

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
 Data File : BF109239.D
 Acq On : 22 Sep 2018 23:16
 Operator : JU/SJ
 Sample : J4777-21 2X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-03-092018-B

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-BF092218.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	474	476	490	rVB	43856	56210	3.56%	0.332%
2	5.310	544	548	551	rBV	1470725	1319192	83.57%	7.781%
3	6.339	719	723	730	rBV	1632870	1431004	90.65%	8.440%
4	6.475	742	746	749	rBV	1635332	1420766	90.00%	8.380%
5	6.539	755	757	763	rBV	24139	21512	1.36%	0.127%
6	6.704	782	785	789	rBV	798186	687001	43.52%	4.052%
7	6.863	808	812	815	rBV	1408010	1116086	70.70%	6.583%
8	7.263	876	880	883	rBV	1018964	851998	53.97%	5.025%
9	7.986	999	1003	1007	rBV	1088598	857685	54.33%	5.059%
10	9.063	1182	1186	1189	rBV	2030138	1578565	100.00%	9.310%
11	9.186	1204	1207	1211	rBV	273412	243447	15.42%	1.436%
12	9.457	1250	1253	1256	rBV	414023	326399	20.68%	1.925%
13	9.686	1289	1292	1294	rBV	26356	21841	1.38%	0.129%
14	9.739	1297	1301	1304	rBV	957569	858976	54.41%	5.066%
15	10.180	1373	1376	1379	rVB	42920	31094	1.97%	0.183%
16	10.404	1410	1414	1416	rBV	24173	27691	1.75%	0.163%
17	10.516	1430	1433	1439	rBV	851966	724073	45.87%	4.271%
18	10.651	1453	1456	1463	rVB	79644	96574	6.12%	0.570%
19	10.851	1487	1490	1493	rBV4	14665	20117	1.27%	0.119%
20	11.098	1529	1532	1535	rBV	87881	75034	4.75%	0.443%
21	11.127	1535	1537	1541	rVB	44453	43674	2.77%	0.258%
22	11.210	1548	1551	1554	rBV	758089	702064	44.47%	4.141%
23	11.233	1554	1555	1559	rVV	100942	67097	4.25%	0.396%
24	11.286	1559	1564	1567	rVB2	36181	38438	2.43%	0.227%
25	11.521	1601	1604	1610	rBV	79366	81205	5.14%	0.479%
26	11.710	1634	1636	1639	rBV	21158	20284	1.28%	0.120%
27	11.739	1639	1641	1646	rVB2	29421	39152	2.48%	0.231%
28	11.821	1652	1655	1658	rBV	45681	46432	2.94%	0.274%
29	11.927	1670	1673	1676	rBV	82859	68189	4.32%	0.402%
30	12.086	1697	1700	1705	rBV7	12313	23154	1.47%	0.137%
31	12.263	1727	1730	1733	rBV3	23962	22064	1.40%	0.130%
32	12.316	1737	1739	1742	rVB	70325	57610	3.65%	0.340%
33	12.416	1753	1756	1760	rBV	228003	198348	12.57%	1.170%
34	12.645	1789	1795	1798	rBV	223927	227254	14.40%	1.340%

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35	12.686	1799	1802	1804	rVV2	56092	41474	2.63%	0.245%
36	12.792	1817	1820	1824	rBV	1219774	1034155	65.51%	6.099%
37	12.868	1830	1833	1835	rBV3	19232	19752	1.25%	0.116%
38	12.974	1848	1851	1855	rVB	44654	45248	2.87%	0.267%
39	13.039	1859	1862	1865	rVB	72949	60584	3.84%	0.357%
40	13.074	1865	1868	1871	rBV	37209	40231	2.55%	0.237%
41	13.168	1881	1884	1886	rVB	30436	24254	1.54%	0.143%
42	13.198	1886	1889	1894	rBV	23628	23240	1.47%	0.137%
43	13.380	1917	1920	1924	rBV	55009	60830	3.85%	0.359%
44	13.474	1934	1936	1941	rBV2	20135	24617	1.56%	0.145%
45	13.586	1952	1955	1958	rBV2	31046	41134	2.61%	0.243%
46	13.680	1969	1971	1973	rBV	21974	20155	1.28%	0.119%
47	13.710	1973	1976	1982	rVB2	61581	72699	4.61%	0.429%
48	13.839	1993	1998	2000	rBV2	717723	762068	48.28%	4.495%
49	13.862	2000	2002	2005	rVB	110201	85001	5.38%	0.501%
50	14.021	2027	2029	2032	rVB	64872	54910	3.48%	0.324%
51	14.327	2078	2081	2083	rBV	63383	68421	4.33%	0.404%
52	14.621	2128	2131	2134	rBV	76504	80487	5.10%	0.475%
53	14.751	2151	2153	2157	rVB	67128	69597	4.41%	0.410%
54	14.839	2165	2168	2178	rBV	95404	203554	12.89%	1.201%
55	14.939	2182	2185	2188	rVB2	101260	111271	7.05%	0.656%
56	15.180	2223	2226	2231	rVB	62572	67102	4.25%	0.396%
57	15.239	2232	2236	2239	rBV	406671	427743	27.10%	2.523%
58	15.692	2309	2313	2318	rVB2	83674	116339	7.37%	0.686%

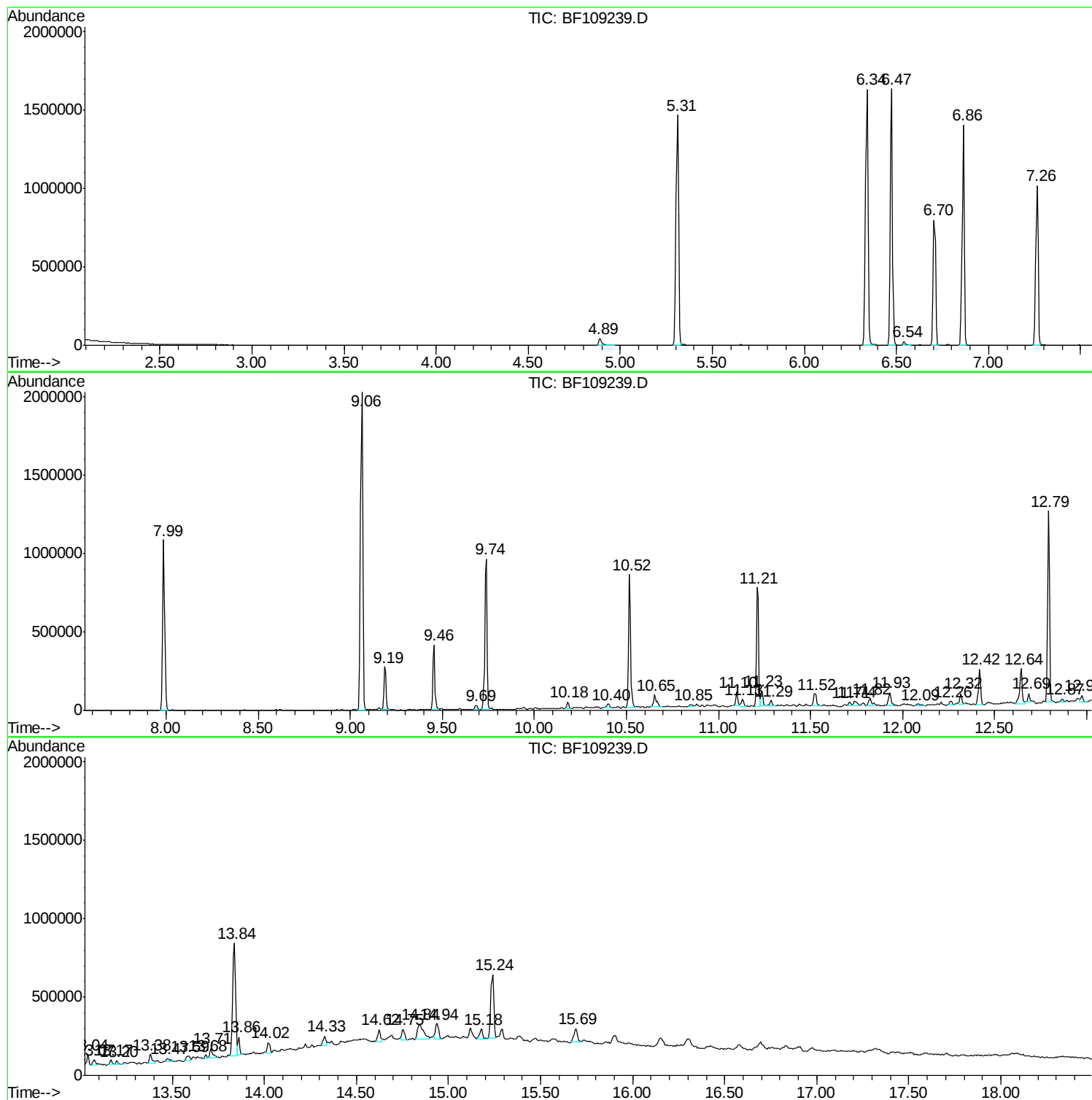
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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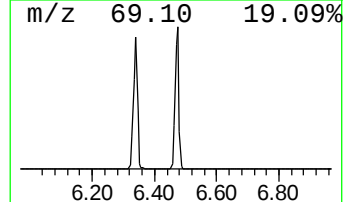
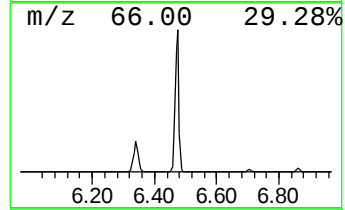
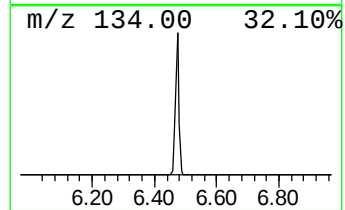
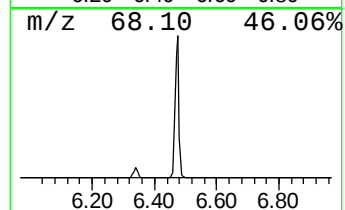
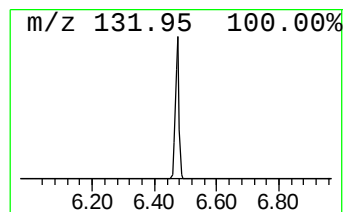
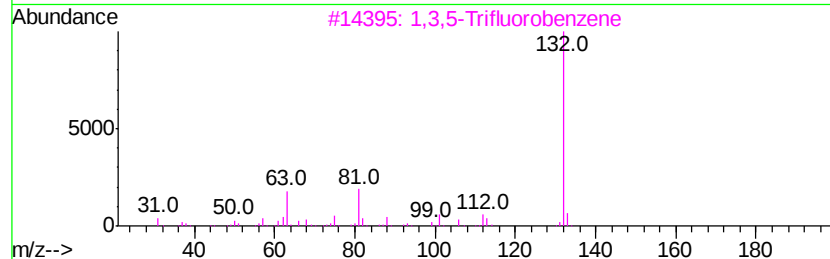
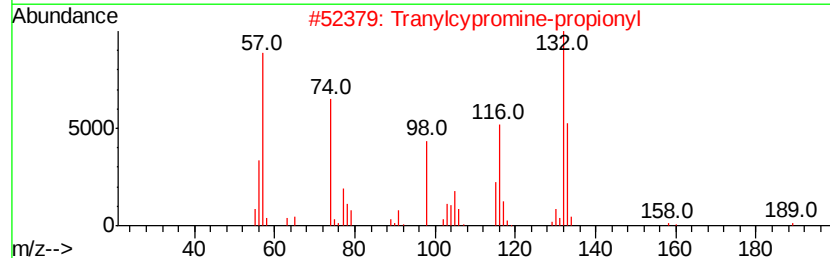
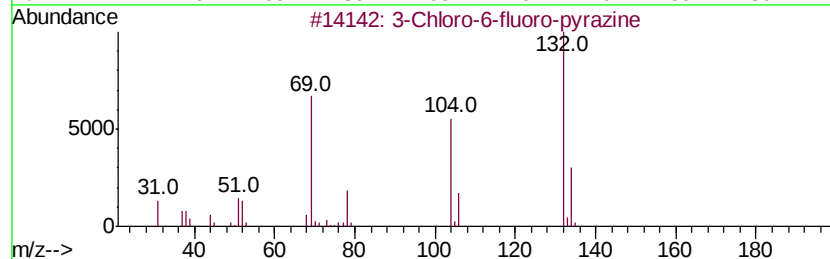
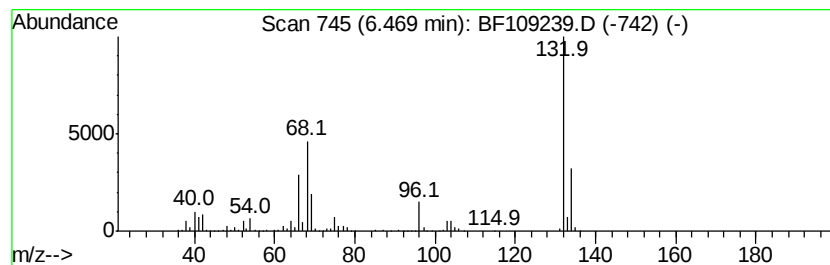
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	41.36 ng	1420770	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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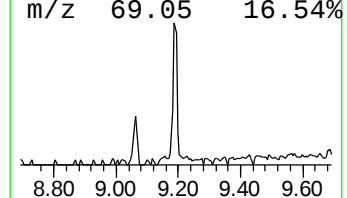
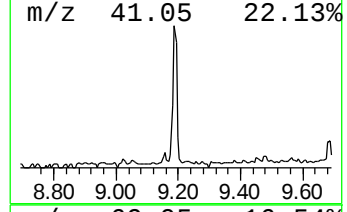
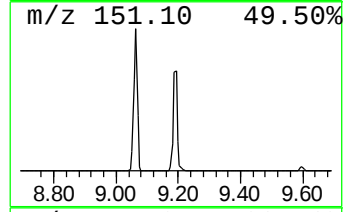
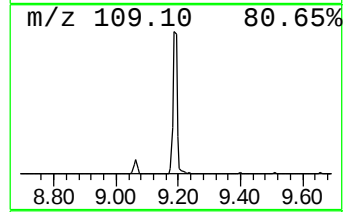
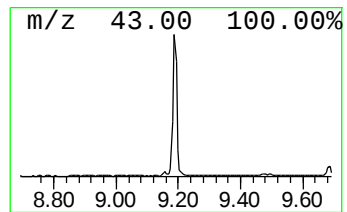
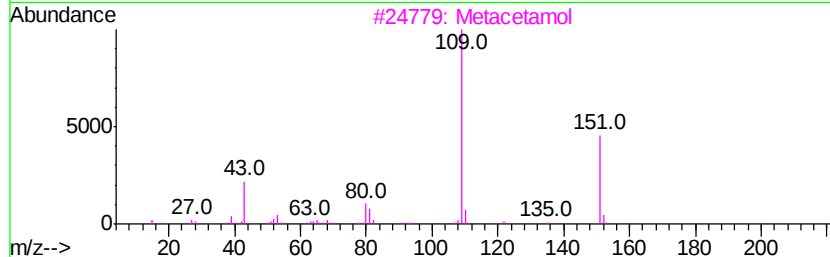
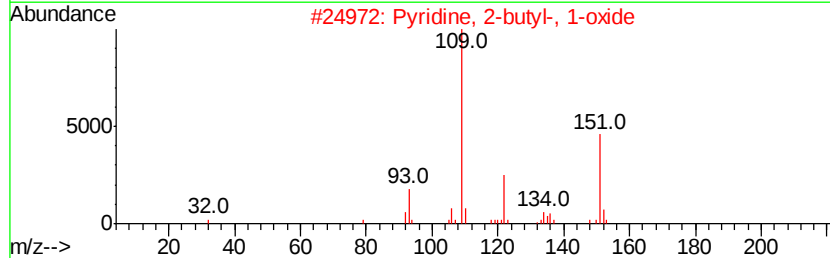
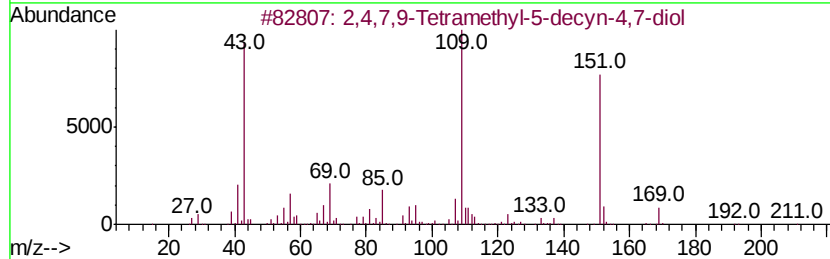
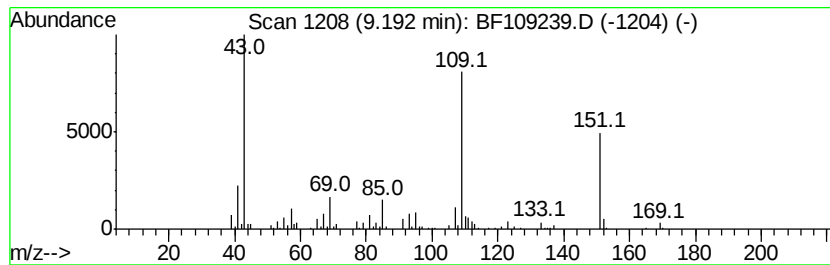
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	5.67 ng	243447	Acenaphthene-d10	9.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2			Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3			Metacetamol	151	C8H9NO2	000621-42-1	58
4			Acetaminophen	151	C8H9NO2	000103-90-2	53
5			p-Isopropoxyaniline	151	C9H13NO	007664-66-6	42



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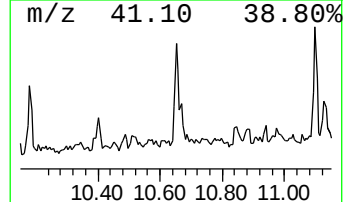
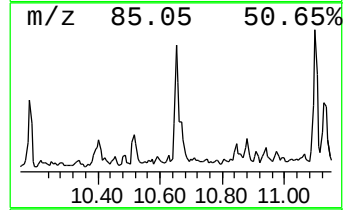
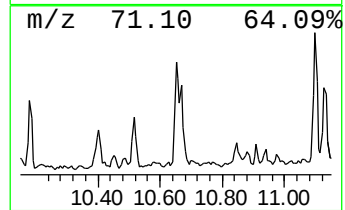
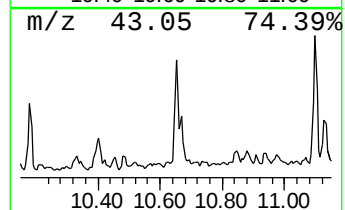
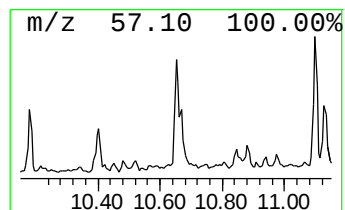
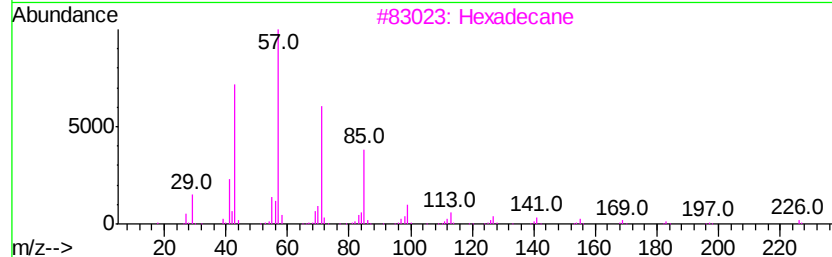
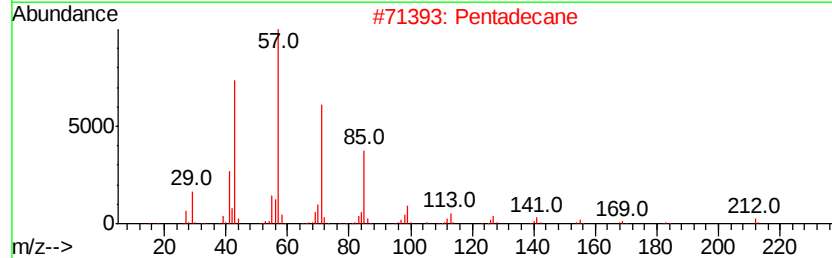
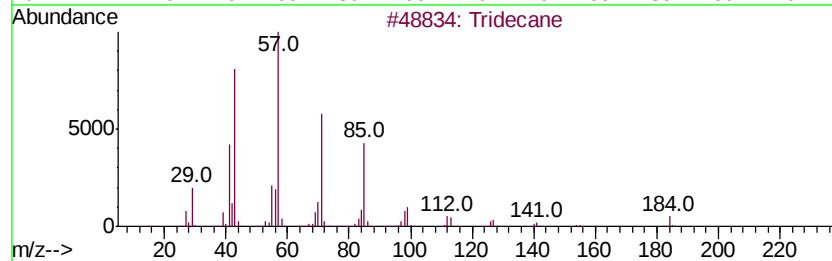
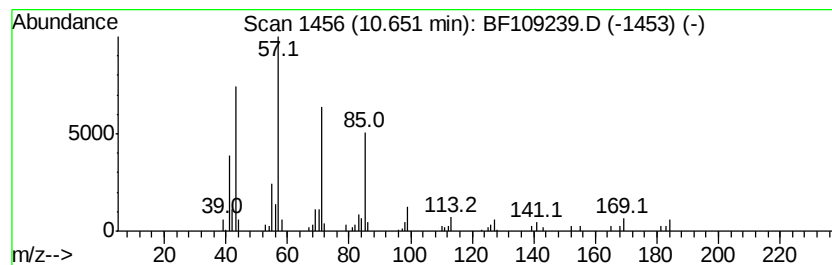
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Peak Number 4 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.65	2.75 ng	96574	Phenanthrene-d10		11.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Octadecane	254	C18H38	000593-45-3	90



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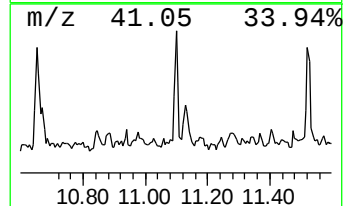
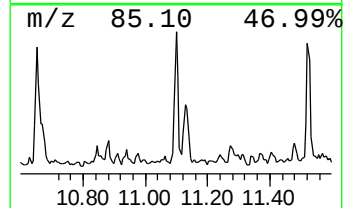
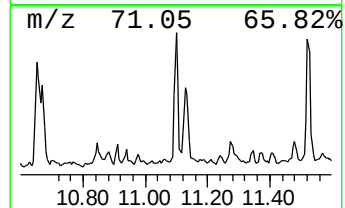
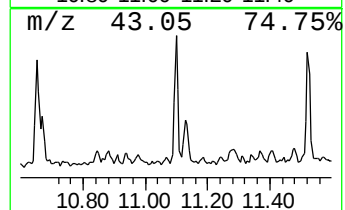
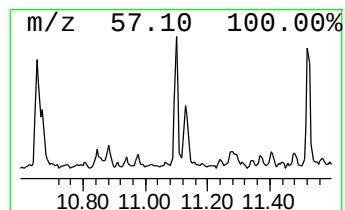
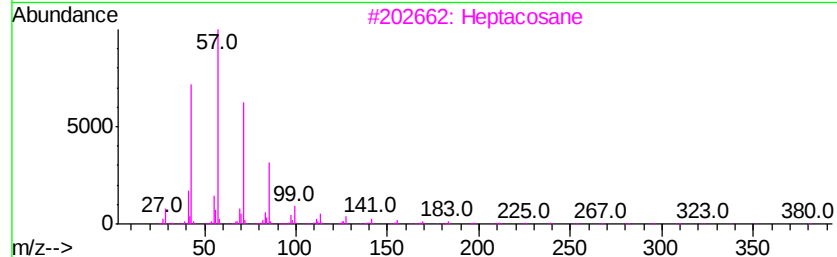
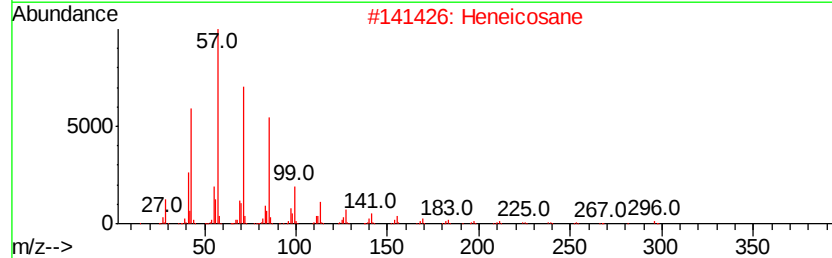
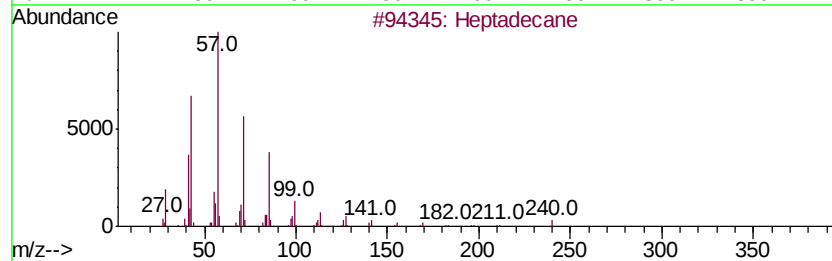
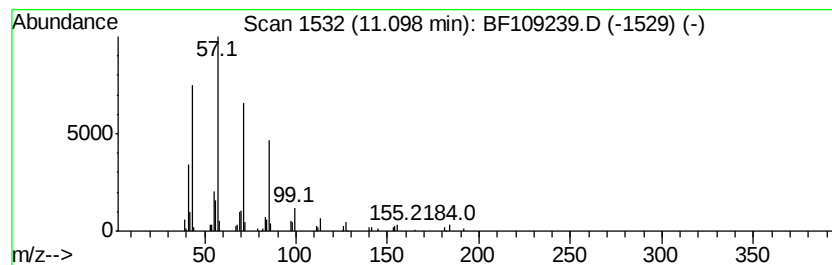
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.14 ng	75034	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Heneicosane		296	C21H44	000629-94-7	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Eicosane		282	C20H42	000112-95-8	87
5	Hexadecane		226	C16H34	000544-76-3	86



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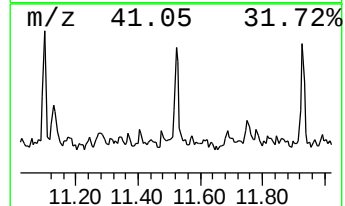
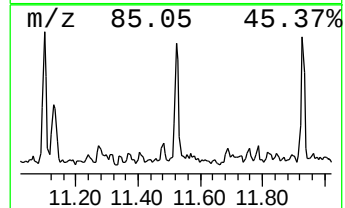
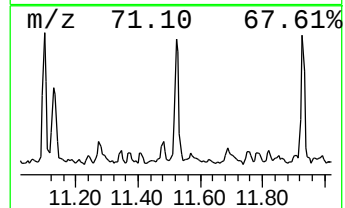
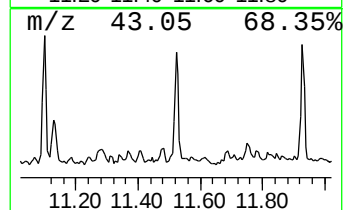
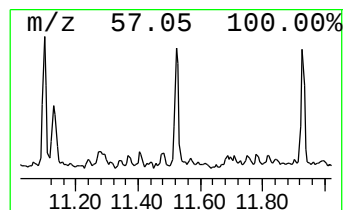
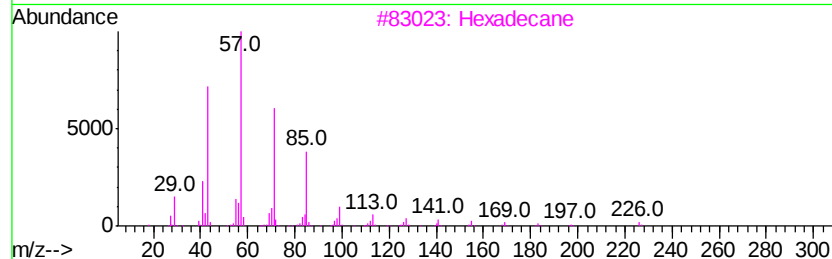
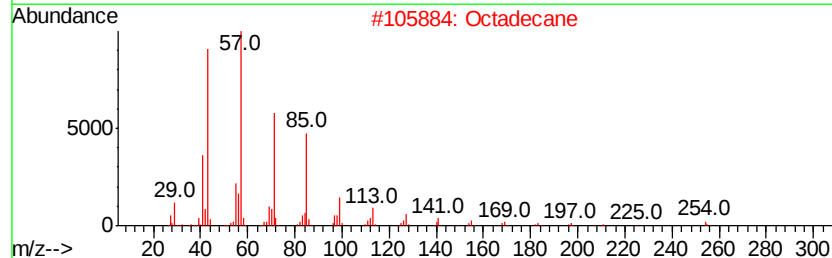
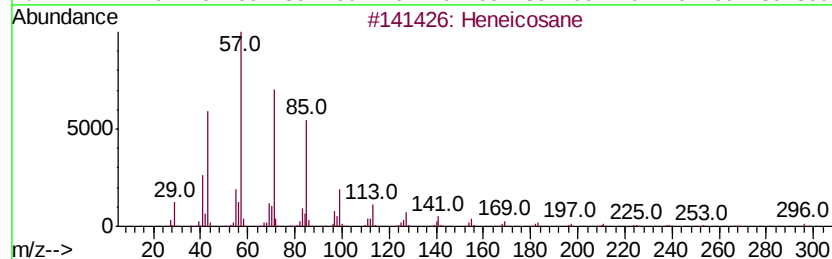
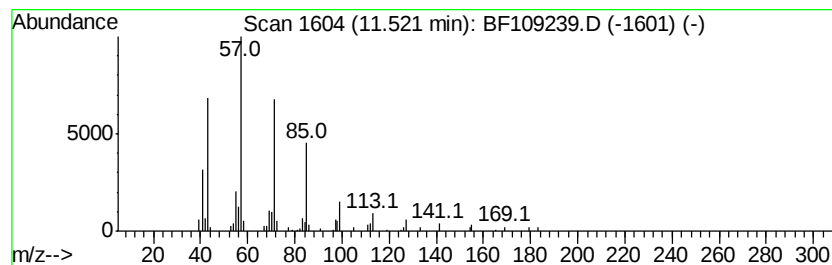
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.31 ng	81205	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Heptadecane		240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109239.D
Acq On : 22 Sep 2018 23:16
Operator : JU/SJ
Sample : J4777-21 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-B

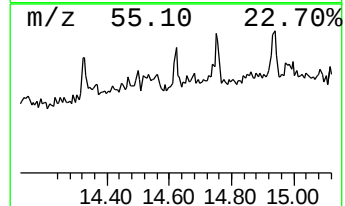
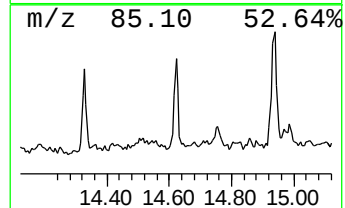
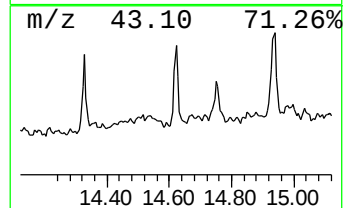
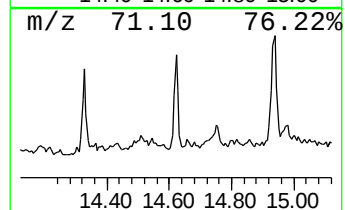
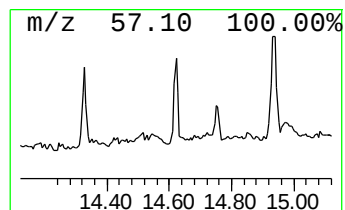
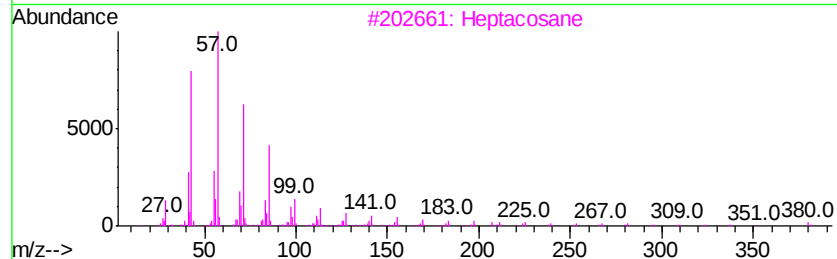
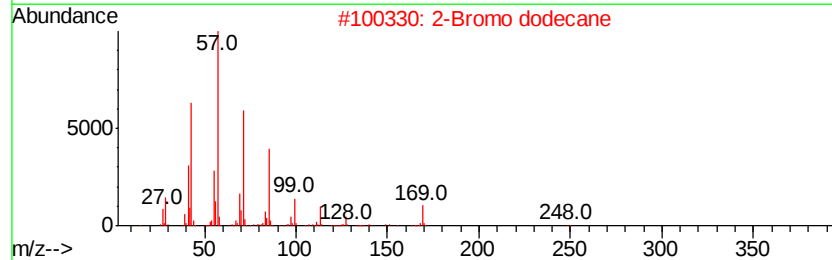
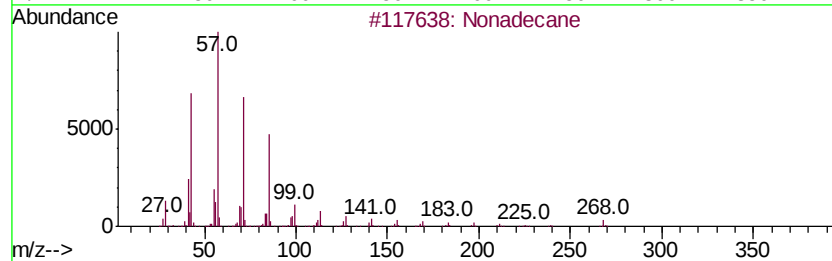
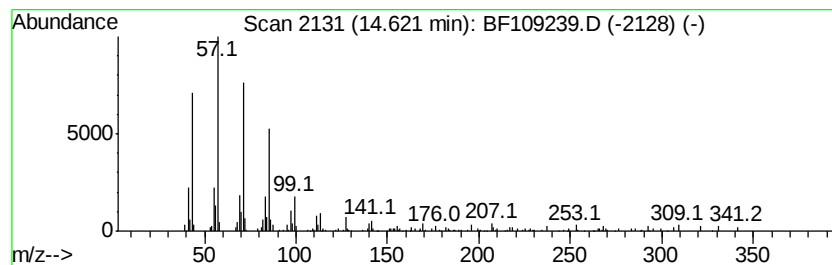
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.76 ng	80487	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	93
3	Heptacosane		380	C27H56	000593-49-7	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109239.D
Acq On : 22 Sep 2018 23:16
Operator : JU/SJ
Sample : J4777-21 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

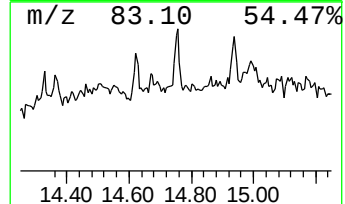
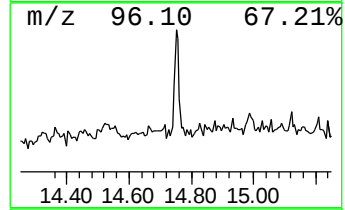
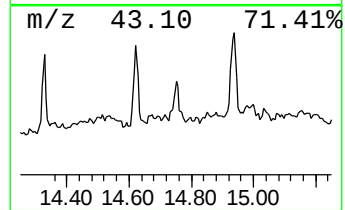
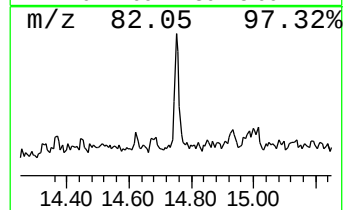
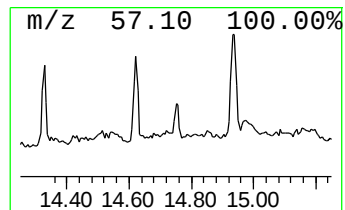
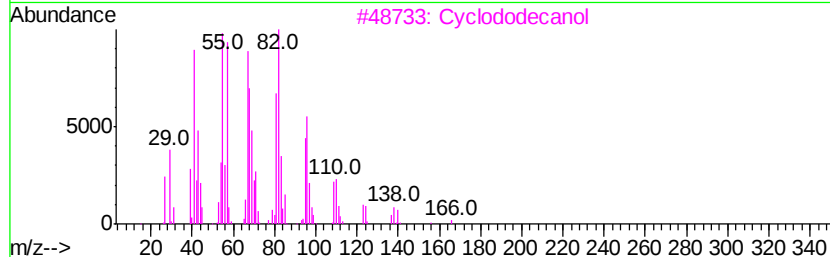
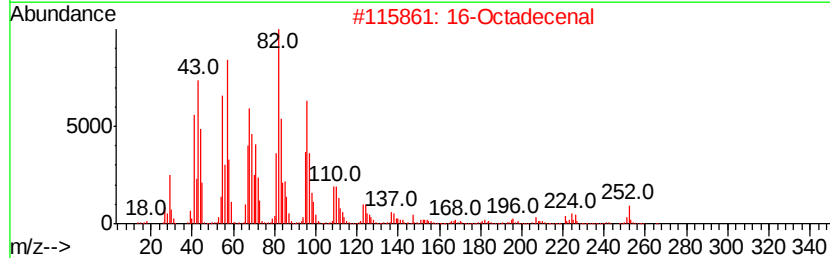
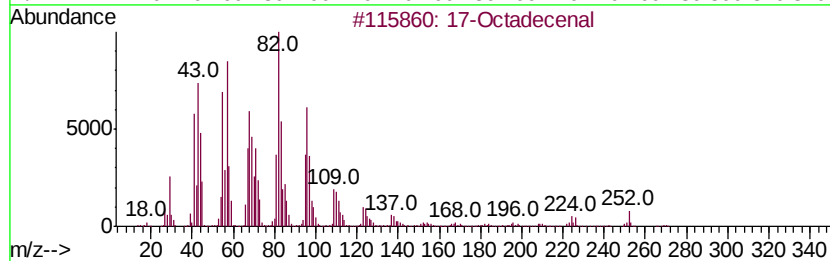
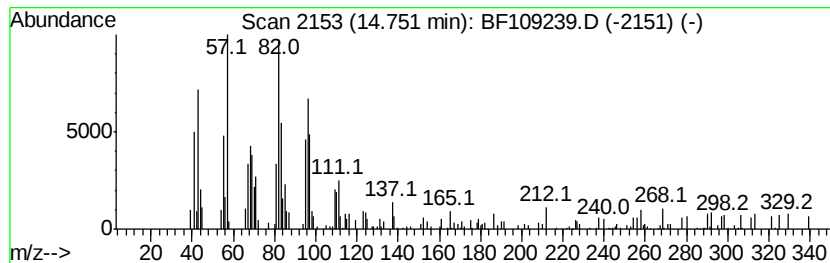
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ClientSampleId :
PL-03-092018-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17-Octadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.75	3.25 ng	69597	Perylene-d12	15.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Octadecenal	266	C18H34O	056554-86-0	81
2	16-Octadecenal	266	C18H34O	056554-87-1	81
3	Cyclododecanol	184	C12H24O	001724-39-6	64
4	Pentadecanal-	226	C15H30O	002765-11-9	58
5	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109239.D
Acq On : 22 Sep 2018 23:16
Operator : JU/SJ
Sample : J4777-21 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-B

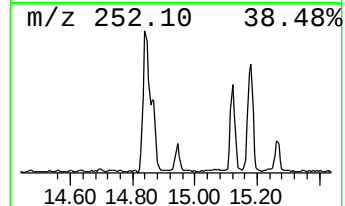
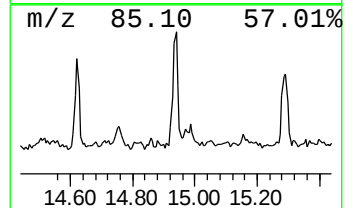
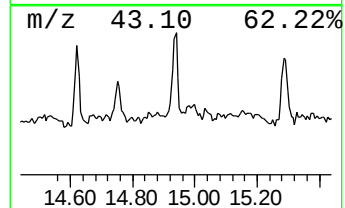
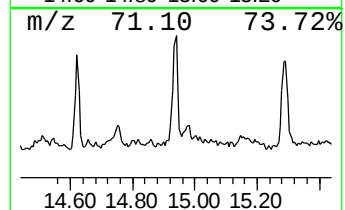
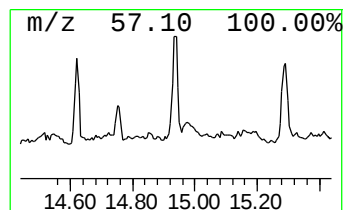
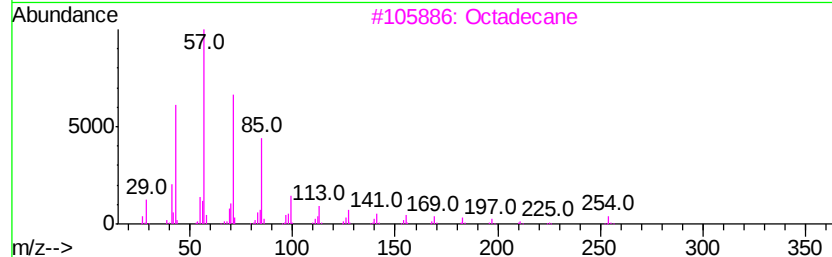
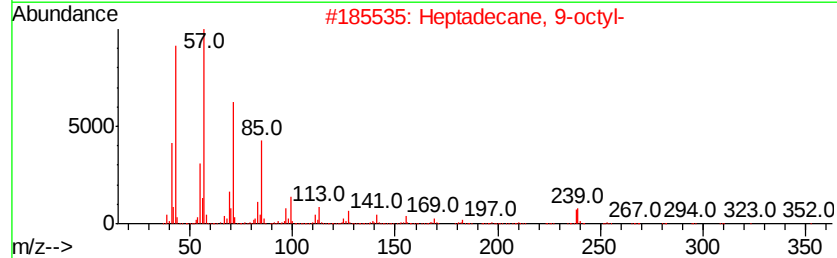
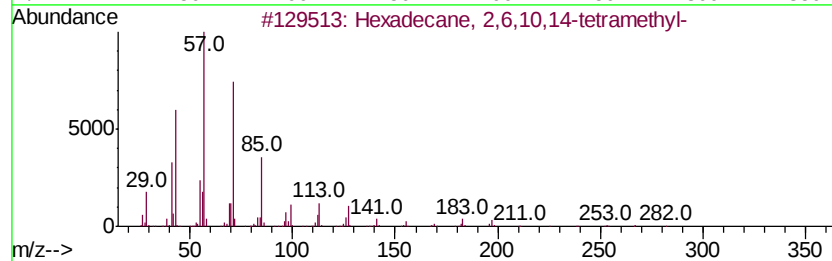
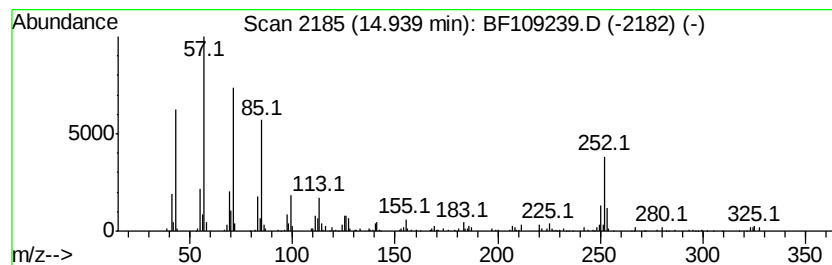
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	5.20 ng	111271	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	60
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	58
3		Octadecane	254	C18H38	000593-45-3	58
4		Tricosane	324	C23H48	000638-67-5	58
5		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
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Operator : JU/SJ
Sample : J4777-21 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

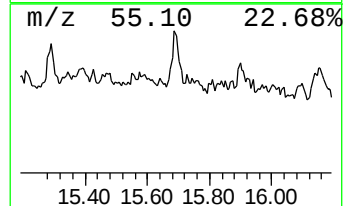
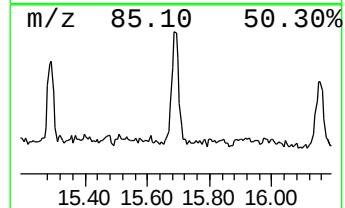
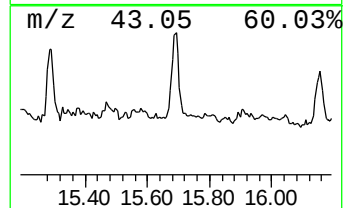
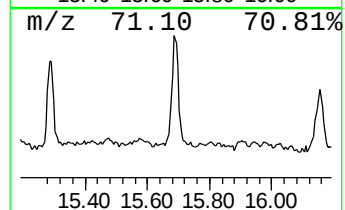
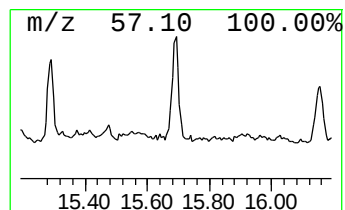
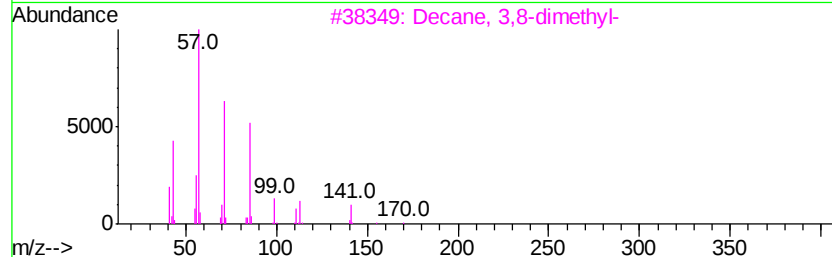
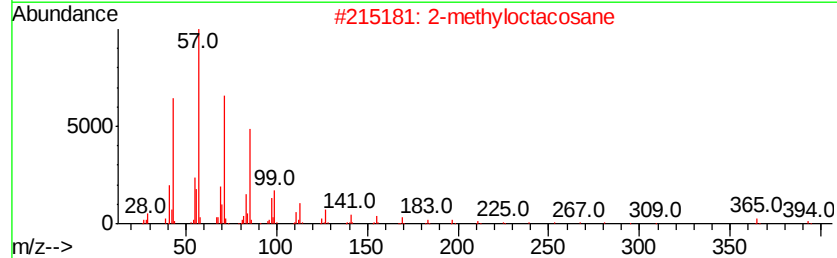
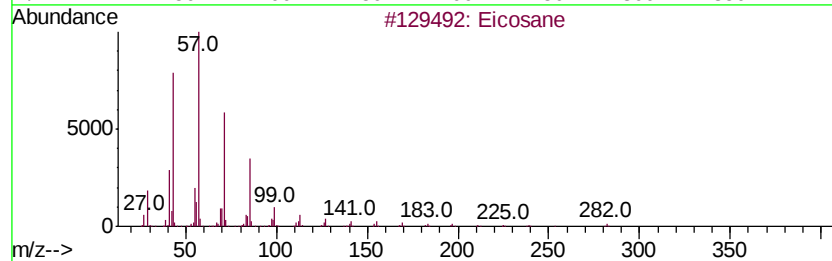
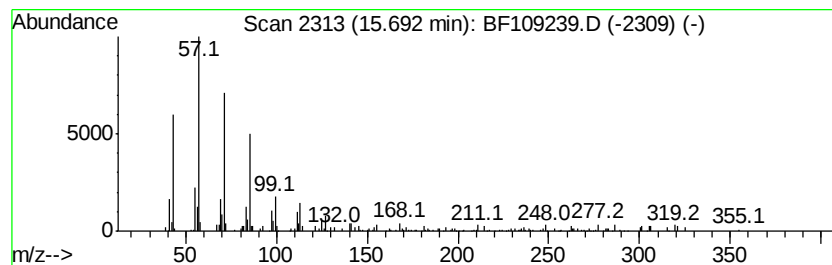
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PL-03-092018-B

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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 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	5.44 ng	116339	Perylene-d12	15.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 90
2	2-methyloctacosane		408 C29H60	1000376-72-8 87
3	Decane, 3,8-dimethyl-		170 C12H26	017312-55-9 87
4	Hentriacontane		437 C31H64	000630-04-6 87
5	Heneicosane		296 C21H44	000629-94-7 83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
Data File : BF109239.D
Acq On : 22 Sep 2018 23:16
Operator : JU/SJ
Sample : J4777-21 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
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2,4,7,9-Tetrameth...	9.19	5.7	ng	243447	3	9.74	858976	20.0
Tridecane	10.65	2.8	ng	96574	4	11.21	702064	20.0
Heptadecane	11.10	2.1	ng	75034	4	11.21	702064	20.0
Heneicosane	11.52	2.3	ng	81205	4	11.21	702064	20.0
Nonadecane	14.62	3.8	ng	80487	6	15.24	427743	20.0
17-Octadecenal	14.75	3.3	ng	69597	6	15.24	427743	20.0
Hexadecane, 2,6,1...	14.94	5.2	ng	111271	6	15.24	427743	20.0
Eicosane	15.69	5.4	ng	116339	6	15.24	427743	20.0