

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
 Data File : BF097709.D
 Acq On : 15 Aug 2017 23:47
 Operator : SJ/JU
 Sample : I4700-07 5X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-01-080917-C

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-BF081517.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	5.375	555	559	563	rBV	763791	664814	8.90%	1.470%
2	6.398	729	733	742	rVB	886178	710069	9.50%	1.570%
3	6.545	754	758	761	rBV	838810	702366	9.40%	1.553%
4	6.781	795	798	802	rBV	1168354	970394	12.99%	2.145%
5	6.939	821	825	828	rVB	563555	500459	6.70%	1.106%
6	7.339	889	893	896	rBV	531163	396649	5.31%	0.877%
7	8.069	1012	1017	1020	rBV	1425780	1306286	17.48%	2.888%
8	8.663	1115	1118	1121	rBV	176952	170315	2.28%	0.377%
9	8.892	1150	1157	1159	rBV3	65145	88103	1.18%	0.195%
10	8.951	1164	1167	1173	rBV6	42540	76463	1.02%	0.169%
11	9.098	1189	1192	1195	rVB3	84458	93831	1.26%	0.207%
12	9.139	1196	1199	1204	rVB	855400	692686	9.27%	1.531%
13	9.233	1210	1215	1219	rBV	342648	359308	4.81%	0.794%
14	9.292	1220	1225	1227	rVV3	64759	76854	1.03%	0.170%
15	9.410	1240	1245	1250	rVB3	161702	170768	2.29%	0.378%
16	9.504	1259	1261	1263	rVV2	89644	77038	1.03%	0.170%
17	9.539	1263	1267	1271	rVV3	172344	300925	4.03%	0.665%
18	9.574	1271	1273	1275	rVV	111322	104068	1.39%	0.230%
19	9.610	1275	1279	1281	rVB3	82974	100484	1.34%	0.222%
20	9.763	1302	1305	1308	rVB	493417	408191	5.46%	0.902%
21	9.822	1309	1315	1318	rBV	1422799	1341457	17.95%	2.966%
22	9.992	1341	1344	1347	rBV2	61741	102458	1.37%	0.227%
23	10.021	1347	1349	1351	rVB	108175	83545	1.12%	0.185%
24	10.080	1356	1359	1363	rVB3	103445	119198	1.60%	0.264%
25	10.257	1386	1389	1392	rVB	567589	502104	6.72%	1.110%
26	10.480	1420	1427	1430	rBV	241500	306217	4.10%	0.677%
27	10.563	1439	1441	1444	rBV2	93888	91625	1.23%	0.203%
28	10.598	1444	1447	1451	rVB2	460209	400189	5.36%	0.885%
29	10.733	1467	1470	1478	rBV	755937	804345	10.77%	1.778%
30	11.057	1523	1525	1531	rVB3	68765	91207	1.22%	0.202%
31	11.180	1543	1546	1549	rBV	639372	517210	6.92%	1.143%
32	11.210	1549	1551	1558	rVB	242657	248573	3.33%	0.550%
33	11.304	1563	1567	1569	rBV	1098222	1008885	13.50%	2.230%
34	11.321	1569	1570	1574	rVB	210576	158137	2.12%	0.350%

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35	11.374	1574	1579	1581	rVB2	84093	104869	1.40%	0.232%
36	11.610	1615	1619	1621	rBV	514059	420538	5.63%	0.930%
37	11.710	1632	1636	1640	rVB	4276501	3969474	53.13%	8.776%
38	11.768	1640	1646	1649	rBV2	61986	93486	1.25%	0.207%
39	11.845	1654	1659	1662	rBV2	400823	431652	5.78%	0.954%
40	11.910	1667	1670	1676	rVB2	93285	157192	2.10%	0.348%
41	12.015	1684	1688	1696	rVB	425470	419948	5.62%	0.928%
42	12.110	1702	1704	1709	rVB2	82879	93271	1.25%	0.206%
43	12.404	1748	1754	1755	rBV	5504192	6699030	89.66%	14.810%
44	12.427	1755	1758	1763	rVV2	5973076	7471218	100.00%	16.518%
45	12.504	1767	1771	1774	rVV2	2267113	2075753	27.78%	4.589%
46	12.557	1777	1780	1788	rVV	1021978	1436281	19.22%	3.175%
47	12.627	1790	1792	1797	rVB	164766	161749	2.16%	0.358%
48	12.739	1806	1811	1814	rVB	592212	591600	7.92%	1.308%
49	12.774	1814	1817	1825	rVB	239859	290397	3.89%	0.642%
50	12.851	1828	1830	1833	rBV3	66656	76161	1.02%	0.168%
51	12.886	1833	1836	1842	rVB	447118	421359	5.64%	0.932%
52	12.939	1842	1845	1847	rBV2	84475	81536	1.09%	0.180%
53	12.986	1850	1853	1857	rVB3	122783	168747	2.26%	0.373%
54	13.062	1862	1866	1868	rBV2	253720	299362	4.01%	0.662%
55	13.086	1868	1870	1871	rVV2	202259	207820	2.78%	0.459%
56	13.145	1875	1880	1883	rVB2	256878	410994	5.50%	0.909%
57	13.227	1891	1894	1895	rBV	246194	233317	3.12%	0.516%
58	13.245	1895	1897	1901	rVV2	399078	425896	5.70%	0.942%
59	13.286	1901	1904	1907	rVV3	415948	423922	5.67%	0.937%
60	13.333	1909	1912	1916	rVV2	171472	193111	2.58%	0.427%
61	13.380	1917	1920	1924	rVV3	176769	221489	2.96%	0.490%
62	13.427	1924	1928	1932	rVB3	277272	312029	4.18%	0.690%
63	13.474	1933	1936	1941	rVB	133050	132614	1.77%	0.293%
64	13.515	1941	1943	1946	rBV3	60258	78214	1.05%	0.173%
65	13.545	1946	1948	1953	rVB5	61901	90775	1.21%	0.201%
66	13.651	1962	1966	1969	rVB2	274717	359354	4.81%	0.794%
67	13.892	2005	2007	2010	rBV	156486	133471	1.79%	0.295%
68	13.933	2010	2014	2017	rVV2	957713	1022926	13.69%	2.262%
69	13.957	2017	2018	2021	rVB	121151	88114	1.18%	0.195%
70	14.409	2091	2095	2097	rBV4	169061	239493	3.21%	0.529%
71	14.727	2147	2149	2155	rVB3	89601	107774	1.44%	0.238%

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Sampling : 1 Min Area: 3 % of largest Peak
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72	14.839	2164	2168	2175	rBV	156950	234604	3.14%	0.519%
73	14.956	2185	2188	2191	rBV	95845	149167	2.00%	0.330%
74	15.056	2203	2205	2212	rVB	137067	143342	1.92%	0.317%
75	15.368	2254	2258	2262	rVB	616056	685947	9.18%	1.517%
76	15.856	2338	2341	2345	rVB	107592	128416	1.72%	0.284%

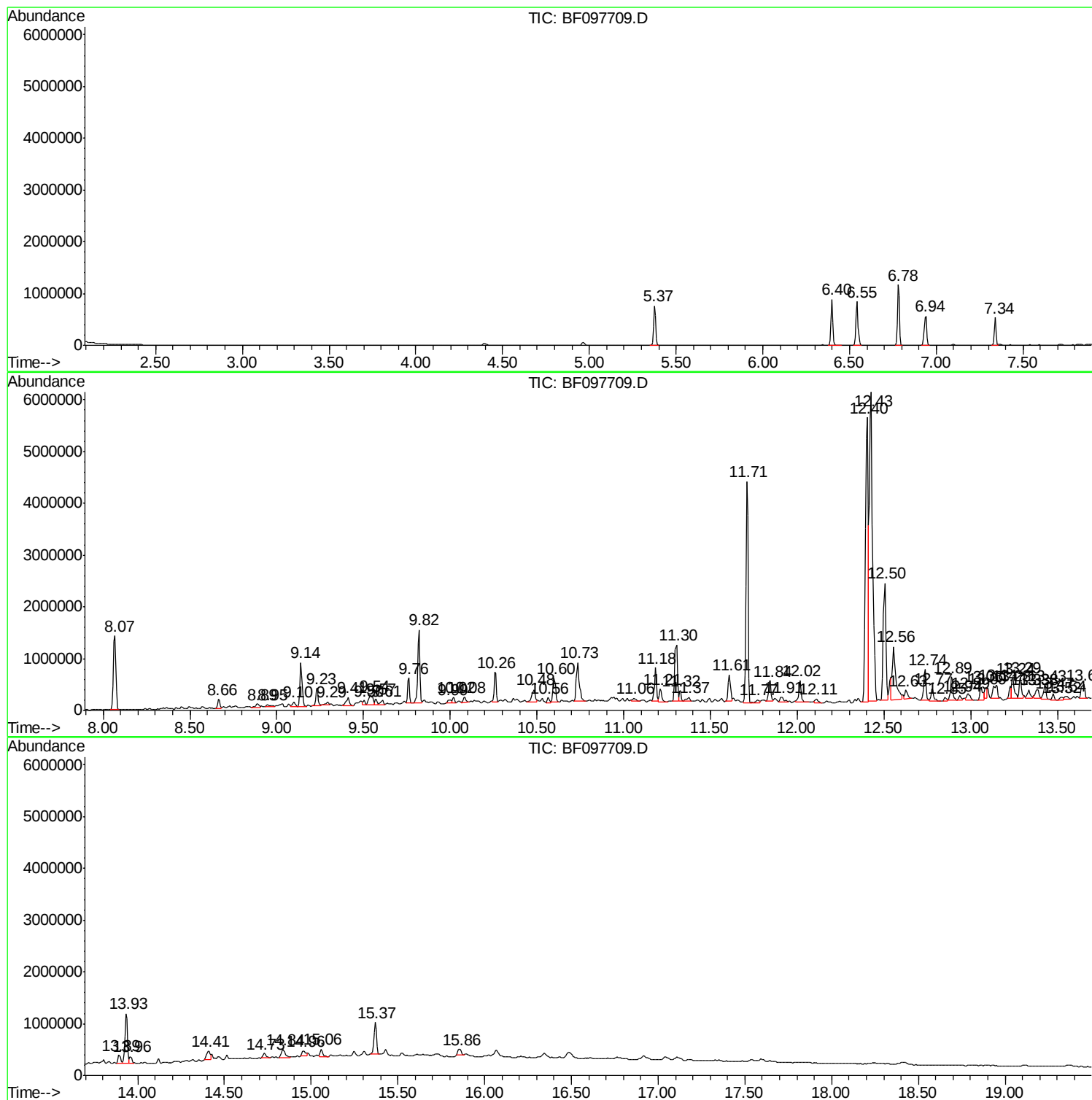
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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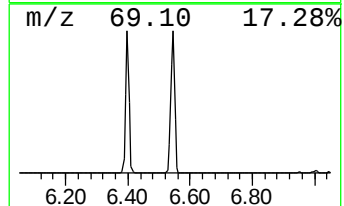
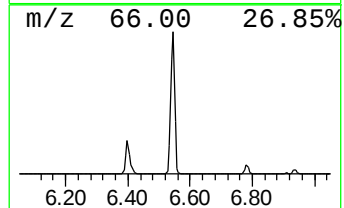
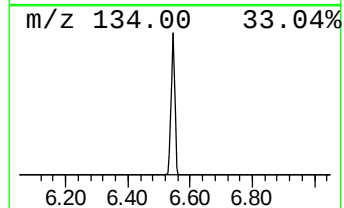
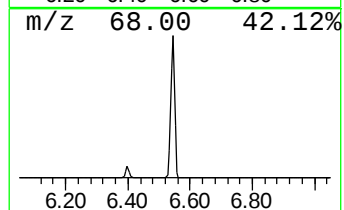
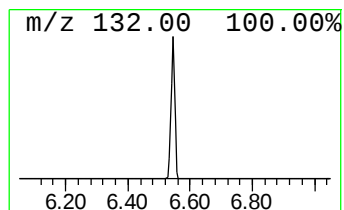
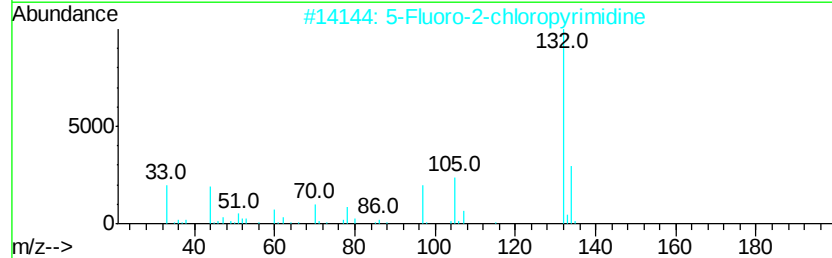
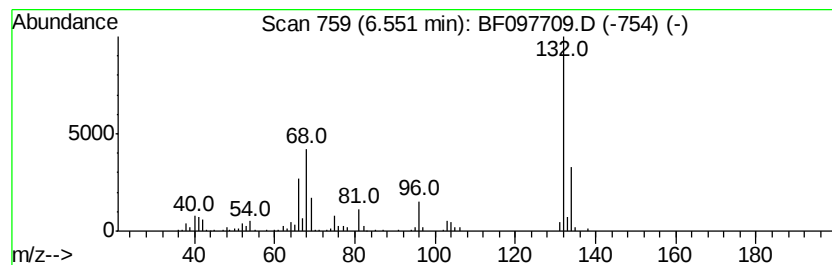
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	14.48 ng	702366	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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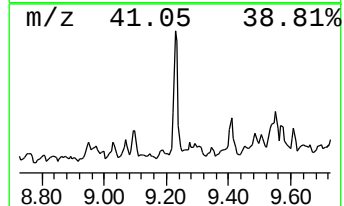
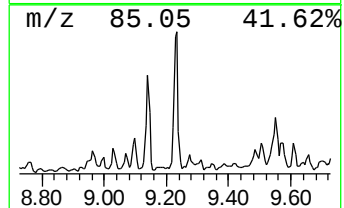
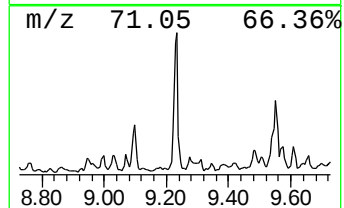
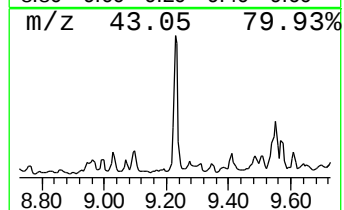
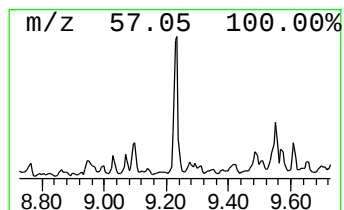
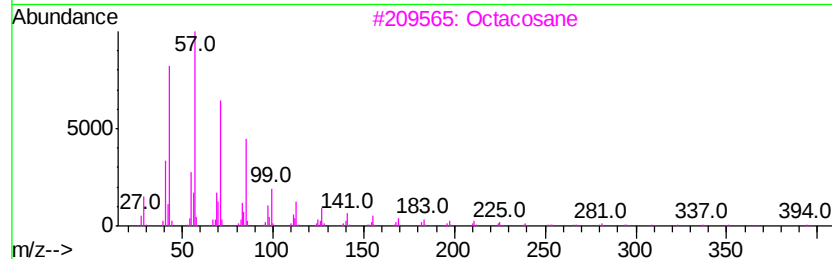
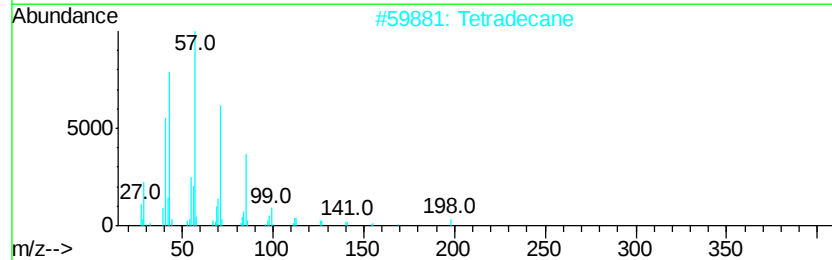
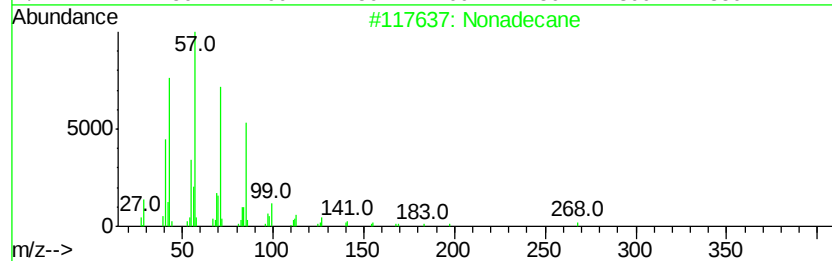
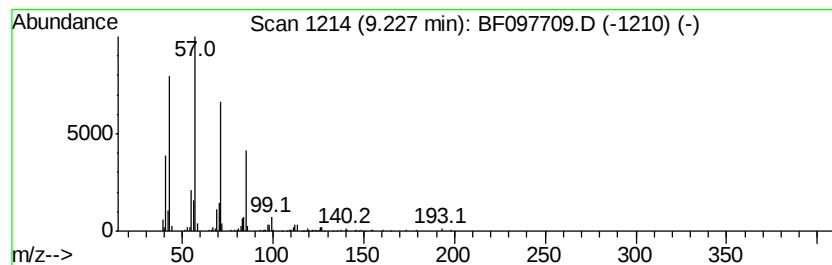
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Nonadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	5.36 ng	359308	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	86
2		Tetradecane	198	C14H30	000629-59-4	72
3		Octacosane	394	C28H58	000630-02-4	72
4		Tridecane, 4-methyl-	198	C14H30	026730-12-1	72
5		Nonane, 5-butyl-	184	C13H28	017312-63-9	72



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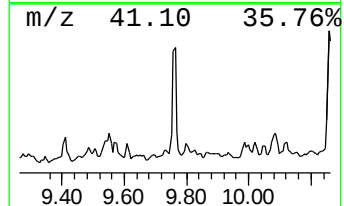
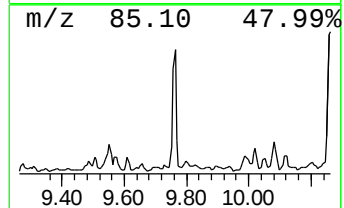
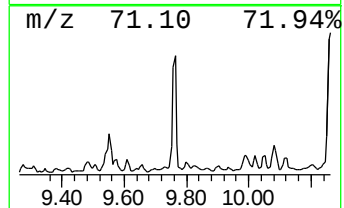
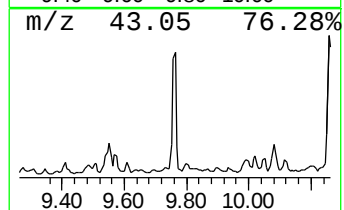
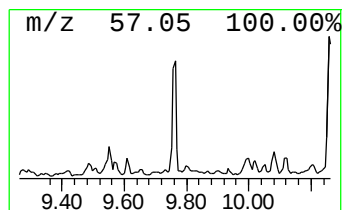
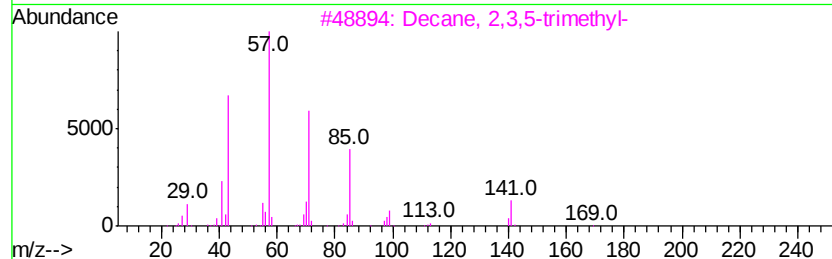
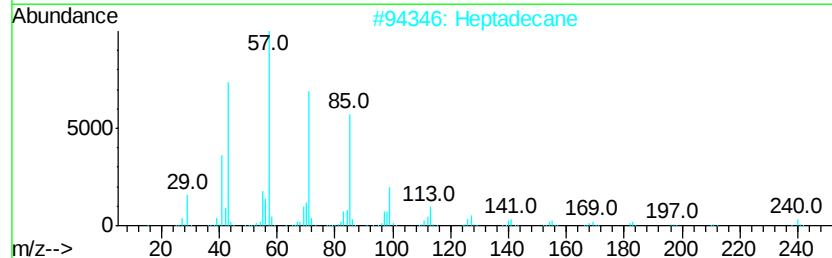
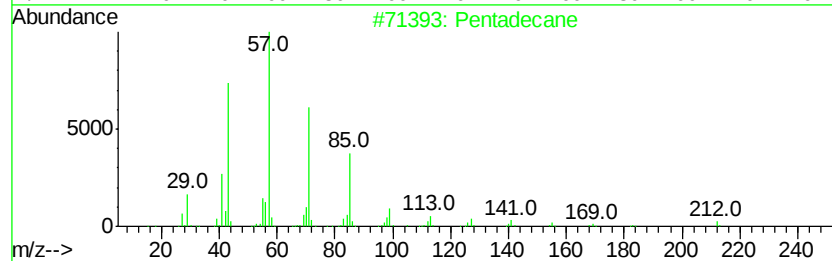
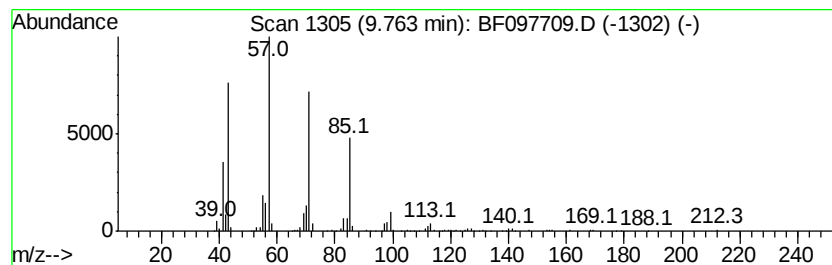
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	6.09 ng	408191	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	90
2		Heptadecane	240	C17H36	000629-78-7	90
3		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	72
5		Hexadecane, 7-methyl-	240	C17H36	026730-20-1	64



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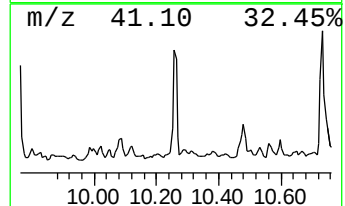
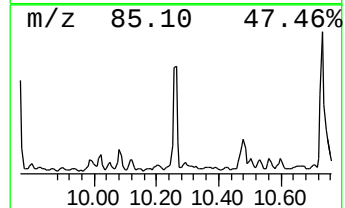
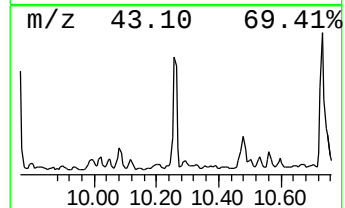
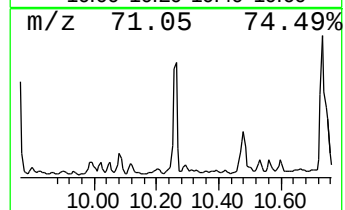
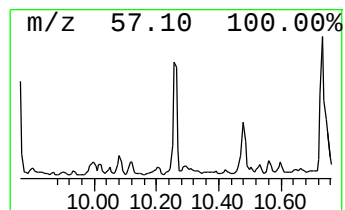
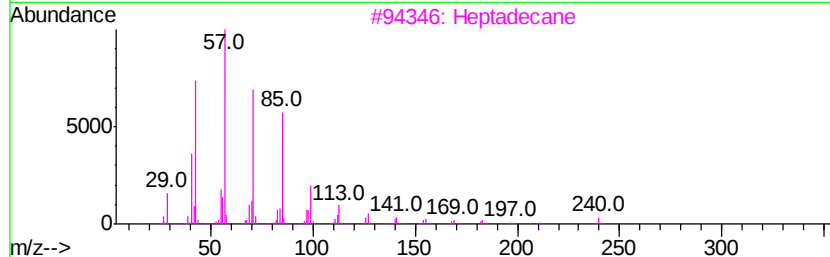
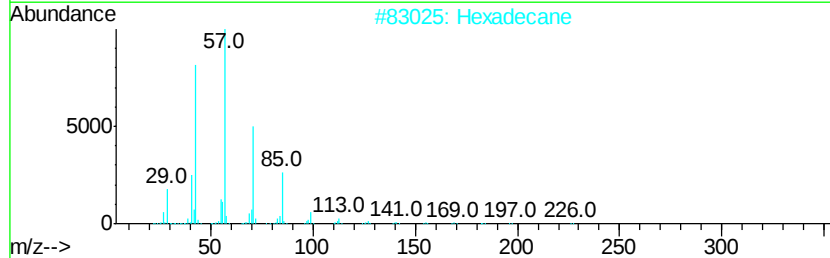
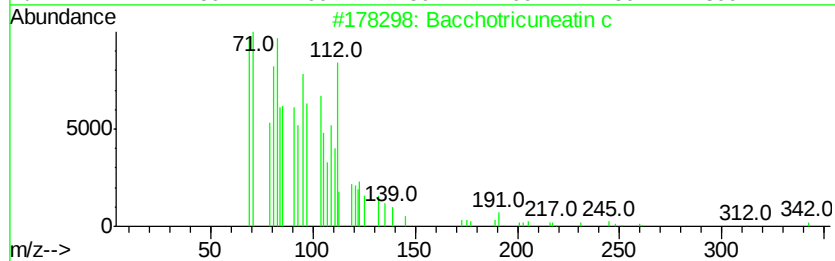
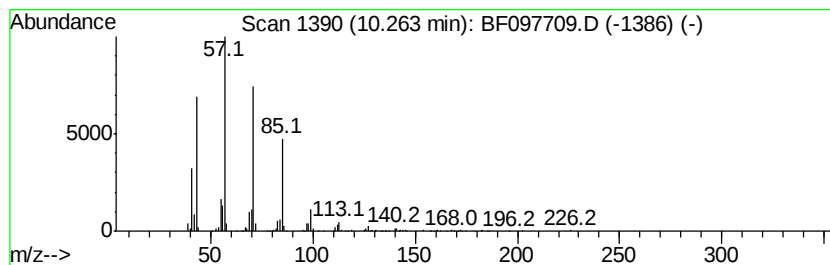
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Bacchotricuneatin c Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	7.49 ng	502104	Acenaphthene-d10	9.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bacchotricuneatin c	342	C20H22O5	066563-30-2	97
2		Hexadecane	226	C16H34	000544-76-3	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-01-080917-C

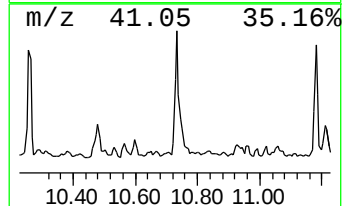
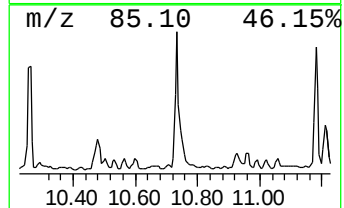
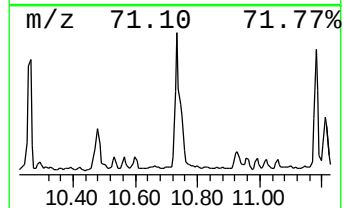
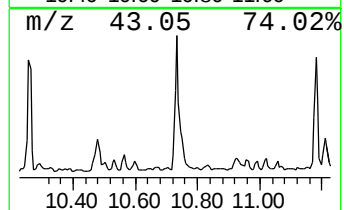
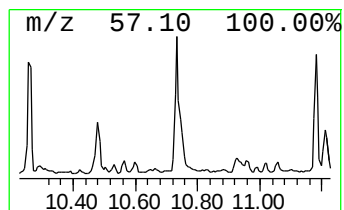
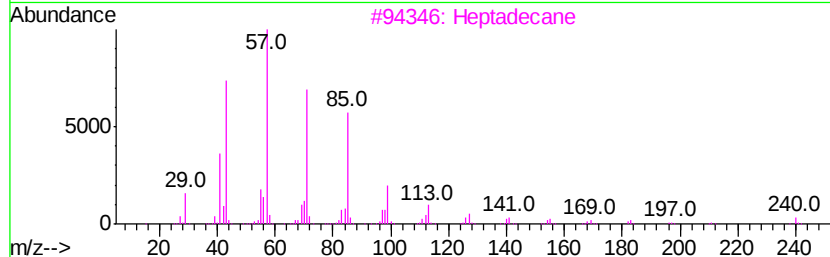
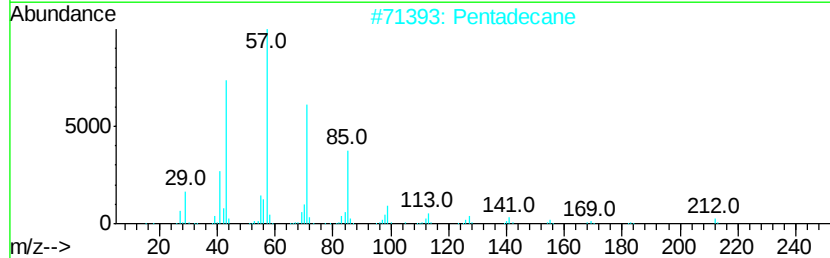
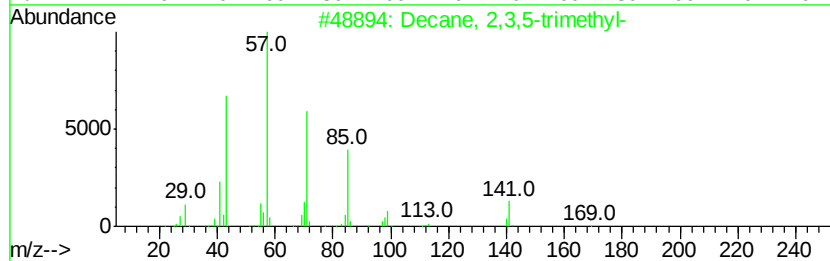
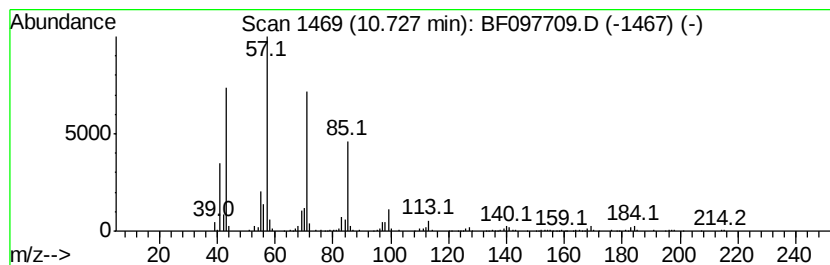
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decane, 2,3,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.73	15.95 ng	804345	Phenanthrene-d10		11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2			Pentadecane	212	C15H32	000629-62-9	90
3			Heptadecane	240	C17H36	000629-78-7	90
4			Tridecane	184	C13H28	000629-50-5	76
5			Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
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NB-01-080917-C

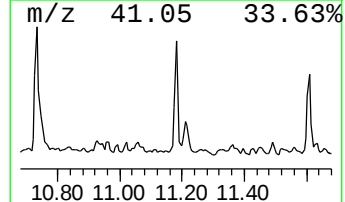
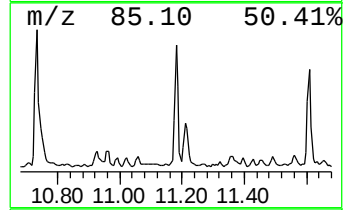
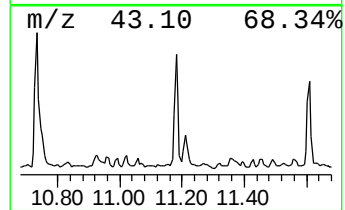
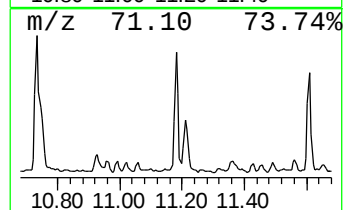
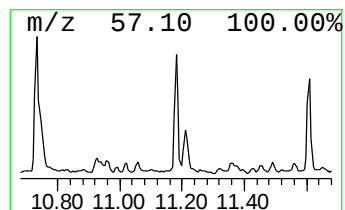
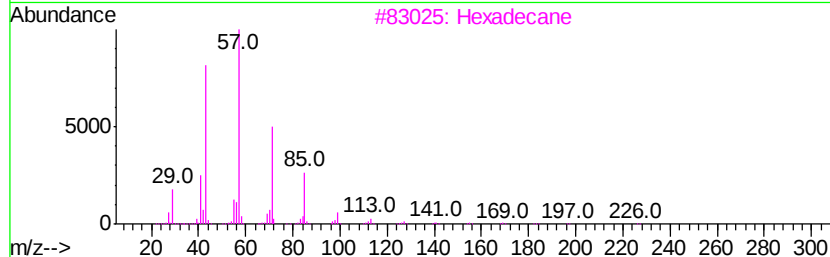
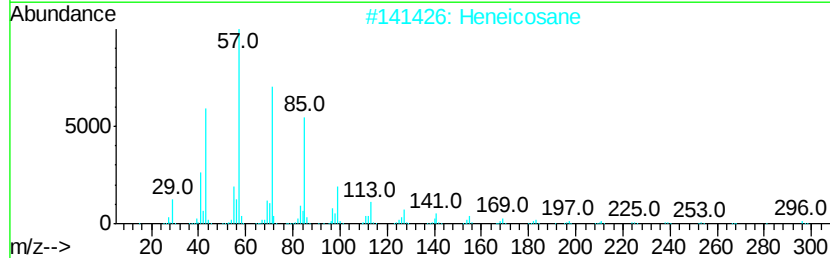
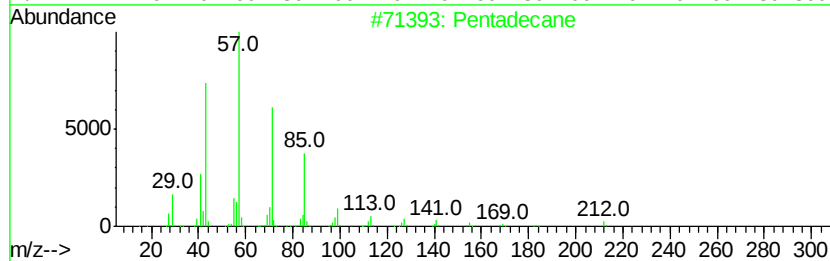
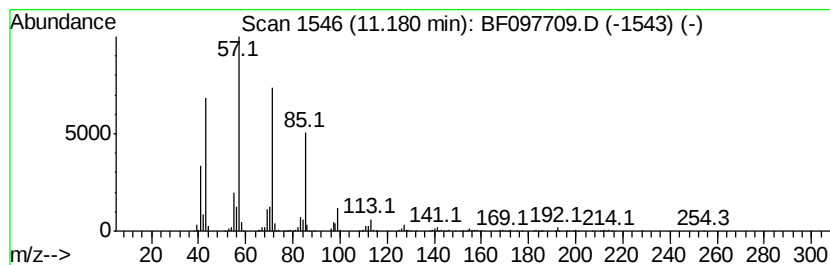
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	10.25 ng	517210	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexadecane	226	C16H34	000544-76-3	80
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	80
5		Undecane	156	C11H24	001120-21-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
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Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

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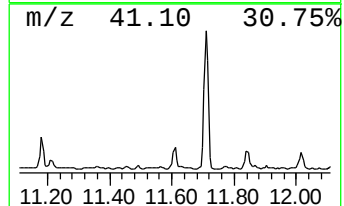
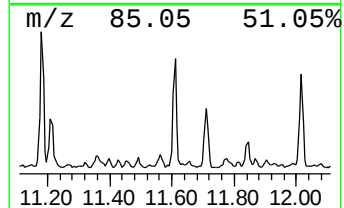
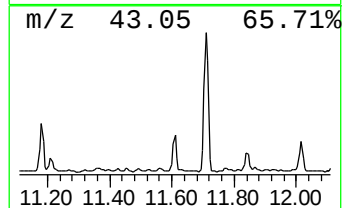
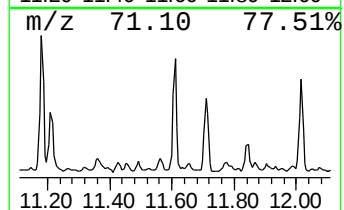
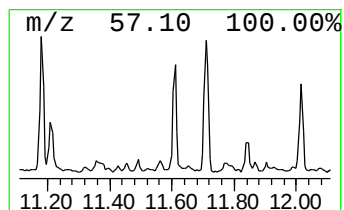
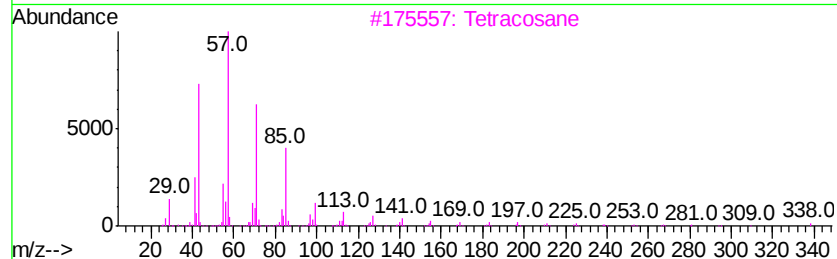
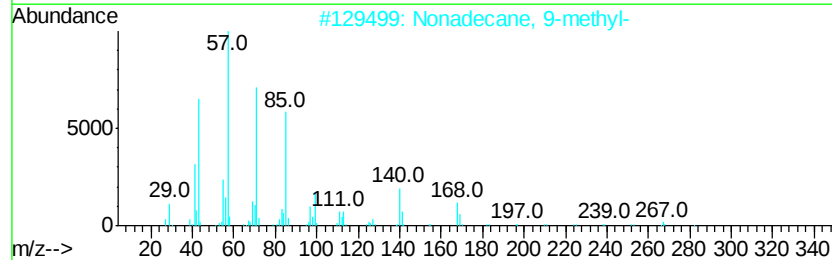
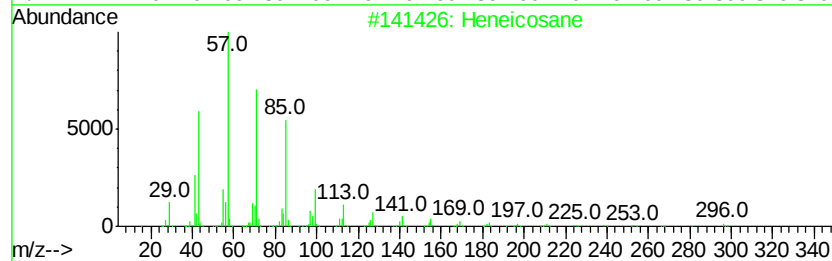
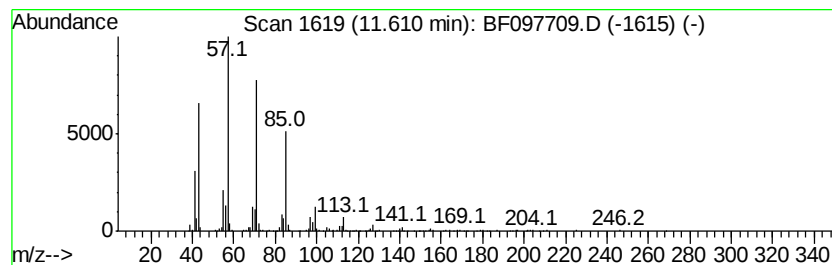
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	8.34 ng	420538	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	83
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
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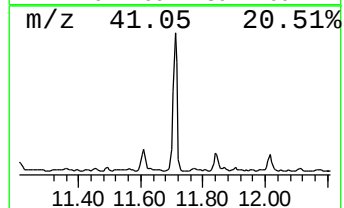
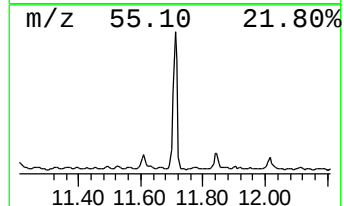
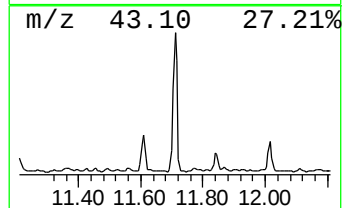
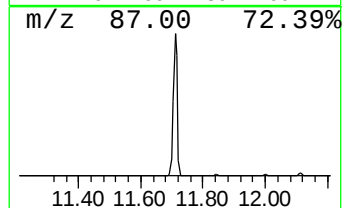
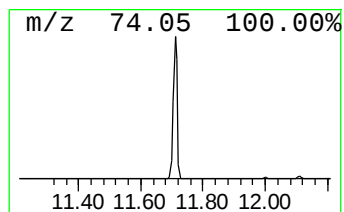
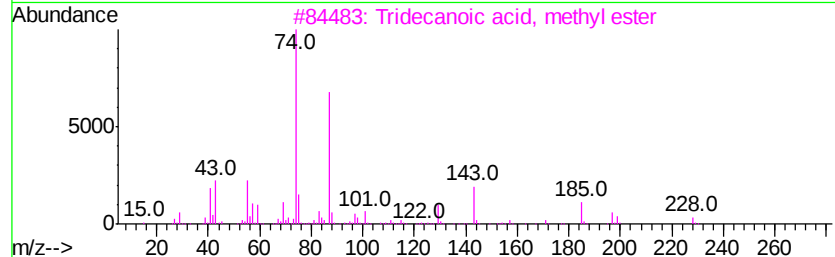
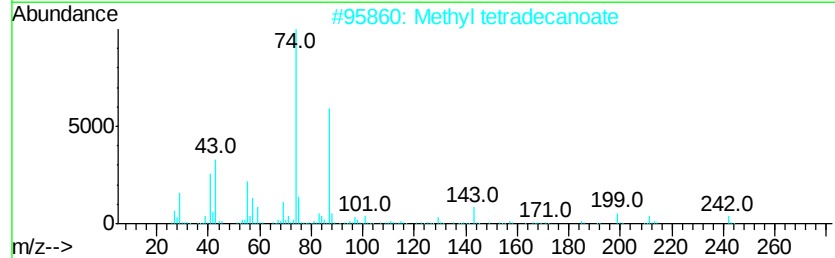
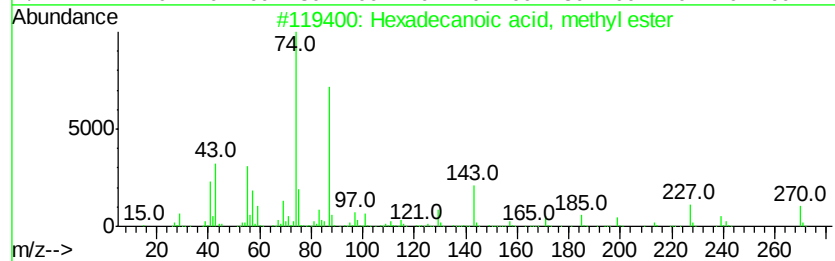
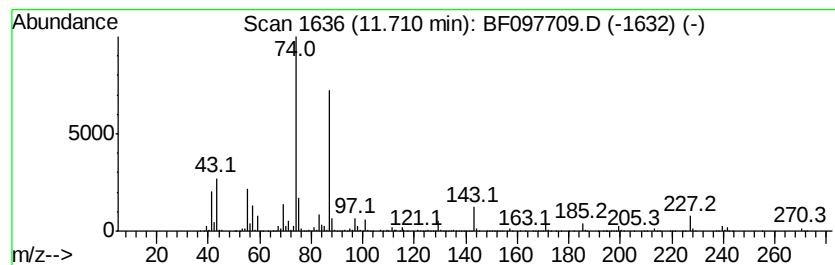
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	78.69 ng	3969470	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

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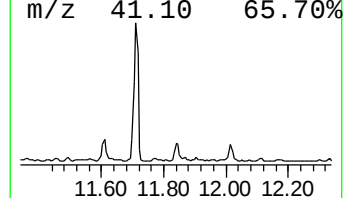
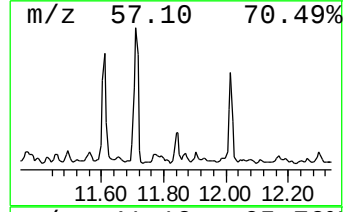
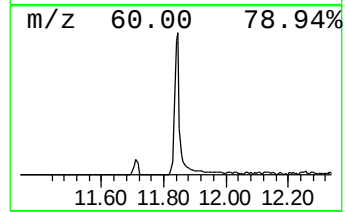
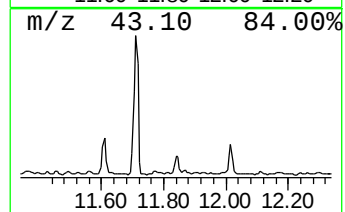
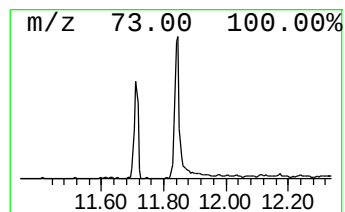
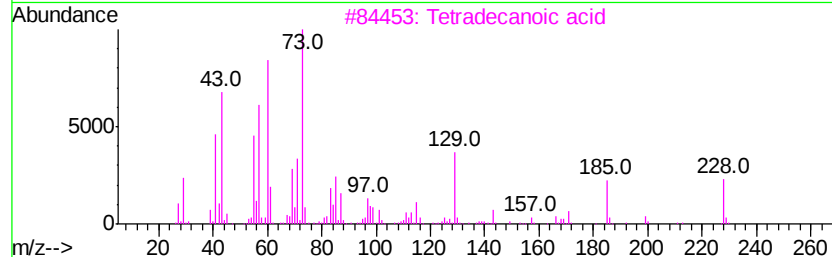
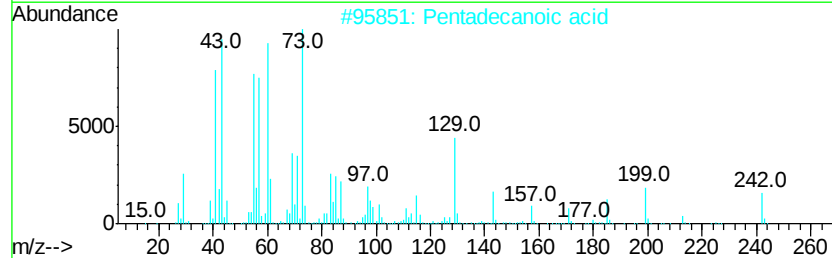
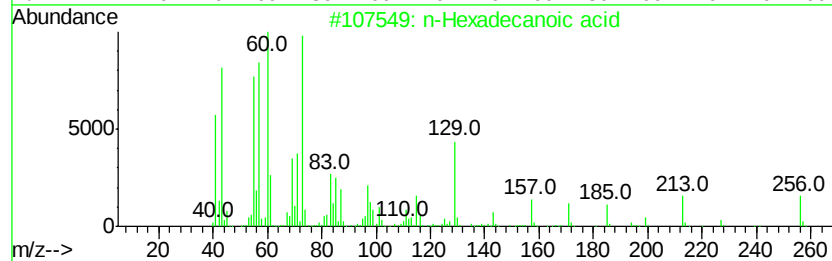
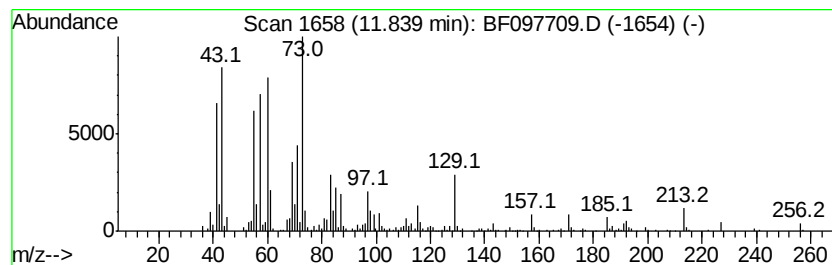
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	8.56 ng	431652	Phenanthrene-d10	11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
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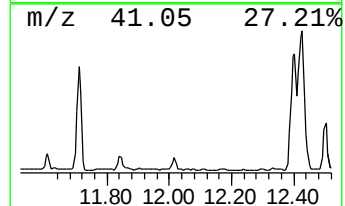
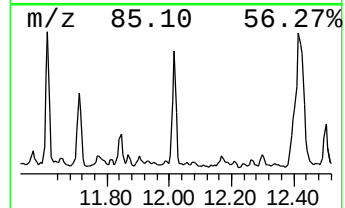
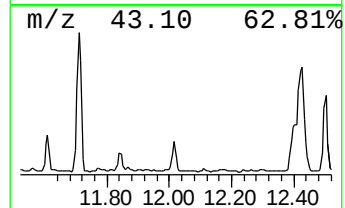
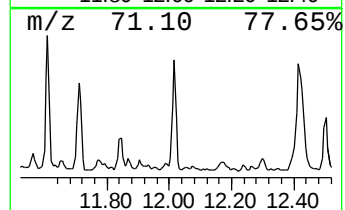
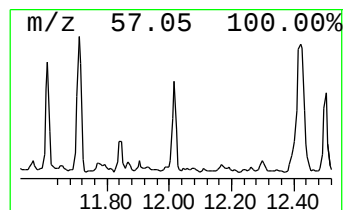
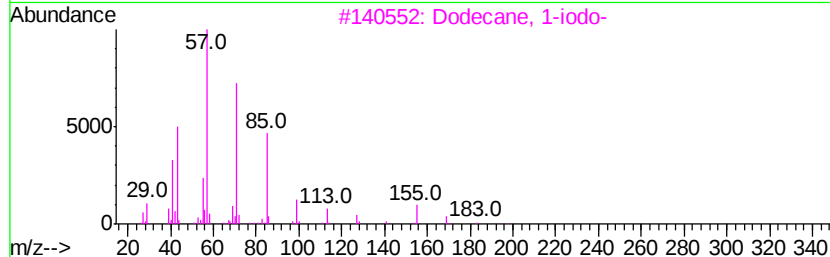
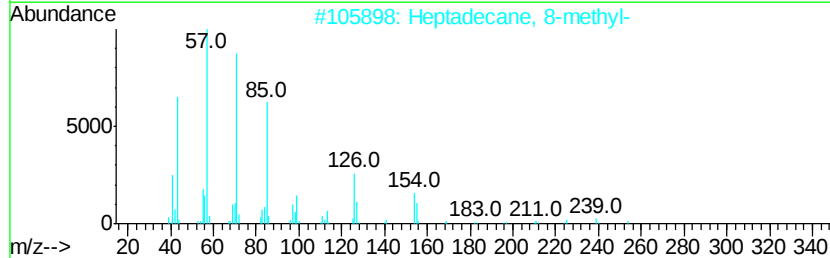
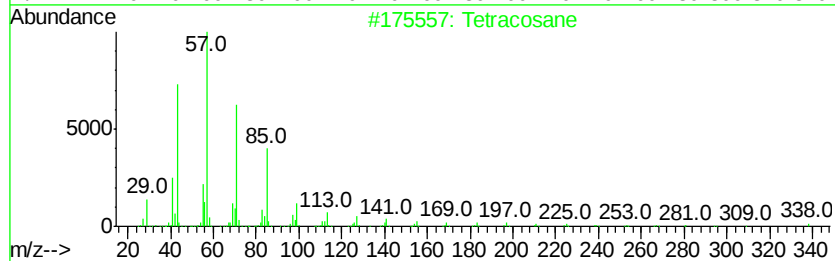
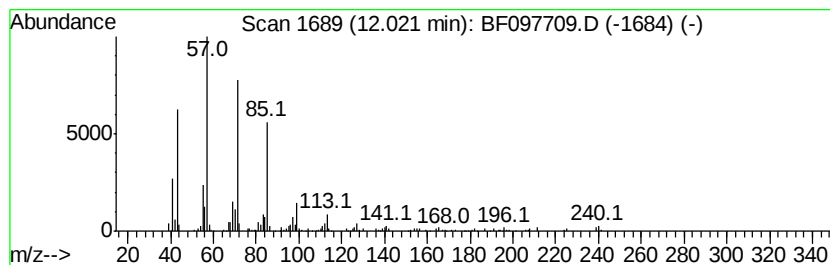
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	8.32 ng	419948	Phenanthrene-d10	11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4			Heptacosane	380	C27H56	000593-49-7	80
5			Hexadecane	226	C16H34	000544-76-3	72



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Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

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ClientSampleId :
NB-01-080917-C

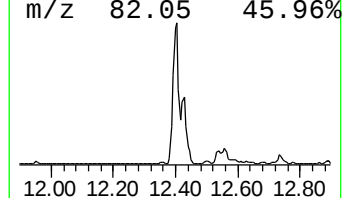
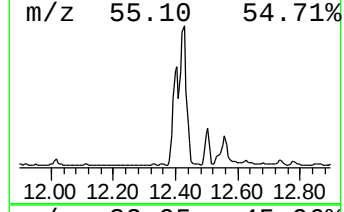
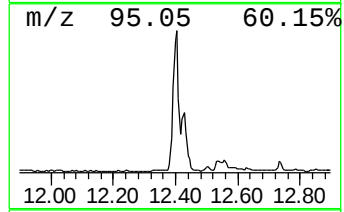
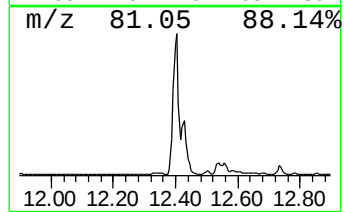
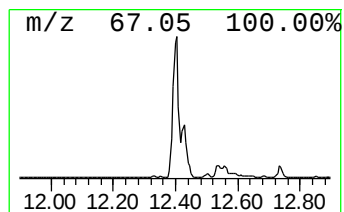
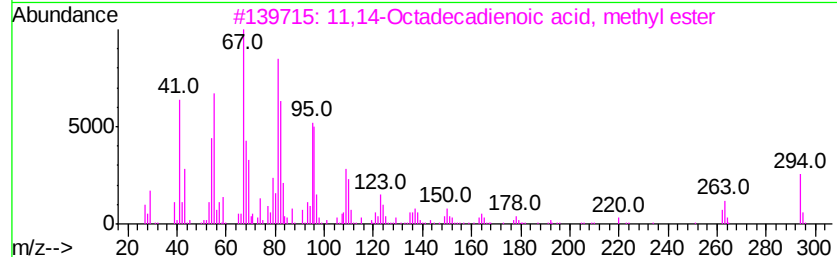
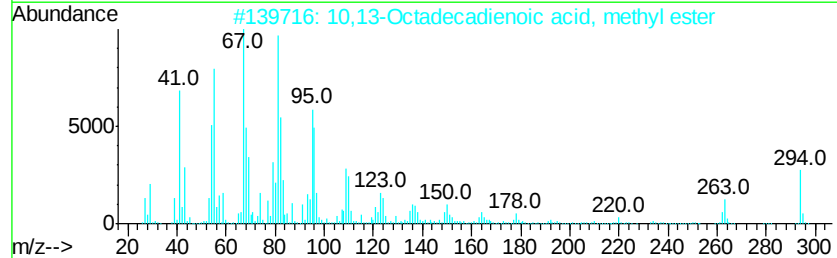
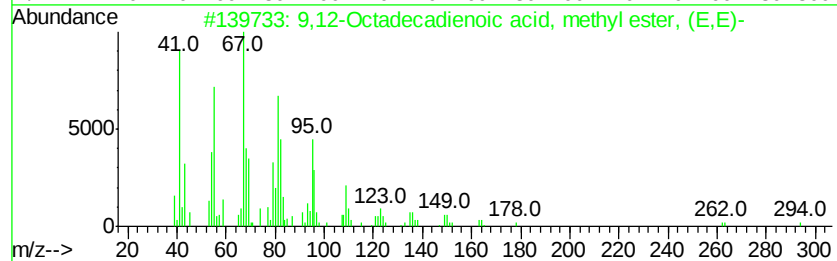
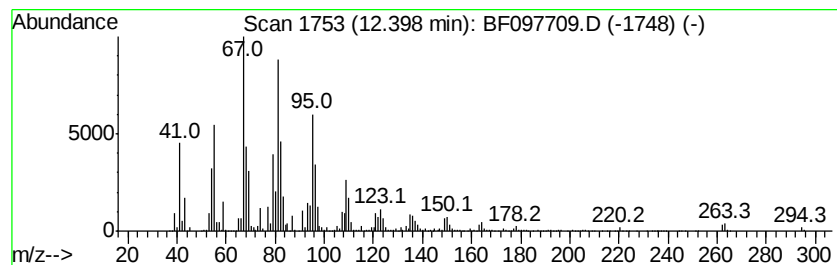
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	132.80 ng	6699030	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97
3		11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	96
4		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5		Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-01-080917-C

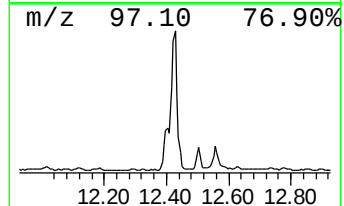
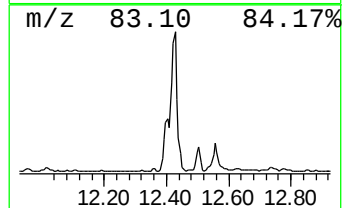
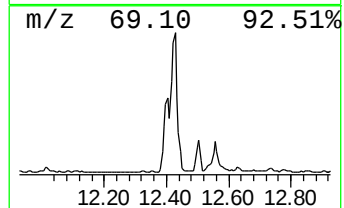
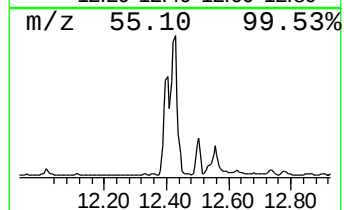
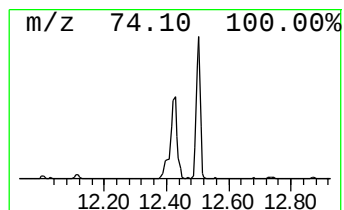
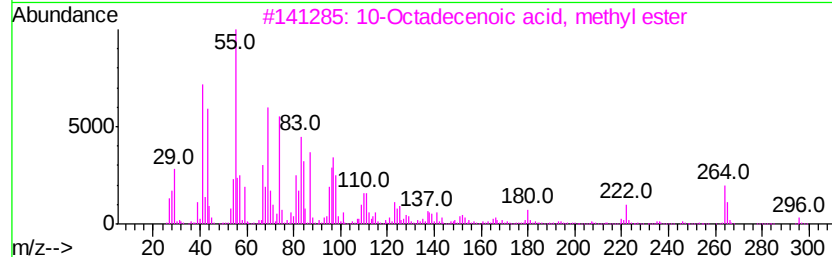
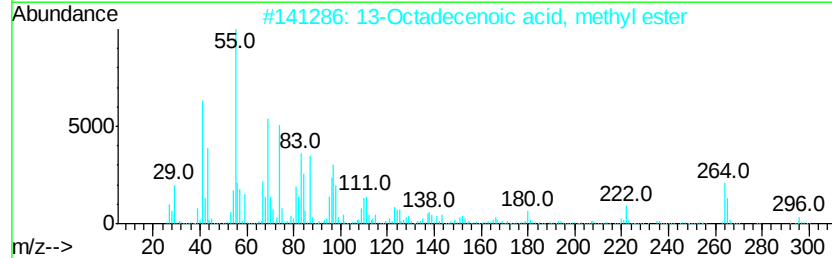
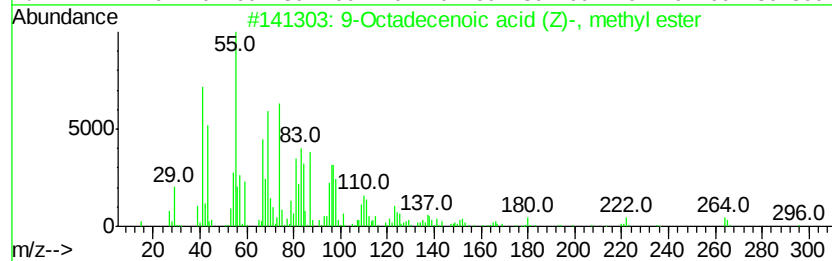
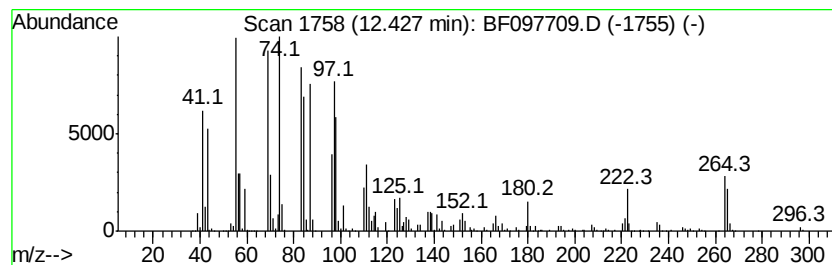
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	148.11 ng	7471220	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
3		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
4		8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	87
5		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

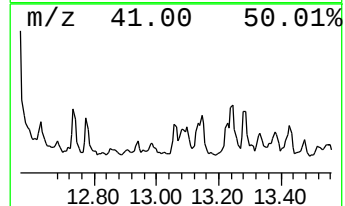
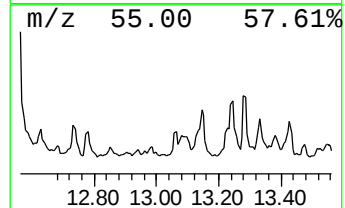
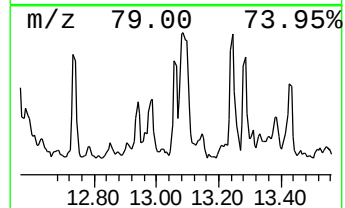
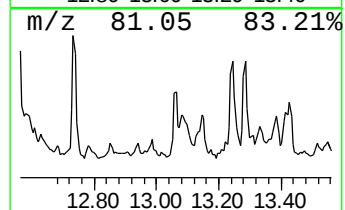
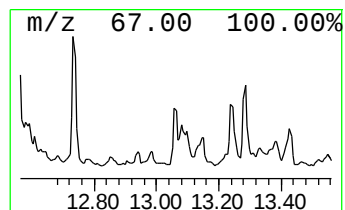
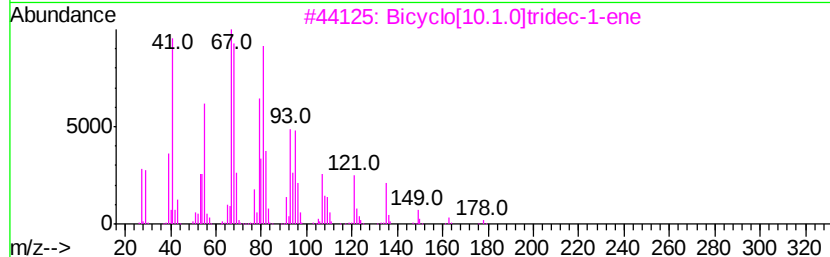
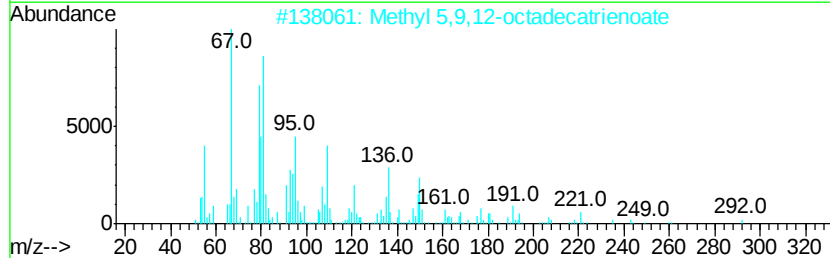
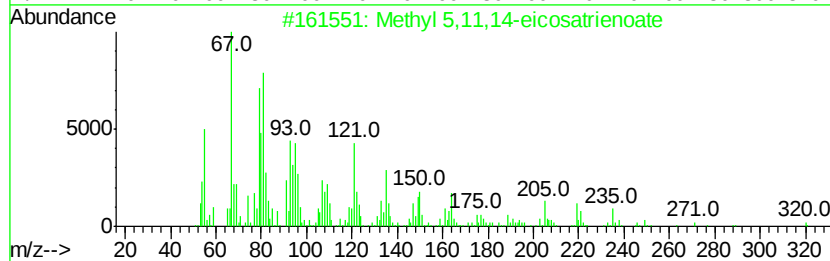
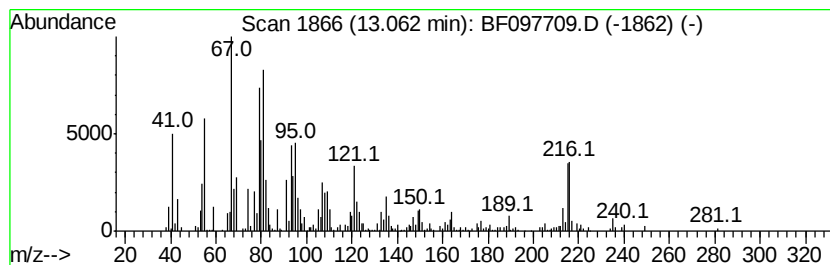
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Methyl 5,11,14-eicosatrienoate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.06	5.85 ng	299362	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 5,11,14-eicosatrienoate	320	C21H36O2	1000336-40-2	80
2	Methyl 5,9,12-octadecatrienoate	292	C19H32O2	1000336-37-5	72
3	Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	70
4	Cis-4-methyl-exo-tricyclo[5.2.1....	150	C11H18	1000215-29-2	62
5	Cyclooctene, 3-ethenyl-	136	C10H16	002213-60-7	55



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

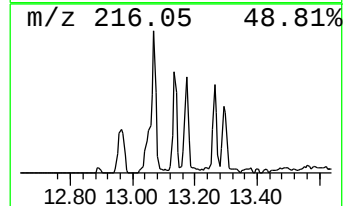
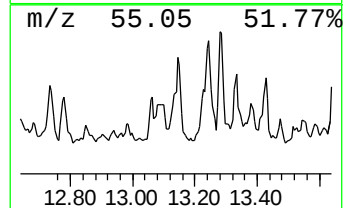
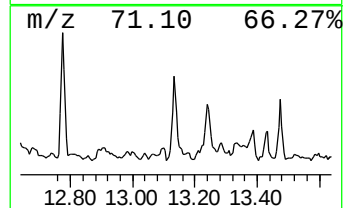
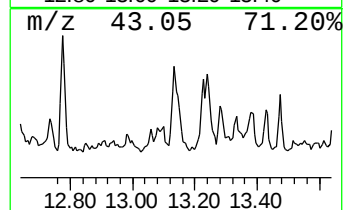
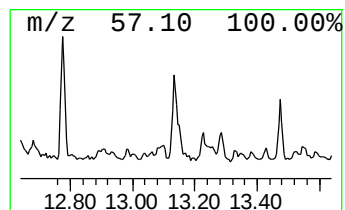
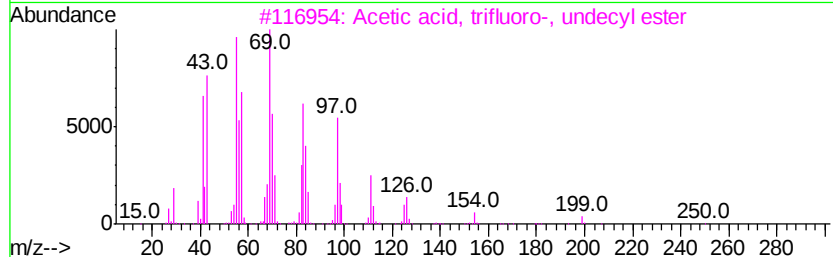
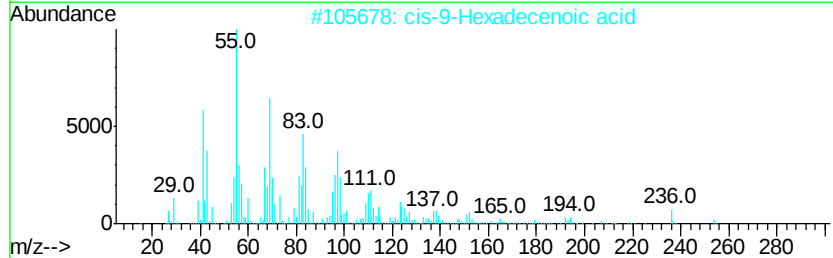
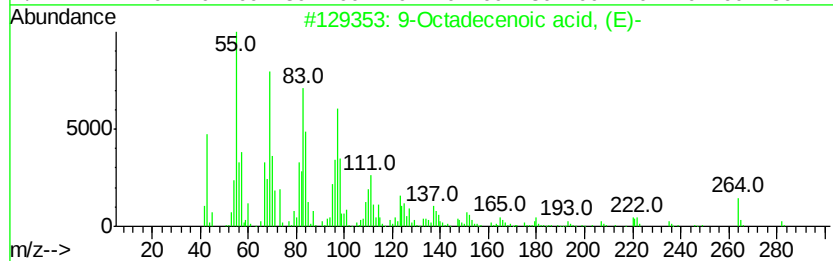
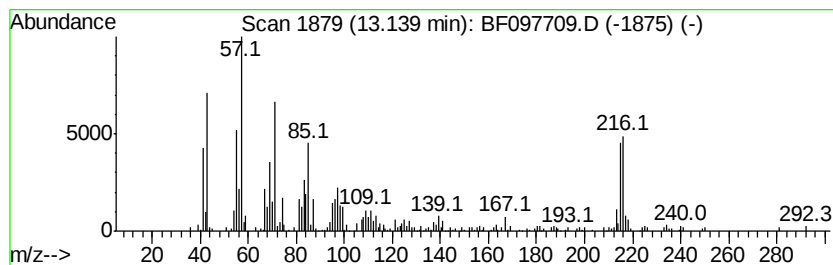
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 9-Octadecenoic acid, (E)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.14	8.04 ng	410994	Chrysene-d12	13.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	74
2		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	64
3		Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	58
4		cis-10-Heptadecenoic acid, methv...	282	C18H34O2	1000333-62-1	49
5		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
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Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

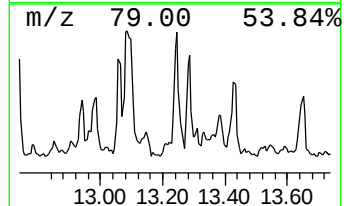
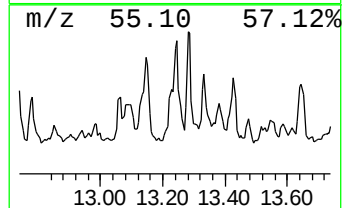
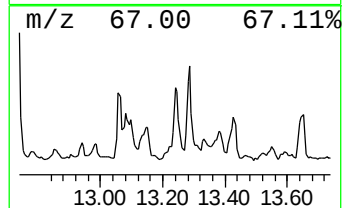
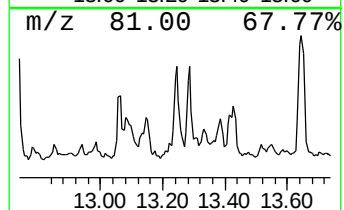
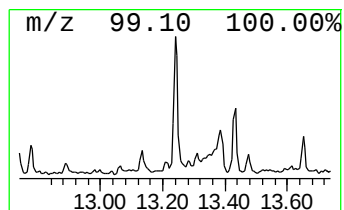
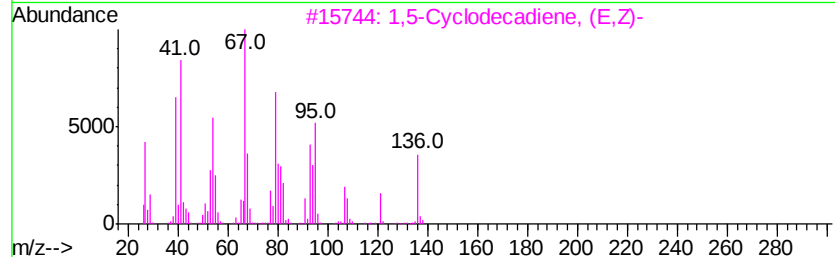
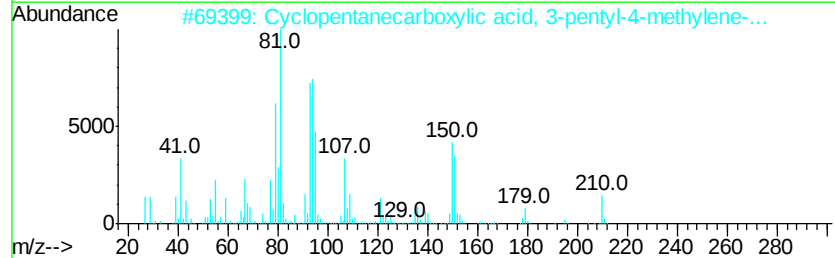
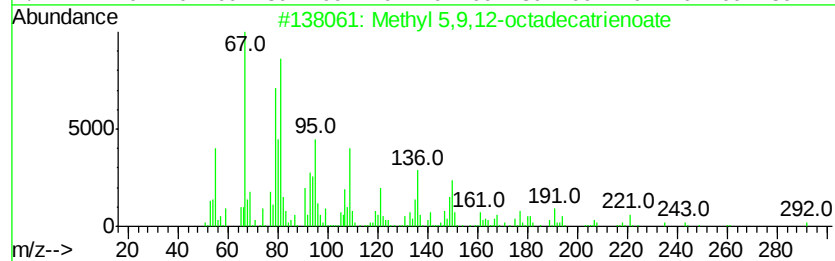
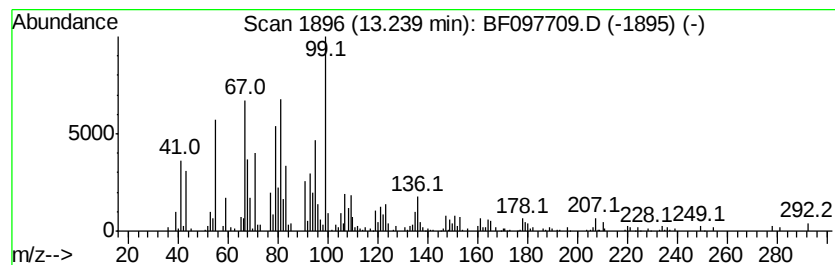
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Methyl 5,9,12-octadecatrien... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.24	8.33 ng	425896	Chrysene-d12	13.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl	5,9,12-octadecatrienoate	292	C19H32O2	1000336-37-5	87
2	Cyclopentanecarboxylic acid, 3-p...		210	C13H22O2	1000154-24-9	70
3	1,5-Cyclodecadiene, (E,Z)-		136	C10H16	001124-78-3	64
4	Bicyclopentylidene		136	C10H16	016189-35-8	60
5	1-Cyclopentylcyclopentene		136	C10H16	004884-21-3	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-01-080917-C

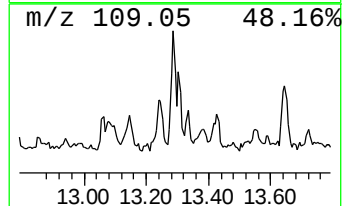
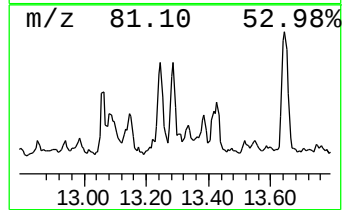
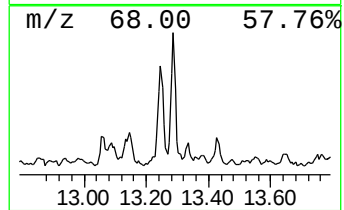
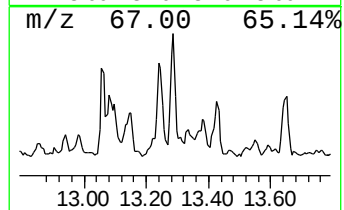
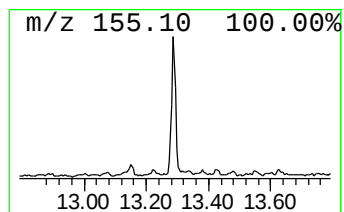
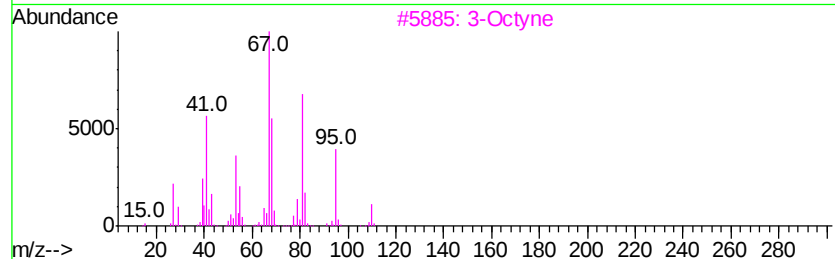
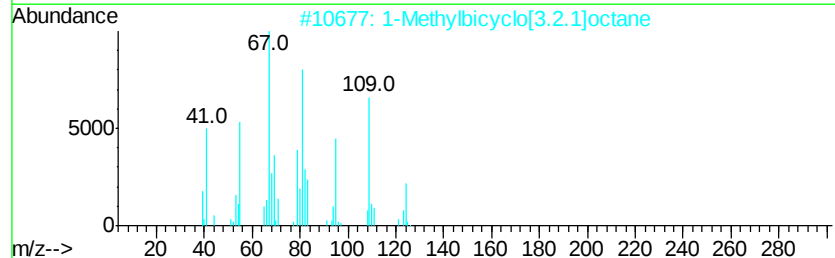
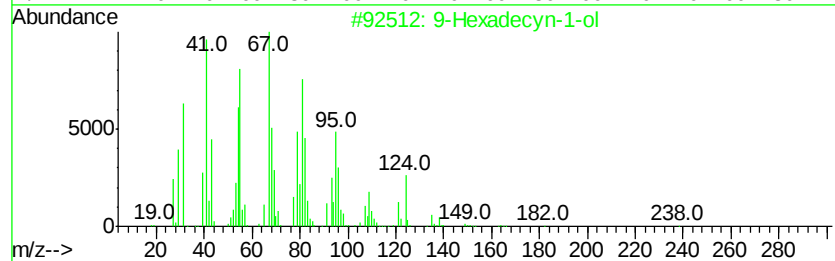
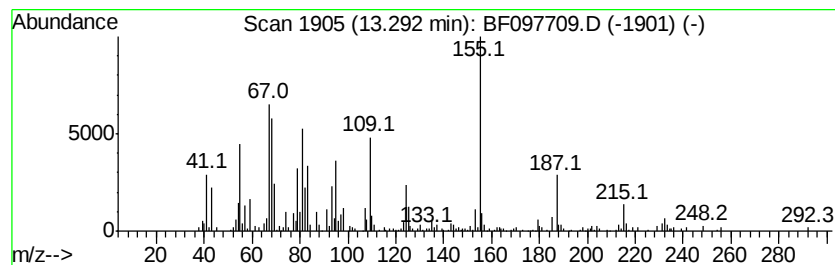
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown13.29 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	8.29 ng	423922	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Hexadecyn-1-ol	238	C16H30O	1000342-40-3	46
2		1-Methylbicyclo[3.2.1]octane	124	C9H16	119972-41-7	43
3		3-Octyne	110	C8H14	015232-76-5	38
4		Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	30
5		3-Dodecyne	166	C12H22	006790-27-8	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097709.D
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Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

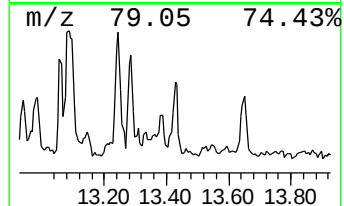
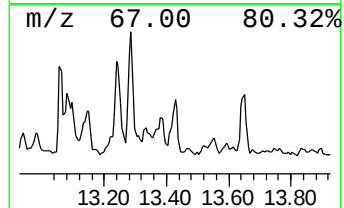
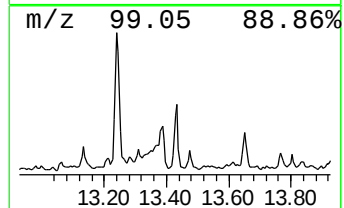
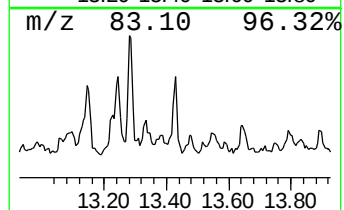
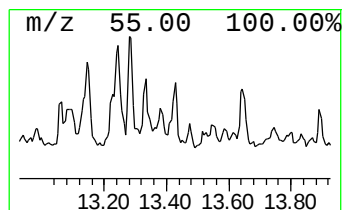
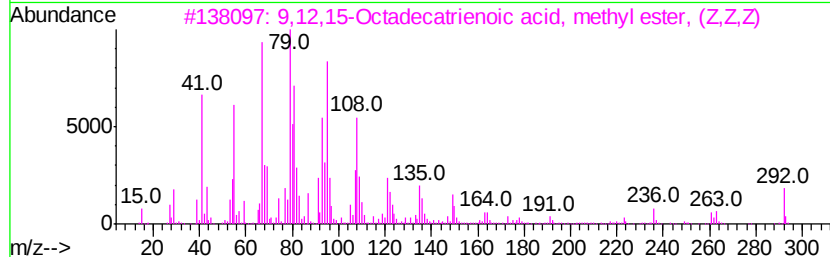
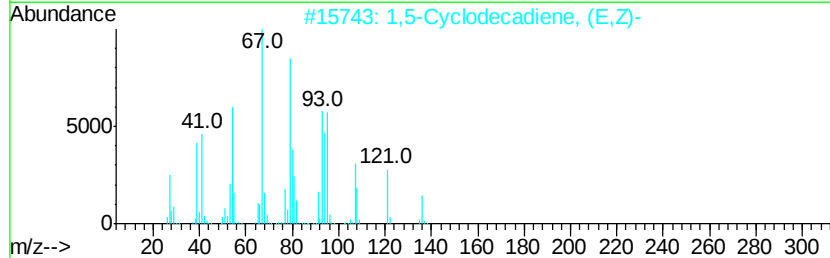
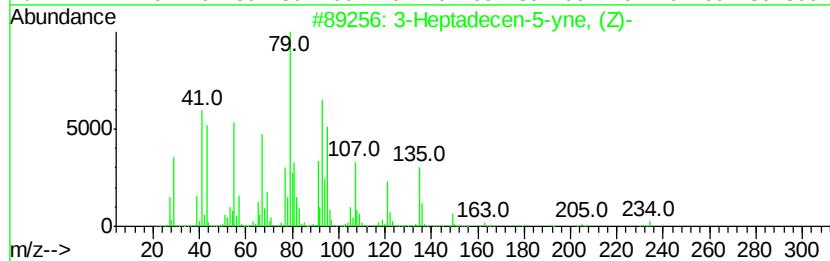
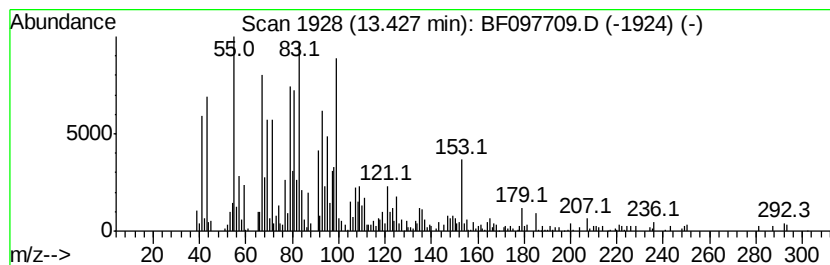
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 3-Heptadecen-5-yne, (Z)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.43	6.10 ng	312029	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptadecen-5-yne, (Z)-	234	C17H30	074744-55-1	55
2	1,5-Cyclodecadiene, (E,Z)-	136	C10H16	001124-78-3	55
3	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	46
4	Methyl 9.cis.,11.trans.t,13.trans...	292	C19H32O2	1000336-42-6	44
5	(1S,15S)-Bicyclo[13.1.0]hexadeca...	236	C16H28O	102572-89-4	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-01-080917-C

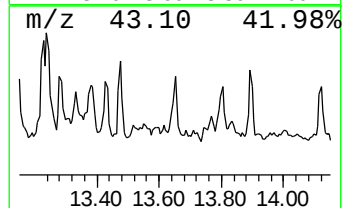
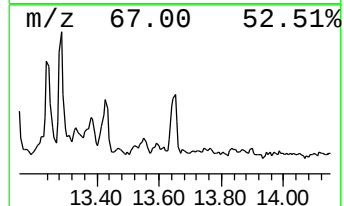
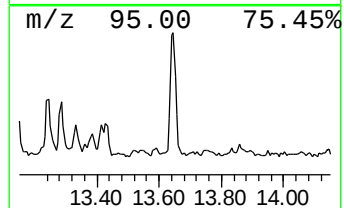
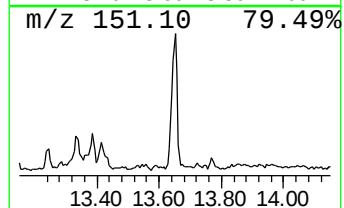
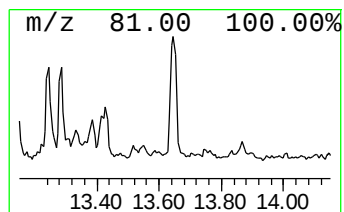
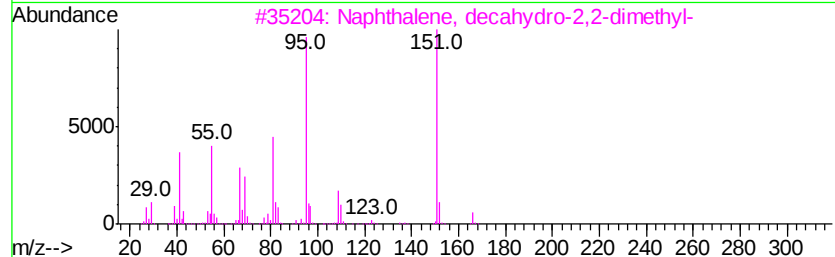
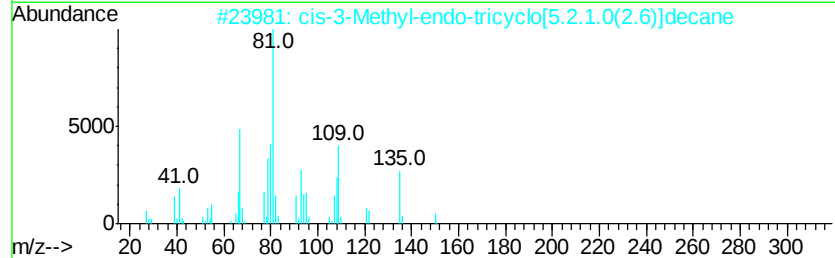
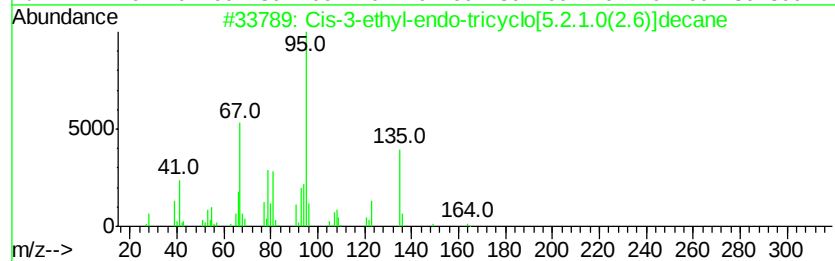
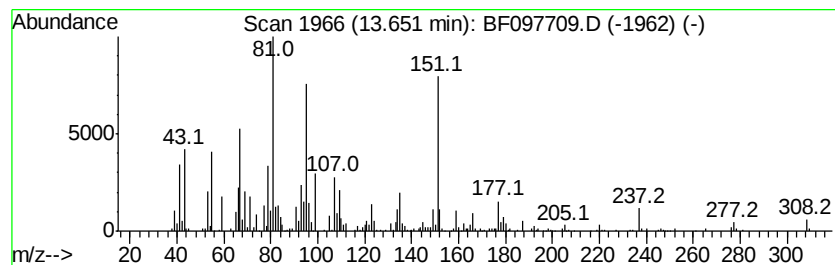
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Cis-3-ethyl-endo-tricyclo[5... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	7.03 ng	359354	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cis-3-ethyl-endo-tricyclo[5.2.1....	164	C12H20	1000215-29-1	89
2		cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	38
3		Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	30
4		Tricyclo[4.2.1.1(2,5)]decan-9-ol...	152	C10H16O	066953-30-8	20
5		2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097709.D
Acq On : 15 Aug 2017 23:47
Operator : SJ/JU
Sample : I4700-07 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-01-080917-C

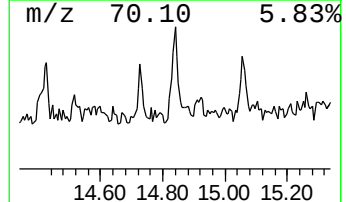
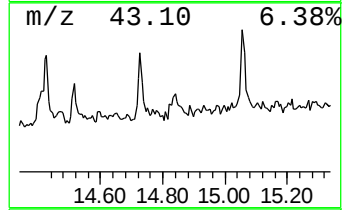
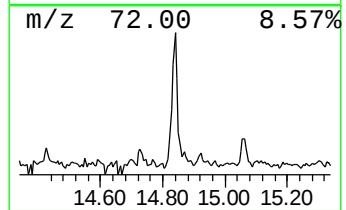
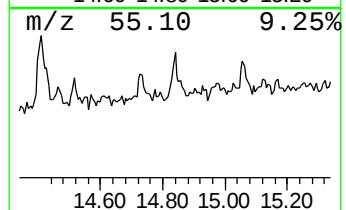
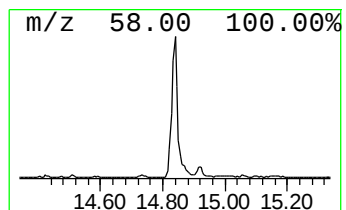
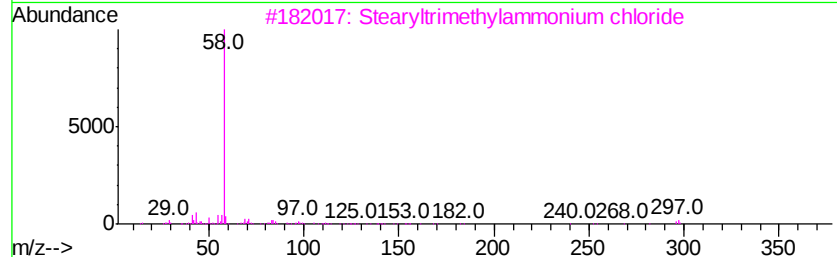
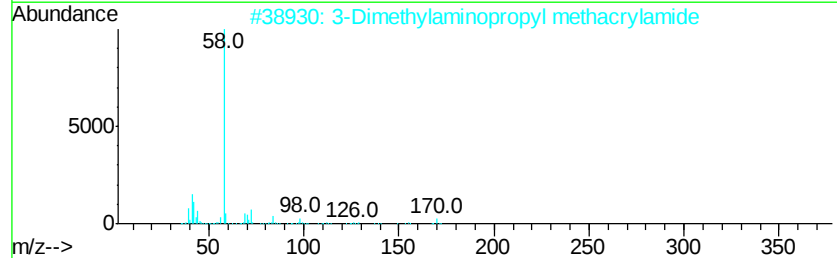
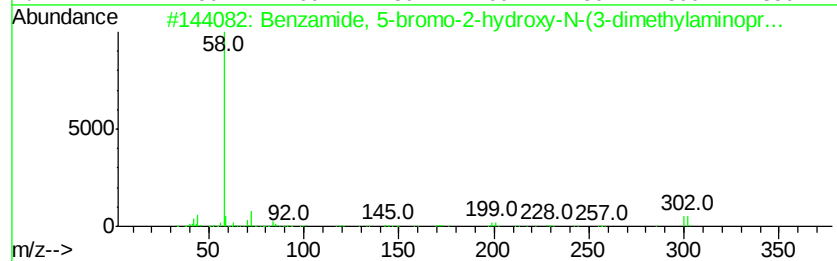
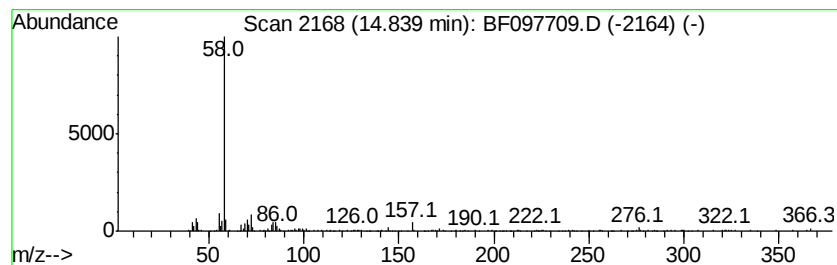
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Benzamide, 5-bromo-2-hydrox... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	6.84 ng	234604	Perylene-d12	15.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, 5-bromo-2-hydroxy-N-(...	300	C12H17BrN2O2	289660-53-3	72
2			3-Dimethylaminopropyl methacryla...	170	C9H18N2O	005205-93-6	64
3			Stearyltrimethylammonium chloride	347	C21H46ClN	000112-03-8	64
4			3-(Dimethylamino)propyl isothioc...	144	C6H12N2S	027421-70-1	64
5			1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
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 Sample : I4700-07 5X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-01-080917-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
unknown6.55	6.55	14.5	ng	702366	1	6.78	970394	20.0
Nonadecane	9.23	5.4	ng	359308	3	9.82	1341460	20.0
Pentadecane	9.76	6.1	ng	408191	3	9.82	1341460	20.0
Bacchotricuneatin c	10.26	7.5	ng	502104	3	9.82	1341460	20.0
Decane, 2,3,5-tri...	10.73	15.9	ng	804345	4	11.30	1008890	20.0
Hexadecane	11.18	10.3	ng	517210	4	11.30	1008890	20.0
Heneicosane	11.61	8.3	ng	420538	4	11.30	1008890	20.0
Hexadecanoic acid...	11.71	78.7	ng	3969470	4	11.30	1008890	20.0
n-Hexadecanoic acid	11.84	8.6	ng	431652	4	11.30	1008890	20.0
Tetracosane	12.02	8.3	ng	419948	4	11.30	1008890	20.0
9,12-Octadecadien...	12.40	132.8	ng	6699030	4	11.30	1008890	20.0
9-Octadecenoic ac...	12.43	148.1	ng	7471220	4	11.30	1008890	20.0
Methyl 5,11,14-ei...	13.06	5.8	ng	299362	5	13.93	1022930	20.0
9-Octadecenoic ac...	13.14	8.0	ng	410994	5	13.93	1022930	20.0
Methyl 5,9,12-oct...	13.24	8.3	ng	425896	5	13.93	1022930	20.0
unknown13.29	13.29	8.3	ng	423922	5	13.93	1022930	20.0
3-Heptadecen-5-yn...	13.43	6.1	ng	312029	5	13.93	1022930	20.0
Cis-3-ethyl-endo-...	13.65	7.0	ng	359354	5	13.93	1022930	20.0
Benzamide, 5-brom...	14.84	6.8	ng	234604	6	15.37	685947	20.0