

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
 Data File : BF097442.D
 Acq On : 7 Aug 2017 21:20
 Operator : SJ/JU
 Sample : I4623-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-WE

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-BF072517.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	4.534	464	467	482	rBV	123057	226080	10.84%	0.993%
2	5.004	543	547	577	rBV	1688248	2085414	100.00%	9.160%
3	6.081	727	730	744	rBV	1713095	1983368	95.11%	8.712%
4	6.187	744	748	759	rVB	1978441	1924199	92.27%	8.452%
5	6.410	783	786	798	rVB	601452	530696	25.45%	2.331%
6	6.563	809	812	823	rBV	1456565	1472366	70.60%	6.467%
7	6.981	880	883	896	rBV	1387229	1432894	68.71%	6.294%
8	7.145	907	911	916	rBV	20758	28681	1.38%	0.126%
9	7.692	1001	1004	1010	rBV	936040	806258	38.66%	3.541%
10	8.775	1183	1188	1191	rBV	2219010	1973908	94.65%	8.670%
11	9.175	1252	1256	1262	rBV	405960	347381	16.66%	1.526%
12	9.434	1297	1300	1304	rBV	786245	683890	32.79%	3.004%
13	9.469	1304	1306	1311	rVB	88474	75577	3.62%	0.332%
14	9.686	1340	1343	1346	rBV2	22391	22677	1.09%	0.100%
15	9.892	1375	1378	1381	rVB	41533	31756	1.52%	0.139%
16	9.981	1391	1393	1397	rBV	57815	51031	2.45%	0.224%
17	10.110	1410	1415	1418	rBV3	18299	23525	1.13%	0.103%
18	10.222	1431	1434	1450	rBV	988873	980382	47.01%	4.306%
19	10.363	1455	1458	1464	rBV	64622	78289	3.75%	0.344%
20	10.804	1530	1533	1536	rBV	59669	57394	2.75%	0.252%
21	10.910	1547	1551	1553	rBV	630496	556694	26.69%	2.445%
22	10.933	1553	1555	1560	rVV	518930	404913	19.42%	1.778%
23	10.986	1560	1564	1569	rVB	114940	105314	5.05%	0.463%
24	11.151	1587	1592	1599	rBV2	43142	52072	2.50%	0.229%
25	11.410	1628	1636	1638	rBV	54937	54897	2.63%	0.241%
26	11.439	1638	1641	1644	rVV	69295	65126	3.12%	0.286%
27	11.469	1644	1646	1652	rVV2	129075	144513	6.93%	0.635%
28	11.516	1652	1654	1657	rVV	94955	98053	4.70%	0.431%
29	11.545	1657	1659	1666	rVB	30295	31018	1.49%	0.136%
30	11.704	1684	1686	1690	rVB	32644	26134	1.25%	0.115%
31	11.745	1690	1693	1697	rBV	24540	24213	1.16%	0.106%
32	11.957	1726	1729	1732	rBV2	20886	21368	1.02%	0.094%
33	12.110	1752	1755	1762	rBV	611416	566002	27.14%	2.486%
34	12.245	1775	1778	1780	rBV	38480	40329	1.93%	0.177%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
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 Max Peaks: 100
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 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.333	1788	1793	1797	rBV	474579	508353	24.38%	2.233%
36	12.392	1801	1803	1811	rVB3	19381	24827	1.19%	0.109%
37	12.492	1812	1820	1823	rBV	1341261	1323528	63.47%	5.813%
38	12.569	1828	1833	1836	rVB2	25428	39132	1.88%	0.172%
39	12.645	1843	1846	1848	rBV2	22237	25226	1.21%	0.111%
40	12.674	1848	1851	1855	rVV	67878	66766	3.20%	0.293%
41	12.733	1859	1861	1864	rVV	60350	53838	2.58%	0.236%
42	12.774	1864	1868	1875	rVB2	46589	72804	3.49%	0.320%
43	12.892	1886	1888	1896	rVB3	20029	25760	1.24%	0.113%
44	13.092	1920	1922	1930	rVB4	15099	21127	1.01%	0.093%
45	13.186	1935	1938	1941	rVB	40146	33811	1.62%	0.149%
46	13.286	1950	1955	1957	rBV3	47733	56603	2.71%	0.249%
47	13.304	1957	1958	1961	rVV	37182	30503	1.46%	0.134%
48	13.357	1965	1967	1971	rVB2	24693	23673	1.14%	0.104%
49	13.392	1971	1973	1975	rBV	42174	36653	1.76%	0.161%
50	13.422	1975	1978	1982	rBV3	18629	29595	1.42%	0.130%
51	13.533	1989	1997	1999	rBV2	674392	910276	43.65%	3.998%
52	13.557	1999	2001	2007	rVB	260481	254400	12.20%	1.117%
53	13.633	2011	2014	2018	rVB	64868	62477	3.00%	0.274%
54	13.704	2018	2026	2028	rBV4	17246	33265	1.60%	0.146%
55	13.886	2054	2057	2059	rBV2	17791	21832	1.05%	0.096%
56	13.921	2059	2063	2066	rVB	47426	49992	2.40%	0.220%
57	14.016	2072	2079	2081	rBV5	19129	34602	1.66%	0.152%
58	14.063	2085	2087	2089	rVB3	25200	21707	1.04%	0.095%
59	14.251	2110	2119	2124	rBV10	29468	59824	2.87%	0.263%
60	14.321	2129	2131	2136	rVB4	17361	22223	1.07%	0.098%
61	14.380	2137	2141	2149	rBV	197768	221505	10.62%	0.973%
62	14.527	2161	2166	2174	rBV	251810	433877	20.81%	1.906%
63	14.616	2178	2181	2184	rVB	45713	42147	2.02%	0.185%
64	14.698	2191	2195	2198	rBV3	20235	31760	1.52%	0.139%
65	14.768	2203	2207	2213	rVB	144209	148257	7.11%	0.651%
66	14.821	2213	2216	2221	rBV	206322	207617	9.96%	0.912%
67	14.868	2221	2224	2228	rVV	379267	465381	22.32%	2.044%
68	14.898	2228	2229	2236	rVB3	63484	75581	3.62%	0.332%
69	15.257	2285	2290	2295	rBV7	17804	36136	1.73%	0.159%
70	16.063	2423	2427	2434	rBV	61450	103443	4.96%	0.454%
71	16.415	2483	2487	2499	rVB2	51671	114897	5.51%	0.505%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.621	2518	2522	2528	rBV7	16332	37375	1.79%	0.164%
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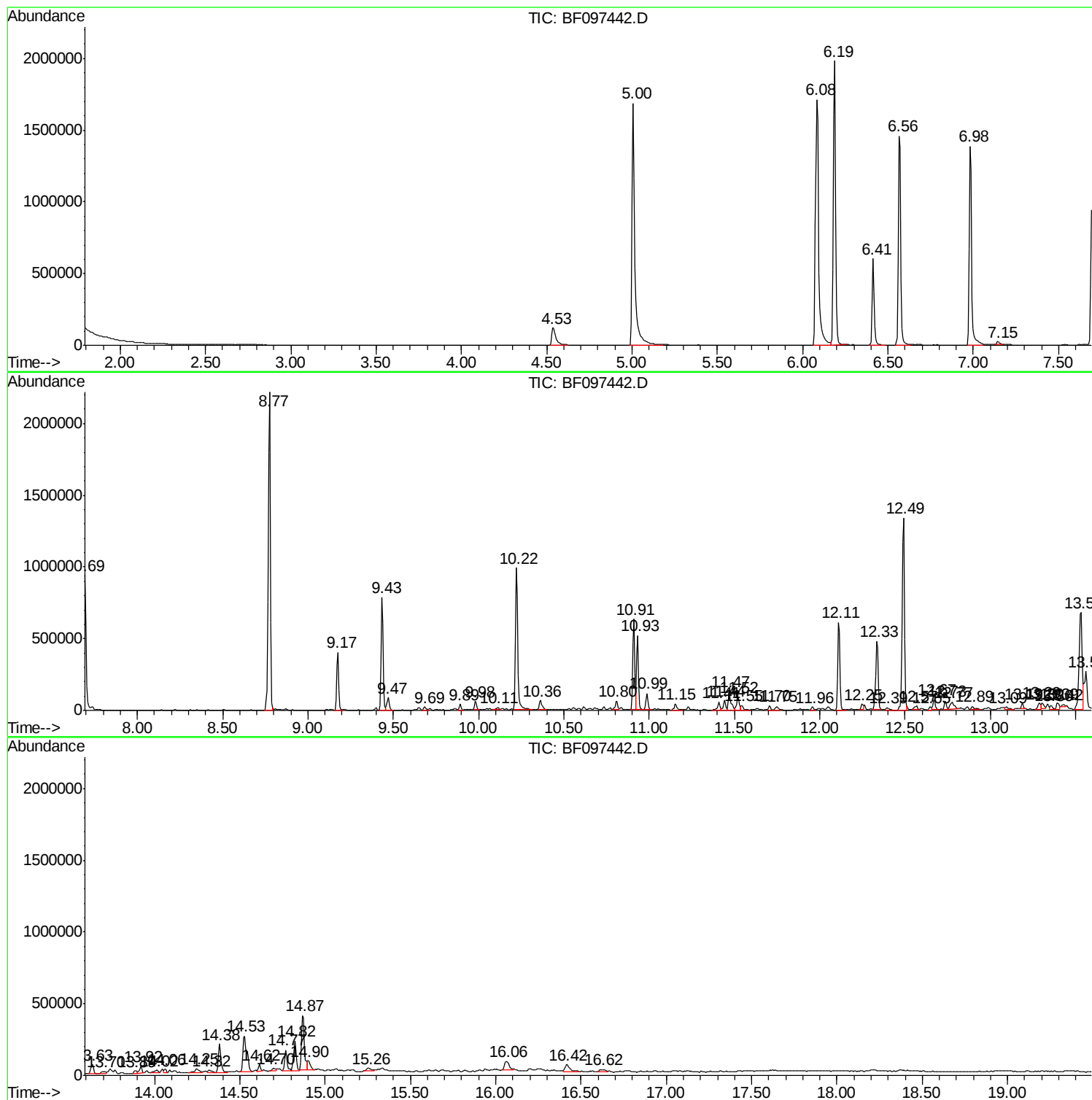
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : I4623-05
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Instrument :
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ClientSampleId :
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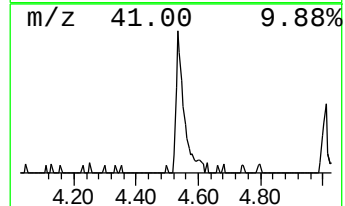
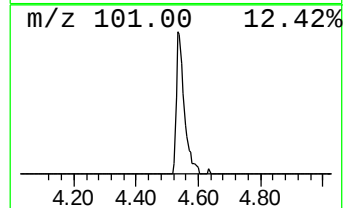
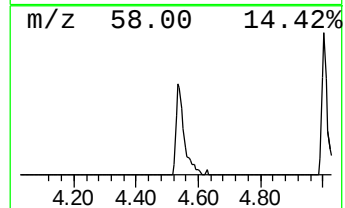
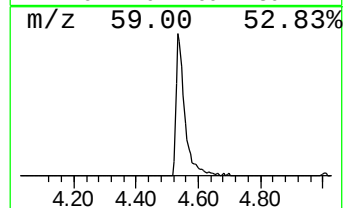
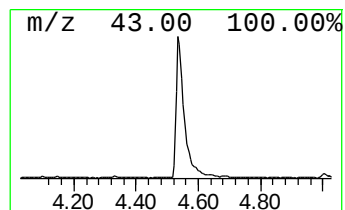
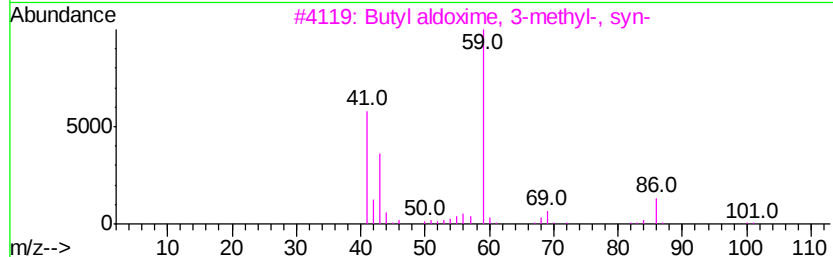
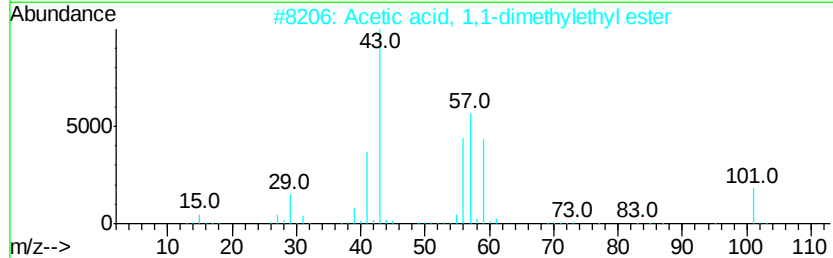
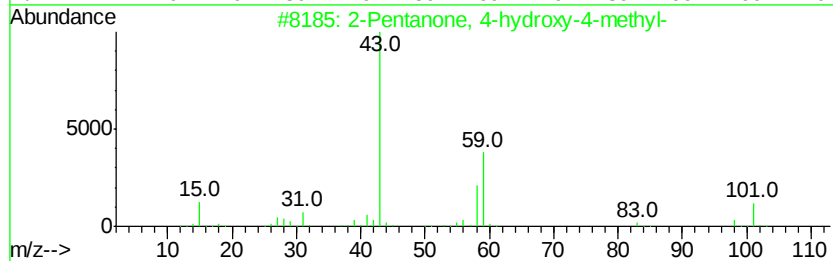
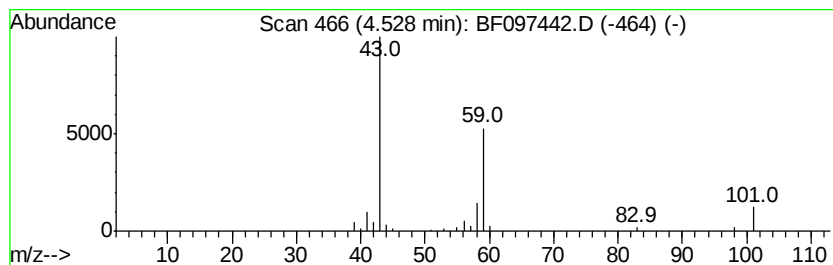
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	8.52 ng	226080	1,4-Dichlorobenzene-d4	6.41

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	38
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
4			5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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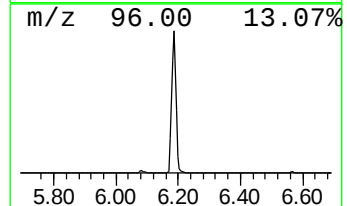
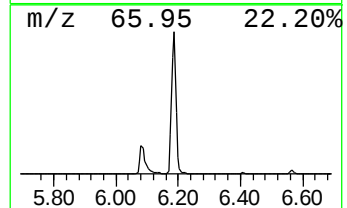
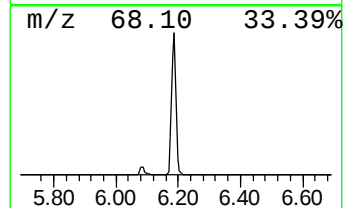
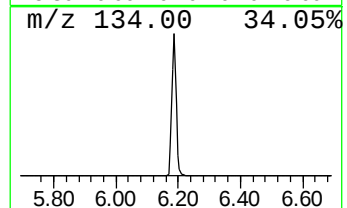
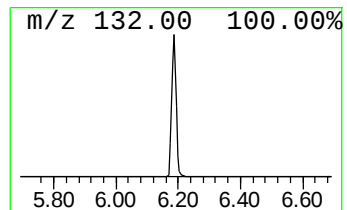
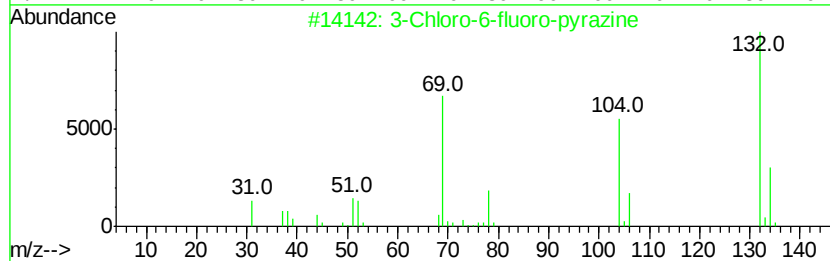
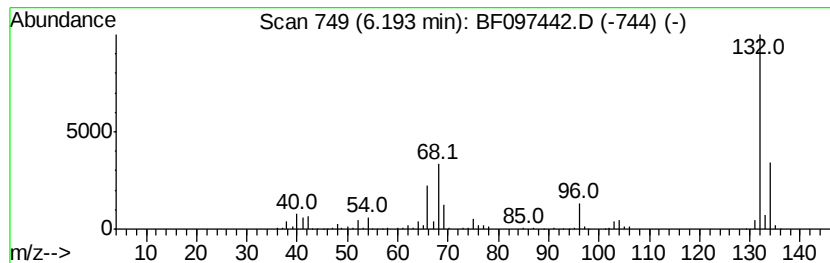
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	72.52 ng	1924200	1,4-Dichlorobenzene-d4	6.41

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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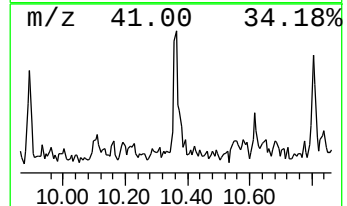
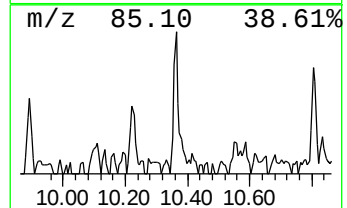
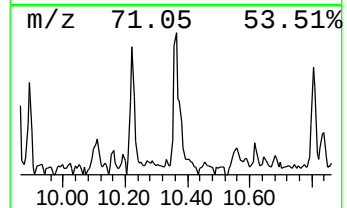
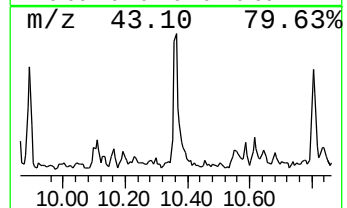
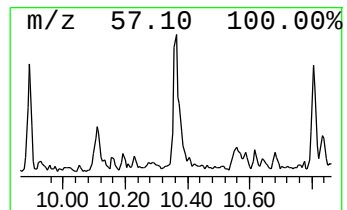
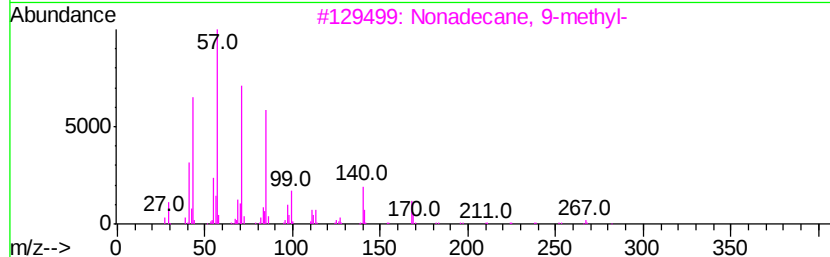
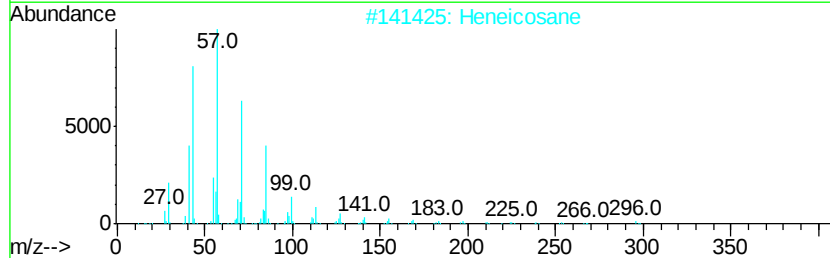
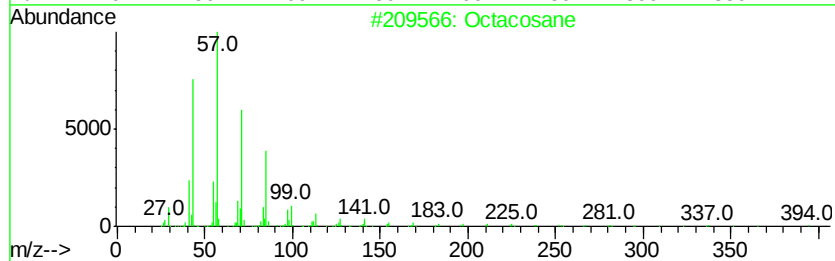
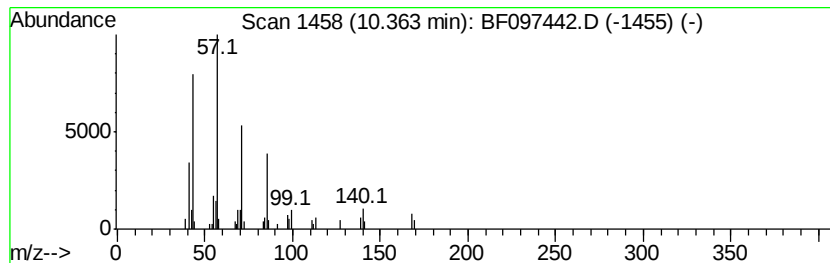
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.36	2.81 ng	78289	Phenanthrene-d10	10.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Heneicosane	296	C21H44	000629-94-7	83
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
4	Pentadecane	212	C15H32	000629-62-9	80
5	Eicosane	282	C20H42	000112-95-8	80



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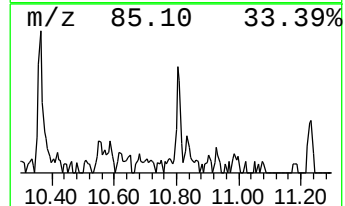
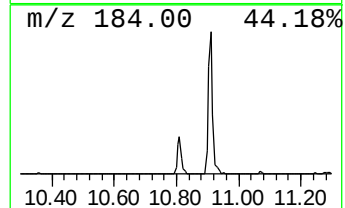
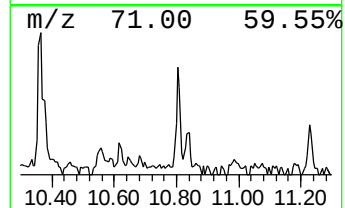
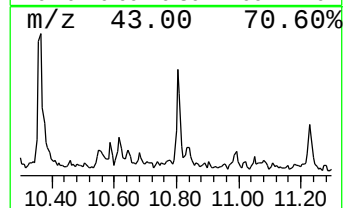
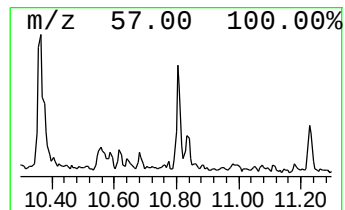
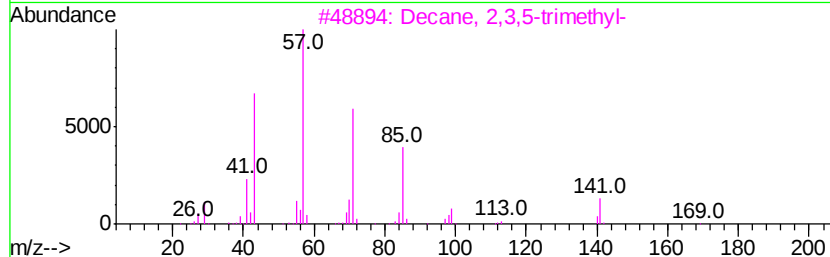
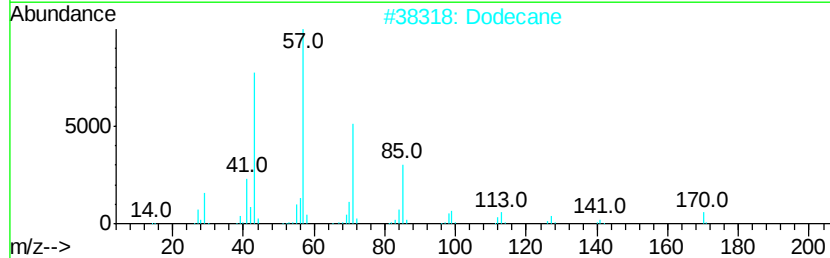
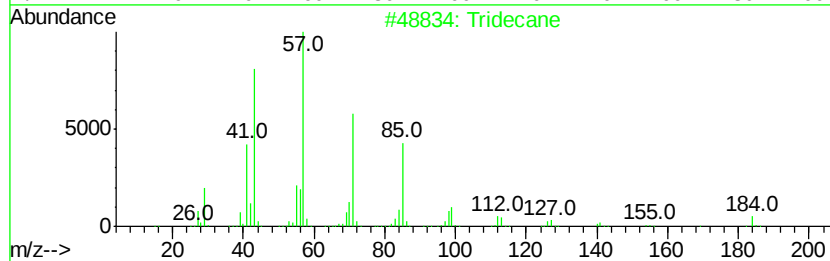
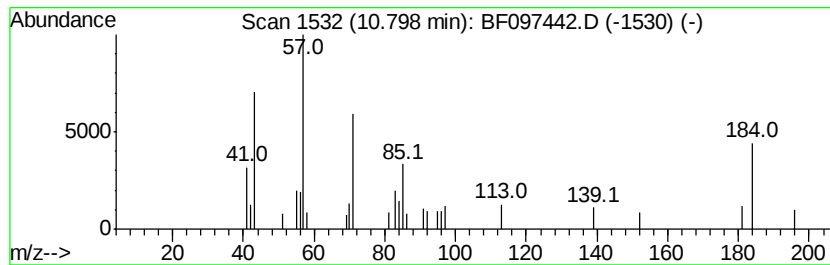
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.06 ng	57394	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	49
2	Dodecane		170	C12H26	000112-40-3	43
3	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	43
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	43
5	Heptadecane		240	C17H36	000629-78-7	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097442.D
Acq On : 7 Aug 2017 21:20
Operator : SJ/JU
Sample : I4623-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-WE

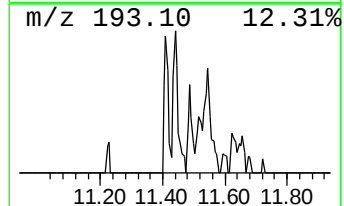
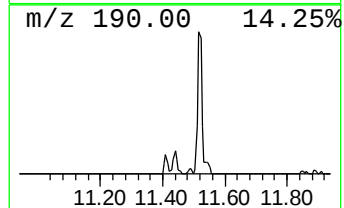
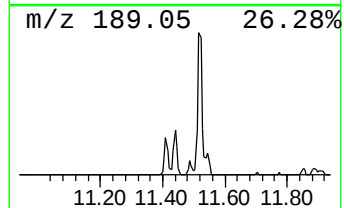
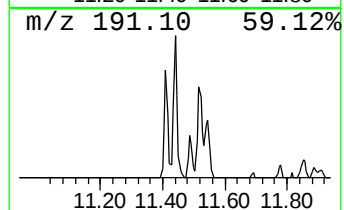
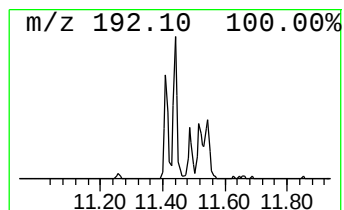
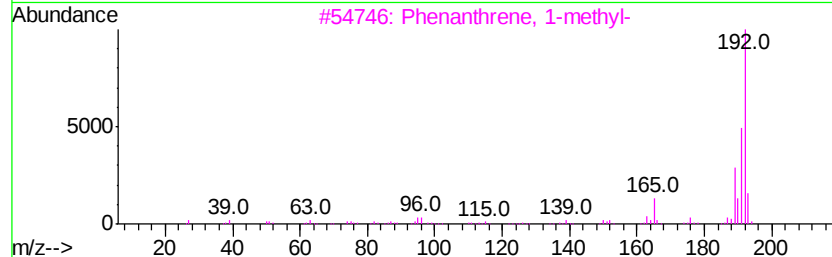
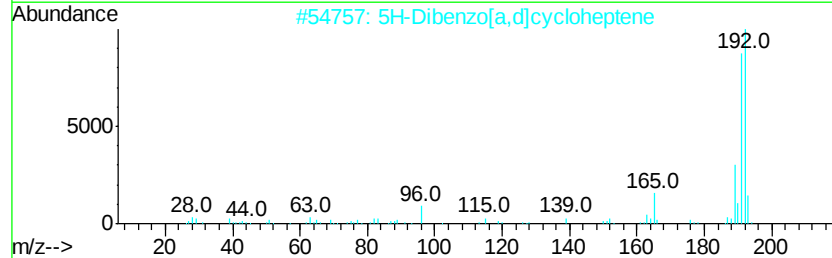
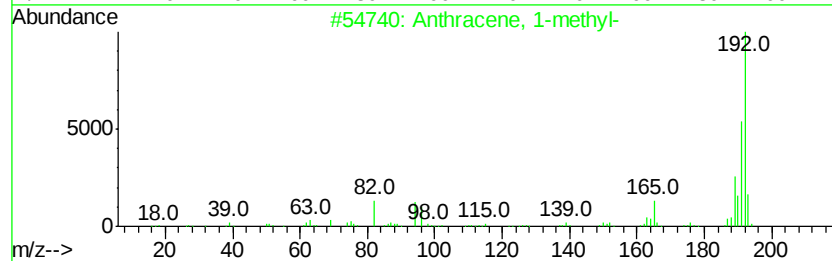
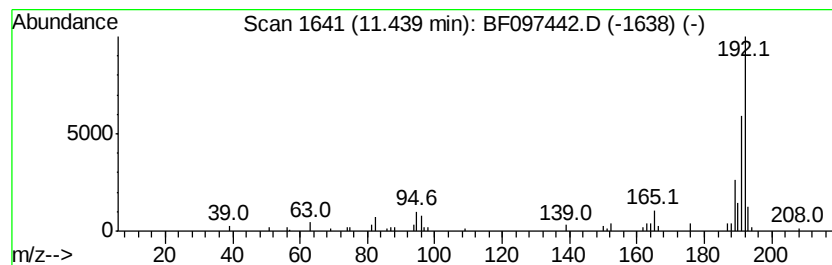
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	2.34 ng	65126	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	94
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
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Sample : I4623-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-WE

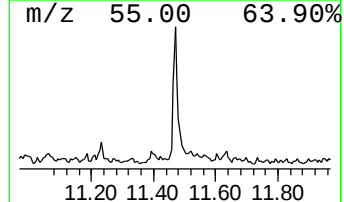
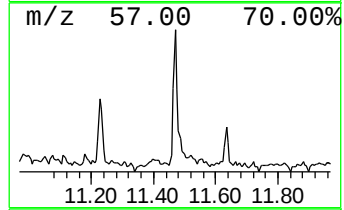
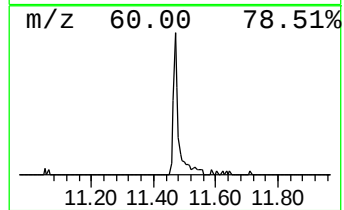
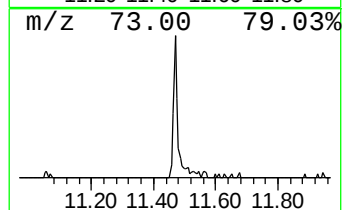
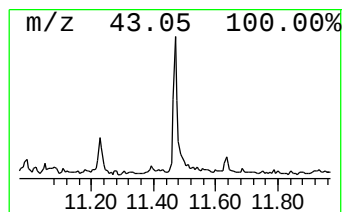
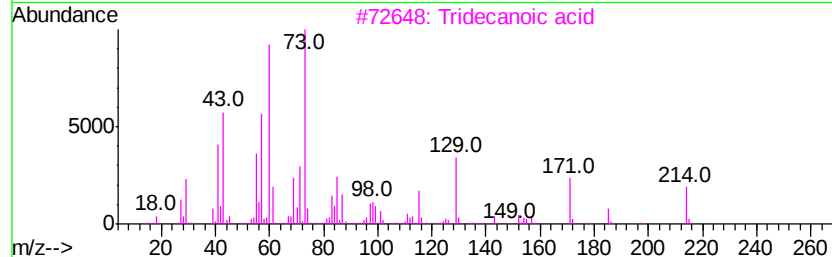
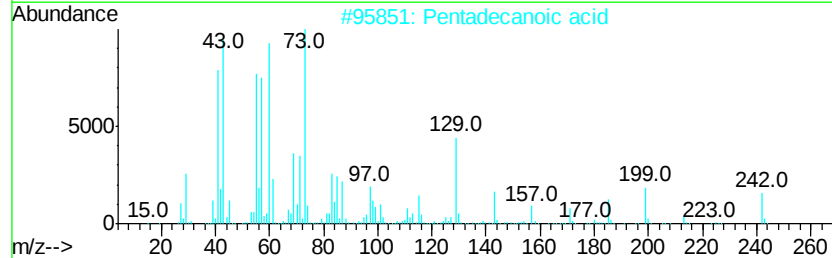
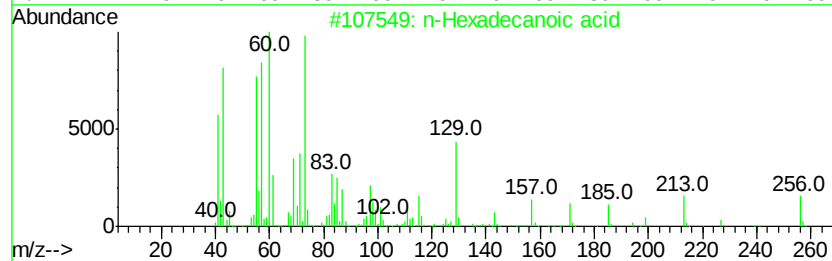
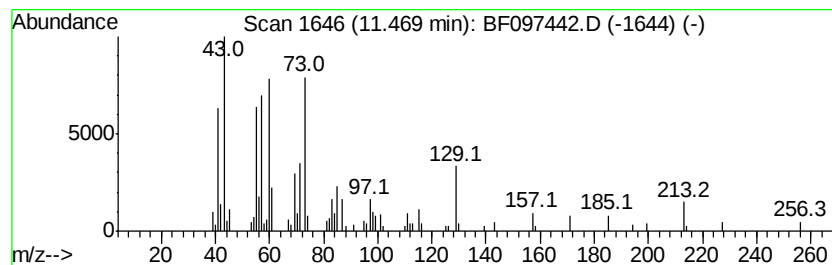
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	5.19 ng	144513	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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Acq On : 7 Aug 2017 21:20
Operator : SJ/JU
Sample : I4623-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

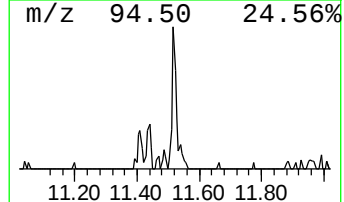
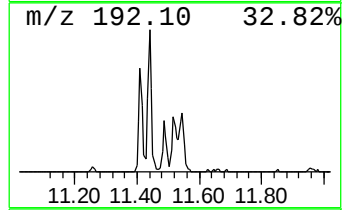
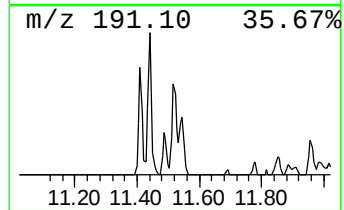
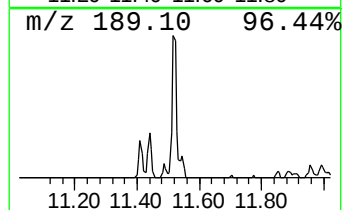
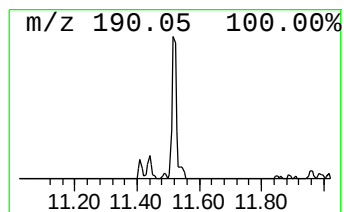
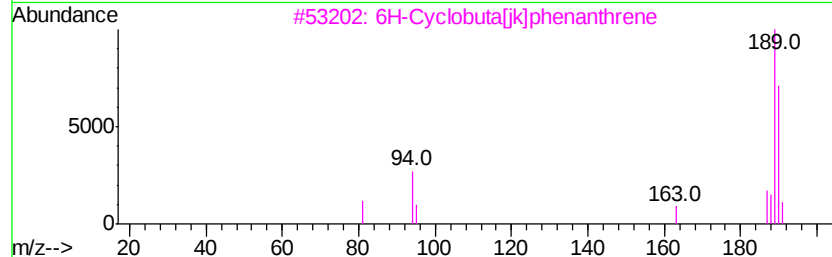
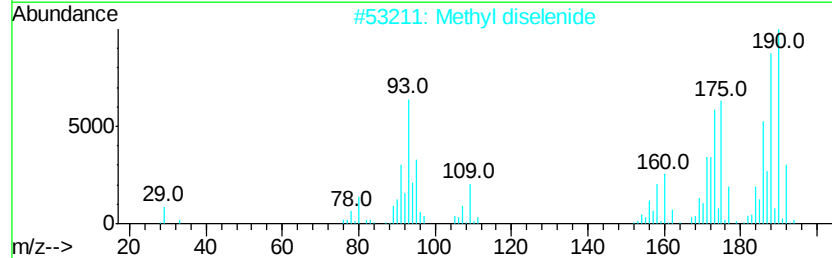
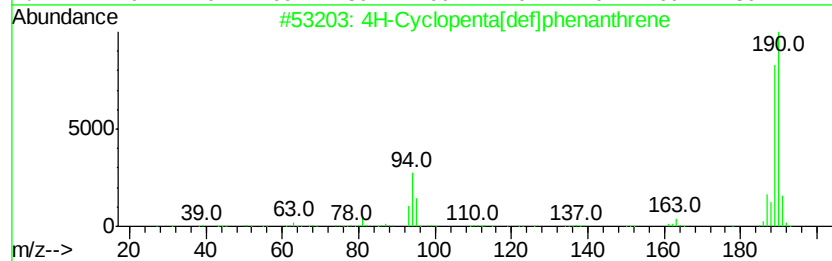
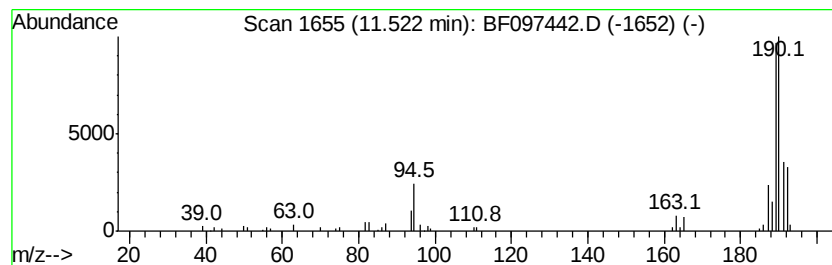
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ClientSampleId :
TEC-WE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.52	3.52 ng	98053	Phenanthrene-d10	10.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	6H-Cyclobuta[ikl]phenanthrene	190	C15H10	083469-43-6	42
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
5	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	37



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Operator : SJ/JU
Sample : I4623-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-WE

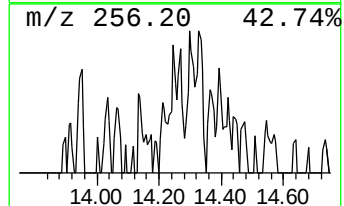
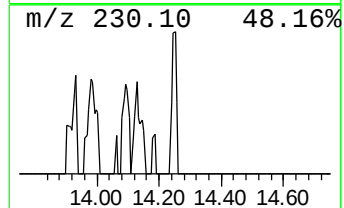
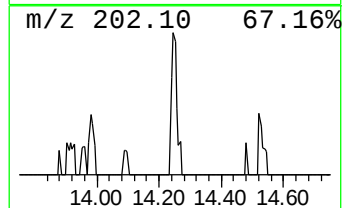
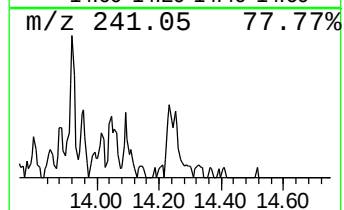
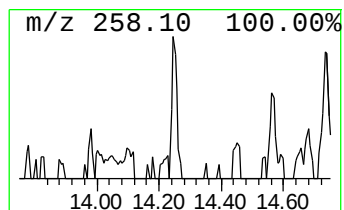
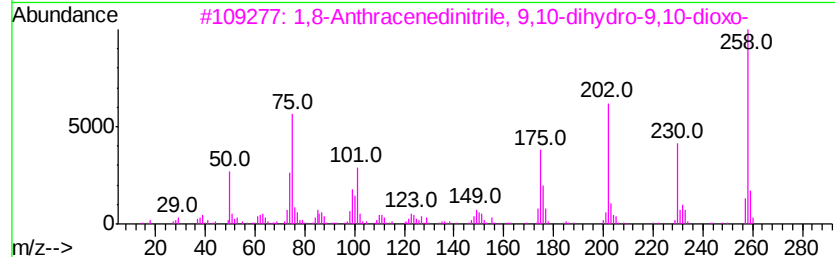
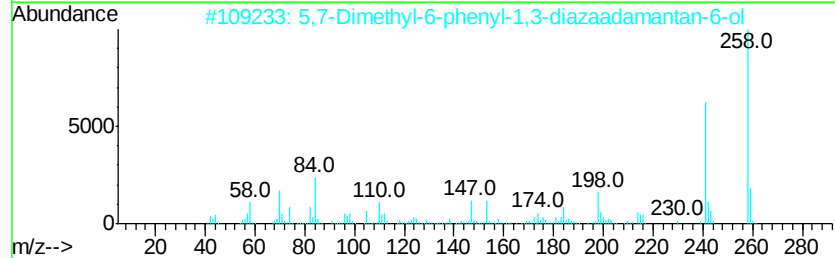
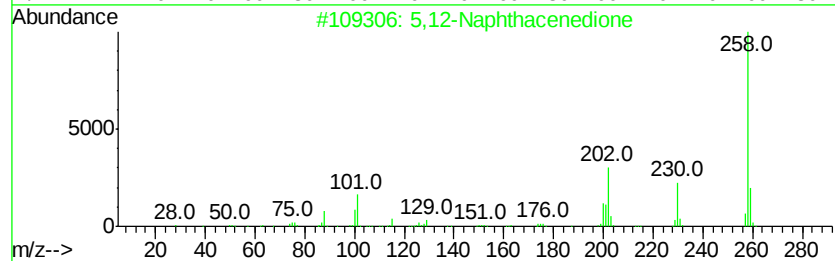
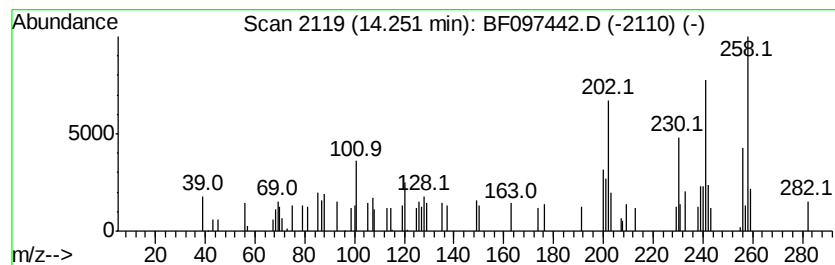
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5,12-Naphthacenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.57 ng	59824	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5,12-Naphthacenedione	258	C18H10O2	001090-13-7	60
2		5,7-Dimethyl-6-phenyl-1,3-diazaa...	258	C16H22N2O	1000216-37-9	38
3		1,8-Anthracenedinitrile, 9,10-di...	258	C16H6N2O2	090866-50-5	35
4		Benz(a)anthracene-7,12-dione	258	C18H10O2	002498-66-0	35
5		1,2-Dihydro-2,4'-biquinoline	258	C18H14N2	1000326-82-7	30



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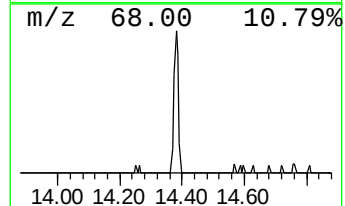
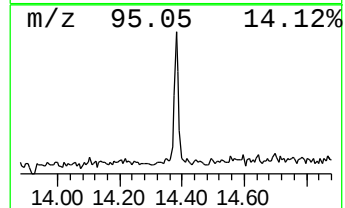
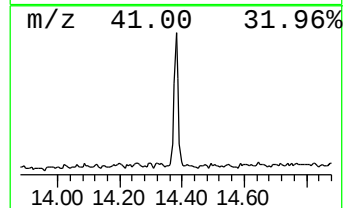
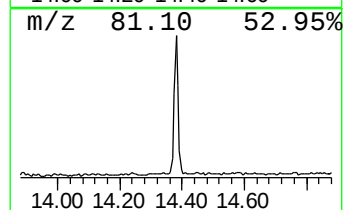
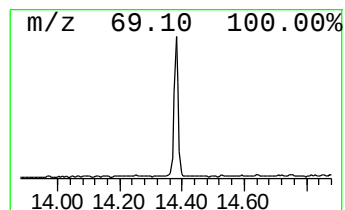
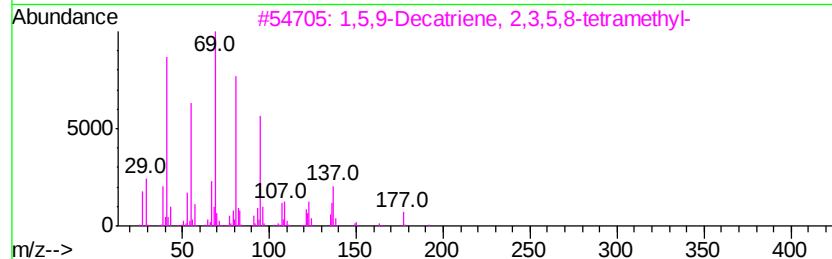
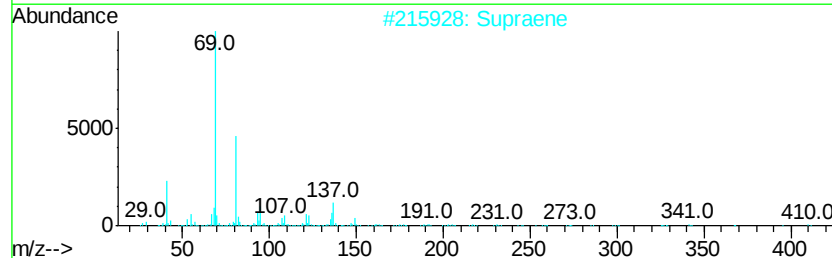
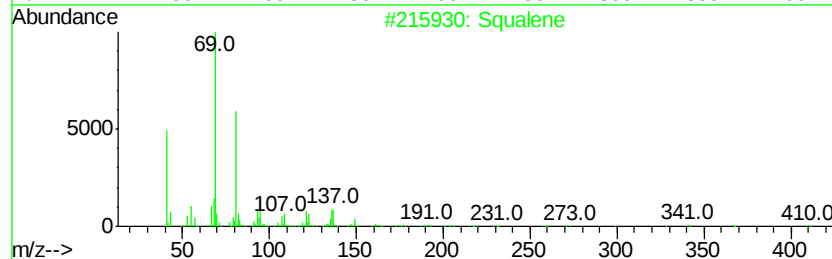
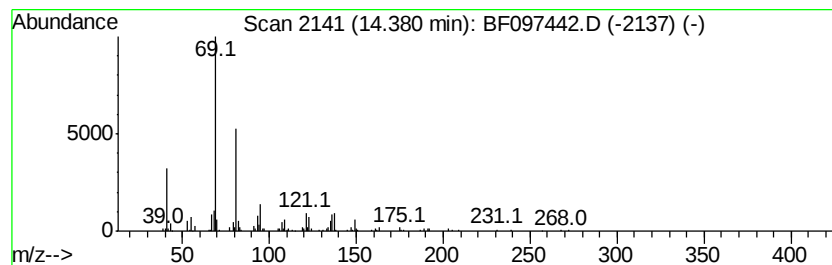
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	9.52 ng	221505	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
4		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
5		Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	50



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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...	4.53	8.5	ng	226080	1	6.41	530696	20.0
unknown6.19	6.19	72.5	ng	1924200	1	6.41	530696	20.0
Octacosane	10.36	2.8	ng	78289	4	10.91	556694	20.0
Tridecane	10.80	2.1	ng	57394	4	10.91	556694	20.0
Anthracene, 1-met...	11.44	2.3	ng	65126	4	10.91	556694	20.0
n-Hexadecanoic acid	11.47	5.2	ng	144513	4	10.91	556694	20.0
4H-Cyclopenta[def...	11.52	3.5	ng	98053	4	10.91	556694	20.0
5,12-Naphthacened...	14.25	2.6	ng	59824	6	14.87	465381	20.0
Squalene	14.38	9.5	ng	221505	6	14.87	465381	20.0