

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
 Data File : BF109002.D
 Acq On : 14 Sep 2018 18:36
 Operator : JU/SJ
 Sample : J4906-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-PIT-8

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-BF091418.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	4.913	434	438	446	rVB	91027	111756	3.83%	0.349%
2	5.325	503	508	512	rBV	2431196	2512458	86.06%	7.855%
3	6.354	677	683	687	rBV	2750421	2706112	92.69%	8.461%
4	6.490	701	706	709	rBV	2742487	2668121	91.39%	8.342%
5	6.719	741	745	748	rBV	1228886	928600	31.81%	2.903%
6	6.878	767	772	775	rBV	2398442	2062043	70.63%	6.447%
7	7.278	835	840	843	rBV	1901902	1710889	58.60%	5.349%
8	8.001	959	963	966	rBV	1446306	1206396	41.32%	3.772%
9	9.078	1141	1146	1149	rBV	3485486	2919394	100.00%	9.127%
10	9.466	1209	1212	1216	rBV	365219	284418	9.74%	0.889%
11	9.748	1256	1260	1264	rBV2	1599548	1405786	48.15%	4.395%
12	10.530	1389	1393	1406	rBV	2129010	2021717	69.25%	6.321%
13	11.225	1507	1511	1514	rBV	1731398	1502415	51.46%	4.697%
14	11.248	1514	1515	1518	rVV	169622	92560	3.17%	0.289%
15	11.295	1518	1523	1527	rVB2	33553	34706	1.19%	0.109%
16	11.724	1593	1596	1598	rBV	58992	47761	1.64%	0.149%
17	11.766	1598	1603	1607	rVV2	190827	227444	7.79%	0.711%
18	11.836	1611	1615	1617	rVV	81816	91656	3.14%	0.287%
19	11.860	1617	1619	1624	rVB	54001	44004	1.51%	0.138%
20	12.019	1644	1646	1648	rBV	45727	37602	1.29%	0.118%
21	12.272	1683	1689	1692	rBV	66608	70475	2.41%	0.220%
22	12.354	1701	1703	1708	rVB5	28460	36264	1.24%	0.113%
23	12.430	1713	1716	1721	rVB	255489	221994	7.60%	0.694%
24	12.654	1749	1754	1757	rBV	355895	322604	11.05%	1.009%
25	12.719	1764	1765	1769	rVB	43966	34485	1.18%	0.108%
26	12.807	1776	1780	1784	rBV	2898325	2804173	96.05%	8.767%
27	12.877	1787	1792	1795	rBV3	50760	66244	2.27%	0.207%
28	12.966	1803	1807	1808	rBV2	41272	47960	1.64%	0.150%
29	12.983	1808	1810	1813	rVB2	67558	60793	2.08%	0.190%
30	13.054	1819	1822	1825	rVB	81864	72375	2.48%	0.226%
31	13.089	1825	1828	1831	rVB	68791	60081	2.06%	0.188%
32	13.177	1841	1843	1846	rVB	53028	47184	1.62%	0.148%
33	13.213	1846	1849	1852	rVB	52144	42035	1.44%	0.131%
34	13.295	1854	1863	1868	rBV6	49236	79804	2.73%	0.250%

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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	13.395	1877	1880	1886	rVB2	81948	93052	3.19%	0.291%
36	13.483	1889	1895	1902	rBV3	36987	57049	1.95%	0.178%
37	13.595	1909	1914	1918	rBV2	40179	63815	2.19%	0.200%
38	13.713	1931	1934	1941	rVB2	224216	331051	11.34%	1.035%
39	13.848	1952	1957	1960	rBV	1309548	1424007	48.78%	4.452%
40	13.871	1960	1961	1968	rVB	167109	145173	4.97%	0.454%
41	14.036	1986	1989	1993	rBV	104472	95495	3.27%	0.299%
42	14.236	2018	2023	2026	rBV	58113	65628	2.25%	0.205%
43	14.265	2026	2028	2032	rVB2	46640	44694	1.53%	0.140%
44	14.342	2032	2041	2046	rBV4	146959	265001	9.08%	0.829%
45	14.636	2088	2091	2095	rVB2	133290	133382	4.57%	0.417%
46	14.707	2100	2103	2107	rVB	100488	95279	3.26%	0.298%
47	14.854	2123	2128	2137	rBV	102320	202280	6.93%	0.632%
48	14.954	2141	2145	2148	rBV	152557	167040	5.72%	0.522%
49	15.136	2172	2176	2180	rVB	76855	82470	2.82%	0.258%
50	15.189	2181	2185	2191	rVB2	120818	143080	4.90%	0.447%
51	15.254	2191	2196	2200	rBV	970848	1089743	37.33%	3.407%
52	15.307	2202	2205	2210	rVB	113712	144098	4.94%	0.451%
53	15.712	2268	2274	2280	rBV2	109987	181720	6.22%	0.568%
54	15.765	2280	2283	2292	rVB7	30383	61338	2.10%	0.192%
55	16.183	2345	2354	2361	rBV3	83097	175348	6.01%	0.548%
56	16.448	2393	2399	2404	rVB8	17004	41237	1.41%	0.129%
57	16.589	2418	2423	2432	rVB2	47458	93539	3.20%	0.292%
58	16.724	2441	2446	2456	rBV5	42993	108862	3.73%	0.340%
59	16.818	2456	2462	2468	rVV3	14850	34536	1.18%	0.108%
60	16.995	2487	2492	2501	rVB	34295	63646	2.18%	0.199%

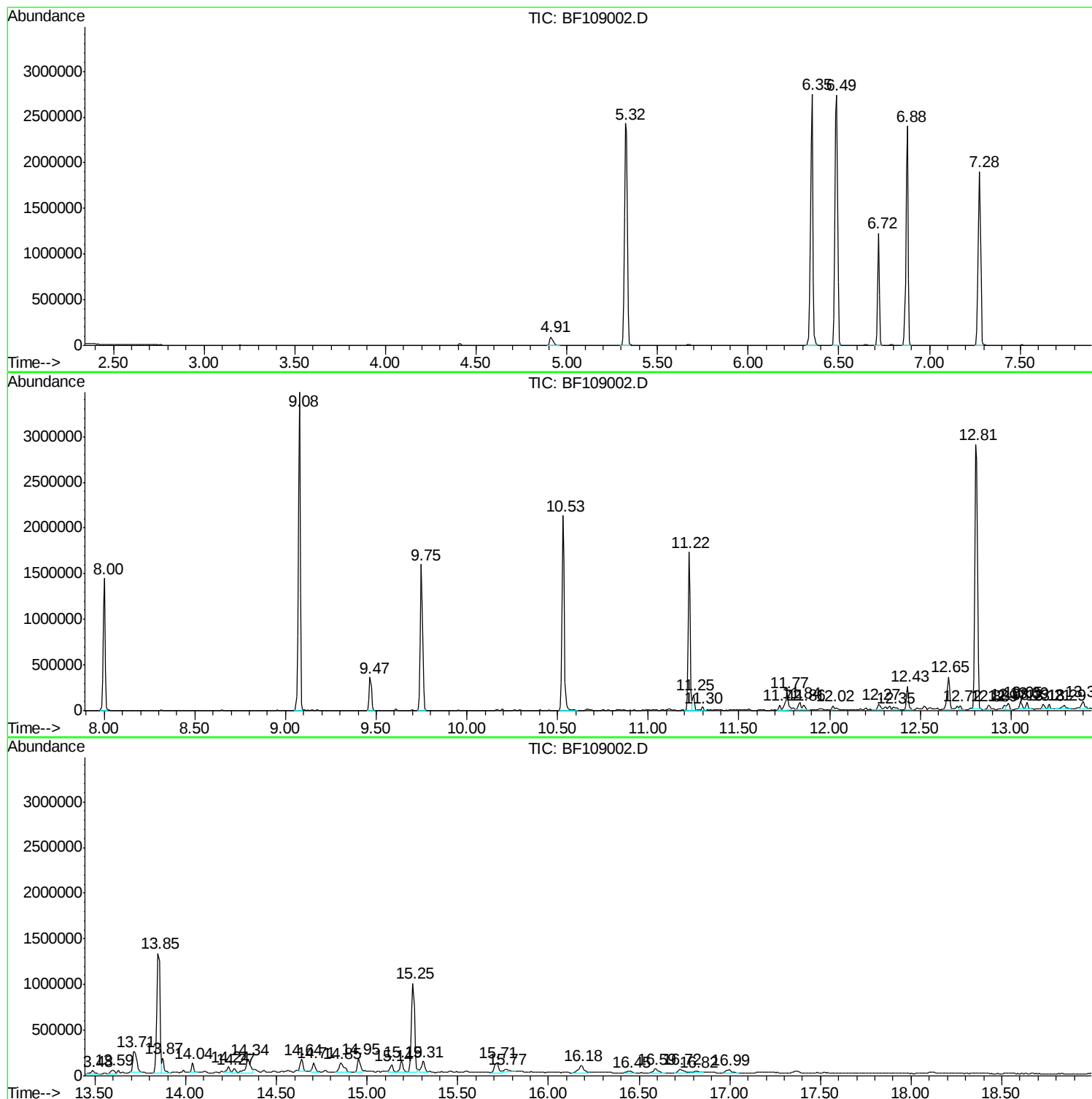
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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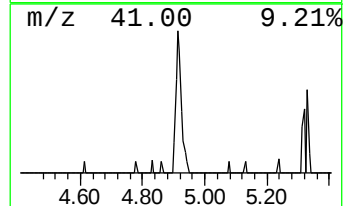
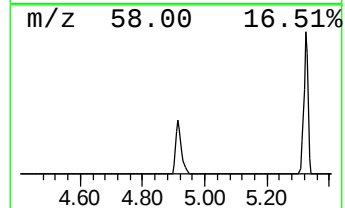
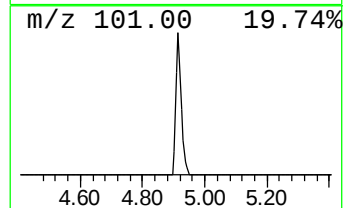
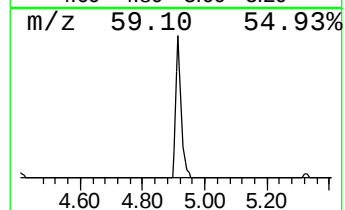
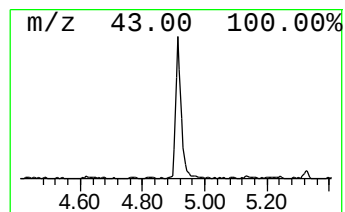
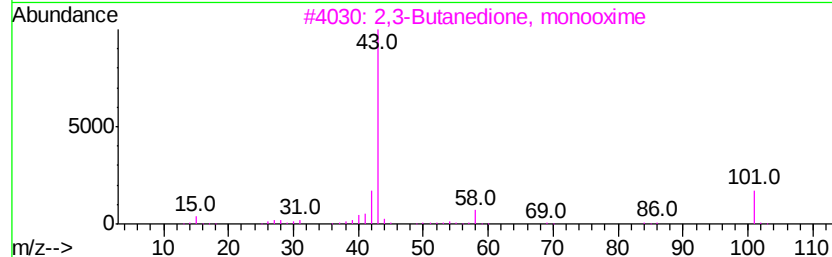
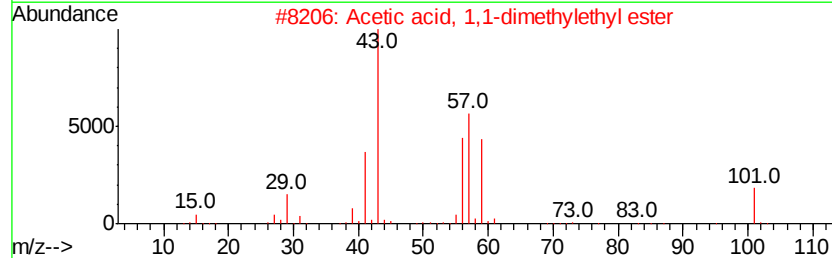
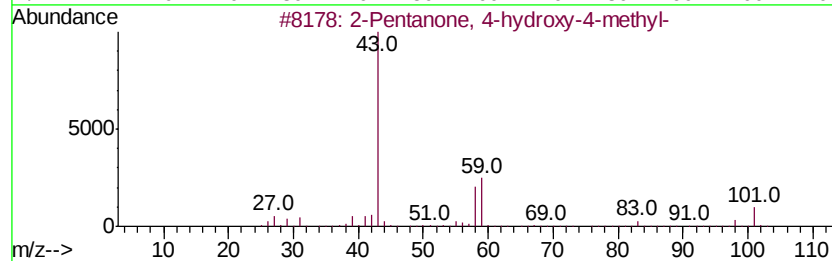
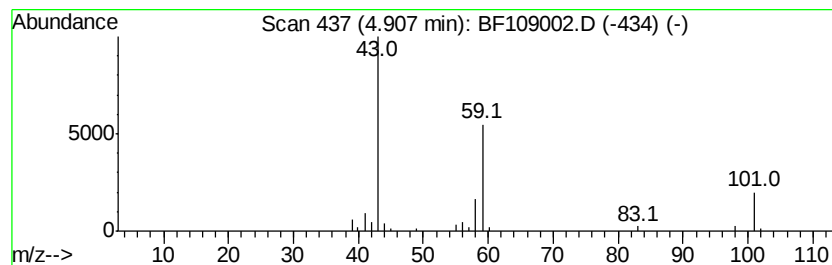
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.41 ng	111756	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol	102	C6H14O	000623-37-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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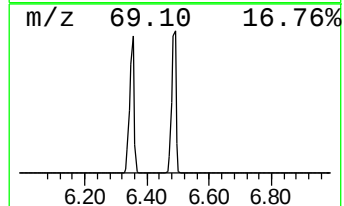
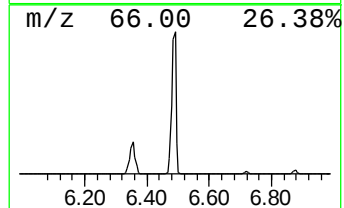
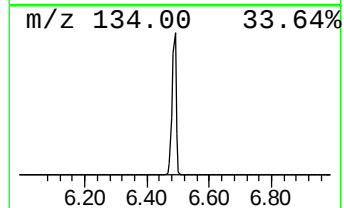
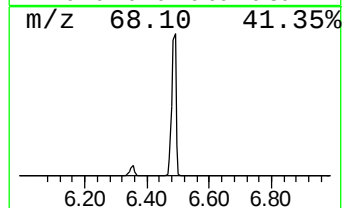
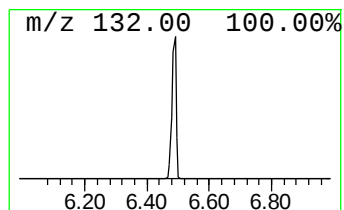
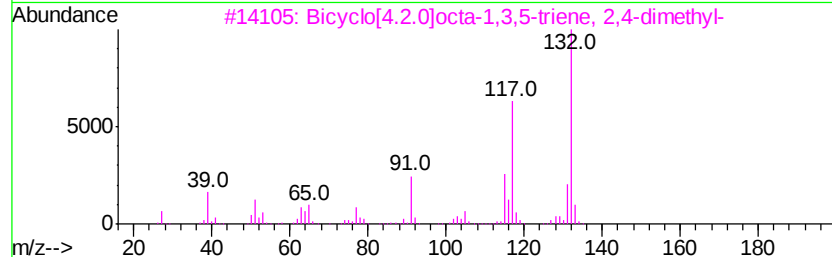
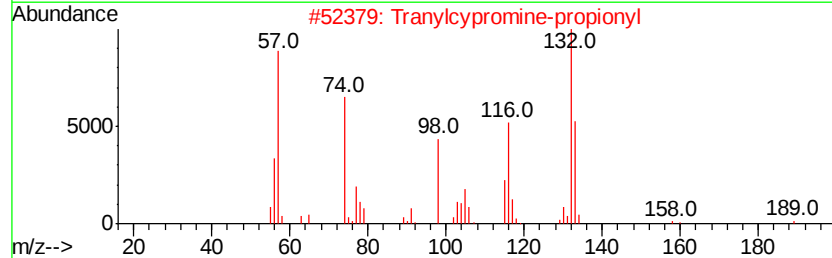
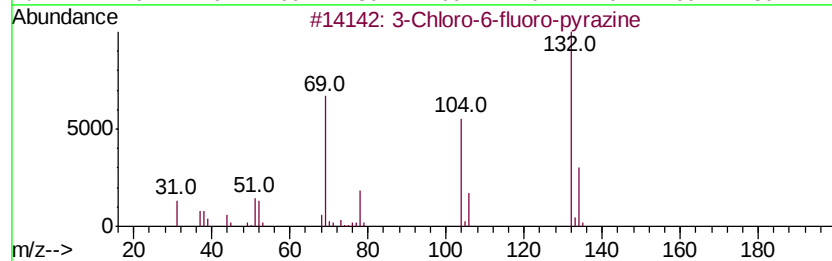
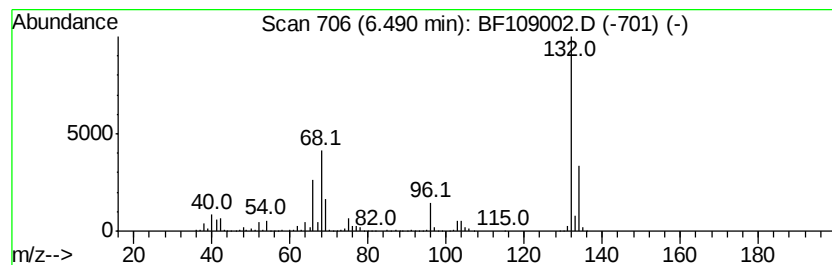
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	57.47 ng	2668120	1,4-Dichlorobenzene-d4	6.72

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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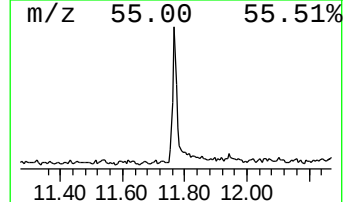
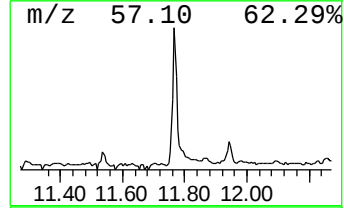
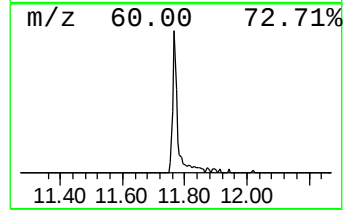
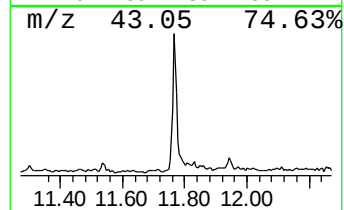
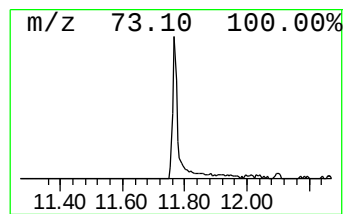
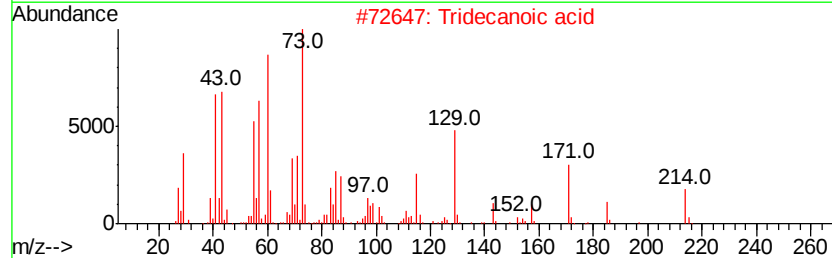
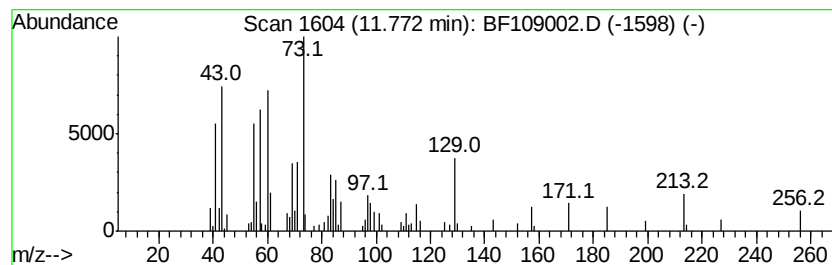
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.03 ng	227444	Phenanthrene-d10	11.22

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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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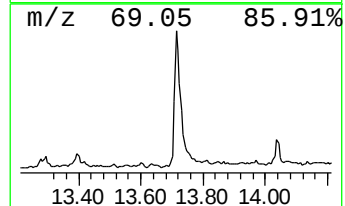
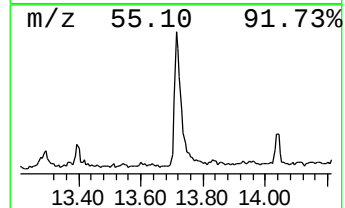
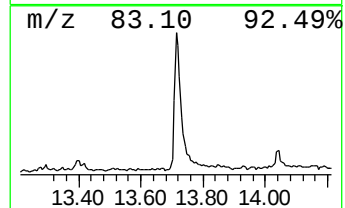
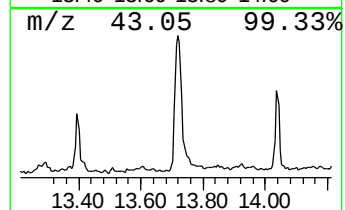
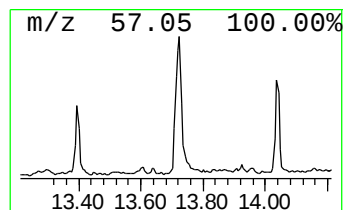
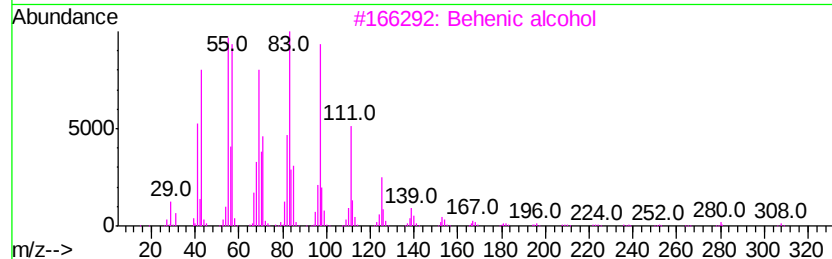
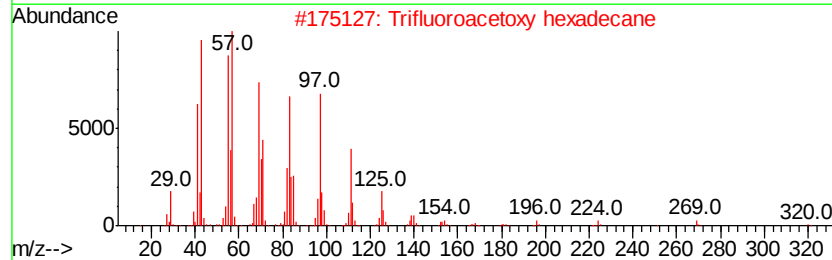
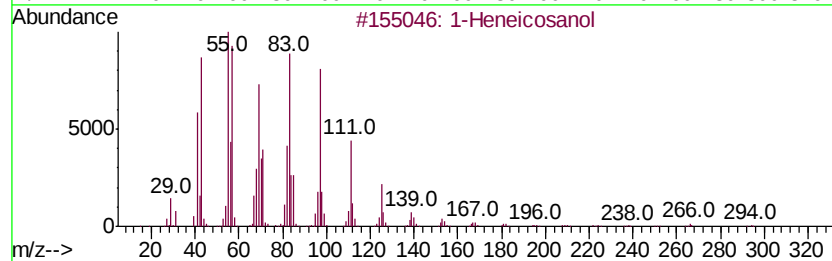
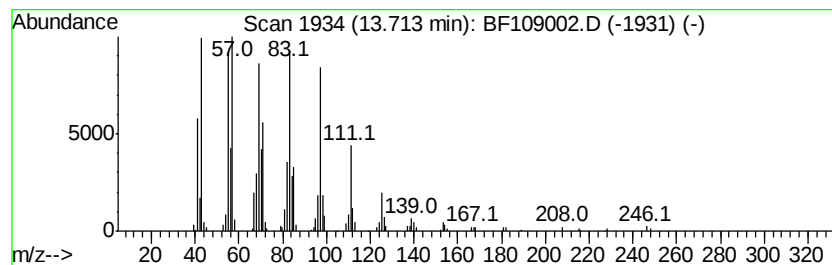
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.65 ng	331051	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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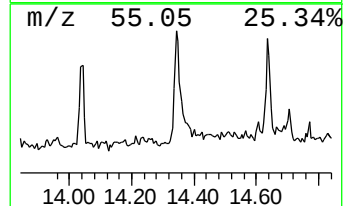
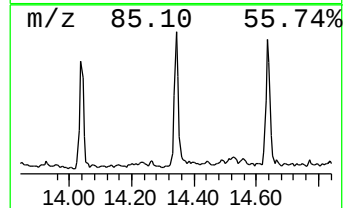
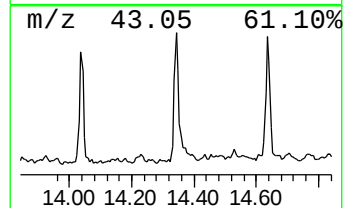
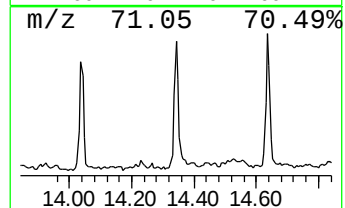
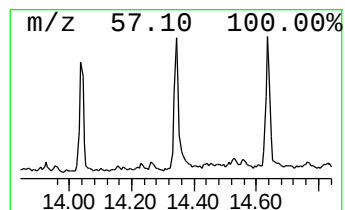
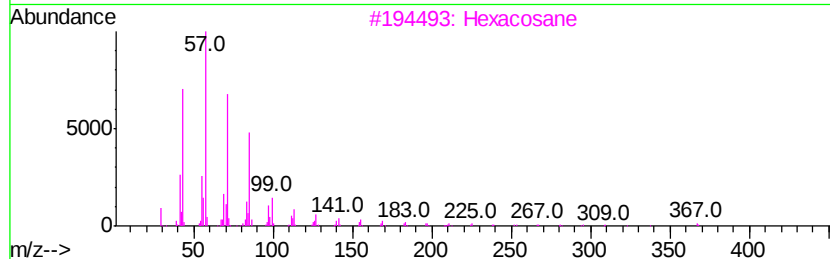
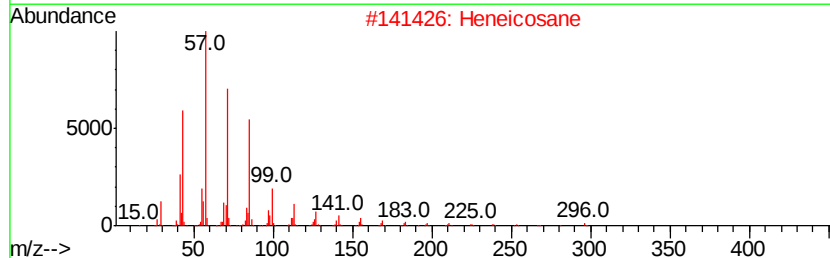
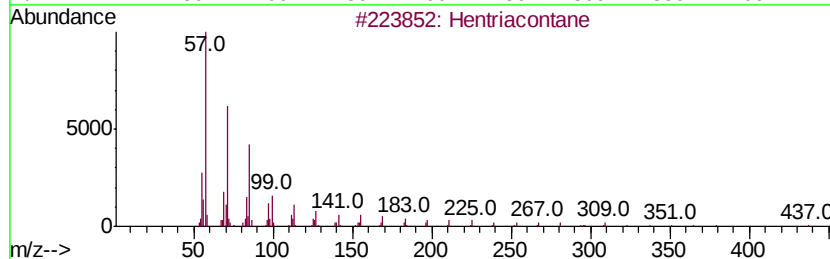
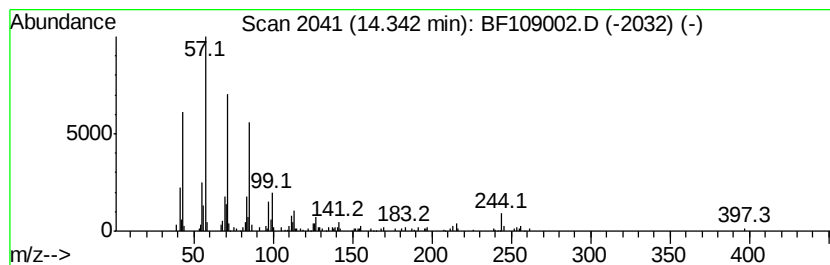
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.72 ng	265001	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	87
2	Heneicosane		296	C21H44	000629-94-7	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Heptadecane		240	C17H36	000629-78-7	83
5	2-methyloctacosane		408	C29H60	1000376-72-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
Operator : JU/SJ
Sample : J4906-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-8

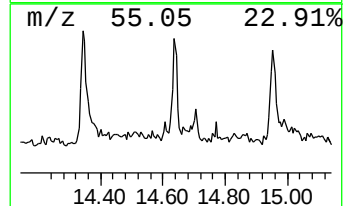
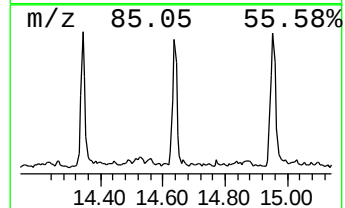
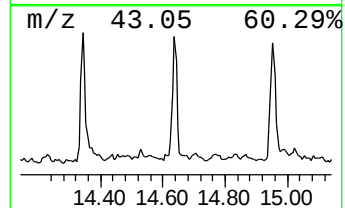
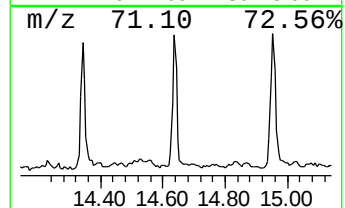
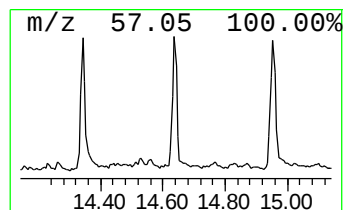
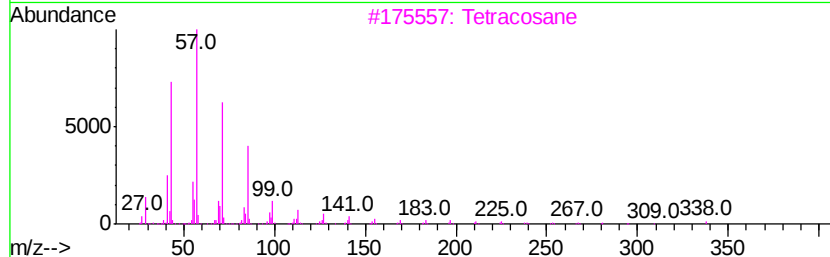
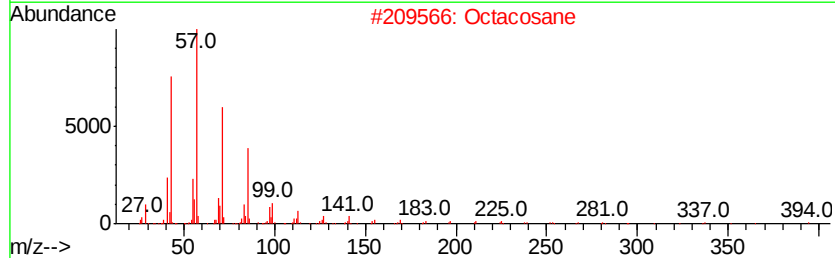
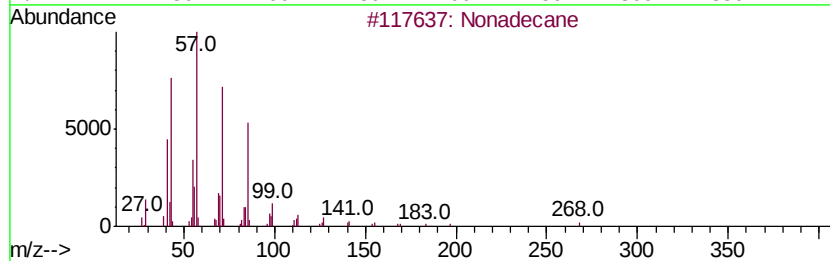
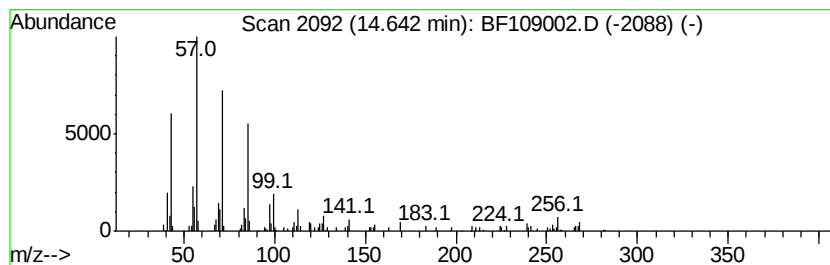
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.45 ng	133382	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-8

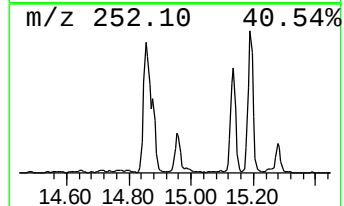
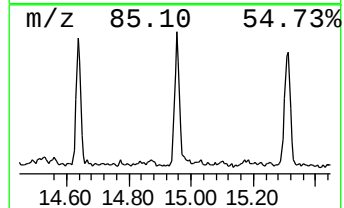
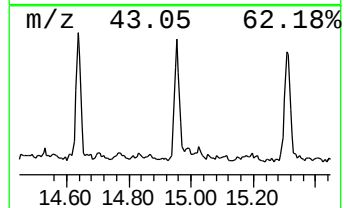
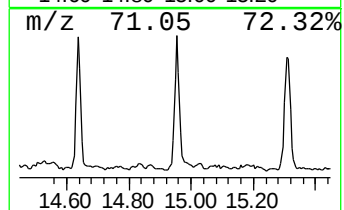
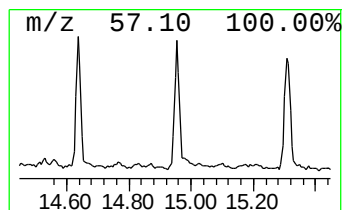
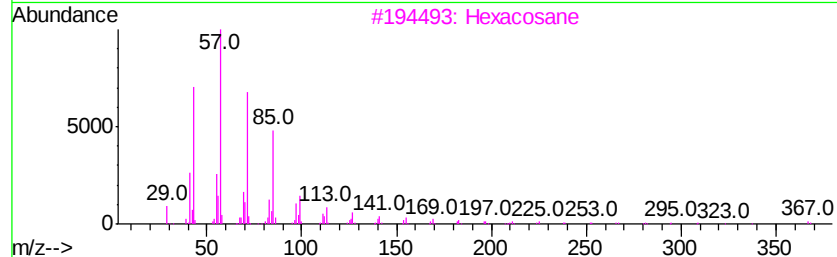
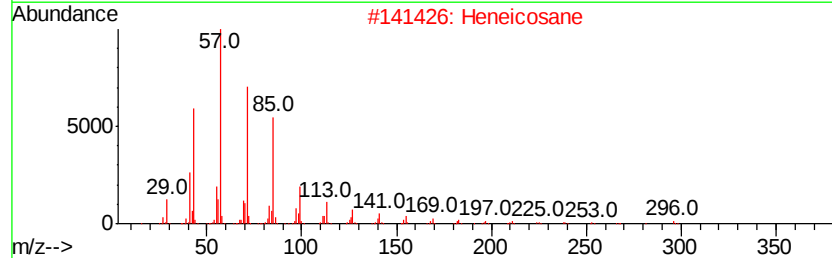
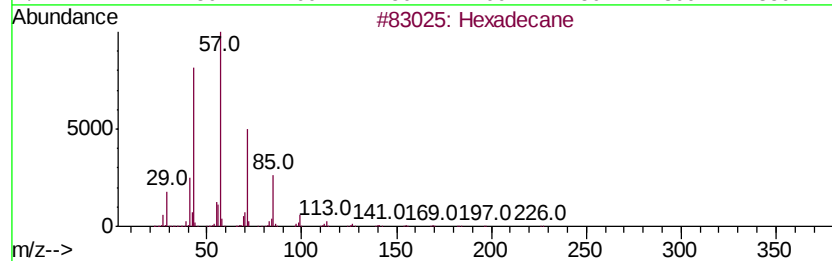
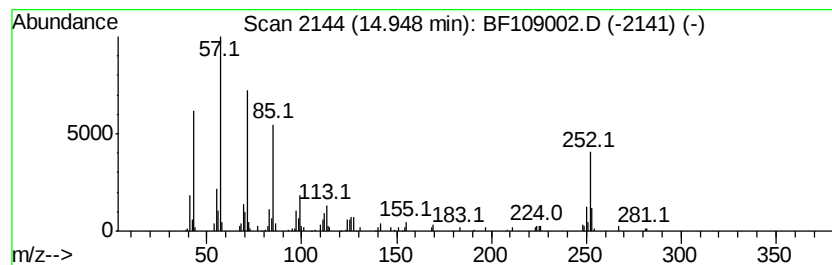
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.07 ng	167040	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Heneicosane		296	C21H44	000629-94-7	60
3	Hexacosane		366	C26H54	000630-01-3	60
4	10-Methylnonadecane		282	C20H42	056862-62-5	58
5	Eicosane		282	C20H42	000112-95-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
Operator : JU/SJ
Sample : J4906-13
Misc :
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Instrument :
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ClientSampleId :
SP-PIT-8

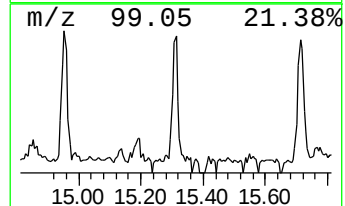
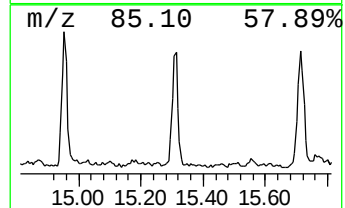
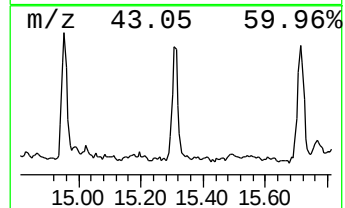
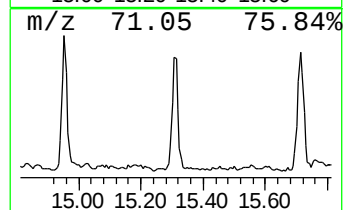
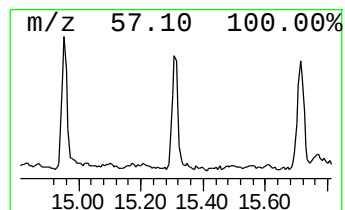
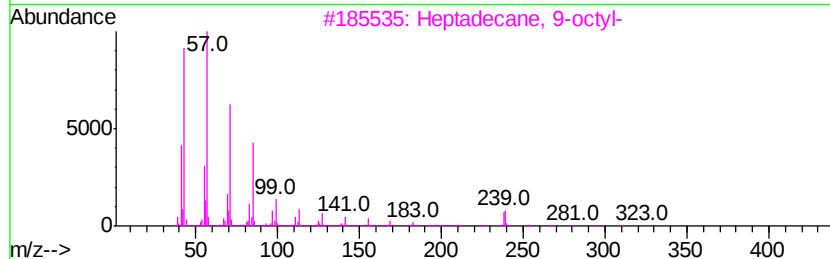
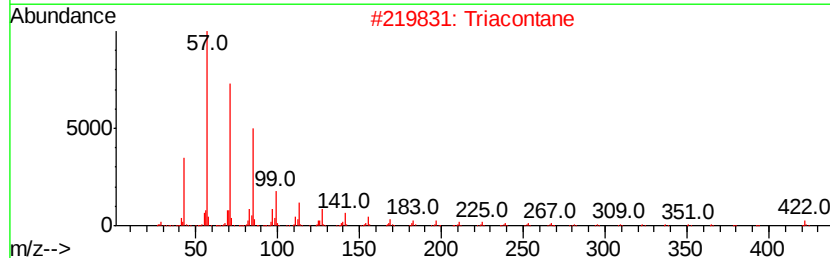
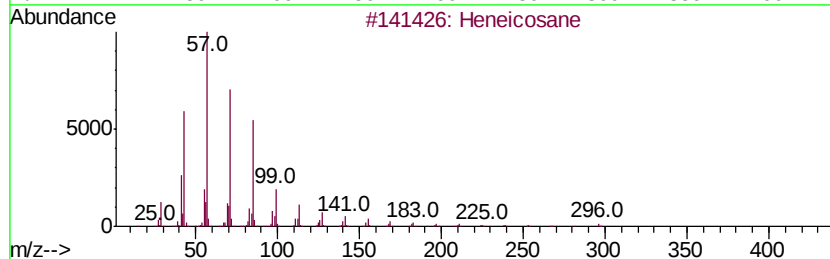
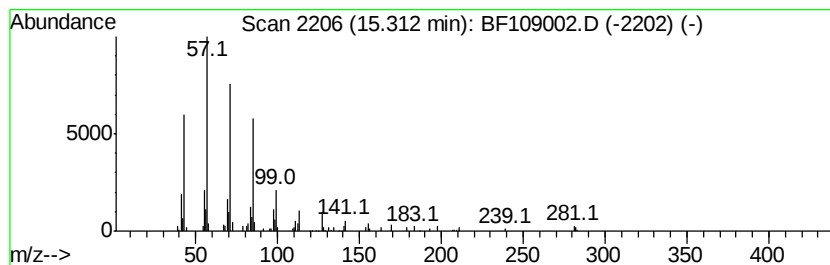
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.64 ng	144098	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Triacontane		422	C30H62	000638-68-6	90
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
Operator : JU/SJ
Sample : J4906-13
Misc :
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Instrument :
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ClientSampleId :
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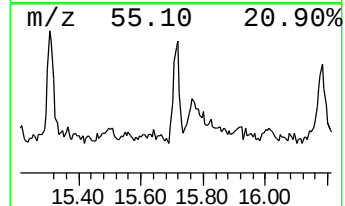
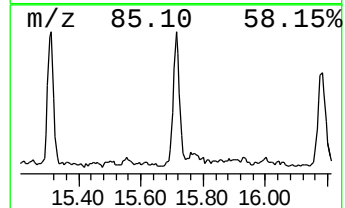
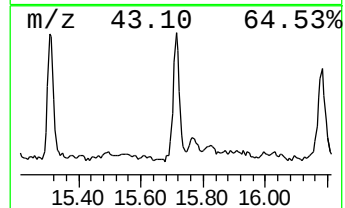
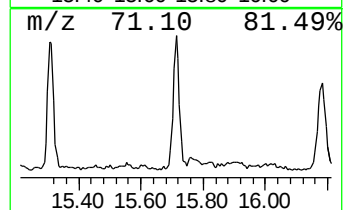
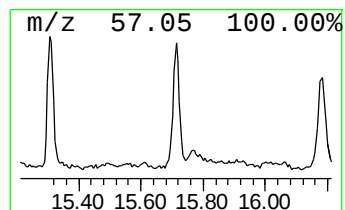
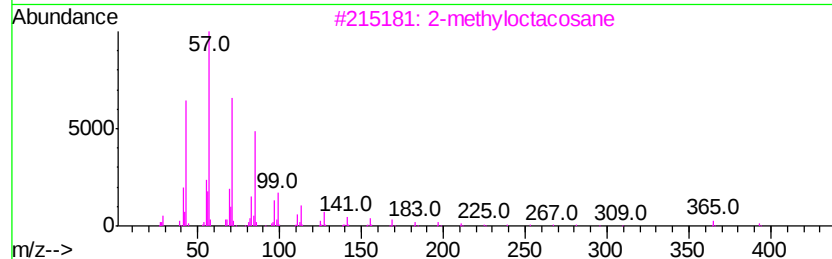
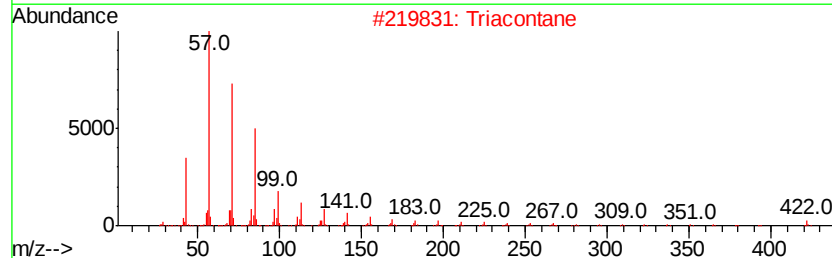
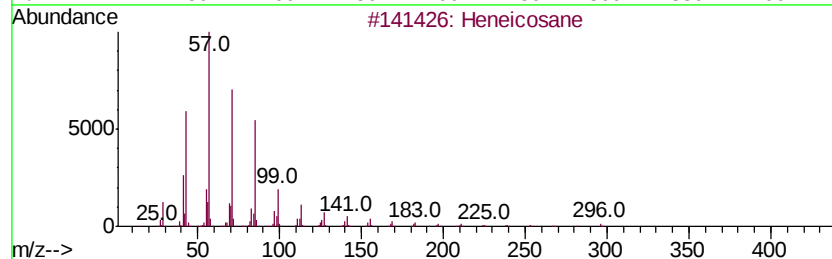
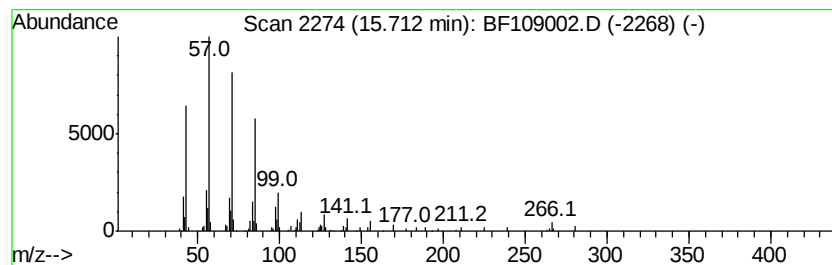
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.34 ng	181720	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacotane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
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Misc :
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SP-PIT-8

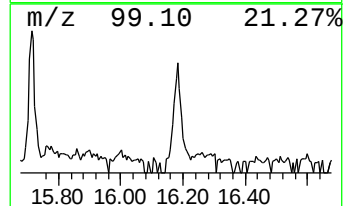
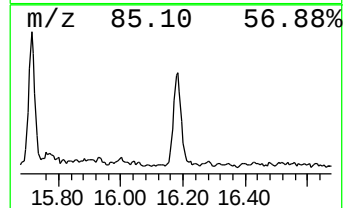
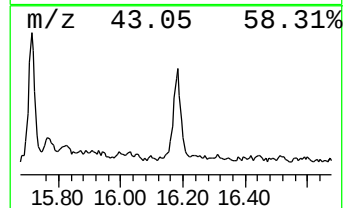
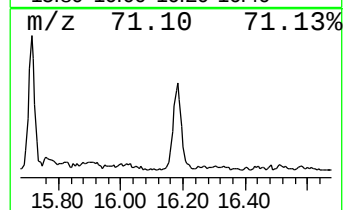
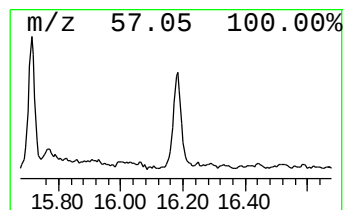
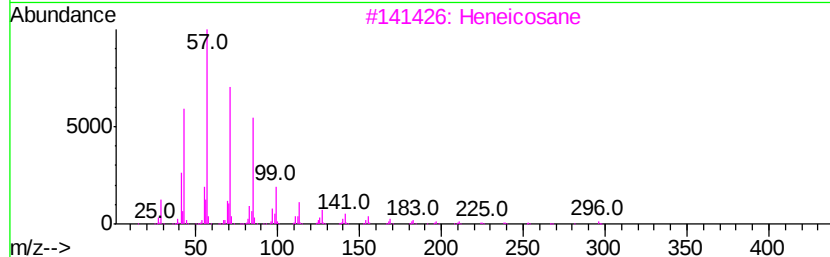
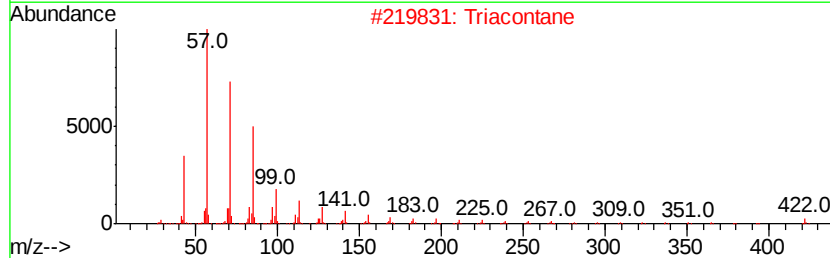
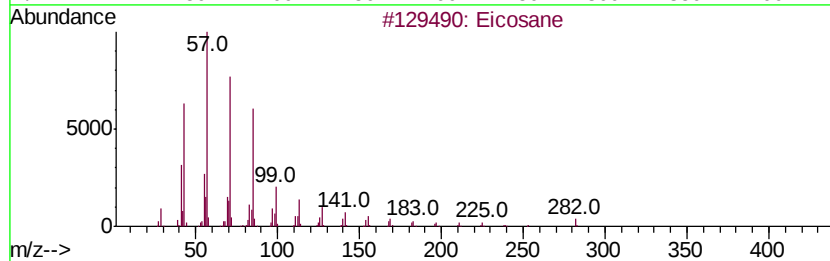
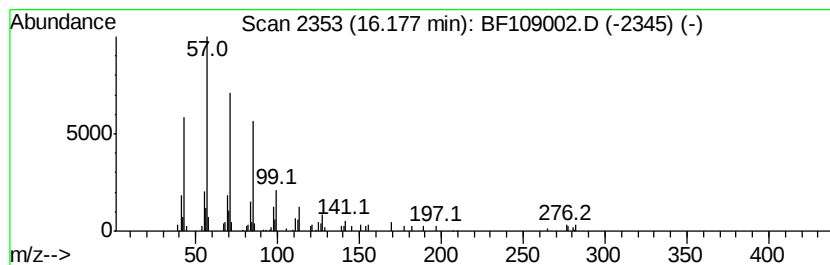
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	3.22 ng	175348	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Triacontane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
Data File : BF109002.D
Acq On : 14 Sep 2018 18:36
Operator : JU/SJ
Sample : J4906-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.49	6.49	57.5	ng	2668120	1	6.72	928600	20.0
n-Hexadecanoic acid	11.77	3.0	ng	227444	4	11.22	1502420	20.0
1-Heneicosanol	13.71	4.7	ng	331051	5	13.85	1424010	20.0
Hentriacontane	14.34	3.7	ng	265001	5	13.85	1424010	20.0
Nonadecane	14.64	2.5	ng	133382	6	15.25	1089740	20.0
Hexadecane	14.95	3.1	ng	167040	6	15.25	1089740	20.0
Heneicosane	15.31	2.6	ng	144098	6	15.25	1089740	20.0
2-methyloctacosane	15.71	3.3	ng	181720	6	15.25	1089740	20.0
Eicosane	16.18	3.2	ng	175348	6	15.25	1089740	20.0