

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121918\
 Data File : BF111600.D
 Acq On : 19 Dec 2018 19:53
 Operator : JU/SJ
 Sample : J6403-33
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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	2.199	16	19	28	rVB2	50703	80298	2.33%	0.175%
2	3.398	220	223	233	rBV	32963	72924	2.12%	0.159%
3	5.110	509	514	522	rVB	151094	189612	5.51%	0.412%
4	5.510	577	582	585	rBV	3283387	3088543	89.69%	6.719%
5	6.516	747	753	757	rBV	3287136	3443582	100.00%	7.491%
6	6.663	773	778	781	rBV	3484275	3234311	93.92%	7.036%
7	6.892	813	817	821	rBV	1373830	1081199	31.40%	2.352%
8	7.051	840	844	847	rVB	3095151	2465124	71.59%	5.362%
9	7.445	907	911	914	rBV	2209186	1993058	57.88%	4.336%
10	8.175	1031	1035	1037	rBV	1713834	1381989	40.13%	3.006%
11	8.192	1037	1038	1042	rVB	80842	54846	1.59%	0.119%
12	8.886	1151	1156	1160	rBV	65130	55422	1.61%	0.121%
13	8.986	1169	1173	1176	rVB	44427	41081	1.19%	0.089%
14	9.251	1213	1218	1221	rVB	3875165	3394178	98.57%	7.383%
15	9.345	1228	1234	1237	rBV2	35264	41751	1.21%	0.091%
16	9.516	1258	1263	1266	rBV2	34522	45074	1.31%	0.098%
17	9.586	1268	1275	1277	rBV	68750	66475	1.93%	0.145%
18	9.639	1281	1284	1287	rVV	462879	373581	10.85%	0.813%
19	9.927	1329	1333	1336	rBV2	1875616	1511447	43.89%	3.288%
20	9.957	1336	1338	1341	rVB	612158	495661	14.39%	1.078%
21	10.127	1362	1367	1371	rVB	190407	171310	4.97%	0.373%
22	10.216	1379	1382	1385	rBV	37144	43221	1.26%	0.094%
23	10.469	1422	1425	1432	rVB	306380	282353	8.20%	0.614%
24	10.539	1432	1437	1438	rBV2	37711	43480	1.26%	0.095%
25	10.627	1450	1452	1456	rVB	52363	49853	1.45%	0.108%
26	10.710	1462	1466	1469	rBV	2863260	2337783	67.89%	5.085%
27	10.833	1484	1487	1489	rBV3	49524	49479	1.44%	0.108%
28	11.022	1513	1519	1521	rBV3	36385	41650	1.21%	0.091%
29	11.210	1549	1551	1555	rVB	41578	41090	1.19%	0.089%
30	11.257	1556	1559	1562	rVV3	29943	44413	1.29%	0.097%
31	11.304	1565	1567	1573	rVB	89115	86796	2.52%	0.189%
32	11.410	1581	1585	1587	rBV	1851605	1599870	46.46%	3.480%
33	11.433	1587	1589	1592	rVV	1332092	984917	28.60%	2.143%
34	11.480	1592	1597	1600	rVV	256088	241428	7.01%	0.525%

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35	11.516	1600	1603	1606	rVB2	46633	47057	1.37%	0.102%
36	11.633	1617	1623	1626	rBV2	93580	119033	3.46%	0.259%
37	11.710	1633	1636	1639	rBV4	41537	38247	1.11%	0.083%
38	11.910	1667	1670	1672	rBV	124936	116917	3.40%	0.254%
39	11.939	1672	1675	1679	rVV	501897	485478	14.10%	1.056%
40	11.980	1679	1682	1685	rVV2	66485	83534	2.43%	0.182%
41	12.021	1685	1689	1691	rVV	241266	235822	6.85%	0.513%
42	12.045	1691	1693	1695	rVB	72001	55792	1.62%	0.121%
43	12.204	1717	1720	1722	rBV	101533	95582	2.78%	0.208%
44	12.357	1743	1746	1749	rBV2	44468	45126	1.31%	0.098%
45	12.457	1760	1763	1766	rBV2	86824	95024	2.76%	0.207%
46	12.504	1767	1771	1775	rVB4	65938	93273	2.71%	0.203%
47	12.539	1775	1777	1783	rVB3	45887	60731	1.76%	0.132%
48	12.621	1787	1791	1794	rBV	1462587	1218210	35.38%	2.650%
49	12.668	1794	1799	1804	rVB3	86152	102972	2.99%	0.224%
50	12.721	1804	1808	1813	rBV3	101886	145411	4.22%	0.316%
51	12.845	1822	1829	1832	rBV	1104110	1204128	34.97%	2.619%
52	12.898	1836	1838	1842	rVB3	77019	82624	2.40%	0.180%
53	12.963	1846	1849	1850	rBV3	67991	57067	1.66%	0.124%
54	12.992	1850	1854	1857	rVB	3679122	3059770	88.85%	6.656%
55	13.063	1862	1866	1869	rBV2	78749	121716	3.53%	0.265%
56	13.127	1874	1877	1879	rBV3	46975	53052	1.54%	0.115%
57	13.151	1879	1881	1882	rVV2	56494	45842	1.33%	0.100%
58	13.174	1882	1885	1888	rVB	169279	153081	4.45%	0.333%
59	13.239	1892	1896	1899	rBV2	165450	169311	4.92%	0.368%
60	13.274	1899	1902	1905	rBV	114192	118242	3.43%	0.257%
61	13.333	1910	1912	1916	rBV5	26696	36980	1.07%	0.080%
62	13.368	1916	1918	1921	rBV2	53573	44479	1.29%	0.097%
63	13.404	1921	1924	1928	rBV2	52955	64972	1.89%	0.141%
64	13.574	1950	1953	1955	rBV2	70638	57968	1.68%	0.126%
65	13.674	1968	1970	1976	rVB	62229	80744	2.34%	0.176%
66	13.792	1985	1990	1992	rBV2	87653	111989	3.25%	0.244%
67	13.821	1992	1995	1997	rVV	91567	91554	2.66%	0.199%
68	13.845	1997	1999	2002	rVV2	74934	96376	2.80%	0.210%
69	13.886	2003	2006	2013	rVB2	439231	476222	13.83%	1.036%
70	14.039	2027	2032	2035	rBV2	1584758	1927234	55.97%	4.192%
71	14.068	2035	2037	2042	rVB	453178	406609	11.81%	0.885%

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72	14.145	2048	2050	2053	rBV	67513	56106	1.63%	0.122%
73	14.221	2060	2063	2066	rVB3	115441	124129	3.60%	0.270%
74	14.257	2066	2069	2073	rBV2	76830	81483	2.37%	0.177%
75	14.427	2096	2098	2101	rVB	100333	80046	2.32%	0.174%
76	14.462	2101	2104	2107	rVB	63911	56898	1.65%	0.124%
77	14.521	2111	2114	2117	rVV2	194130	209751	6.09%	0.456%
78	14.574	2121	2123	2127	rVB3	84273	81557	2.37%	0.177%
79	14.833	2164	2167	2176	rVB	165478	203236	5.90%	0.442%
80	15.080	2205	2209	2212	rBV	426697	635424	18.45%	1.382%
81	15.180	2222	2226	2233	rVB3	239105	393429	11.42%	0.856%
82	15.386	2257	2261	2268	rVB	265854	336614	9.78%	0.732%
83	15.451	2268	2272	2277	rVV	375552	466465	13.55%	1.015%
84	15.515	2278	2283	2287	rVV	1116205	1372178	39.85%	2.985%
85	15.568	2289	2292	2299	rVB	227943	299277	8.69%	0.651%
86	16.009	2362	2367	2371	rBV	169124	268368	7.79%	0.584%
87	16.527	2452	2455	2461	rVB3	58202	96399	2.80%	0.210%
88	16.980	2527	2532	2541	rVB3	180066	366877	10.65%	0.798%
89	17.427	2603	2608	2614	rVB	119579	215826	6.27%	0.469%

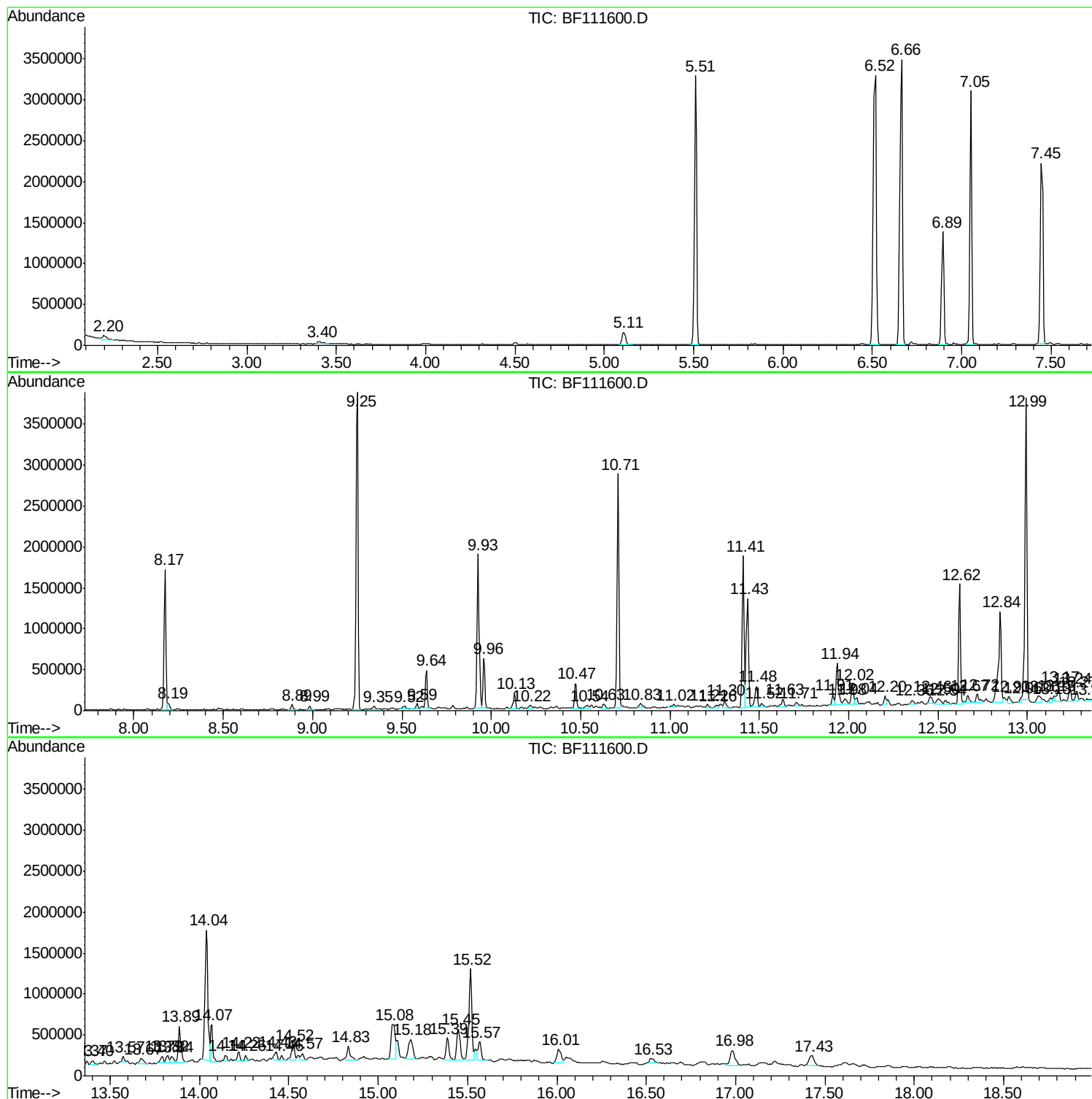
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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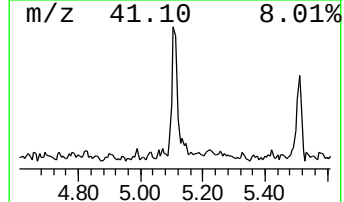
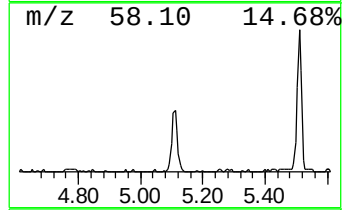
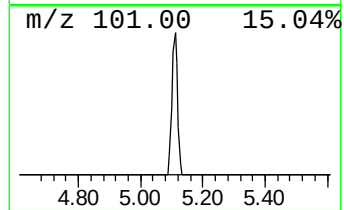
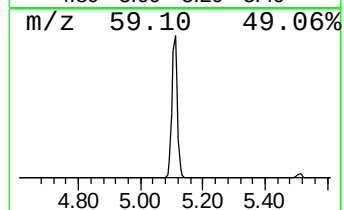
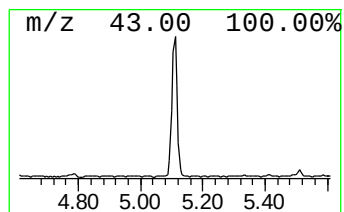
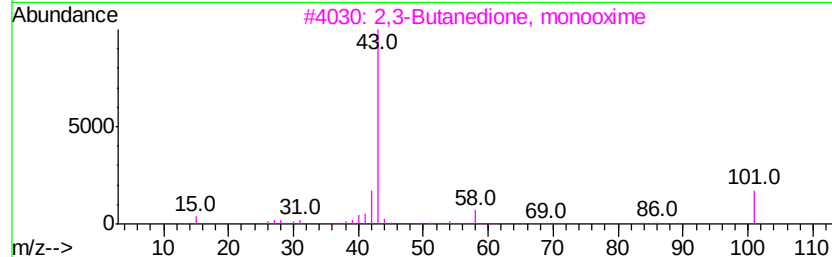
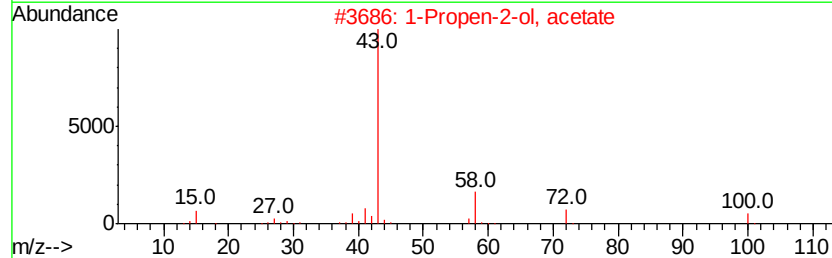
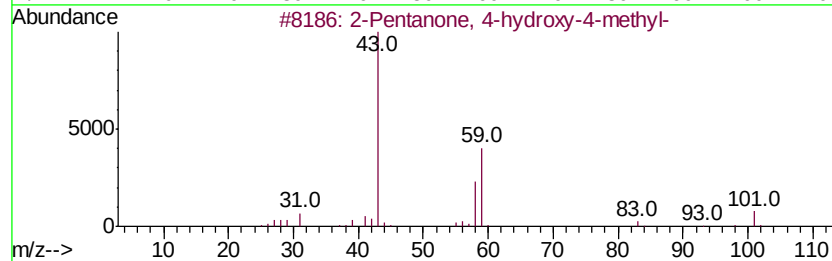
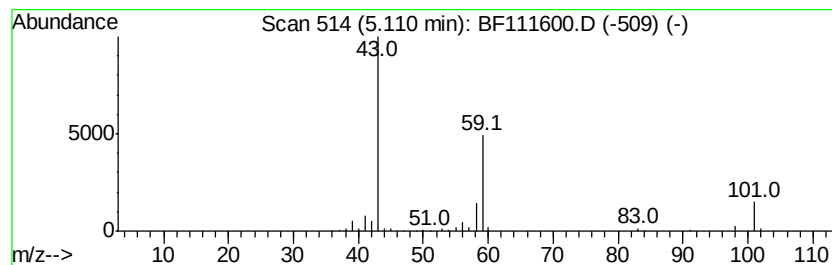
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.51 ng	189612	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Allyl acetate	100	C5H8O2	000591-87-7	9
5			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9



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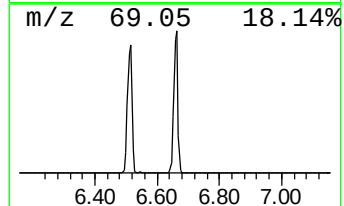
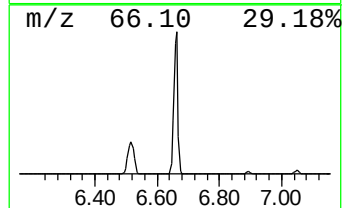
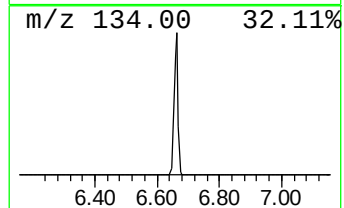
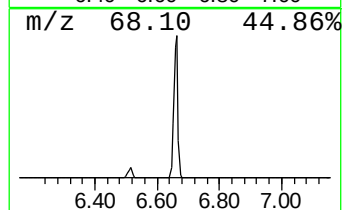
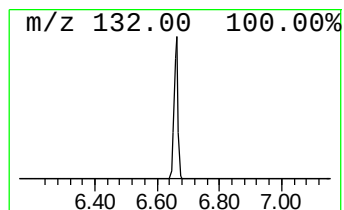
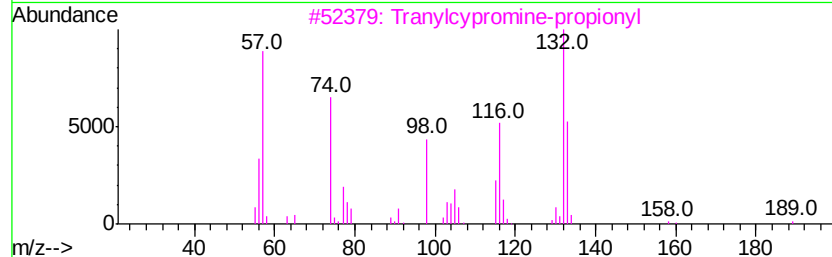
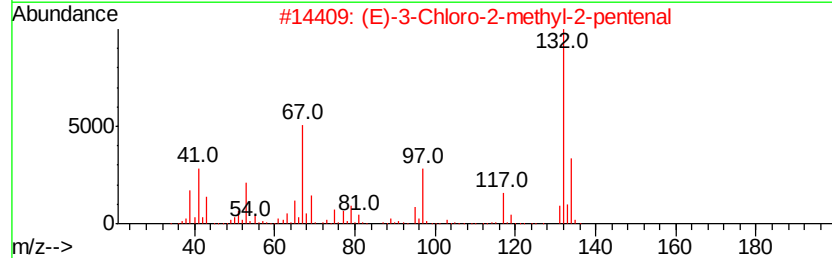
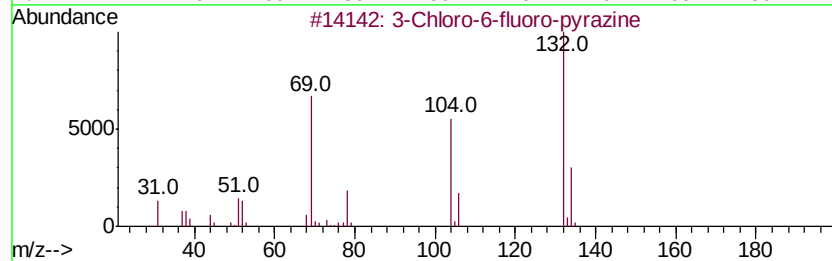
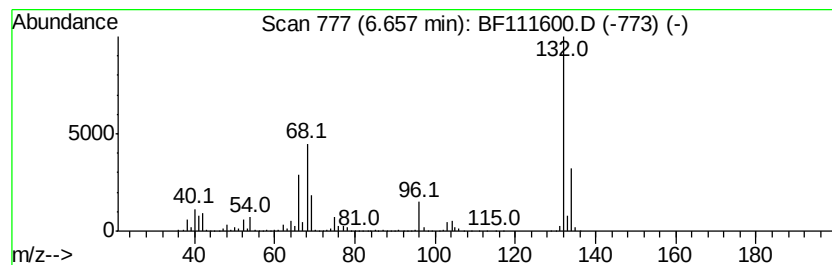
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	59.83 ng	3234310	1,4-Dichlorobenzene-d4	6.89

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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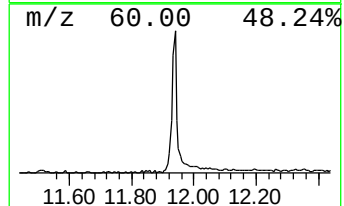
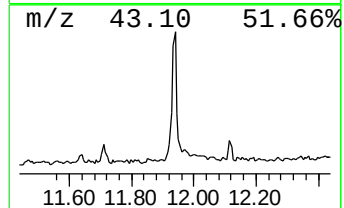
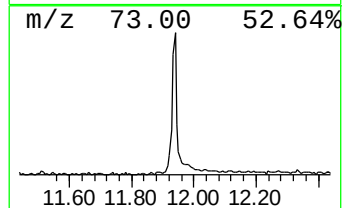
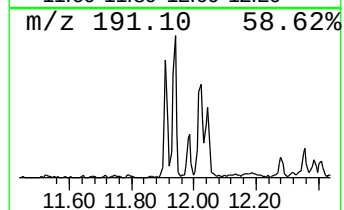
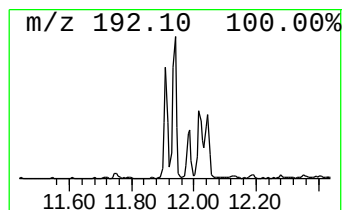
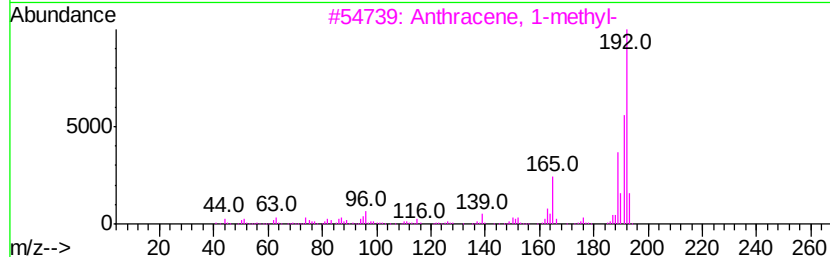
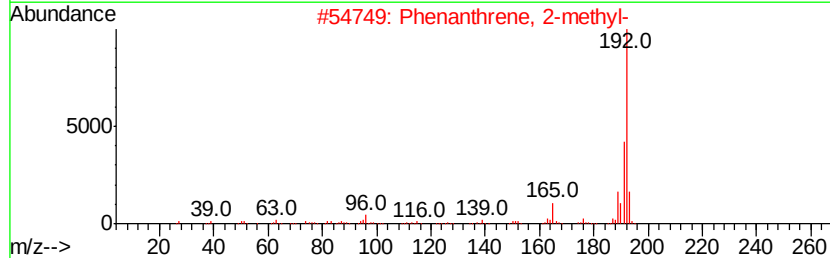
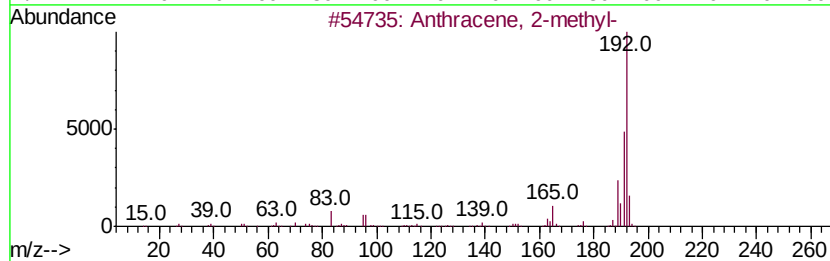
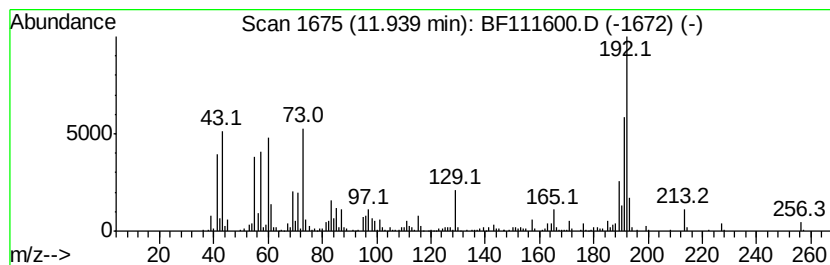
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.94	6.07 ng	485478	Phenanthrene-d10	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



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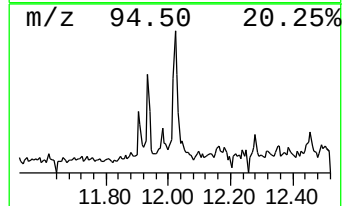
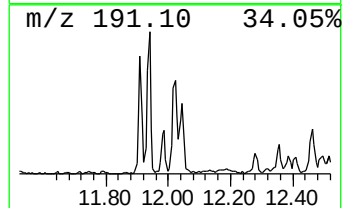
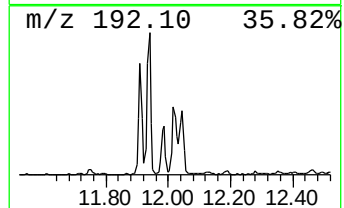
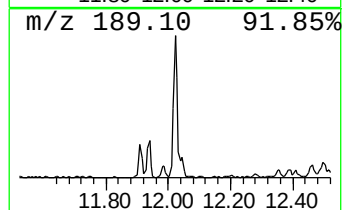
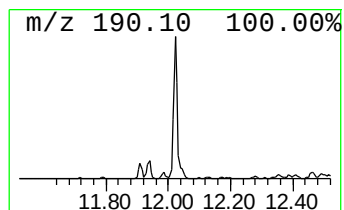
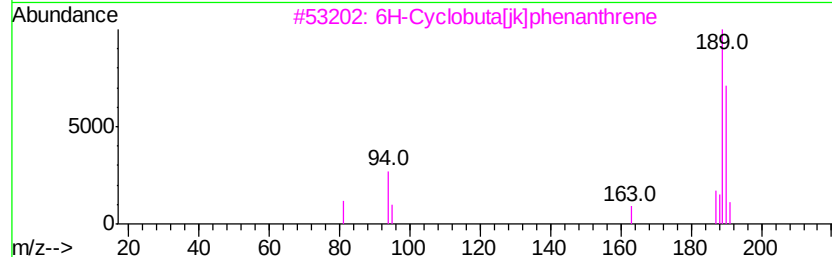
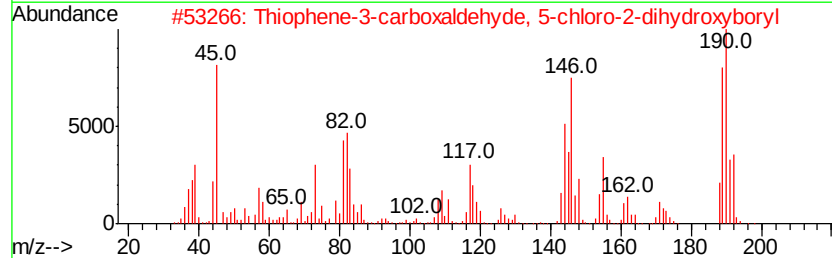
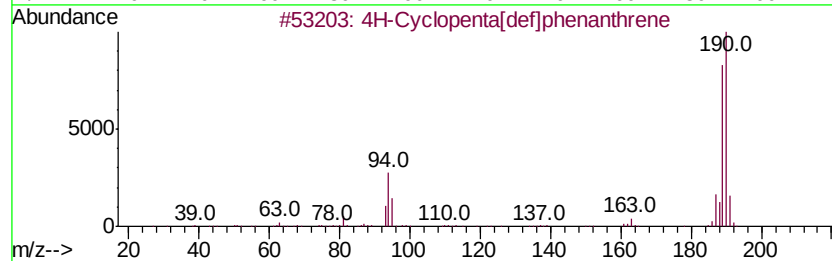
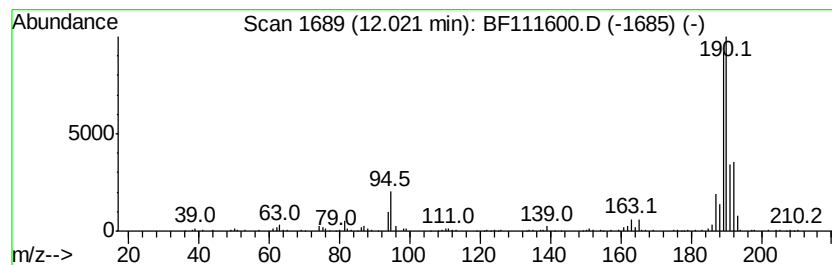
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.95 ng	235822	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3		6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	50
4		2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
Data File : BF111600.D
Acq On : 19 Dec 2018 19:53
Operator : JU/SJ
Sample : J6403-33
Misc :
ALS Vial : 4 Sample Multiplier: 1

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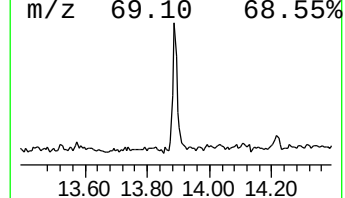
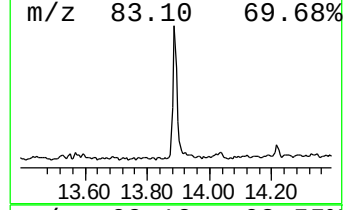
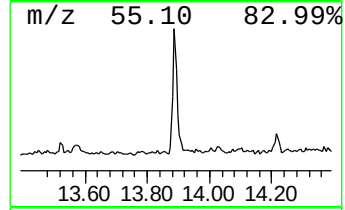
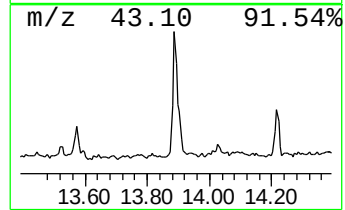
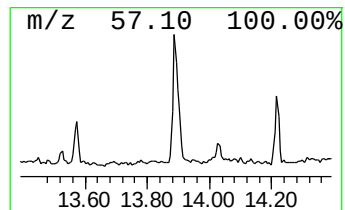
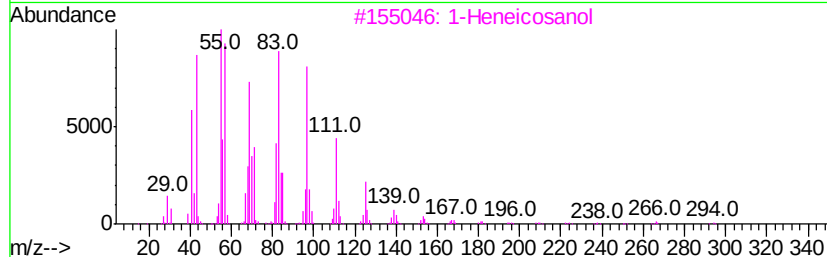
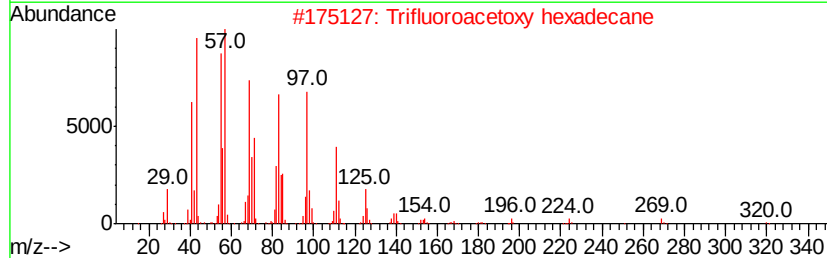
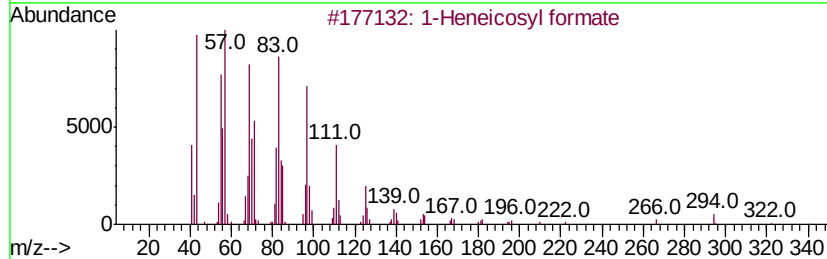
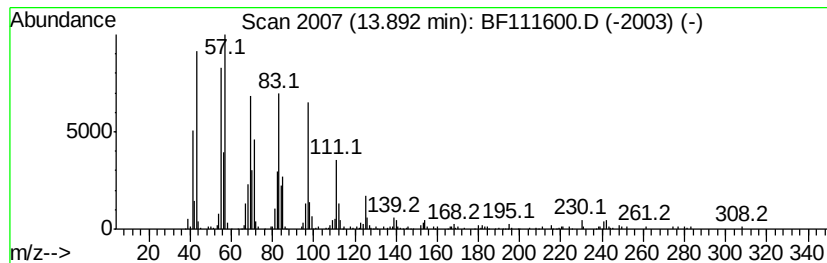
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	4.94 ng	476222	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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Sample : J6403-33
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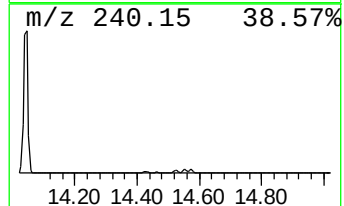
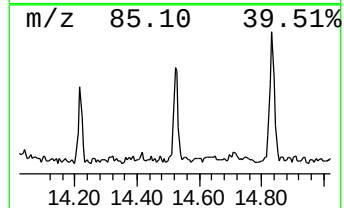
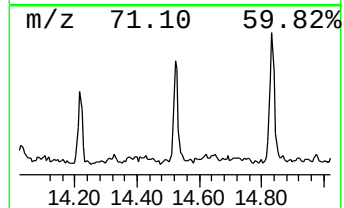
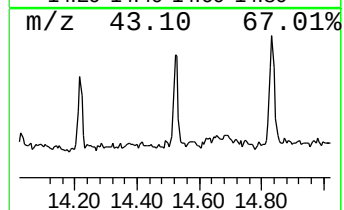
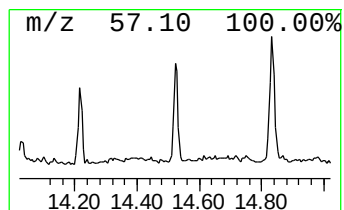
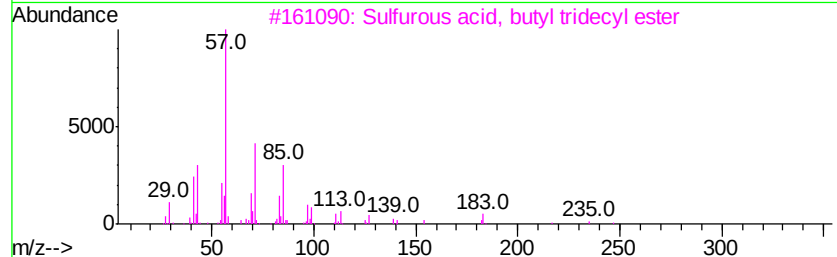
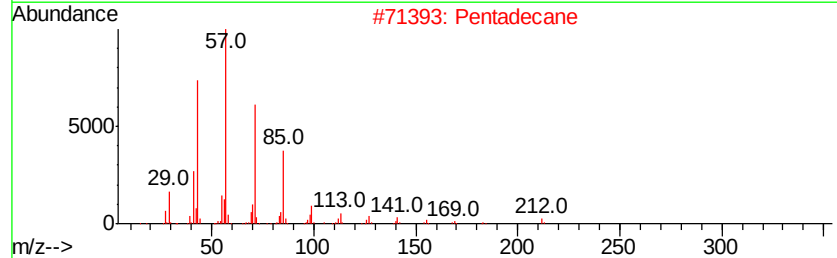
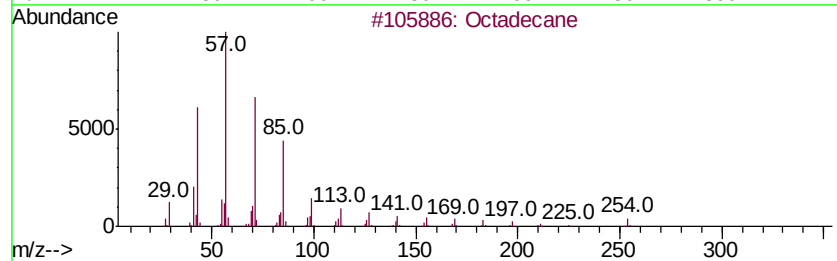
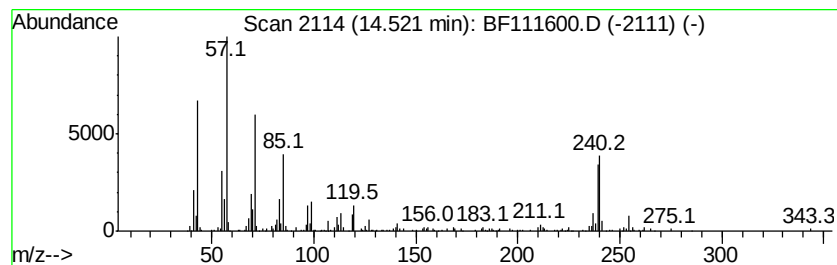
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.52	2.18 ng	209751	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	64
2	Pentadecane	212	C15H32	000629-62-9	64
3	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	50
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	50
5	Hentriacontane	437	C31H64	000630-04-6	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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 Operator : JU/SJ
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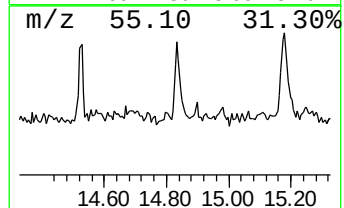
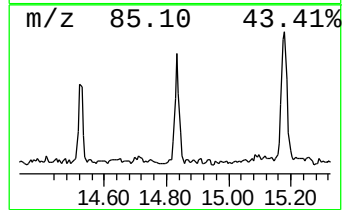
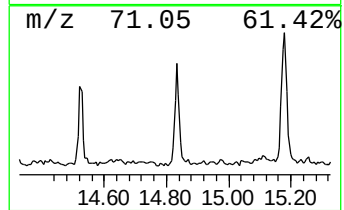
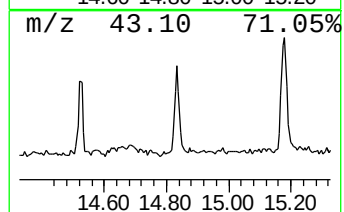
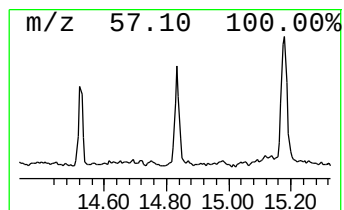
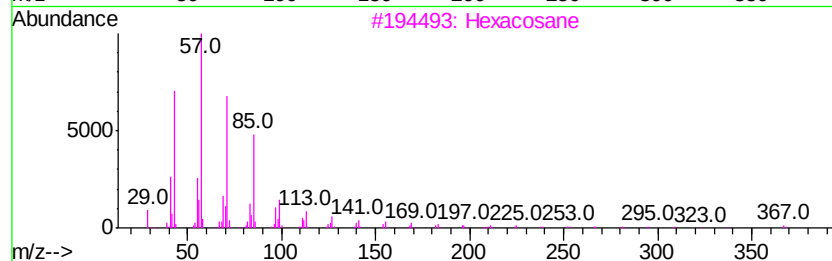
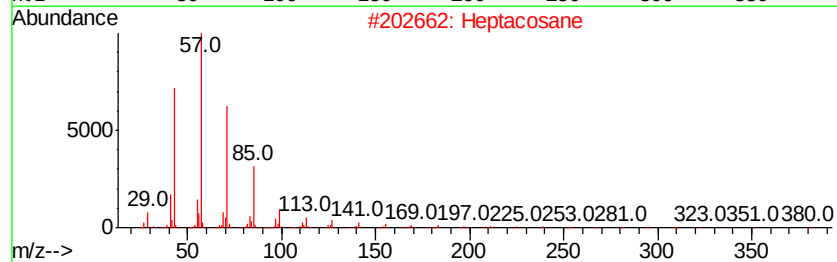
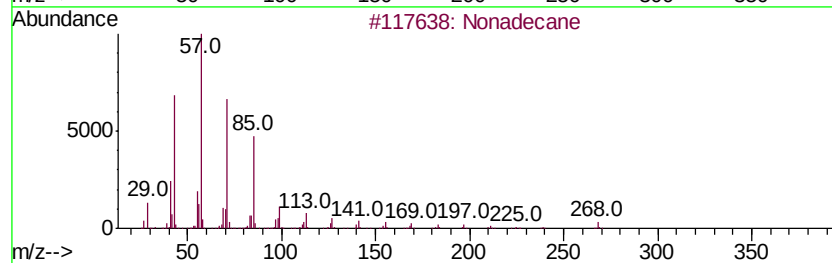
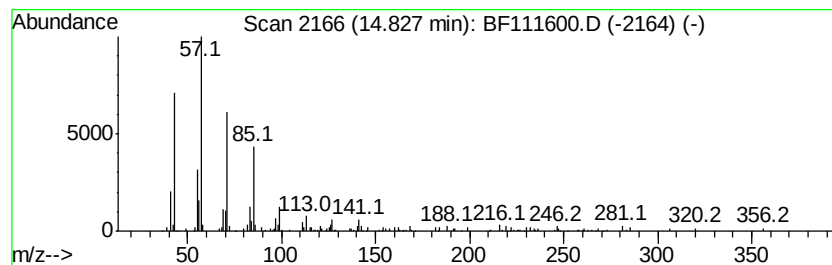
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.96 ng	203236	Perylene-d12	15.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	96
2	Heptacosane		380	C27H56	000593-49-7	90
3	Hexacosane		366	C26H54	000630-01-3	90
4	Octacosane		394	C28H58	000630-02-4	90
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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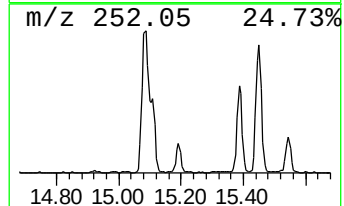
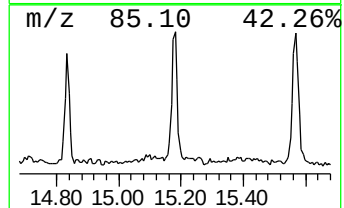
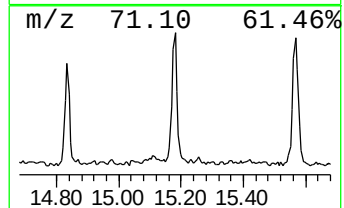
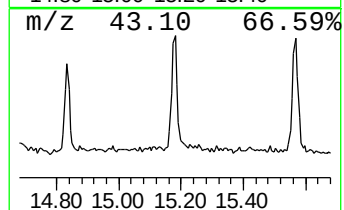
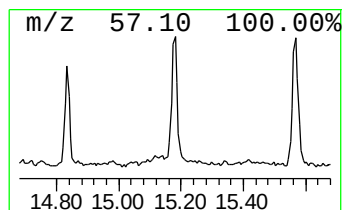
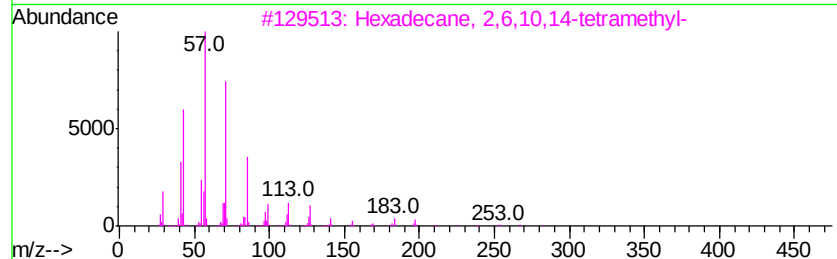
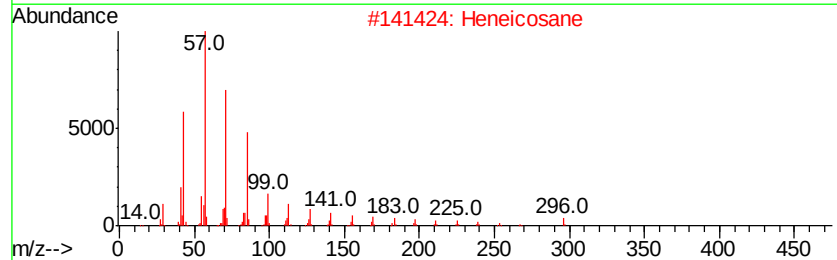
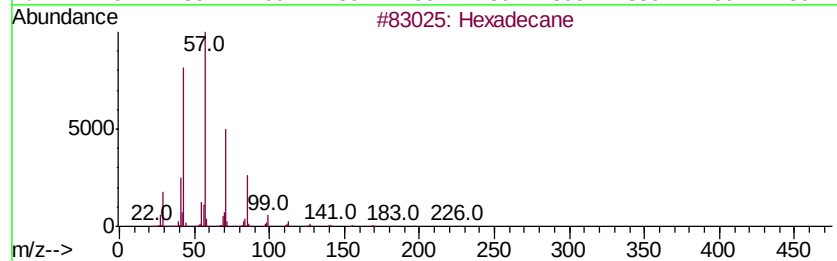
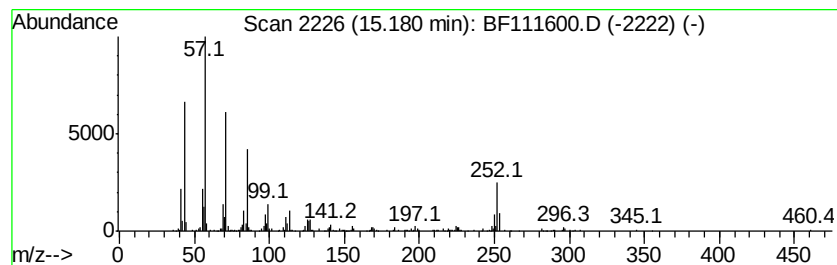
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	5.73 ng	393429	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	95
2	Heneicosane	296 C21H44	000629-94-7	91
3	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	90
4	Eicosane, 2-methyl-	296 C21H44	001560-84-5	76
5	Heptacosane	380 C27H56	000593-49-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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Acq On : 19 Dec 2018 19:53
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Misc :
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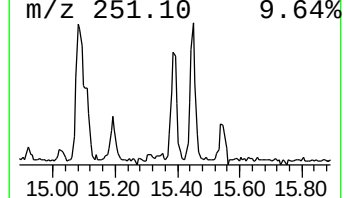
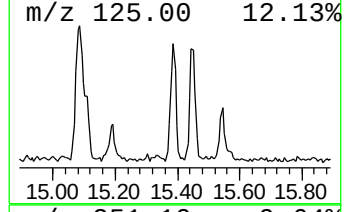
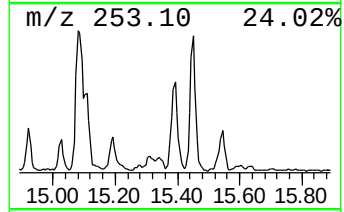
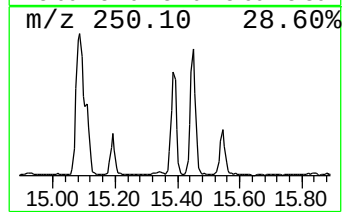
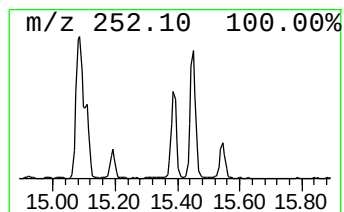
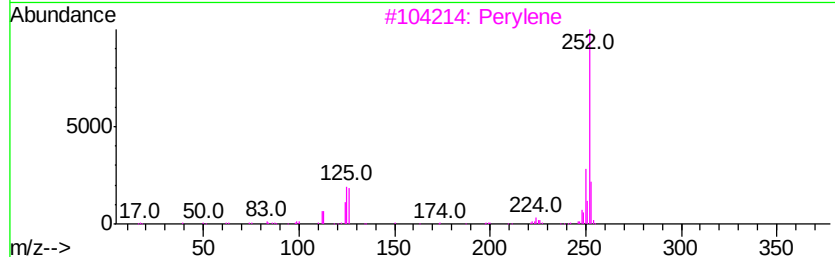
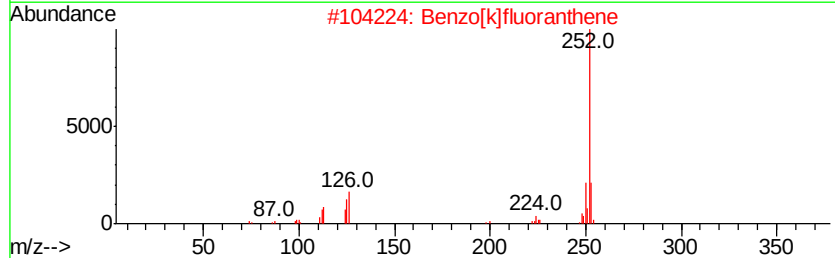
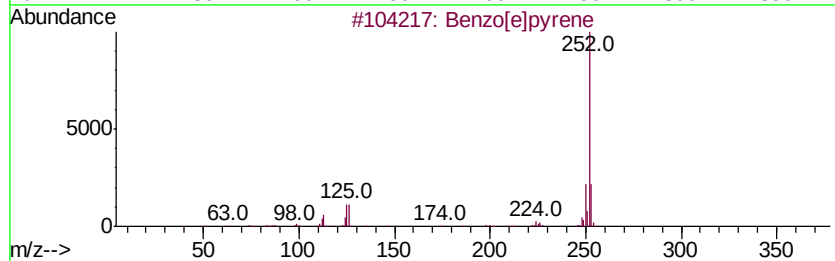
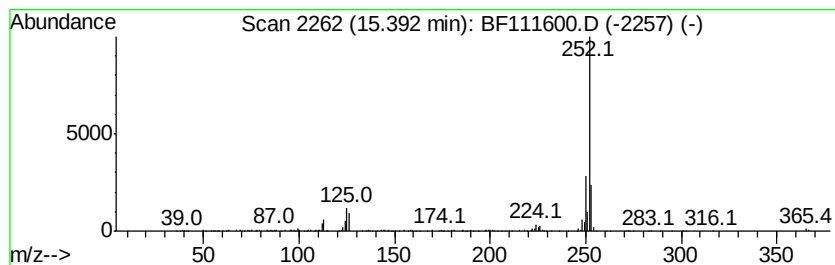
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	4.91 ng	336614	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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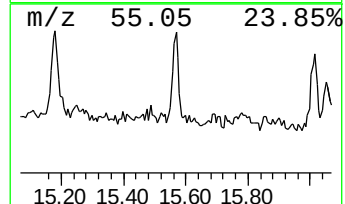
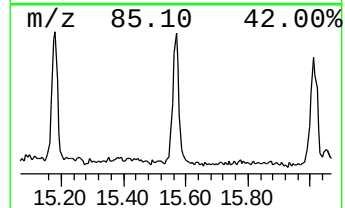
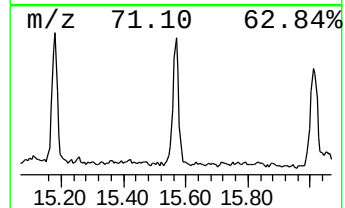
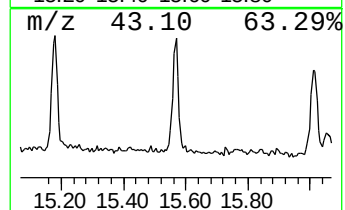
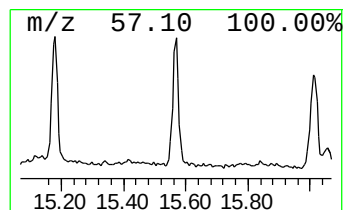
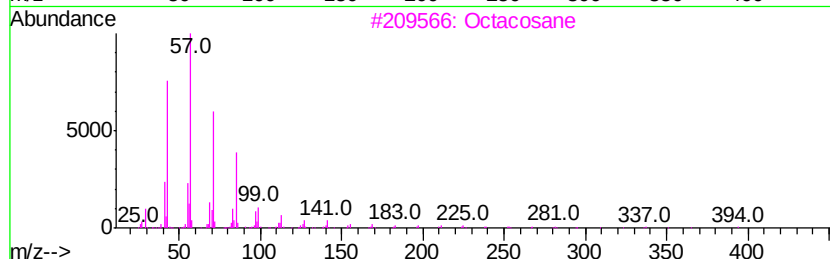
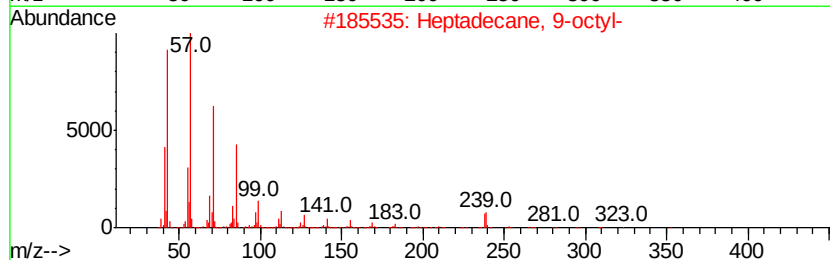
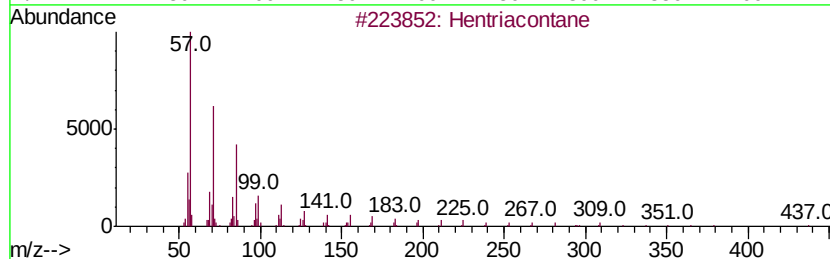
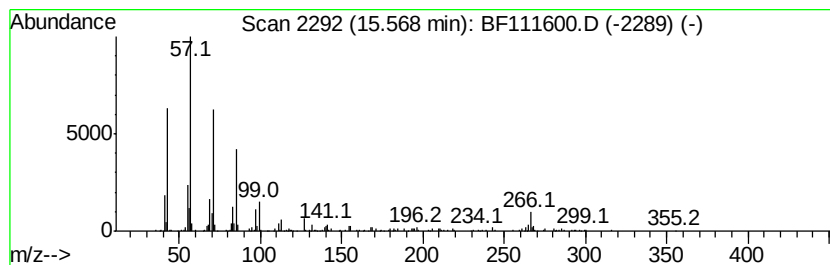
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	4.36 ng	299277	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	83
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3		Octacosane	394	C28H58	000630-02-4	80
4		Heneicosane	296	C21H44	000629-94-7	76
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76



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Sample : J6403-33
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5-A

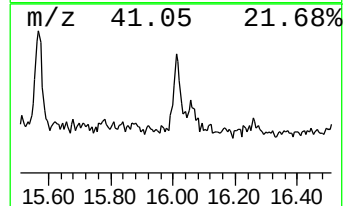
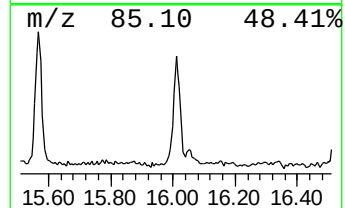
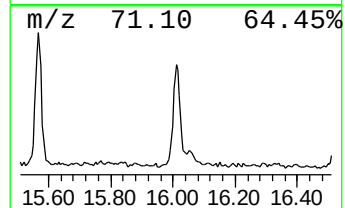
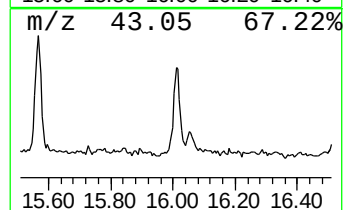
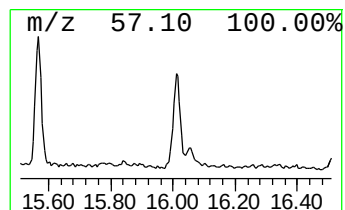
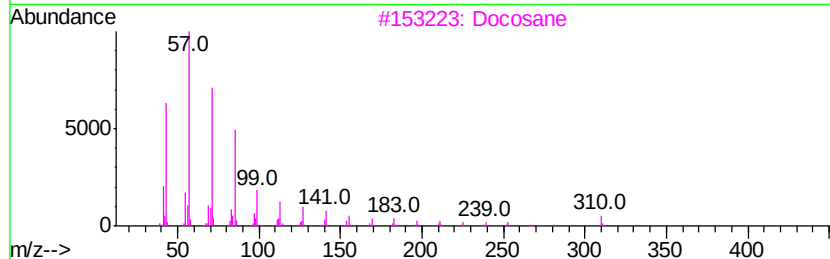
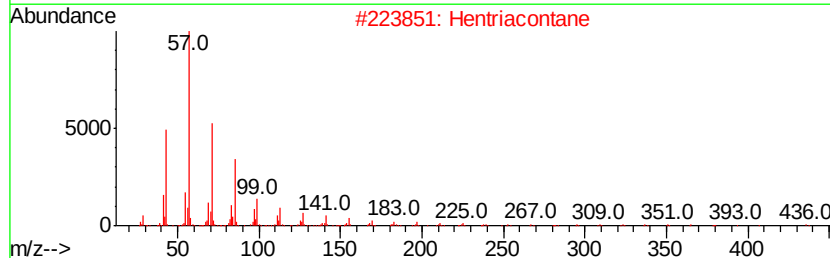
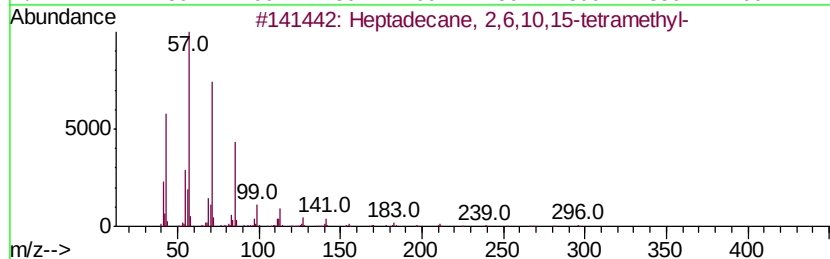
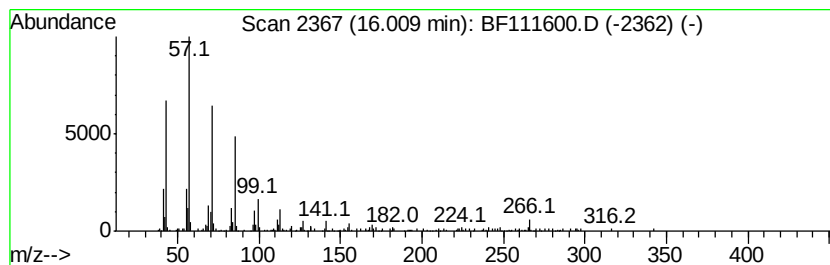
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.91 ng	268368	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Docosane	310	C22H46	000629-97-0	87
4		Triacontane	422	C30H62	000638-68-6	86
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121918\
Data File : BF111600.D
Acq On : 19 Dec 2018 19:53
Operator : JU/SJ
Sample : J6403-33
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	5.11	3.5	ng	189612	1	6.89	1081200	20.0
unknown6.66	6.66	59.8	ng	3234310	1	6.89	1081200	20.0
Anthracene, 2-met...	11.94	6.1	ng	485478	4	11.41	1599870	20.0
4H-Cyclopenta[def...	12.02	3.0	ng	235822	4	11.41	1599870	20.0
1-Heneicosyl formate	13.89	4.9	ng	476222	5	14.04	1927230	20.0
Octadecane	14.52	2.2	ng	209751	5	14.04	1927230	20.0
Nonadecane	14.83	3.0	ng	203236	6	15.52	1372180	20.0
Hexadecane	15.18	5.7	ng	393429	6	15.52	1372180	20.0
Benzo[e]pyrene	15.39	4.9	ng	336614	6	15.52	1372180	20.0
Hentriacontane	15.57	4.4	ng	299277	6	15.52	1372180	20.0
Heptadecane, 2,6,...	16.01	3.9	ng	268368	6	15.52	1372180	20.0