

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
 Data File : BF103762.D
 Acq On : 19 Mar 2018 18:16
 Operator : JU/SJ
 Sample : J1755-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OK-01-031618

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-BF031518.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	5.581	590	594	597	rBV	721279	643419	5.65%	1.436%
2	6.581	760	764	769	rVB	694274	663043	5.83%	1.480%
3	6.734	786	790	793	rVV	833794	678870	5.97%	1.515%
4	6.969	826	830	833	rVB	1145574	892020	7.84%	1.991%
5	7.122	851	856	859	rBV	673176	566585	4.98%	1.265%
6	7.522	922	924	927	rVV	437822	419504	3.69%	0.936%
7	7.551	927	929	933	rVB	205113	159264	1.40%	0.355%
8	8.222	1039	1043	1045	rBV	280939	250744	2.20%	0.560%
9	8.251	1045	1048	1051	rVV	1483618	1184364	10.41%	2.644%
10	8.298	1053	1056	1059	rVB2	197051	169978	1.49%	0.379%
11	8.534	1092	1096	1100	rVB3	142359	151065	1.33%	0.337%
12	8.657	1114	1117	1120	rVB2	170425	126842	1.11%	0.283%
13	8.751	1130	1133	1135	rBV	180895	139440	1.23%	0.311%
14	8.828	1141	1146	1151	rBV	394821	354587	3.12%	0.791%
15	8.910	1158	1160	1166	rVB5	80327	127874	1.12%	0.285%
16	9.069	1181	1187	1189	rBV2	170263	170911	1.50%	0.381%
17	9.257	1217	1219	1222	rVB2	160181	120942	1.06%	0.270%
18	9.322	1227	1230	1234	rVB	1030211	775341	6.81%	1.731%
19	9.392	1239	1242	1246	rBV	419639	384946	3.38%	0.859%
20	9.581	1272	1274	1280	rVB4	79423	118027	1.04%	0.263%
21	9.663	1280	1288	1291	rBV4	127535	260621	2.29%	0.582%
22	9.716	1294	1297	1300	rBV2	214931	207070	1.82%	0.462%
23	9.928	1330	1333	1336	rVB	450072	364058	3.20%	0.813%
24	10.010	1341	1347	1350	rVB	1422394	1208120	10.62%	2.697%
25	10.245	1384	1387	1392	rBV2	131615	148251	1.30%	0.331%
26	10.428	1412	1418	1421	rBV	444629	404124	3.55%	0.902%
27	10.645	1450	1455	1458	rBV	156734	196936	1.73%	0.440%
28	10.798	1478	1481	1485	rBV	437174	370956	3.26%	0.828%
29	10.898	1495	1498	1504	rBV	358815	431319	3.79%	0.963%
30	11.351	1572	1575	1577	rBV	309087	240145	2.11%	0.536%
31	11.380	1577	1580	1587	rVB2	149960	213893	1.88%	0.477%
32	11.504	1597	1601	1603	rBV	1178161	1059931	9.32%	2.366%
33	11.527	1603	1605	1608	rVB	347490	286700	2.52%	0.640%
34	11.780	1645	1648	1650	rBV	213327	186585	1.64%	0.416%

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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

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35	11.886	1661	1666	1669	rBV	4491875	4196318	36.88%	9.366%
36	12.016	1683	1688	1696	rBV4	393985	604516	5.31%	1.349%
37	12.186	1714	1717	1723	rBV	204795	224649	1.97%	0.501%
38	12.586	1776	1785	1787	rBV	5845470	11377927	100.00%	25.396%
39	12.604	1787	1788	1793	rVV2	5661480	5544486	48.73%	12.376%
40	12.680	1797	1801	1804	rVB	2049998	1896738	16.67%	4.234%
41	12.722	1804	1808	1813	rBV	568641	911966	8.02%	2.036%
42	12.804	1819	1822	1828	rVB2	345107	349869	3.07%	0.781%
43	12.951	1844	1847	1853	rVB	539399	515320	4.53%	1.150%
44	13.086	1867	1870	1873	rVB	683447	634678	5.58%	1.417%
45	13.304	1905	1907	1909	rBV	140918	130309	1.15%	0.291%
46	13.327	1909	1911	1917	rVB3	161136	184307	1.62%	0.411%
47	13.404	1918	1924	1926	rBV2	199957	249511	2.19%	0.557%
48	14.074	2035	2038	2043	rBV	216169	233780	2.05%	0.522%
49	14.151	2047	2051	2054	rVV2	961153	1076028	9.46%	2.402%
50	14.174	2054	2055	2063	rVB	179736	182607	1.60%	0.408%
51	14.298	2073	2076	2081	rBV2	162477	165251	1.45%	0.369%
52	14.610	2126	2129	2132	rVB	167174	153697	1.35%	0.343%
53	14.933	2181	2184	2187	rBV	145342	148695	1.31%	0.332%
54	15.063	2202	2206	2215	rVB	375265	598524	5.26%	1.336%
55	15.292	2242	2245	2249	rVB	176643	190402	1.67%	0.425%
56	15.692	2309	2313	2320	rVB2	629435	879151	7.73%	1.962%
57	16.445	2438	2441	2448	rVB2	199280	353078	3.10%	0.788%
58	16.909	2517	2520	2526	rVB2	191738	323085	2.84%	0.721%

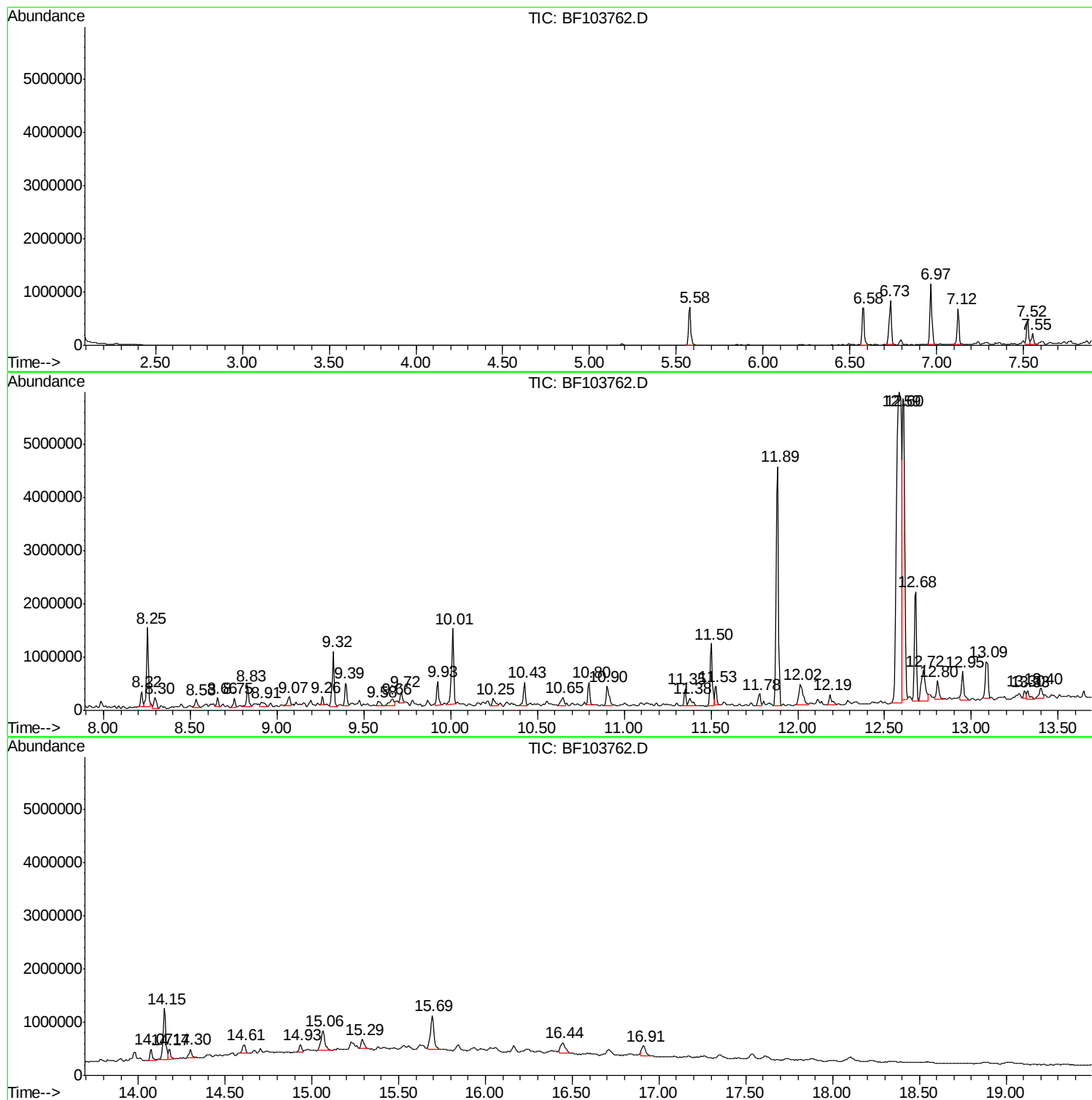
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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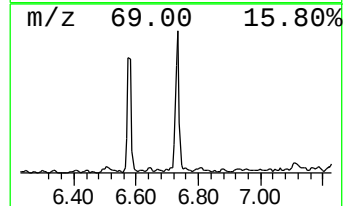
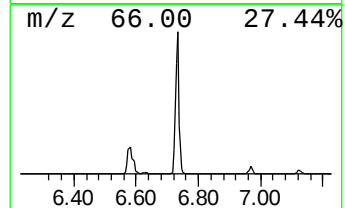
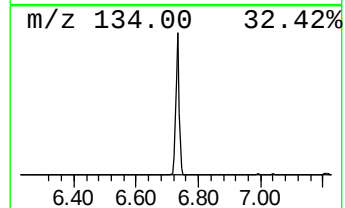
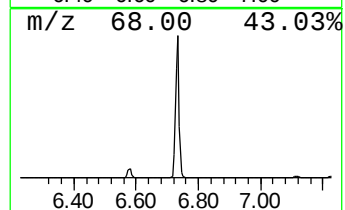
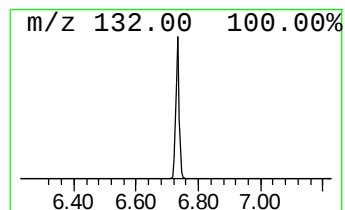
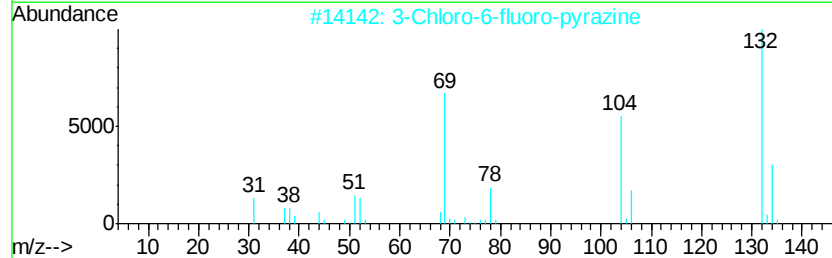
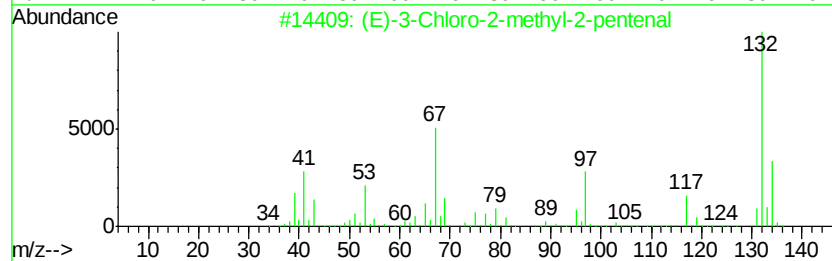
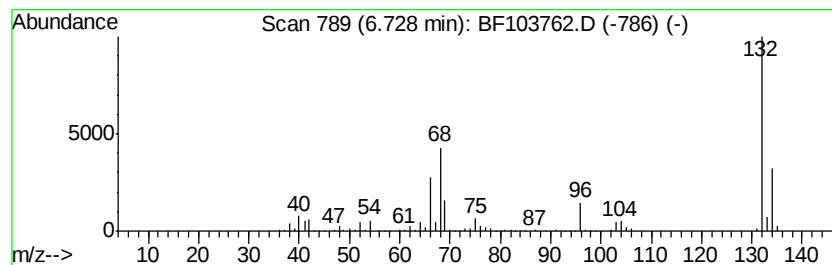
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	15.22 ng	678870	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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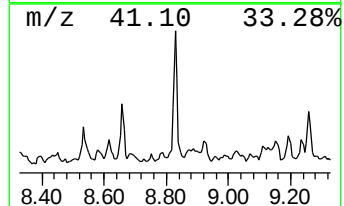
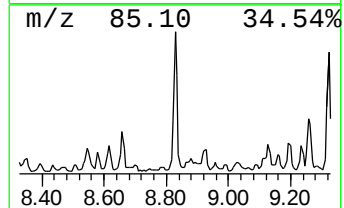
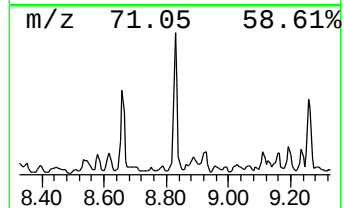
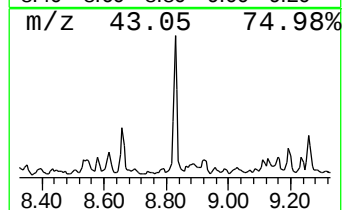
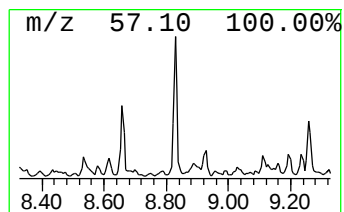
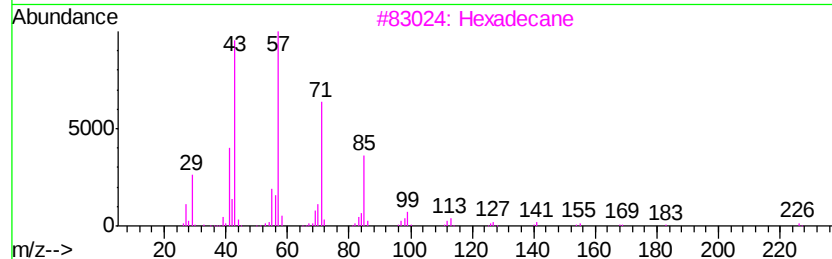
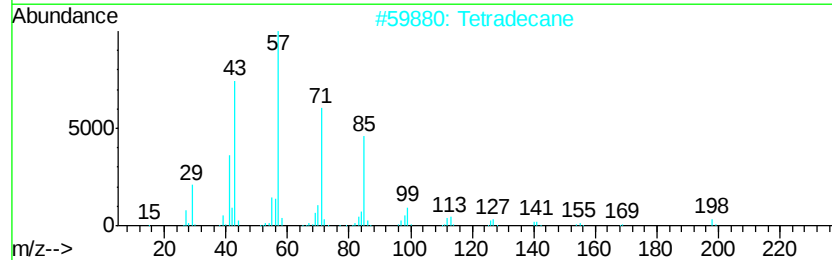
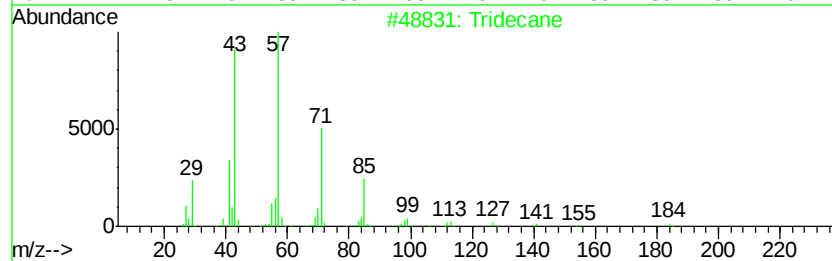
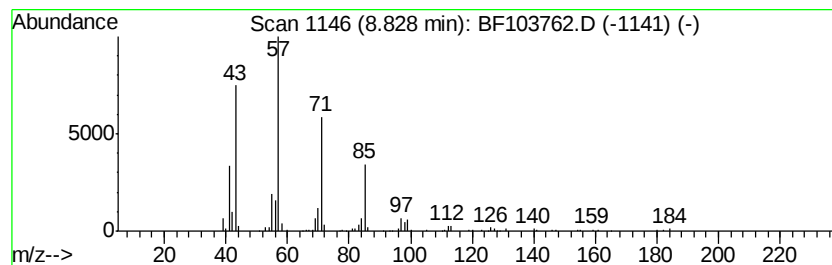
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	5.99 ng	354587	Napthalene-d8	8.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tridecane	184 C13H28	000629-50-5	87
2	Tetradecane	198 C14H30	000629-59-4	86
3	Hexadecane	226 C16H34	000544-76-3	86
4	Undecane, 2,3-dimethyl-	184 C13H28	017312-77-5	86
5	Nonadecane	268 C19H40	000629-92-5	83



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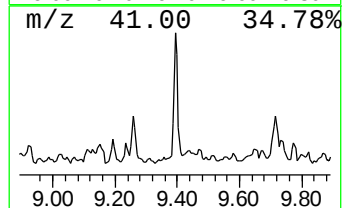
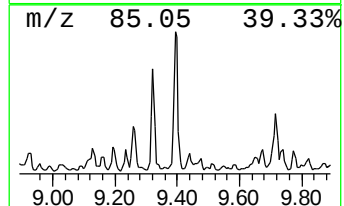
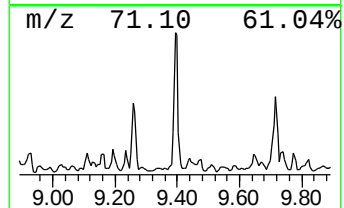
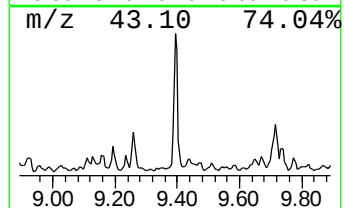
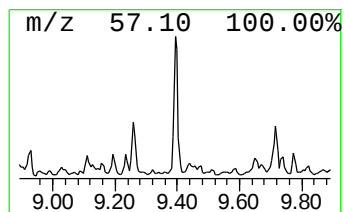
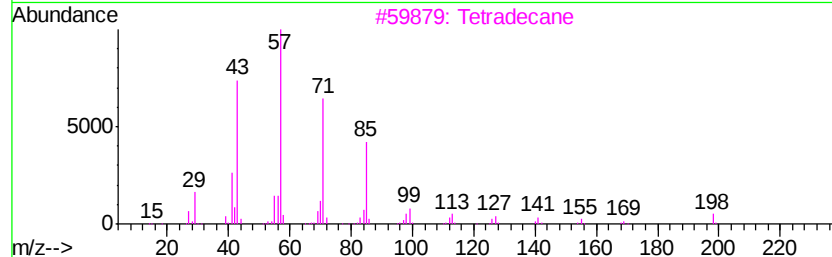
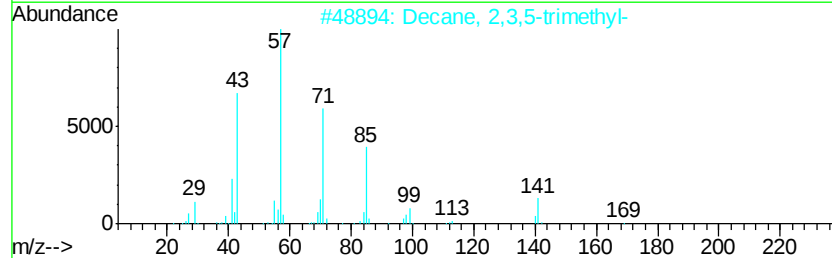
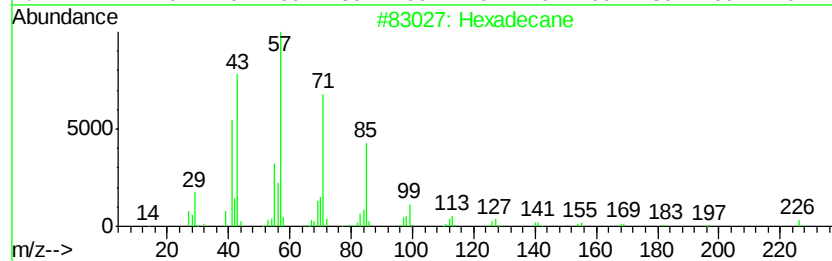
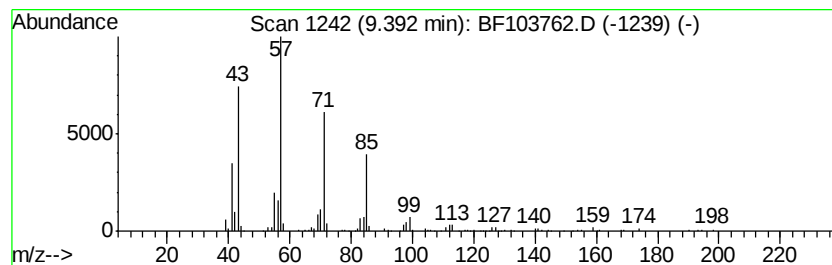
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	6.37 ng	384946	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3		Tetradecane	198	C14H30	000629-59-4	87
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	86
5		Bacchotricuneatin c	342	C20H22O5	066563-30-2	76



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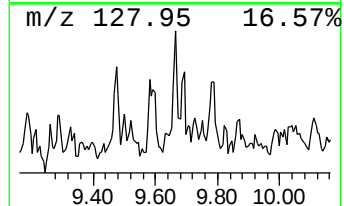
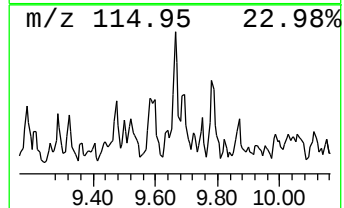
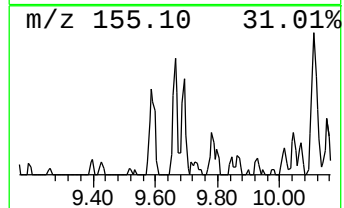
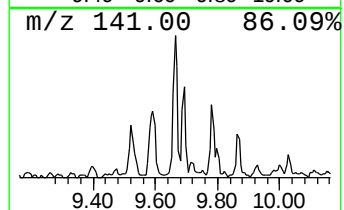
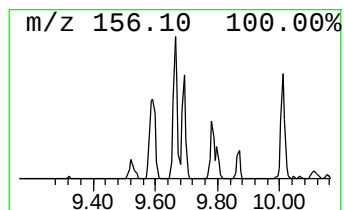
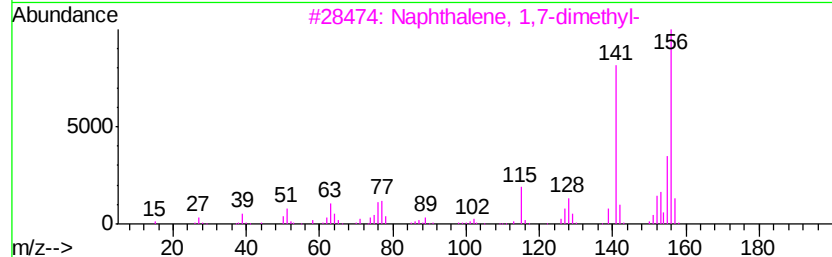
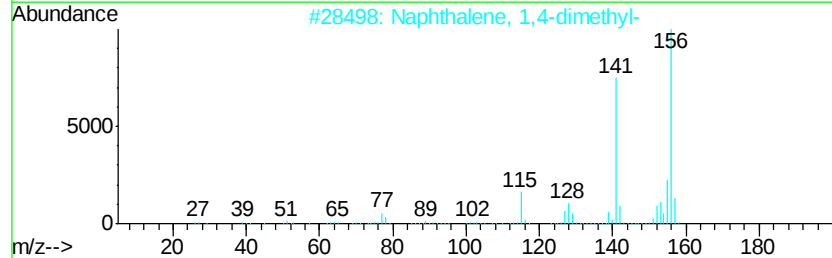
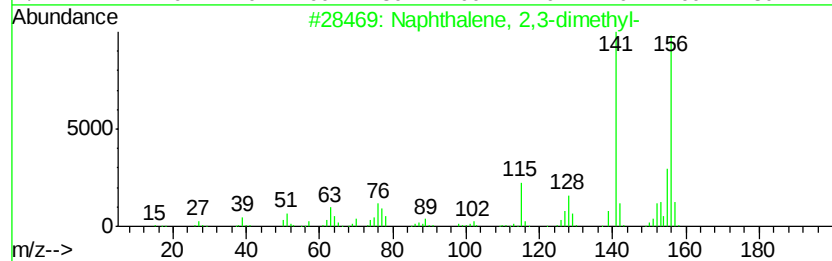
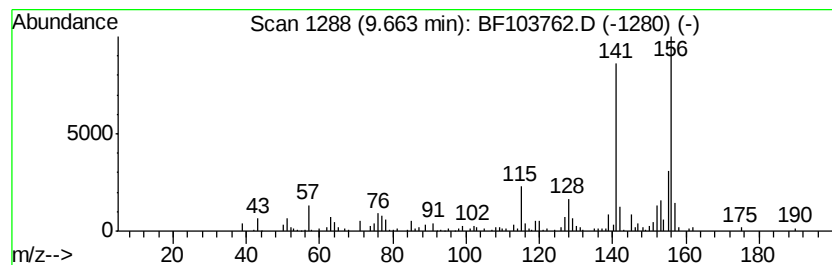
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	4.31 ng	260621	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2		Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
3		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
4		Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95
5		Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95



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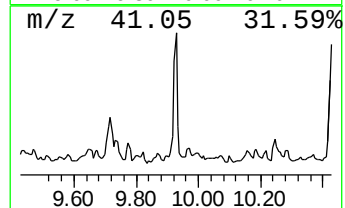
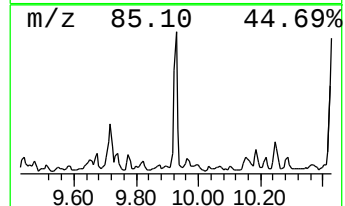
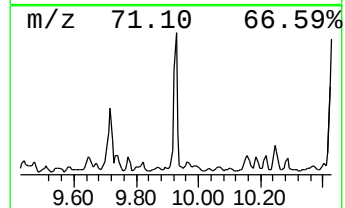
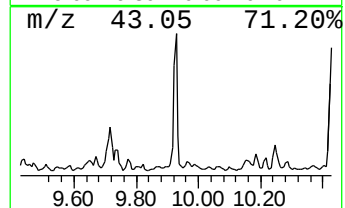
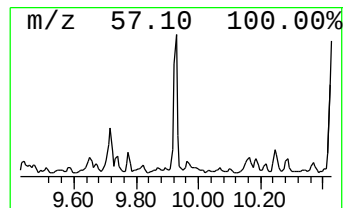
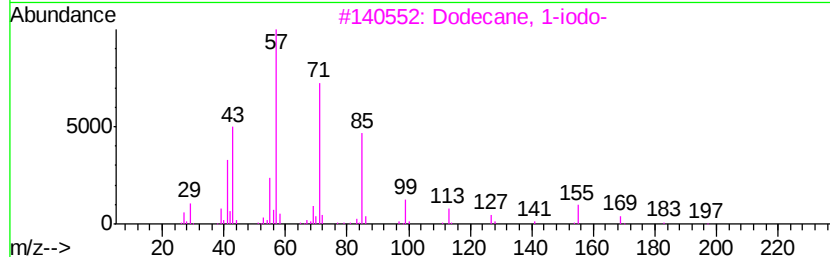
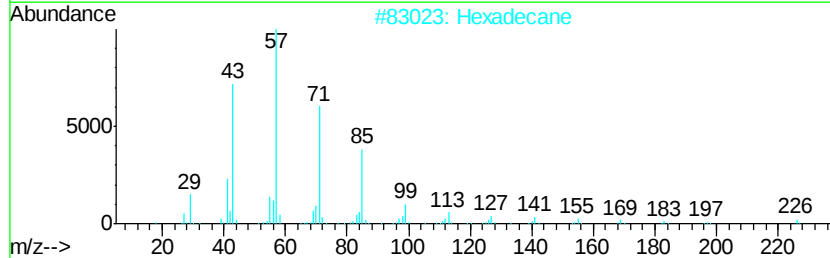
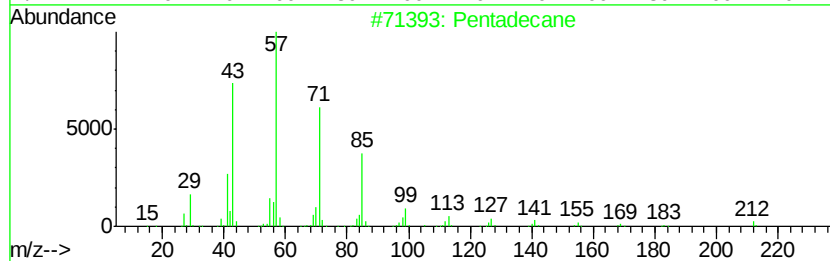
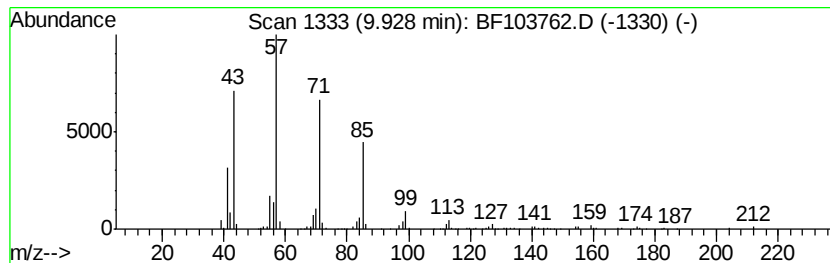
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	6.03 ng	364058	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	91
2		Hexadecane	226	C16H34	000544-76-3	80
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
4		Tridecane	184	C13H28	000629-50-5	72
5		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103762.D
Acq On : 19 Mar 2018 18:16
Operator : JU/SJ
Sample : J1755-03
Misc :
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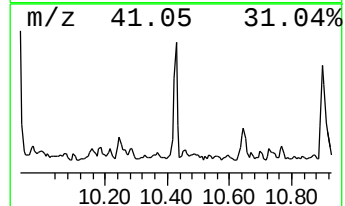
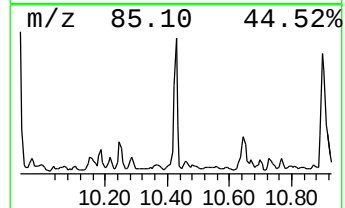
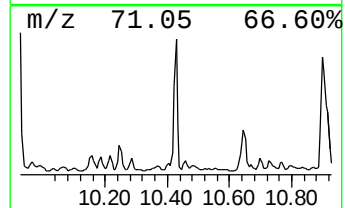
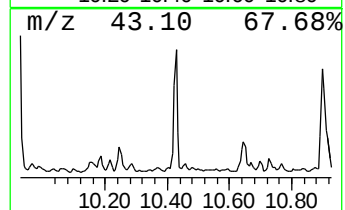
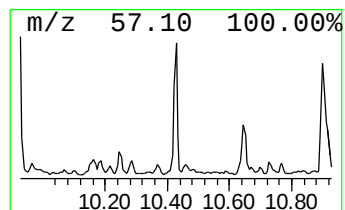
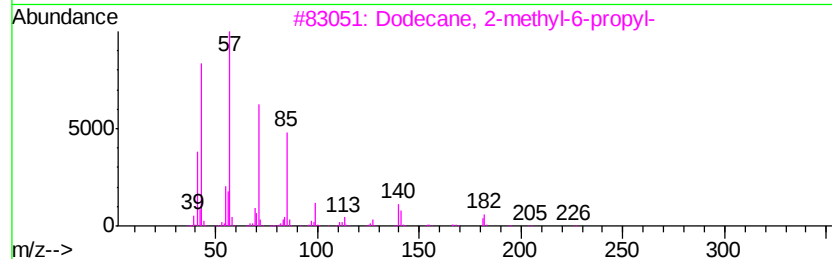
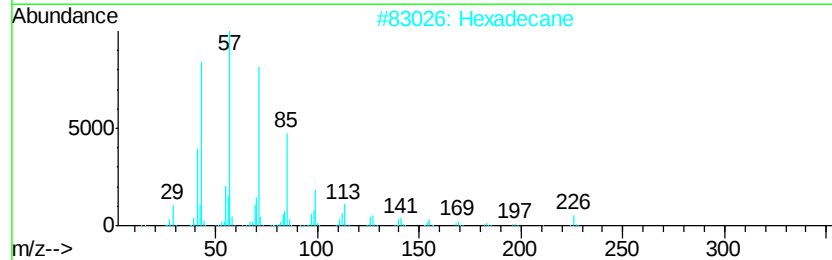
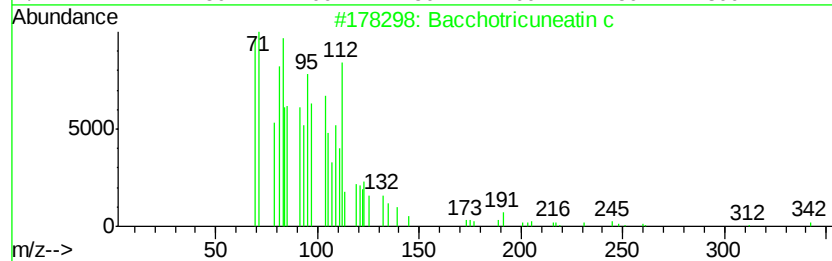
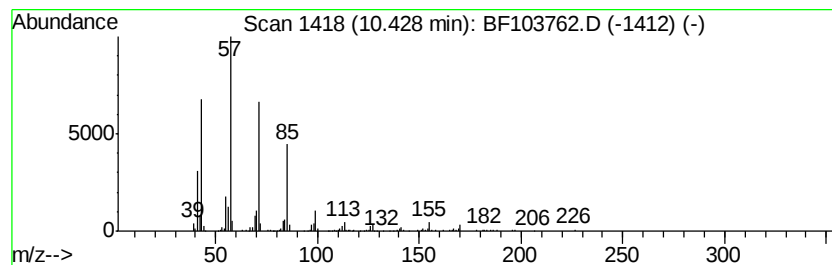
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bacchotricuneatin c Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	6.69 ng	404124	Acenaphthene-d10		10.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	96
2	Hexadecane	226	C16H34	000544-76-3	95
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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ClientSampleId :
OK-01-031618

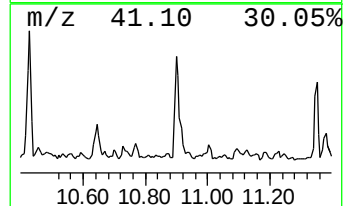
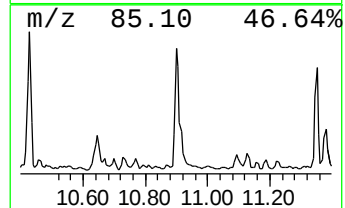
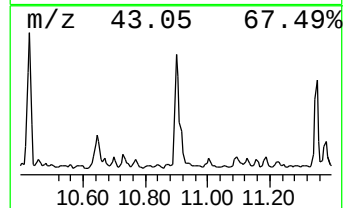
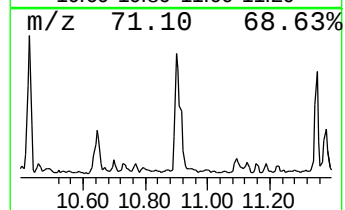
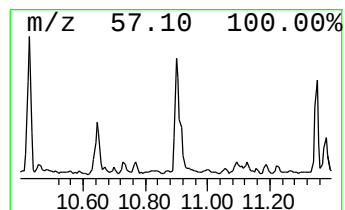
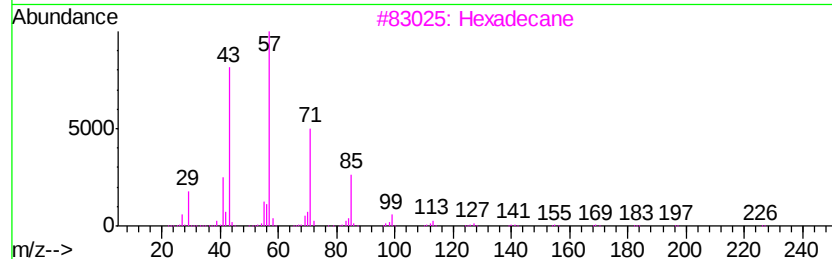
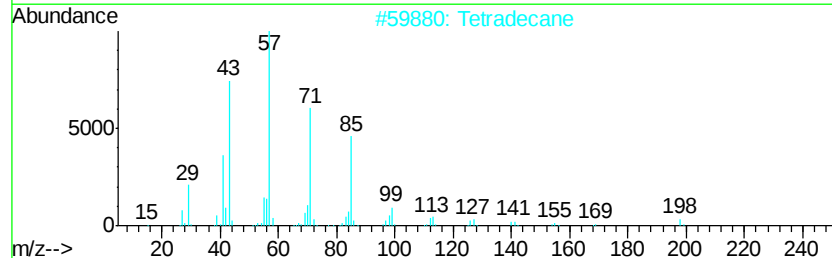
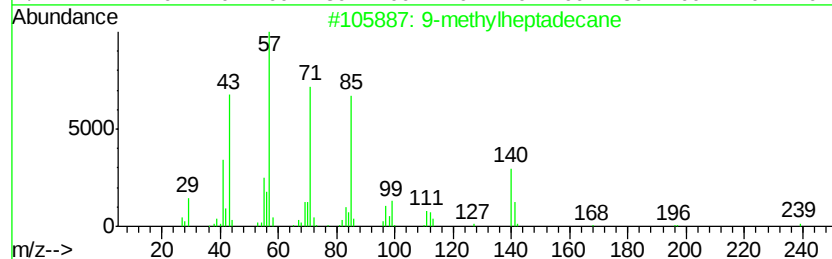
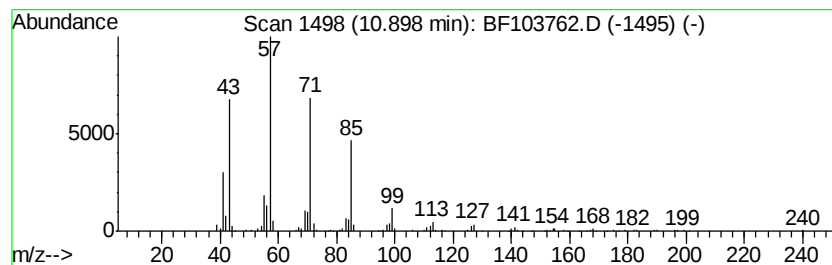
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-methylheptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.90	8.14 ng	431319	Phenanthrene-d10		11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-methylheptadecane		254	C18H38	026741-18-4	86
2	Tetradecane		198	C14H30	000629-59-4	86
3	Hexadecane		226	C16H34	000544-76-3	80
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	80
5	Nonane, 5-butyl-		184	C13H28	017312-63-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103762.D
Acq On : 19 Mar 2018 18:16
Operator : JU/SJ
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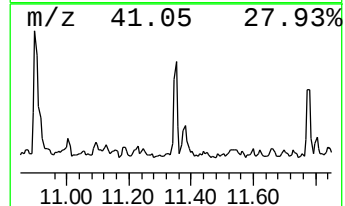
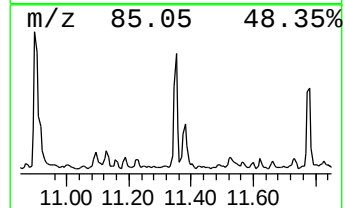
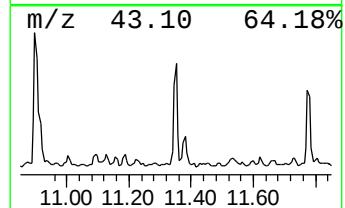
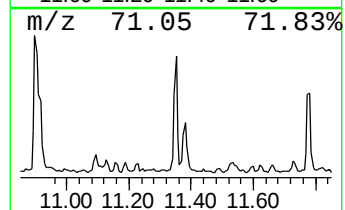
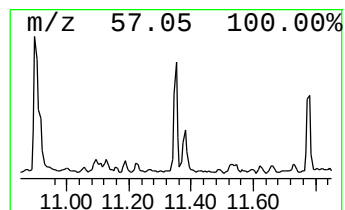
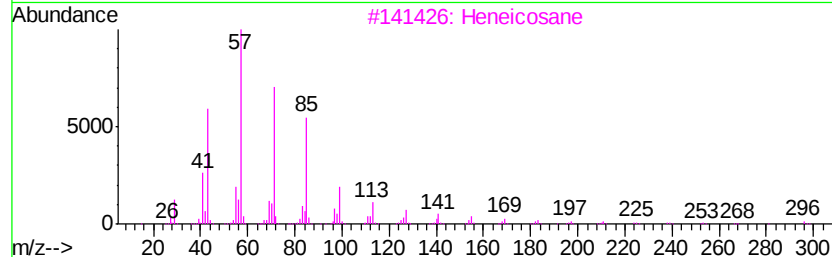
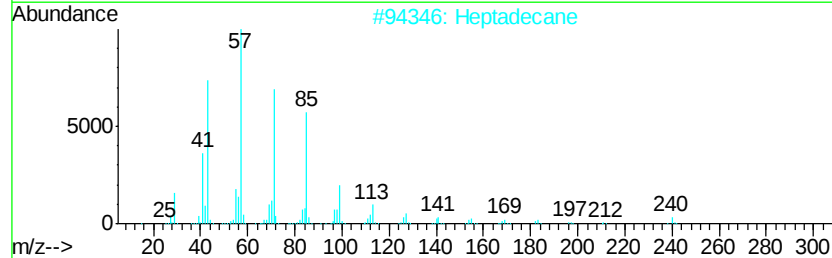
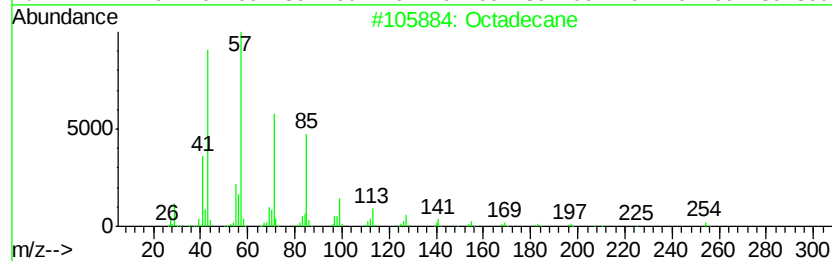
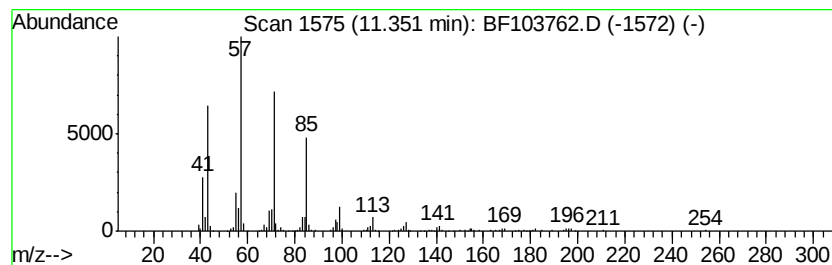
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	4.53 ng	240145	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Pentadecane	212	C15H32	000629-62-9	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103762.D
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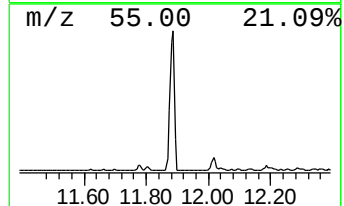
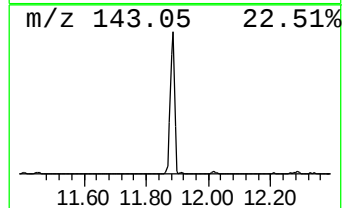
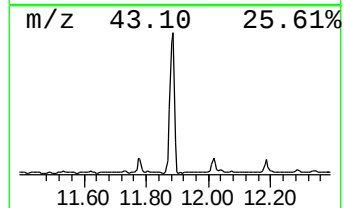
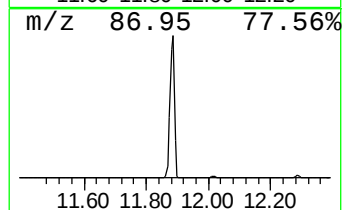
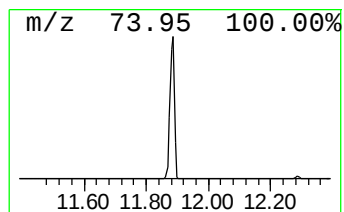
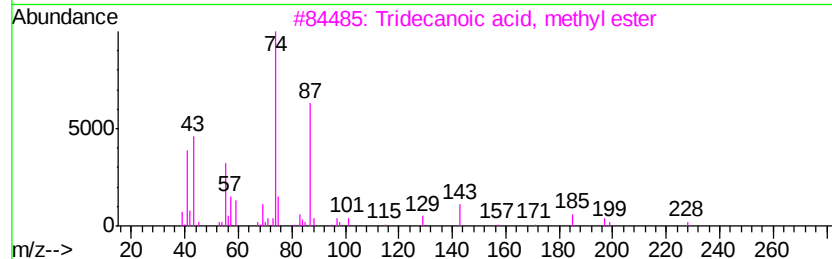
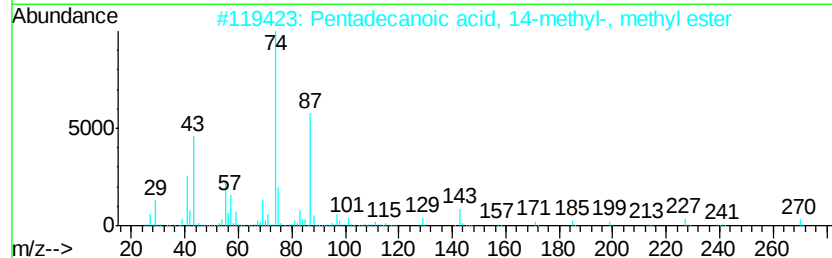
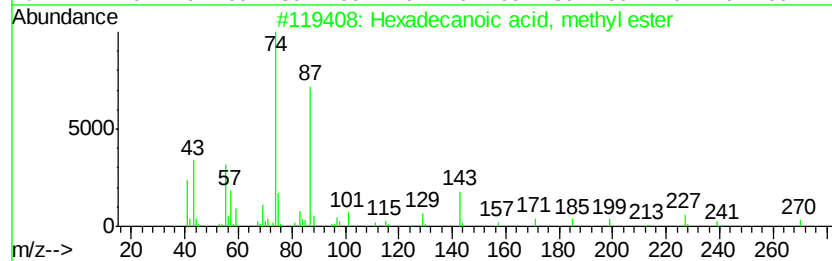
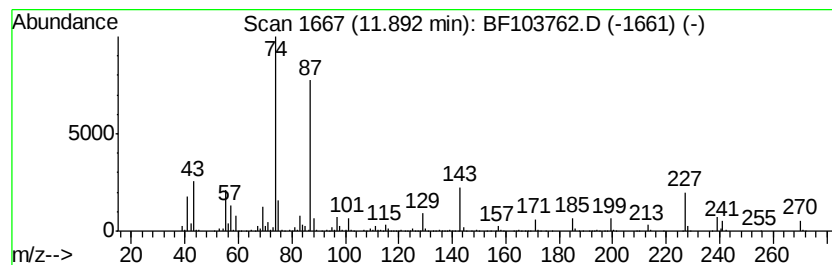
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	79.18 ng	4196320	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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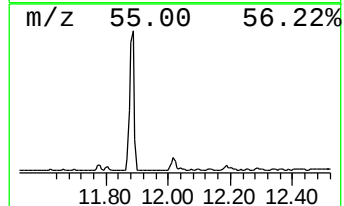
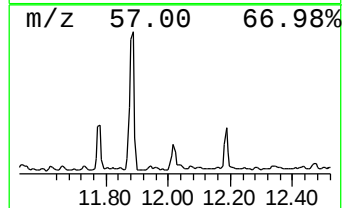
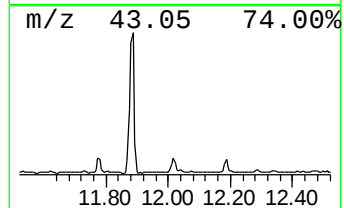
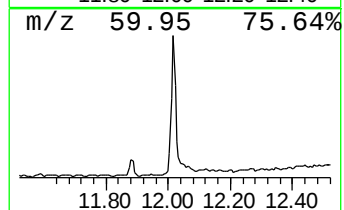
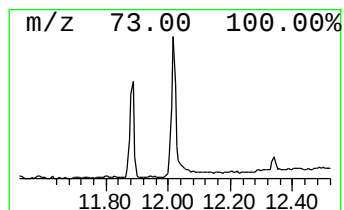
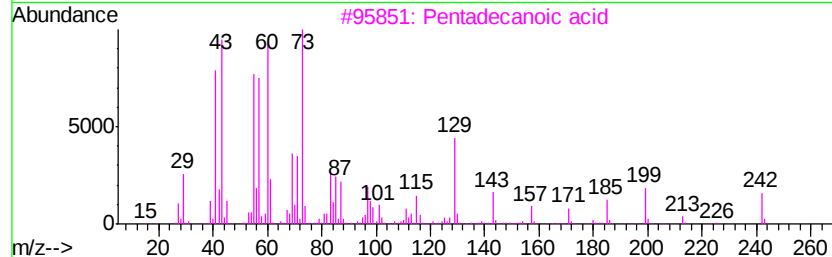
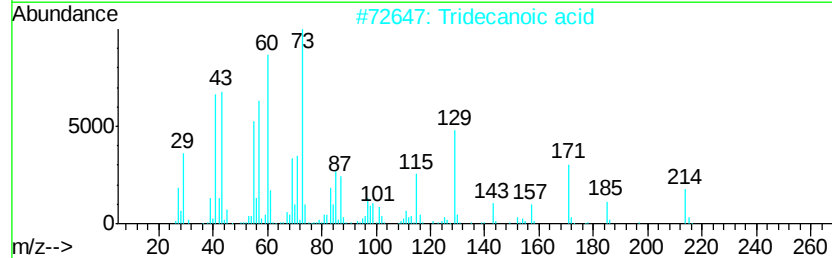
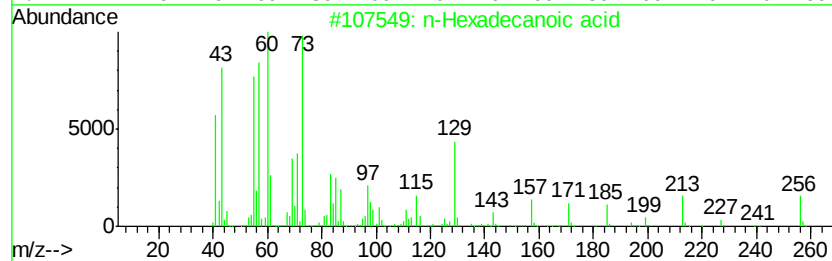
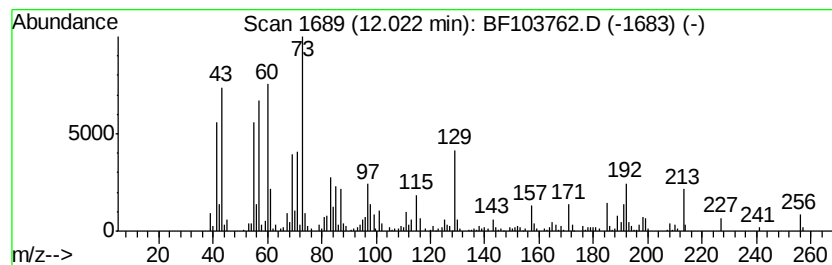
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	11.41 ng	604516	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Tetradecane	198	C14H30	000629-59-4	43



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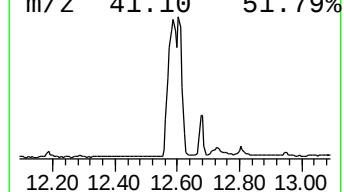
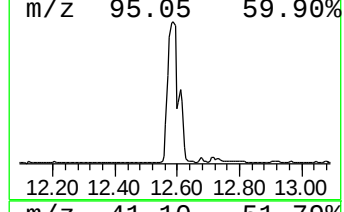
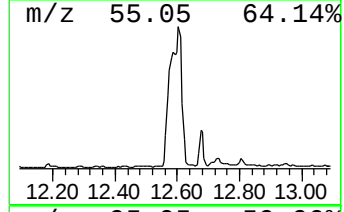
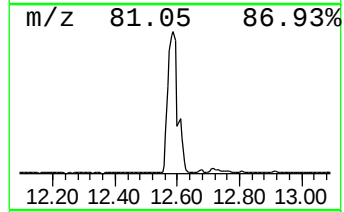
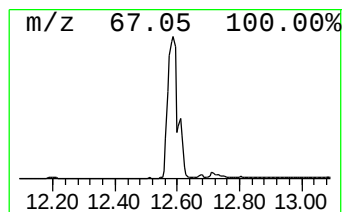
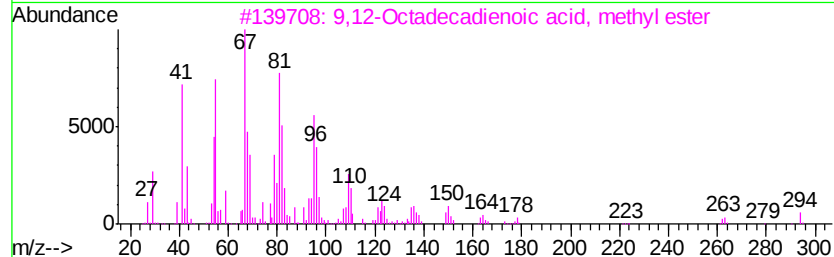
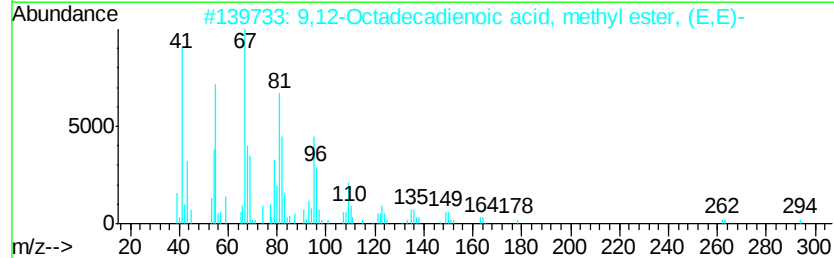
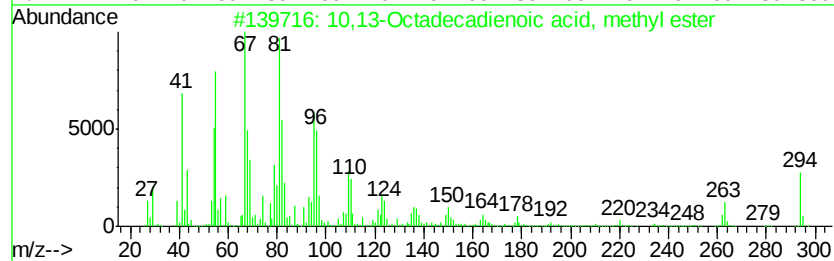
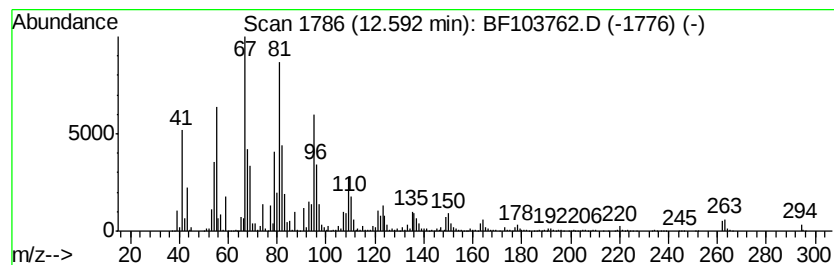
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	214.69 ng	11377900	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3		9,12-Octadecadienoic acid, methv...	294	C19H34O2	002462-85-3	99
4		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99



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Acq On : 19 Mar 2018 18:16
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	104.62 ng	5544490	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	93
4		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
5		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91

