

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
 Data File : BF100803.D
 Acq On : 22 Nov 2017 2:26
 Operator : SJ/JU
 Sample : I6466-07
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHAP-2-E(0-1)

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-BF110817.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	5.099	508	512	521	rBV	227835	284301	15.70%	1.703%
2	5.493	574	579	582	rBV	1563165	1476444	81.55%	8.846%
3	6.498	745	750	762	rVB	1427817	1595403	88.12%	9.559%
4	6.640	770	774	778	rBV	1604415	1563665	86.37%	9.369%
5	6.875	810	814	817	rBV	526133	480157	26.52%	2.877%
6	7.028	836	840	843	rBV	1473801	1268373	70.06%	7.600%
7	7.434	904	909	912	rBV	1067989	977974	54.02%	5.860%
8	8.151	1028	1031	1035	rBV	718340	610422	33.72%	3.657%
9	8.704	1122	1125	1129	rBV	101308	84791	4.68%	0.508%
10	9.228	1209	1214	1217	rBV	2123071	1810457	100.00%	10.848%
11	9.616	1277	1280	1284	rBV	64520	57165	3.16%	0.343%
12	9.910	1326	1330	1334	rBV	745586	633514	34.99%	3.796%
13	10.622	1447	1451	1454	rBV	393228	327558	18.09%	1.963%
14	10.698	1460	1464	1467	rBV	972591	825912	45.62%	4.949%
15	10.804	1479	1482	1483	rBV	27119	24966	1.38%	0.150%
16	11.251	1555	1558	1560	rBV	29704	22388	1.24%	0.134%
17	11.280	1560	1563	1569	rVB4	22032	32305	1.78%	0.194%
18	11.392	1579	1582	1585	rBV	565359	554337	30.62%	3.321%
19	11.416	1585	1586	1590	rVB	92365	64940	3.59%	0.389%
20	11.675	1628	1630	1635	rVV2	28941	25198	1.39%	0.151%
21	11.728	1635	1639	1643	rVB6	15057	22875	1.26%	0.137%
22	11.910	1664	1670	1676	rBV2	58955	111571	6.16%	0.669%
23	12.004	1683	1686	1689	rBV2	32406	37235	2.06%	0.223%
24	12.028	1689	1690	1694	rVB2	28027	20279	1.12%	0.122%
25	12.080	1694	1699	1704	rBV2	31251	38829	2.14%	0.233%
26	12.186	1715	1717	1721	rBV	19352	21937	1.21%	0.131%
27	12.445	1758	1761	1763	rBV	32267	30268	1.67%	0.181%
28	12.475	1763	1766	1769	rVV3	35493	37232	2.06%	0.223%
29	12.527	1773	1775	1780	rBV3	18503	26433	1.46%	0.158%
30	12.610	1785	1789	1793	rBV	167962	159287	8.80%	0.954%
31	12.792	1817	1820	1822	rVB3	24341	20368	1.13%	0.122%
32	12.839	1822	1828	1834	rVV	206896	236848	13.08%	1.419%
33	12.892	1834	1837	1840	rVB2	25074	26249	1.45%	0.157%
34	12.980	1847	1852	1855	rBV	1207102	1121946	61.97%	6.722%

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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	13.051	1861	1864	1869	rBV6	30611	42196	2.33%	0.253%
36	13.163	1881	1883	1887	rVB2	29362	24292	1.34%	0.146%
37	13.198	1887	1889	1892	rBV2	27104	24099	1.33%	0.144%
38	13.269	1898	1901	1904	rBV2	41534	40075	2.21%	0.240%
39	13.363	1914	1917	1919	rBV	25589	21730	1.20%	0.130%
40	13.392	1919	1922	1925	rVV	24273	22730	1.26%	0.136%
41	13.539	1944	1947	1950	rBV3	24430	28781	1.59%	0.172%
42	13.669	1967	1969	1973	rVB	30791	33388	1.84%	0.200%
43	13.780	1984	1988	1991	rBV6	25671	40633	2.24%	0.243%
44	13.833	1995	1997	1999	rBV	23750	25471	1.41%	0.153%
45	13.863	1999	2002	2008	rVB2	100113	124397	6.87%	0.745%
46	14.033	2026	2031	2034	rBV2	549212	609850	33.68%	3.654%
47	14.057	2034	2035	2043	rVB	115814	98901	5.46%	0.593%
48	14.186	2054	2057	2060	rBV4	28622	32585	1.80%	0.195%
49	14.492	2106	2109	2115	rBV4	43016	69336	3.83%	0.415%
50	15.074	2205	2208	2212	rBV	99769	155469	8.59%	0.932%
51	15.133	2216	2218	2222	rVB3	36914	31958	1.77%	0.191%
52	15.380	2258	2260	2265	rVB	61266	73353	4.05%	0.440%
53	15.445	2268	2271	2277	rVV	97536	127976	7.07%	0.767%
54	15.510	2278	2282	2292	rVB	312681	430840	23.80%	2.581%

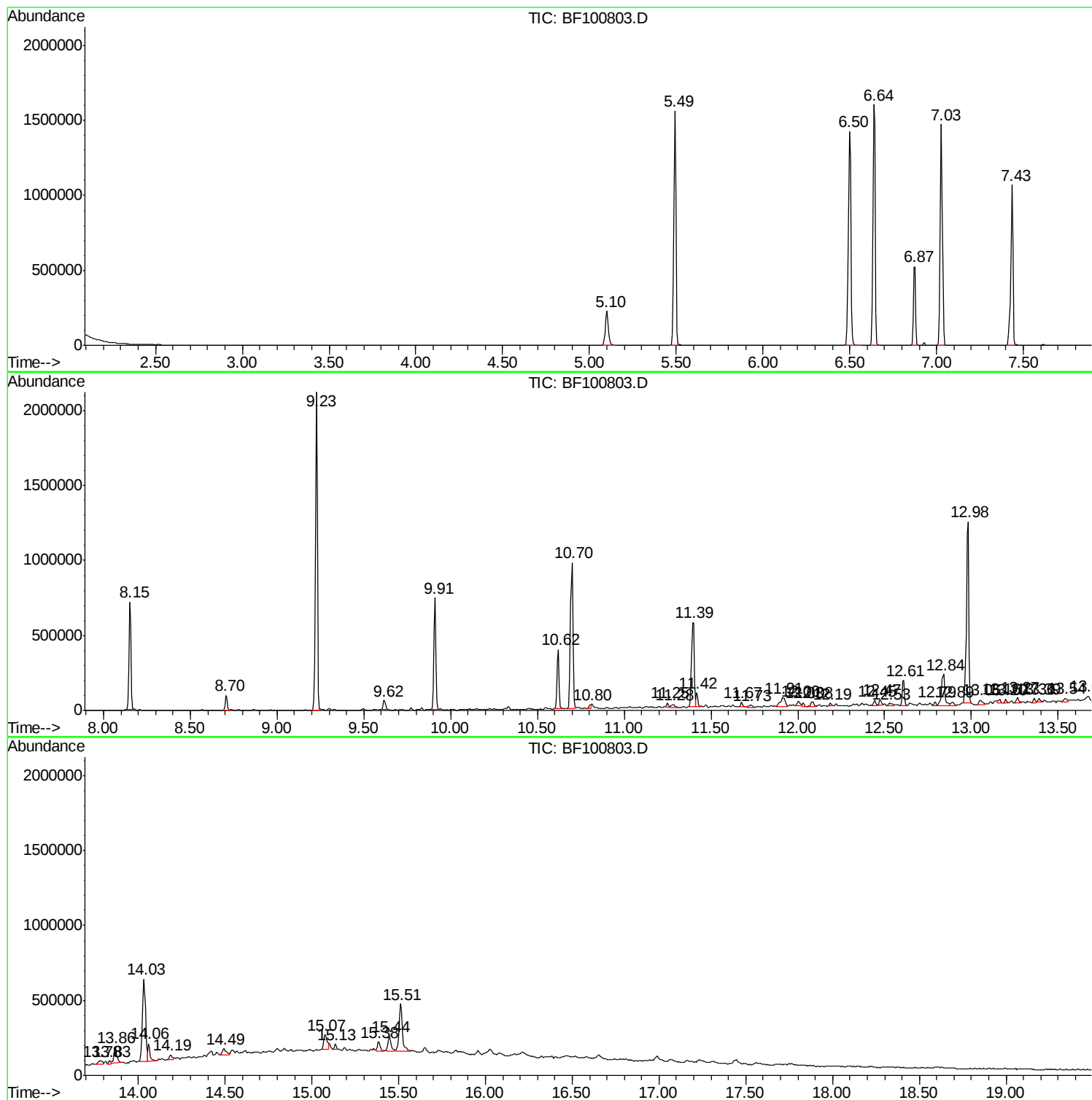
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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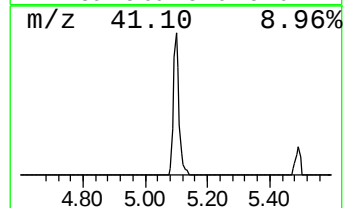
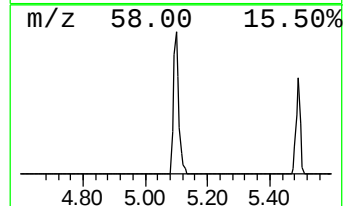
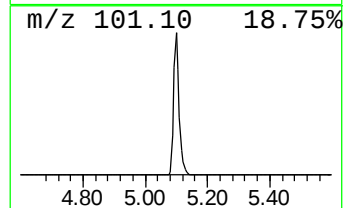
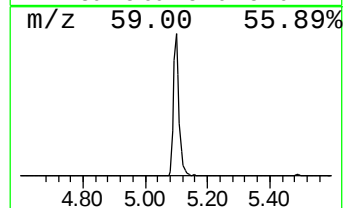
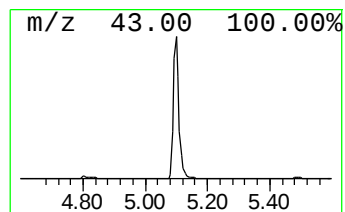
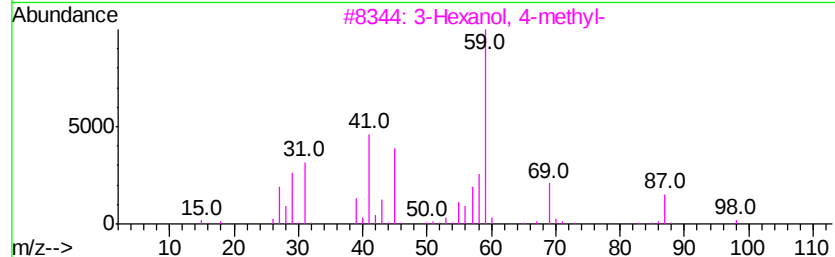
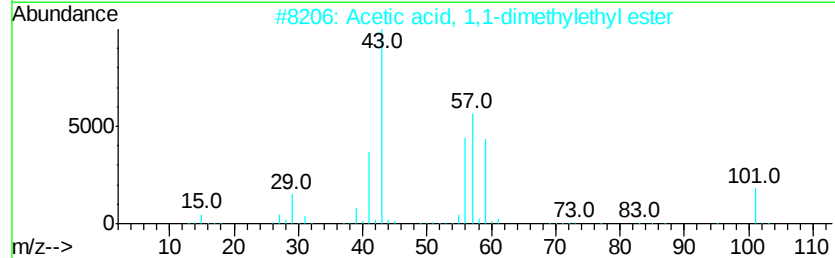
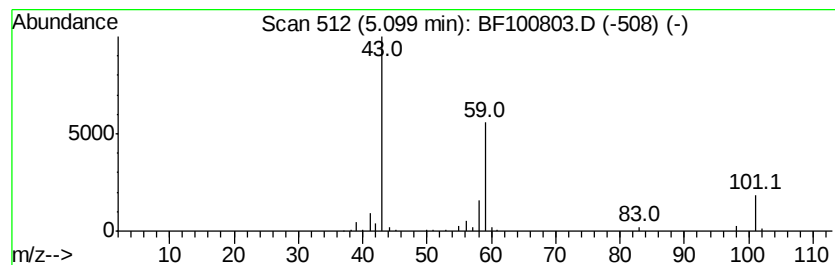
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	11.84 ng	284301	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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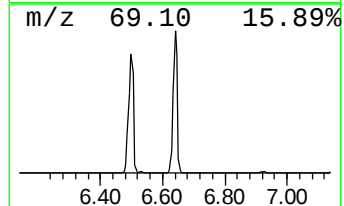
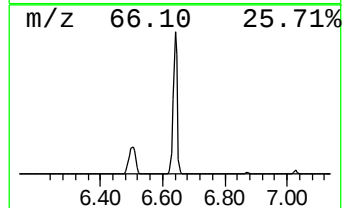
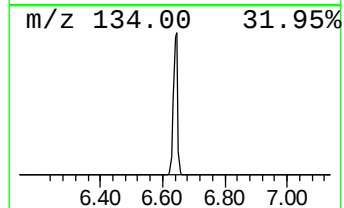
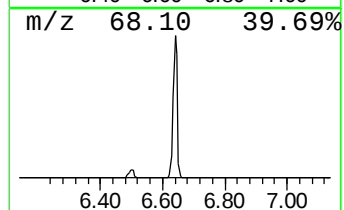
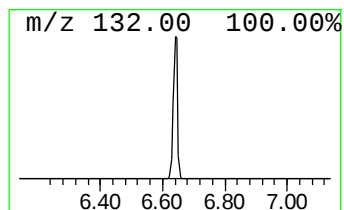
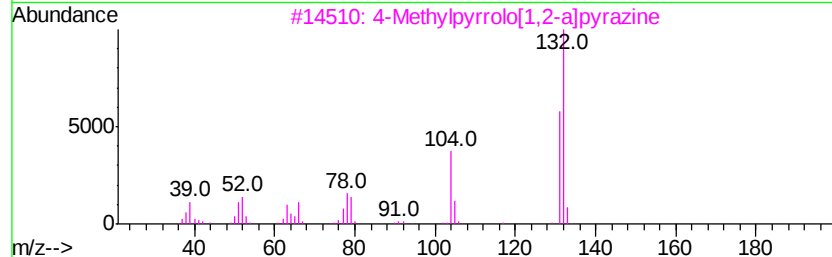
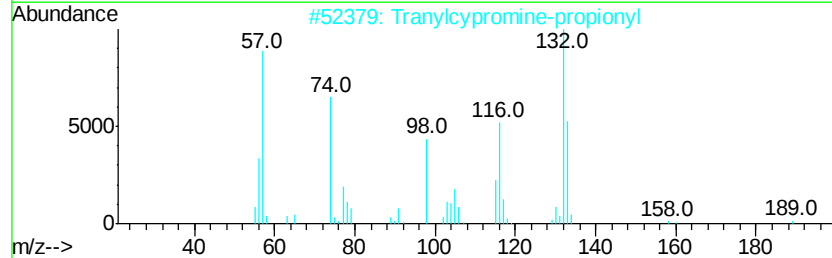
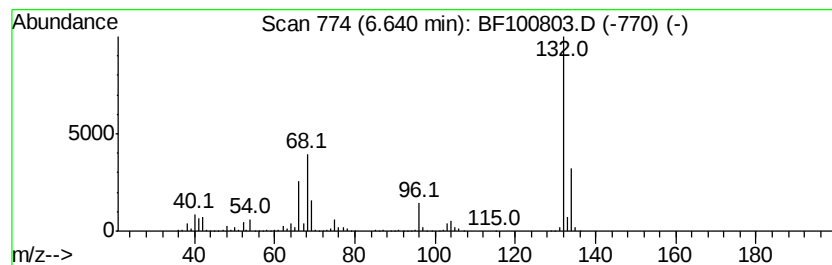
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	65.13 ng	1563670	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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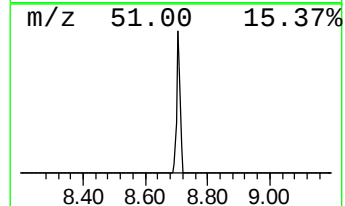
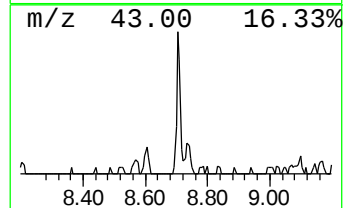
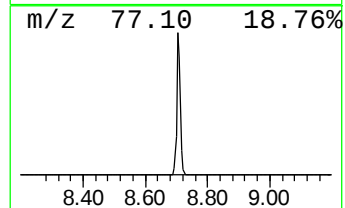
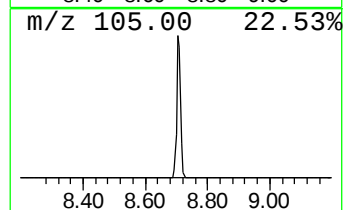
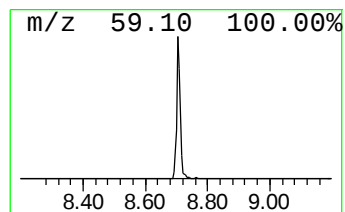
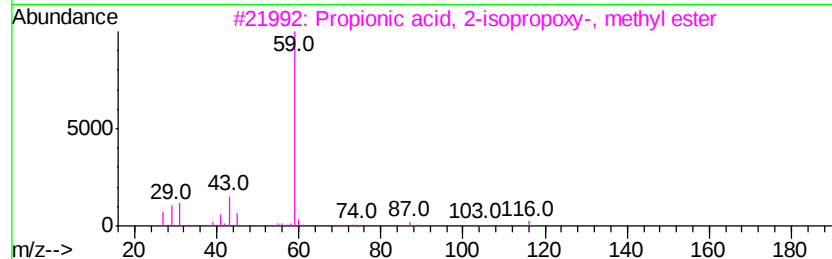
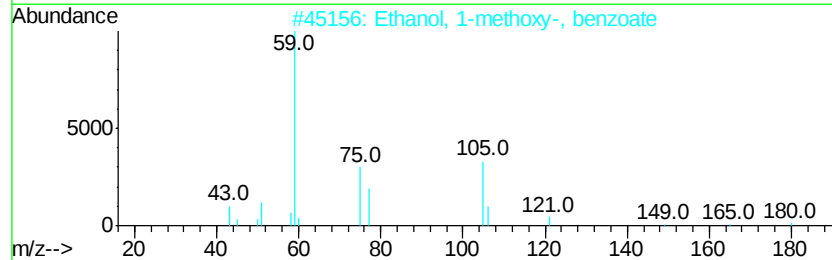
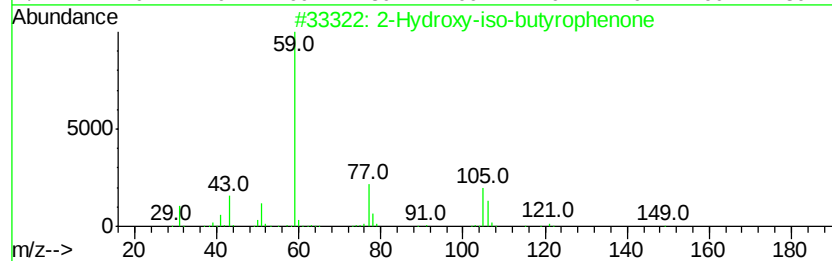
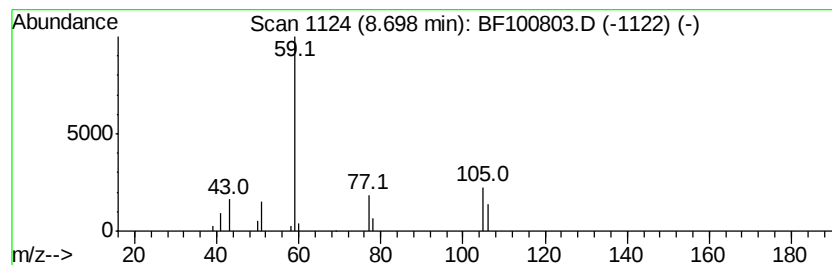
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	2.78 ng	84791	Napthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3		Propionic acid, 2-isopropoxy-, methyl ester	146	C7H14O3	1000151-15-1	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



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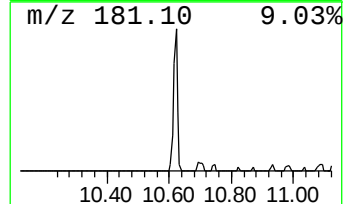
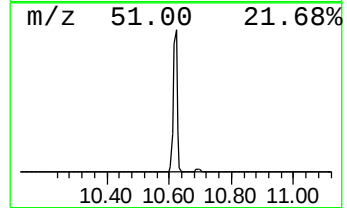
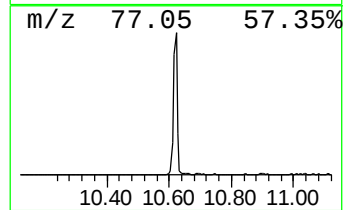
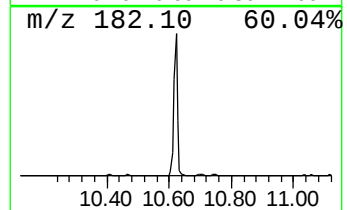
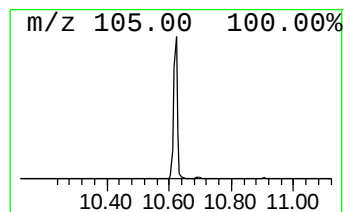
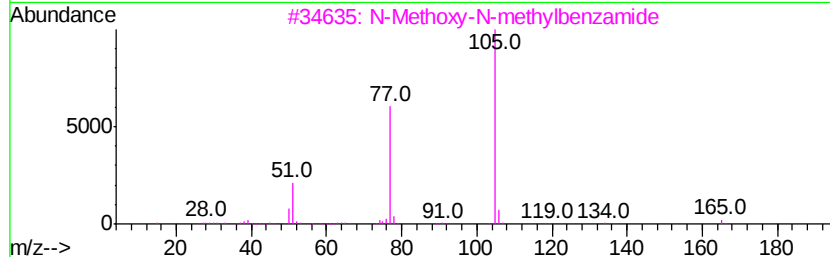
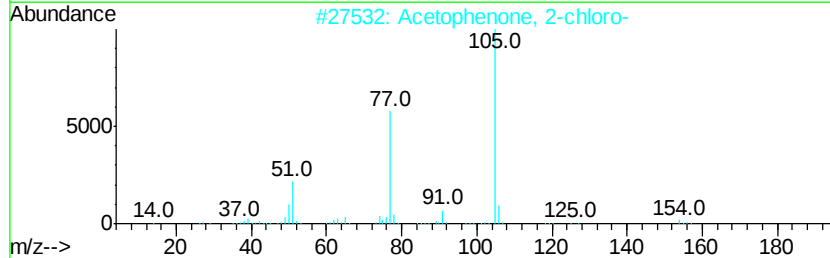
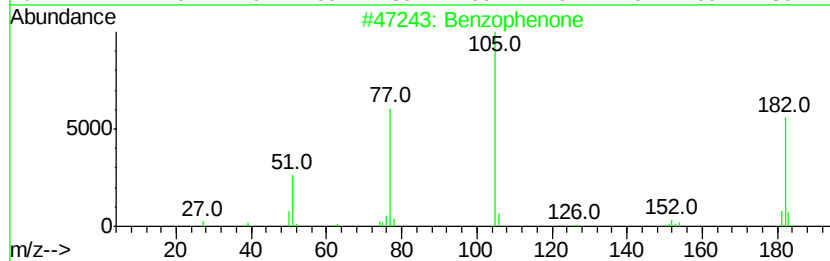
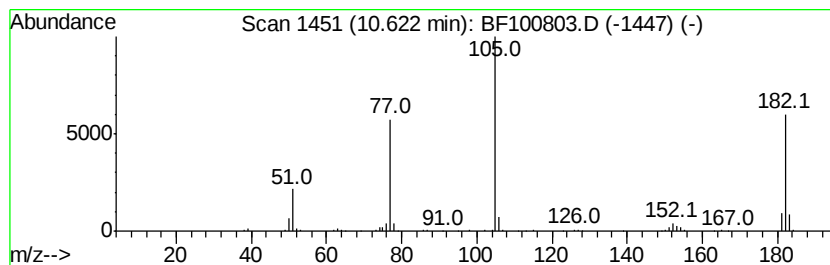
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	10.34 ng	327558	Acenaphthene-d10	9.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3		N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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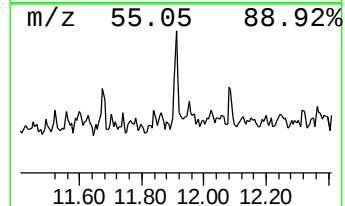
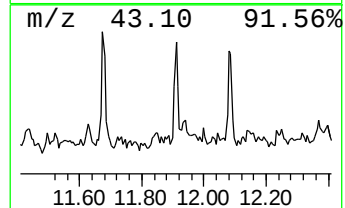
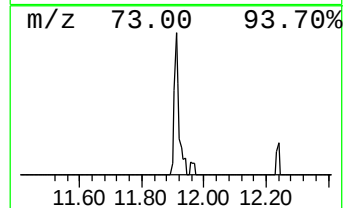
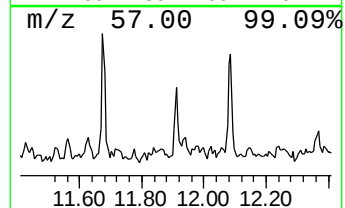
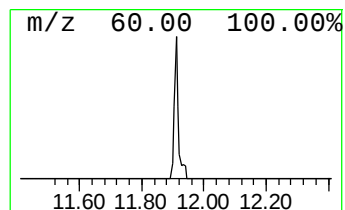
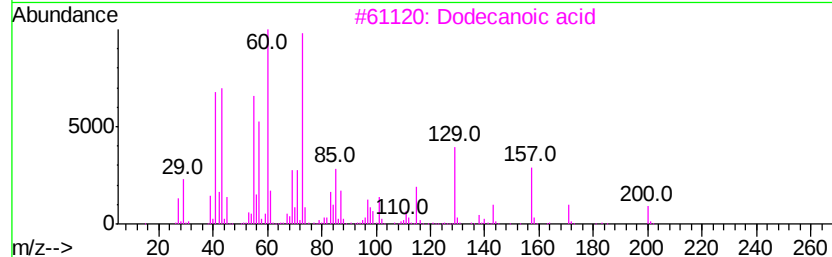
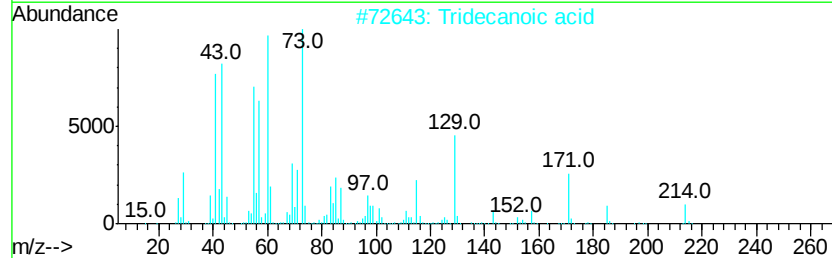
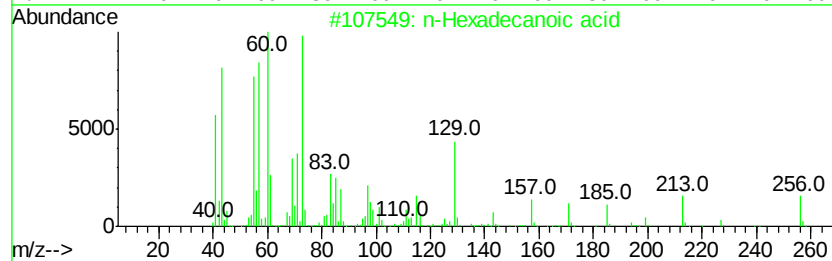
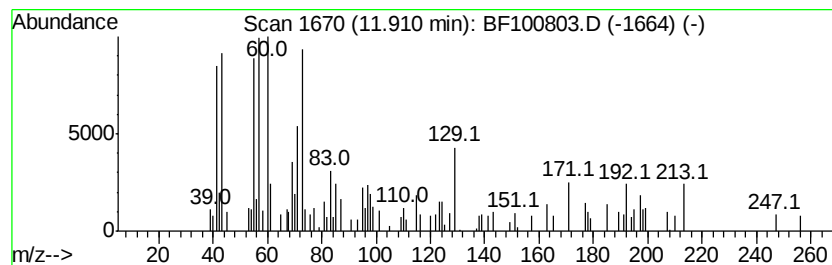
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	4.03 ng	111571	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
2		Tridecanoic acid	214	C13H26O2	000638-53-9	52
3		Dodecanoic acid	200	C12H24O2	000143-07-7	43
4		Undecanoic acid	186	C11H22O2	000112-37-8	35
5		3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100803.D
Acq On : 22 Nov 2017 2:26
Operator : SJ/JU
Sample : I6466-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHAP-2-E(0-1)

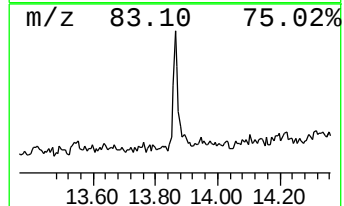
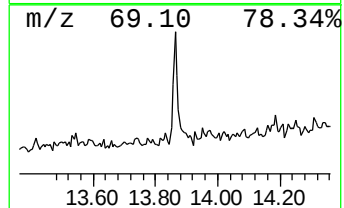
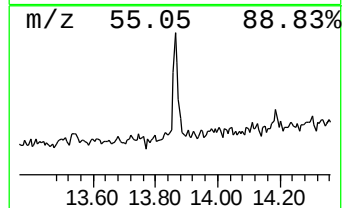
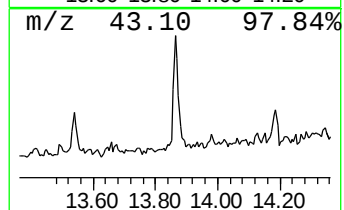
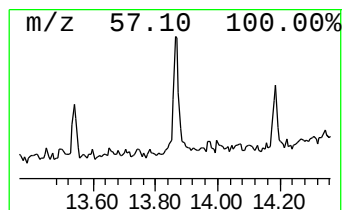
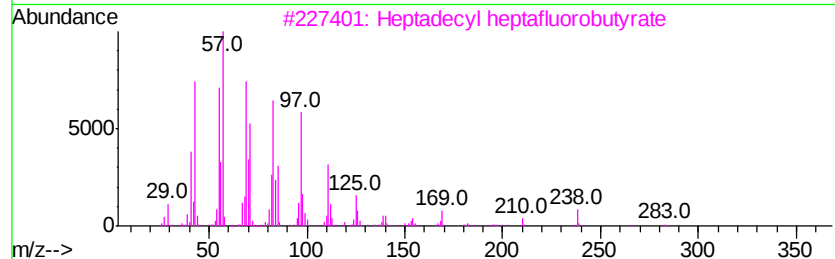
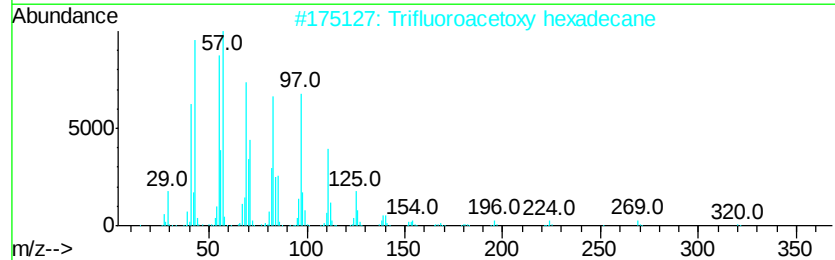
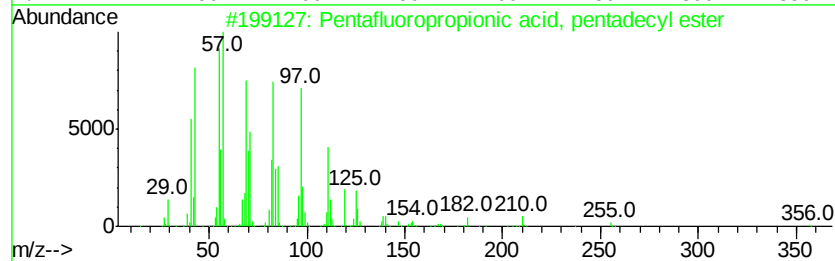
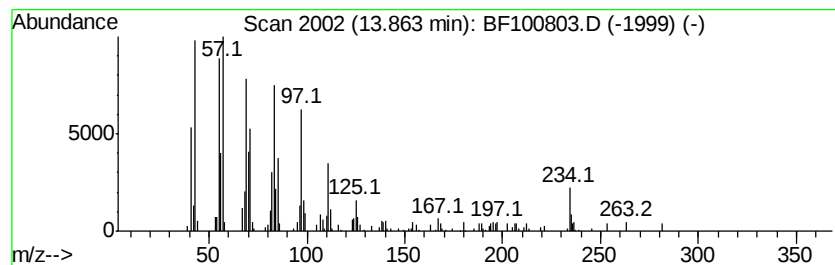
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.08 ng	124397	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



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Acq On : 22 Nov 2017 2:26
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Sample : I6466-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

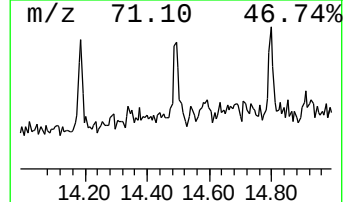
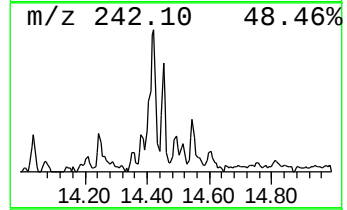
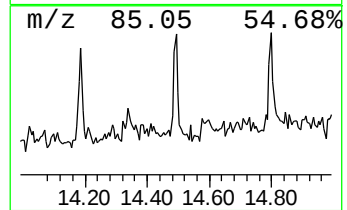
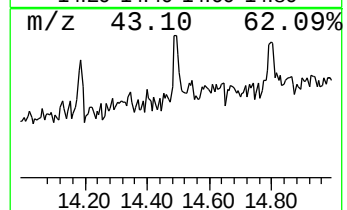
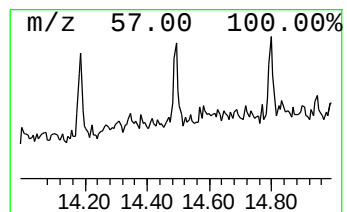
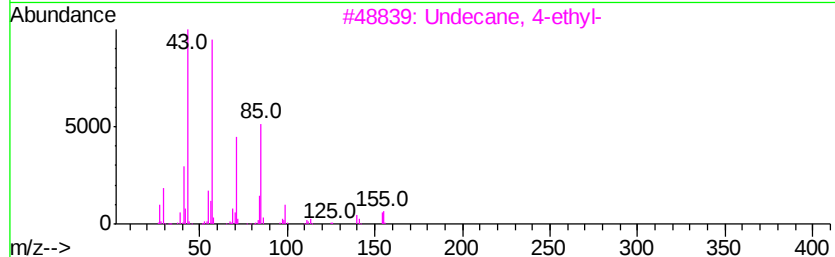
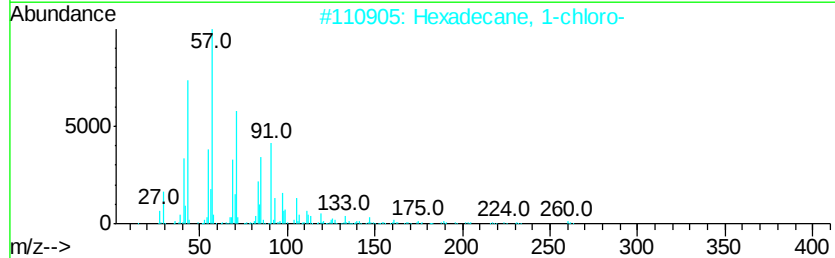
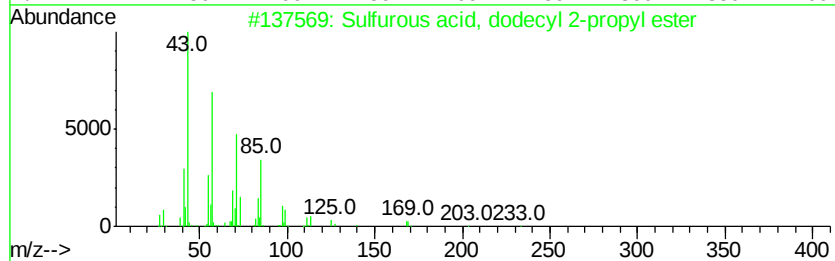
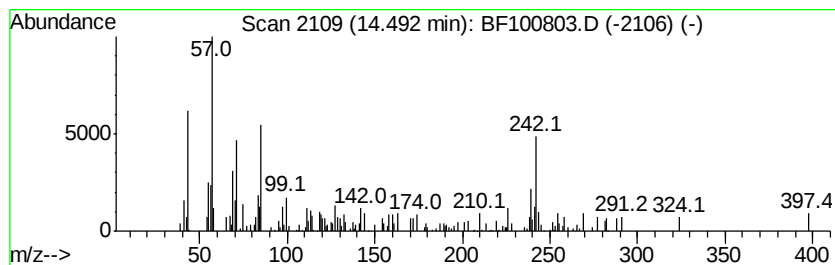
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ClientSampleId :
CHAP-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.49 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.27 ng	69336	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfurous acid, dodecyl 2-propyl...	292 C15H32O3S	1000309-12-3 35
2		Hexadecane, 1-chloro-	260 C16H33Cl	004860-03-1 35
3		Undecane, 4-ethyl-	184 C13H28	017312-59-3 35
4		Sulfurous acid, 2-ethylhexyl iso...	278 C14H30O3S	1000309-19-0 35
5		Sulfurous acid, hexyl nonyl ester	292 C15H32O3S	1000309-13-1 35



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Sample : I6466-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHAP-2-E(0-1)

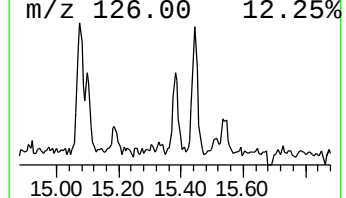
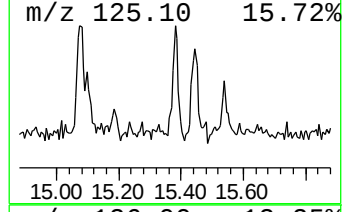
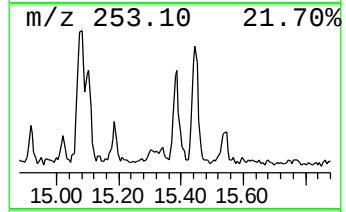
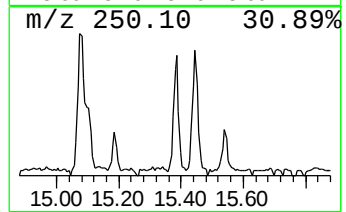
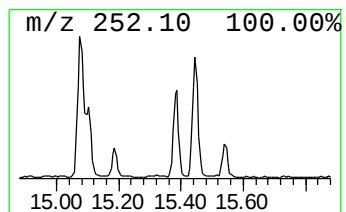
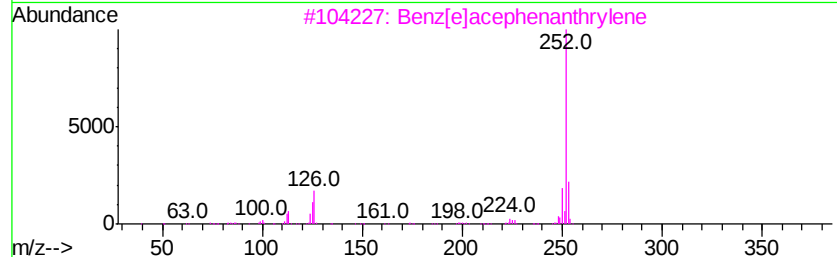
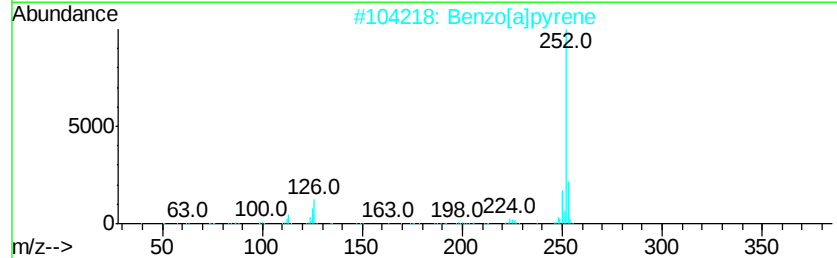
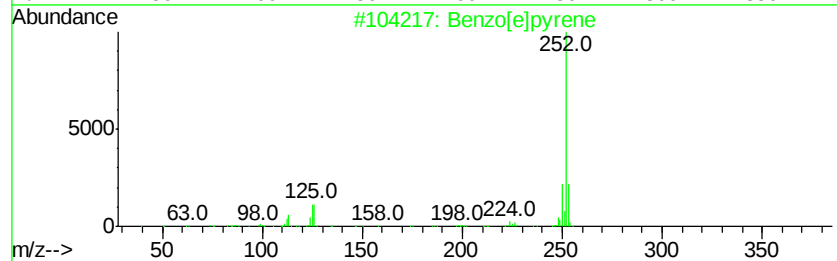
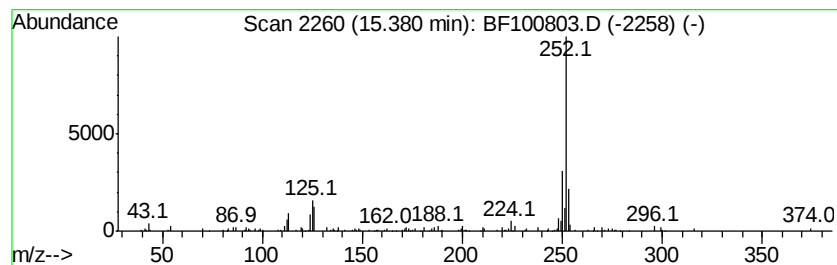
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	3.41 ng	73353	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[a]pyrene	252	C20H12	000050-32-8	95
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
4		Benzo[i]fluoranthene	252	C20H12	000205-82-3	93
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



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ALS Vial : 31 Sample Multiplier: 1

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BNA_F
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CHAP-2-E(0-1)

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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...	5.10	11.8	ng	284301	1	6.87	480157	20.0
unknown6.64	6.64	65.1	ng	1563670	1	6.87	480157	20.0
2-Hydroxy-iso-but...	8.70	2.8	ng	84791	2	8.15	610422	20.0
Benzophenone	10.62	10.3	ng	327558	3	9.91	633514	20.0
n-Hexadecanoic acid	11.91	4.0	ng	111571	4	11.40	554337	20.0
Pentafluoropropio...	13.86	4.1	ng	124397	5	14.03	609850	20.0
unknown14.49	14.49	2.3	ng	69336	5	14.03	609850	20.0
Benzo[e]pyrene	15.38	3.4	ng	73353	6	15.51	430840	20.0