812191	639966	46.50%	3.395%
84	12.480	1762	1767	1771	rBV2	645231	700813	50.92%	3.717%
85	12.592	1784	1786	1791	rBV4	45686	53007	3.85%	0.281%
86	12.710	1801	1806	1809	rBV	566203	556726	40.45%	2.953%
87	12.857	1828	1831	1834	rVB	590638	517484	37.60%	2.745%
88	13.104	1870	1873	1876	rBV	99109	88630	6.44%	0.470%
89	13.904	2005	2009	2012	rBV2	919395	951235	69.11%	5.046%
90	15.327	2247	2251	2254	rBV	528403	615532	44.72%	3.265%

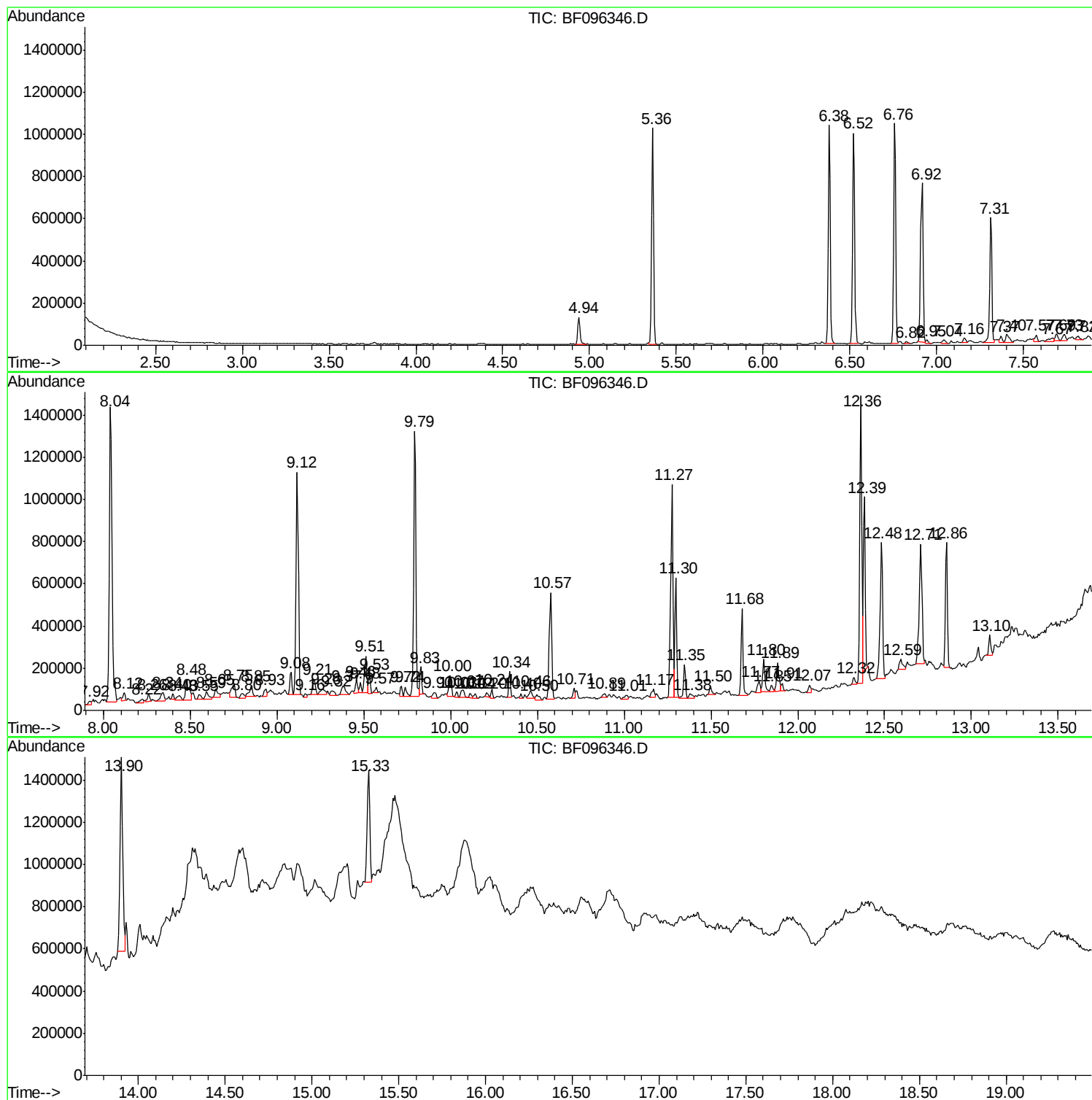
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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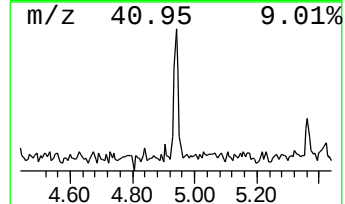
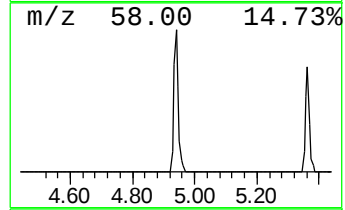
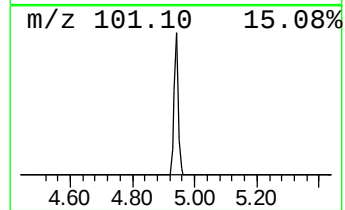
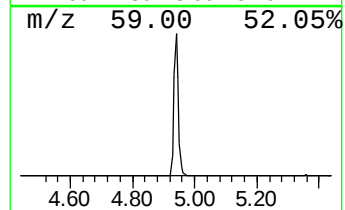
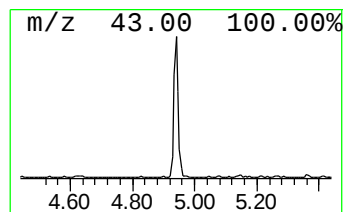
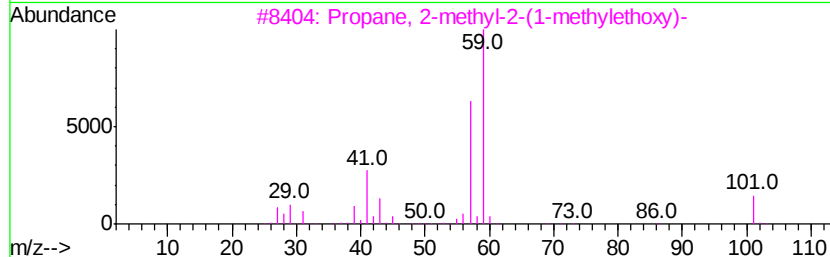
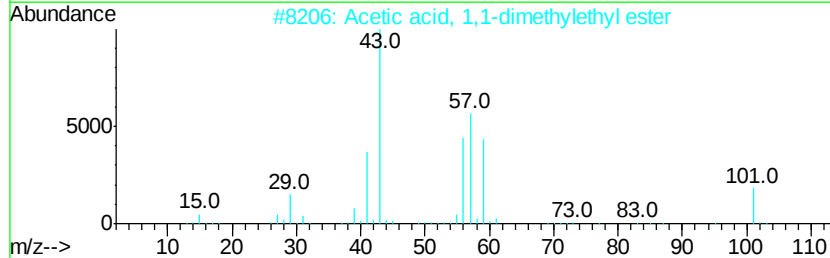
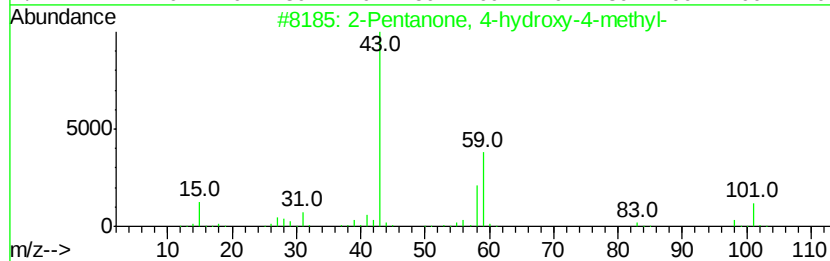
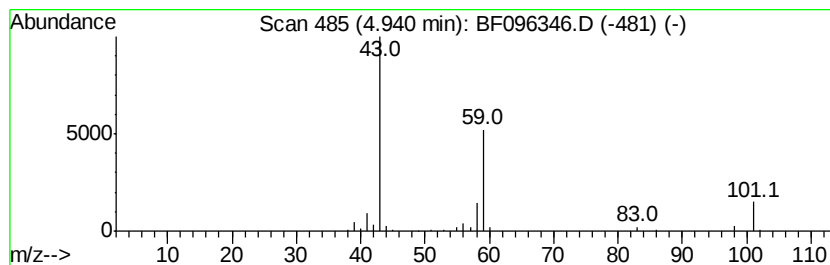
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.81 ng	129189	1,4-Dichlorobenzene-d4	6.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
4	3-Hexanol	102	C6H14O	000623-37-0	33	
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	



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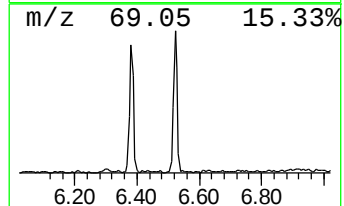
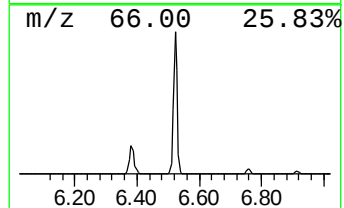
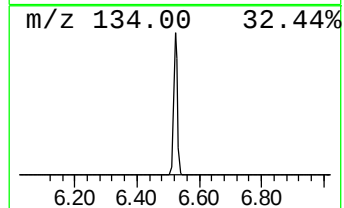
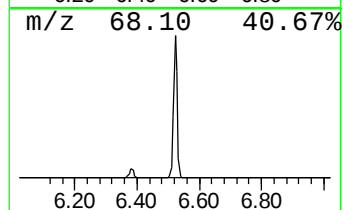
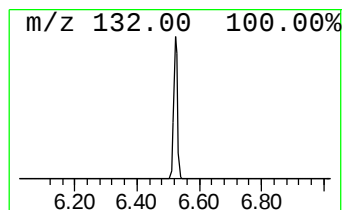
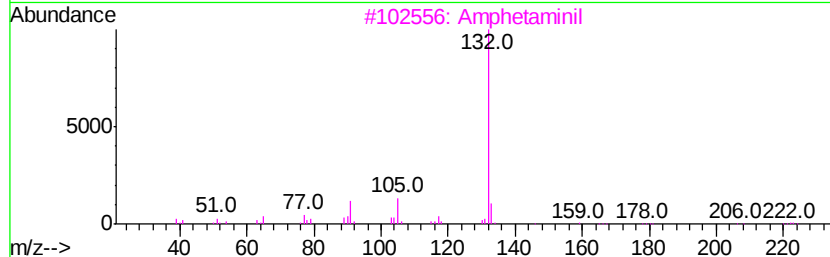
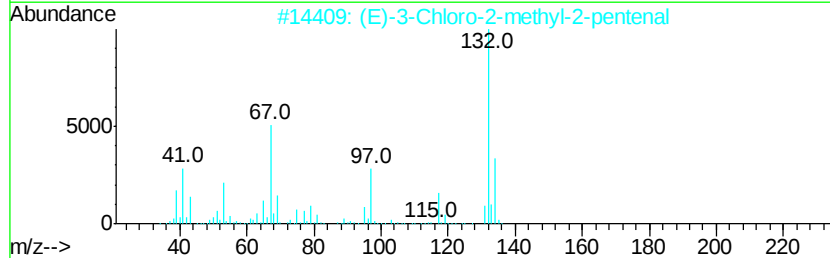
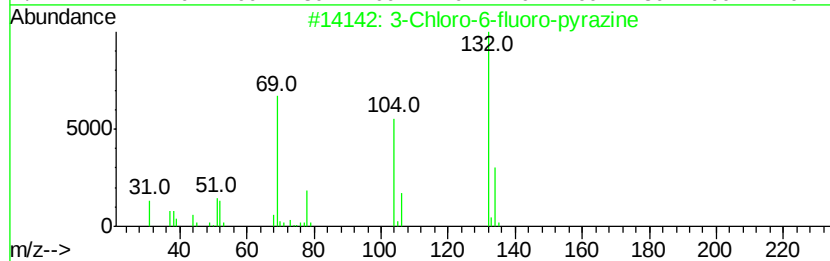
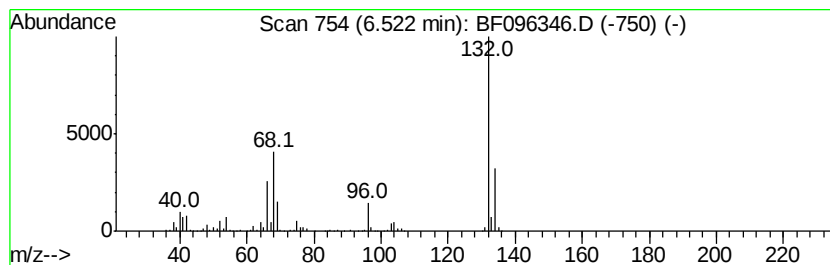
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	19.06 ng	874621	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Amphetaminil	250	C17H18N2	017590-01-1	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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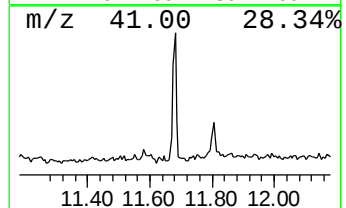
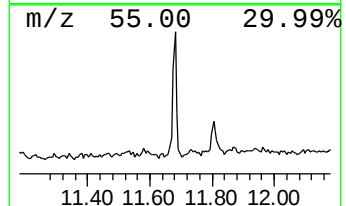
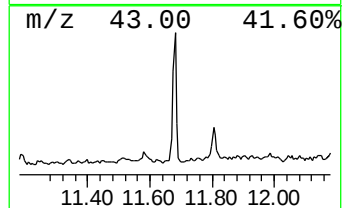
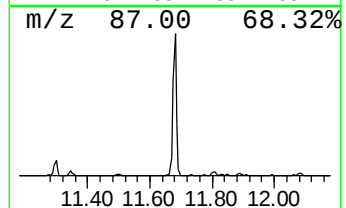
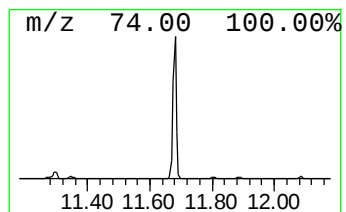
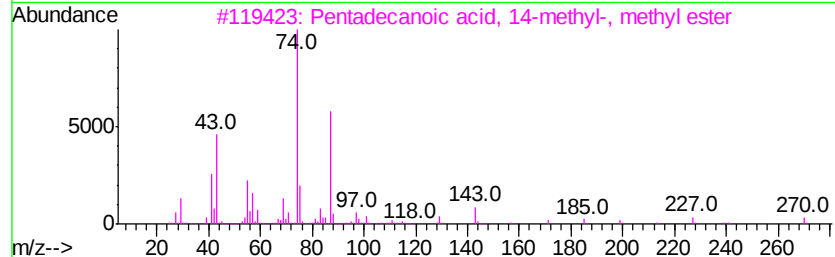
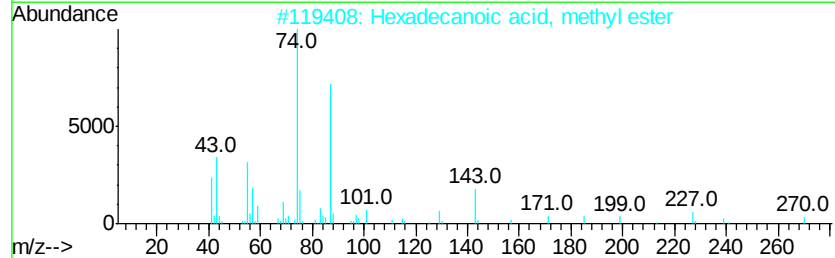
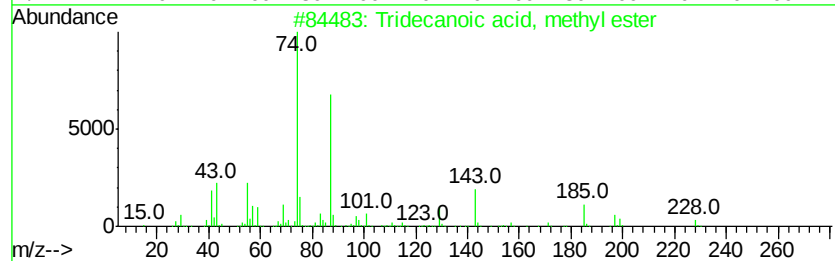
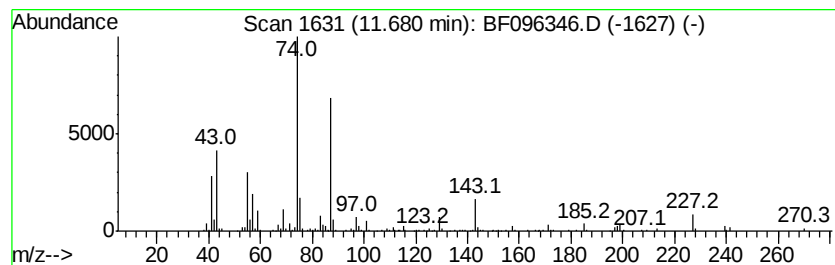
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	7.60 ng	334894	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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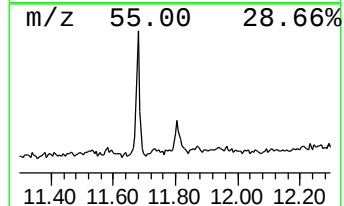
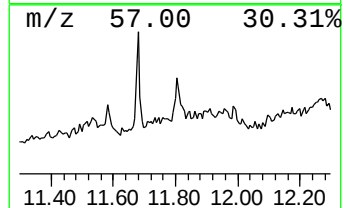
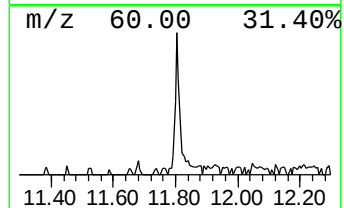
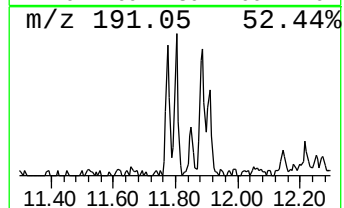
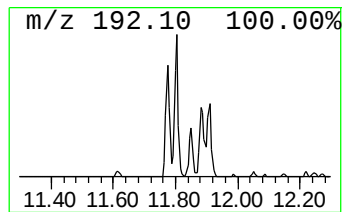
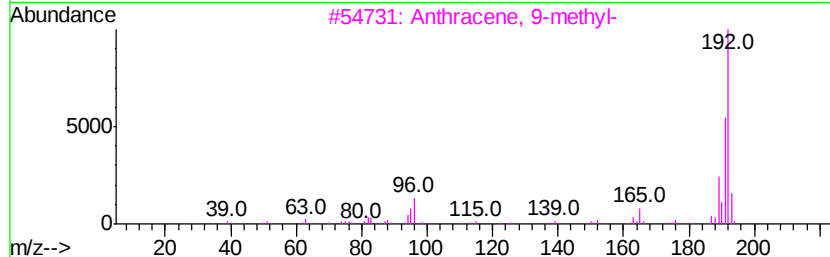
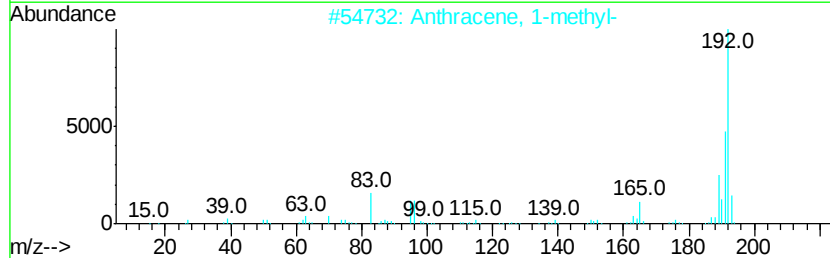
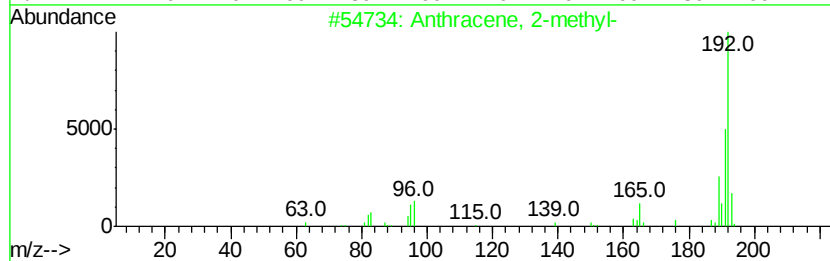
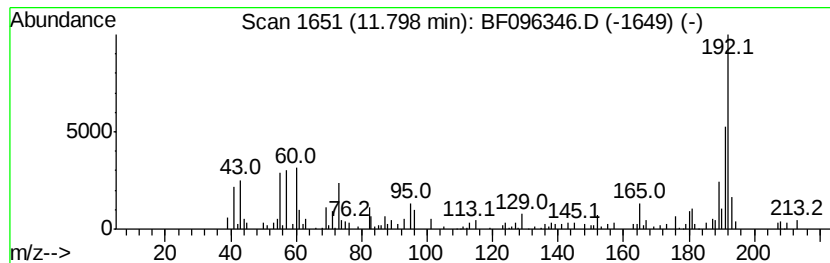
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.40 ng	149679	Phenanthrene-d10	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
3		Anthracene, 9-methyl-	192	C15H12	000779-02-2	83
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
5		Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096346.D
Acq On : 30 Jun 2017 19:51
Operator : SJ/MA
Sample : I3959-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

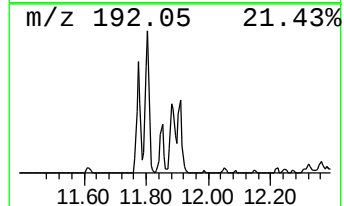
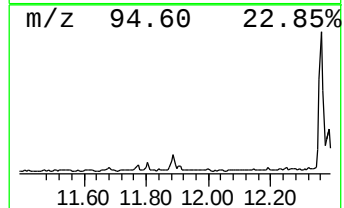
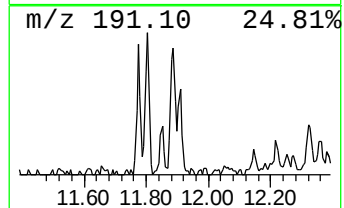
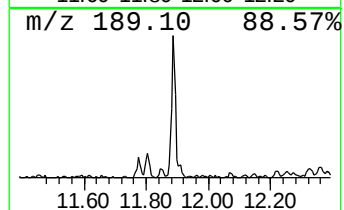
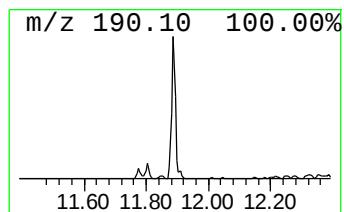
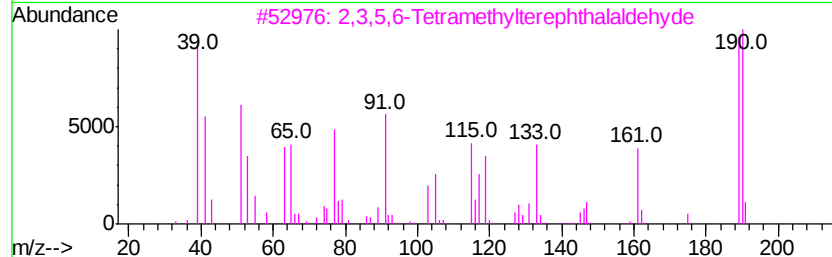
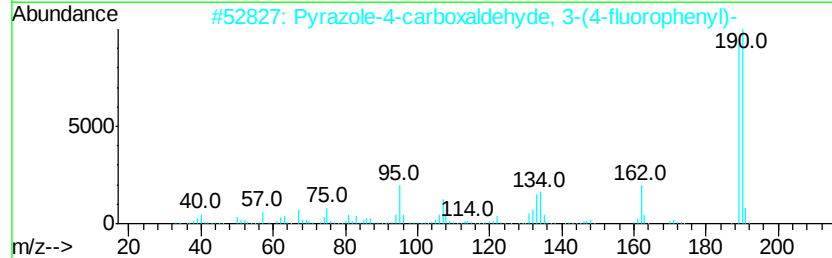
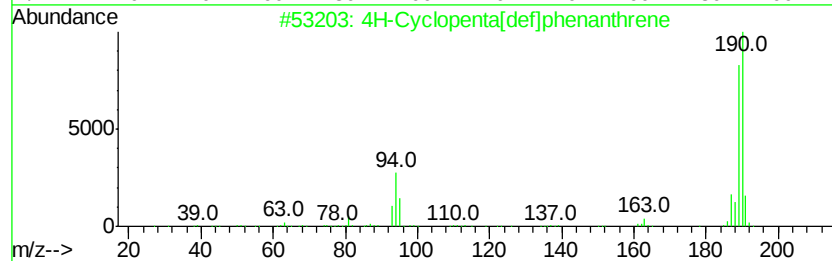
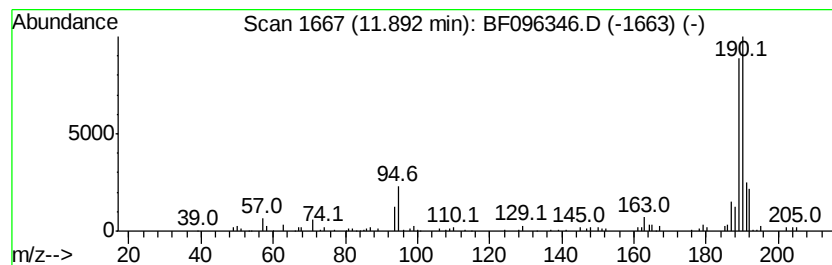
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ClientSampleId :
BU-03-062717-A

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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 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.89	2.88 ng	126714	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	46
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-062717-A

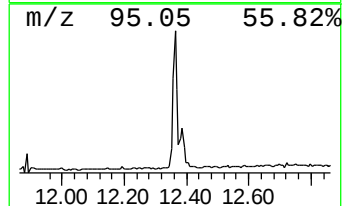
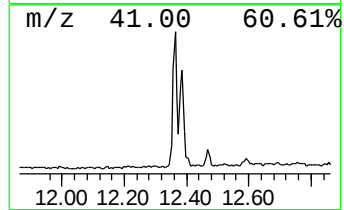
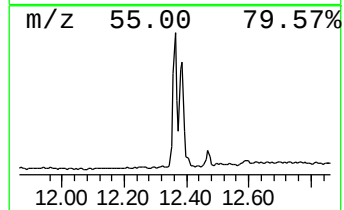
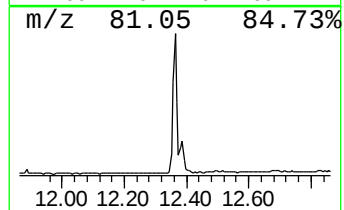
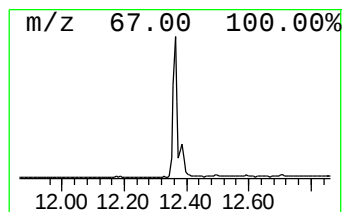
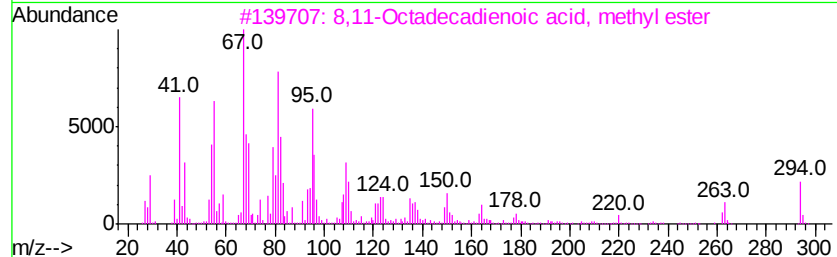
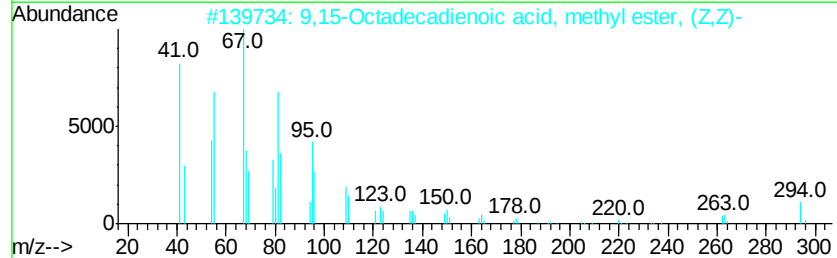
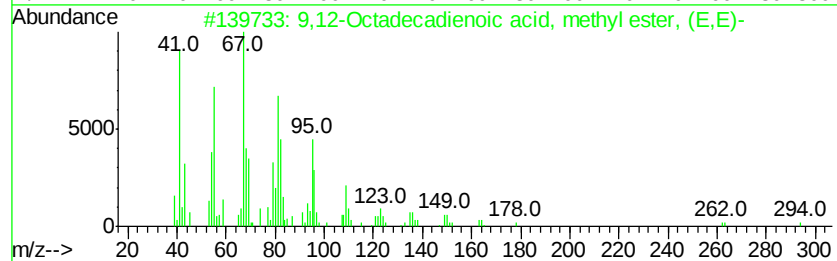
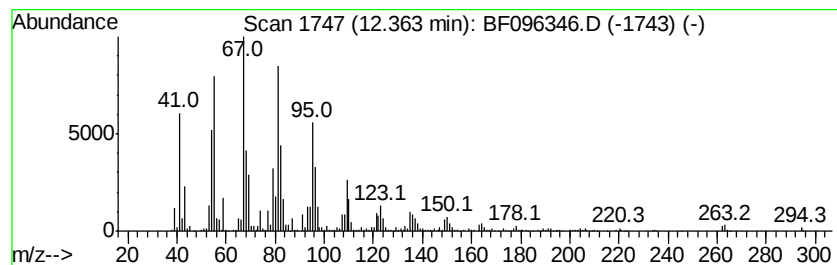
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	28.14 ng	1239180	Phenanthrene-d10	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3		8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98
4		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98



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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-062717-A

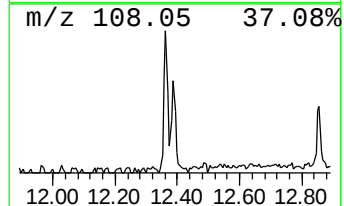
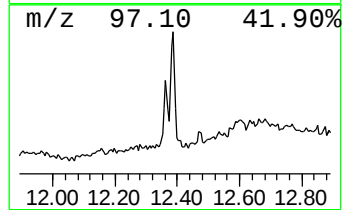
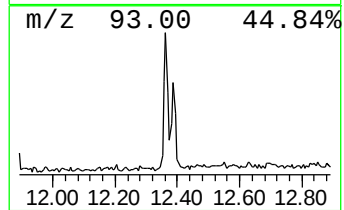
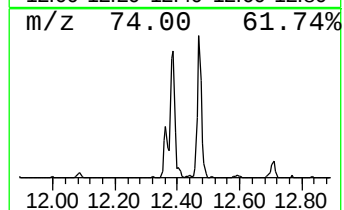
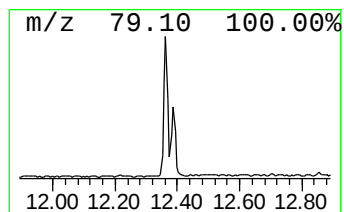
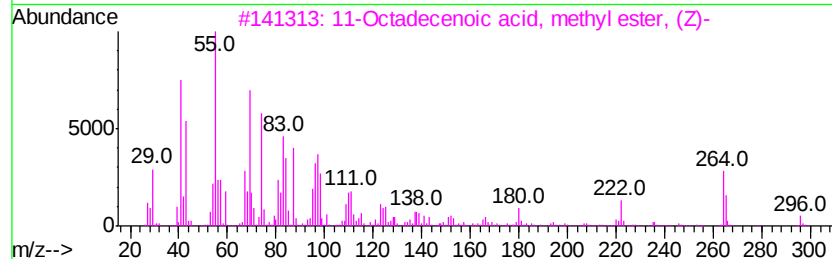
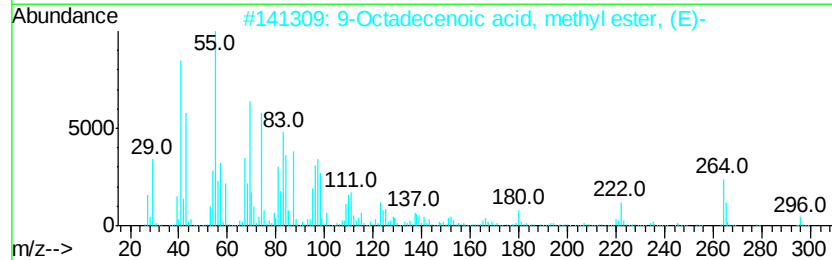
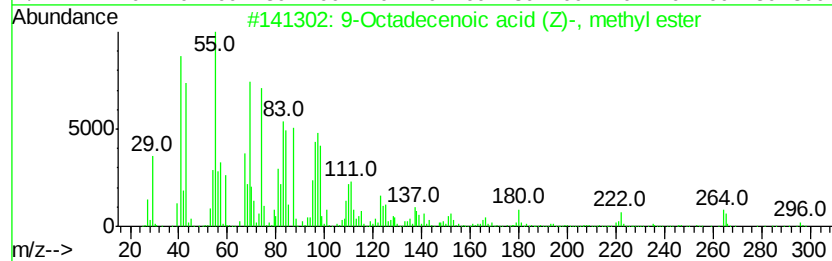
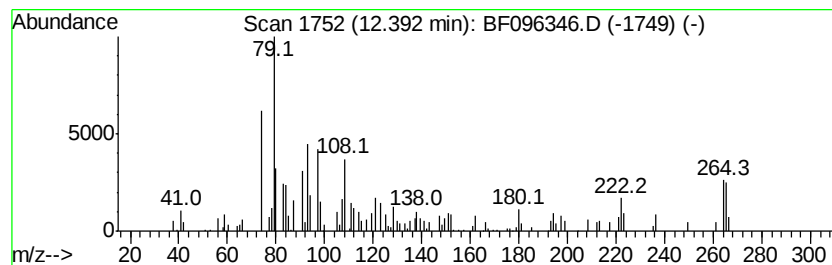
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	14.53 ng	639966	Phenanthrene-d10	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3		11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99



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Sample : I3959-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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
2-Pentanone, 4-hy...	4.94	2.8	ng	129189	1	6.76	917950	20.0
unknown6.52	6.52	19.1	ng	874621	1	6.76	917950	20.0
Tridecanoic acid,...	11.68	7.6	ng	334894	4	11.27	880762	20.0
Anthracene, 2-met...	11.80	3.4	ng	149679	4	11.27	880762	20.0
4H-Cyclopenta[def...	11.89	2.9	ng	126714	4	11.27	880762	20.0
9,12-Octadecadien...	12.36	28.1	ng	1239180	4	11.27	880762	20.0
9-Octadecenoic ac...	12.39	14.5	ng	639966	4	11.27	880762	20.0