

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
 Data File : BF098927.D
 Acq On : 29 Sep 2017 00:48
 Operator : SJ/JU
 Sample : I5457-11 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-3-092617

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-BF092317.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	21	25	40	rVB2	113787	211670	12.28%	0.898%
2	2.340	40	43	51	rVB	33530	51918	3.01%	0.220%
3	4.540	413	417	421	rBV	22745	24774	1.44%	0.105%
4	5.139	515	519	534	rVB	324122	359915	20.88%	1.527%
5	5.539	579	587	590	rBV	1835253	1713217	99.38%	7.269%
6	6.539	752	757	764	rBV	1785188	1654595	95.98%	7.020%
7	6.686	777	782	785	rBV	1929113	1723916	100.00%	7.314%
8	6.739	788	791	796	rVV	65048	58889	3.42%	0.250%
9	6.916	817	821	824	rBV	1126468	898995	52.15%	3.814%
10	7.069	843	847	851	rBV	1444413	1349620	78.29%	5.726%
11	7.475	911	916	919	rBV	1207112	993046	57.60%	4.213%
12	8.198	1035	1039	1042	rBV	1399226	1088827	63.16%	4.620%
13	9.269	1216	1221	1224	rBV	2054426	1650666	95.75%	7.004%
14	9.663	1284	1288	1293	rVB	271840	239302	13.88%	1.015%
15	9.816	1310	1314	1317	rBV	64730	58755	3.41%	0.249%
16	9.874	1319	1324	1327	rVB2	32132	32650	1.89%	0.139%
17	9.957	1329	1338	1341	rBV	1034937	1010586	58.62%	4.288%
18	10.310	1393	1398	1402	rBV5	28751	36191	2.10%	0.154%
19	10.374	1406	1409	1412	rVB	50601	42758	2.48%	0.181%
20	10.498	1427	1430	1436	rVB2	26169	27942	1.62%	0.119%
21	10.739	1467	1471	1482	rVB	833712	738204	42.82%	3.132%
22	10.845	1486	1489	1499	rBV	84839	102736	5.96%	0.436%
23	11.045	1518	1523	1526	rBV5	17636	27651	1.60%	0.117%
24	11.245	1554	1557	1560	rVB2	23662	22580	1.31%	0.096%
25	11.292	1561	1565	1568	rVV2	46955	45456	2.64%	0.193%
26	11.339	1568	1573	1576	rVB2	23005	38106	2.21%	0.162%
27	11.386	1576	1581	1586	rBV3	16772	24408	1.42%	0.104%
28	11.439	1586	1590	1592	rBV2	976507	835709	48.48%	3.546%
29	11.463	1592	1594	1598	rVV	441210	363901	21.11%	1.544%
30	11.516	1600	1603	1606	rVV	126568	100563	5.83%	0.427%
31	11.545	1606	1608	1615	rVB3	17851	21949	1.27%	0.093%
32	11.668	1622	1629	1632	rBV2	53978	65822	3.82%	0.279%
33	11.721	1635	1638	1639	rBV2	24628	20161	1.17%	0.086%
34	11.951	1672	1677	1679	rBV2	103382	155750	9.03%	0.661%

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35	11.968	1679	1680	1683	rVV	104132	58878	3.42%	0.250%
36	12.015	1686	1688	1691	rVB	41715	30539	1.77%	0.130%
37	12.057	1691	1695	1697	rBV2	104537	122925	7.13%	0.522%
38	12.127	1704	1707	1709	rBV2	26985	24323	1.41%	0.103%
39	12.233	1722	1725	1728	rBV	64801	66562	3.86%	0.282%
40	12.263	1728	1730	1732	rVB	36742	30580	1.77%	0.130%
41	12.492	1766	1769	1771	rBV	49750	50536	2.93%	0.214%
42	12.521	1771	1774	1777	rVV4	28911	41622	2.41%	0.177%
43	12.574	1781	1783	1788	rVB	58886	58304	3.38%	0.247%
44	12.657	1793	1797	1800	rBV	936382	820248	47.58%	3.480%
45	12.751	1809	1813	1815	rBV2	39506	49382	2.86%	0.210%
46	12.886	1829	1836	1839	rBV	879066	870926	50.52%	3.695%
47	12.933	1841	1844	1848	rVB2	41361	49048	2.85%	0.208%
48	13.021	1853	1859	1862	rBV	1356458	1210741	70.23%	5.137%
49	13.104	1868	1873	1876	rBV2	62272	113339	6.57%	0.481%
50	13.210	1889	1891	1895	rVB	106822	89249	5.18%	0.379%
51	13.274	1900	1902	1905	rBV	54149	45736	2.65%	0.194%
52	13.315	1906	1909	1911	rVB2	66743	65074	3.77%	0.276%
53	13.715	1974	1977	1981	rVB	98627	97004	5.63%	0.412%
54	13.833	1993	1997	1999	rBV2	79206	101232	5.87%	0.430%
55	13.857	1999	2001	2003	rBV	55585	41189	2.39%	0.175%
56	13.886	2003	2006	2007	rBV	48799	51859	3.01%	0.220%
57	13.909	2007	2010	2011	rBV3	81583	78792	4.57%	0.334%
58	14.080	2035	2039	2042	rBV2	980049	1242111	72.05%	5.270%
59	14.109	2042	2044	2049	rVB	416251	337880	19.60%	1.434%
60	14.186	2055	2057	2061	rBV	68389	57558	3.34%	0.244%
61	15.139	2215	2219	2222	rBV	344655	545418	31.64%	2.314%
62	15.451	2269	2272	2278	rVB	189505	243895	14.15%	1.035%
63	15.509	2279	2282	2289	rBV	268077	339556	19.70%	1.441%
64	15.580	2290	2294	2297	rBV	534598	637052	36.95%	2.703%
65	17.086	2547	2550	2557	rVB2	125759	205768	11.94%	0.873%

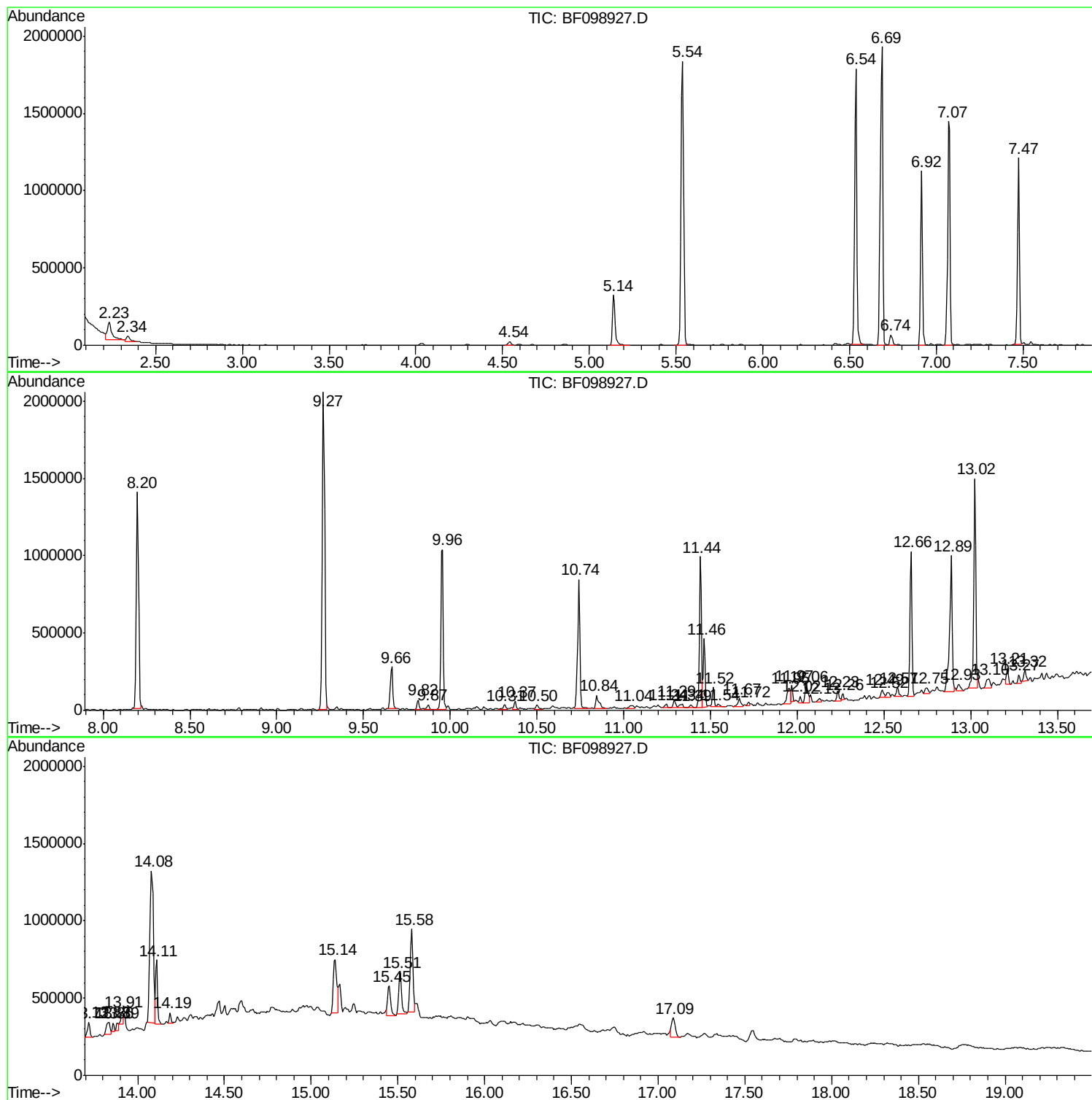
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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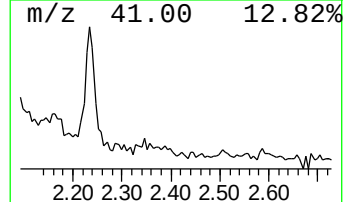
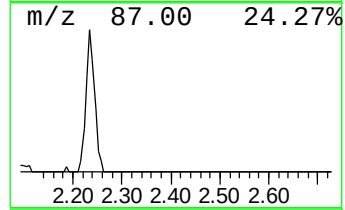
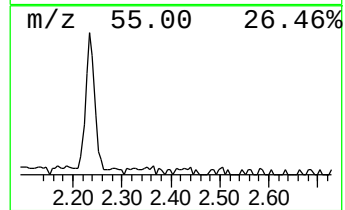
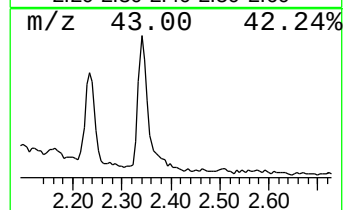
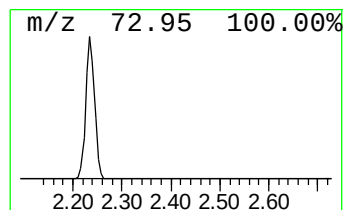
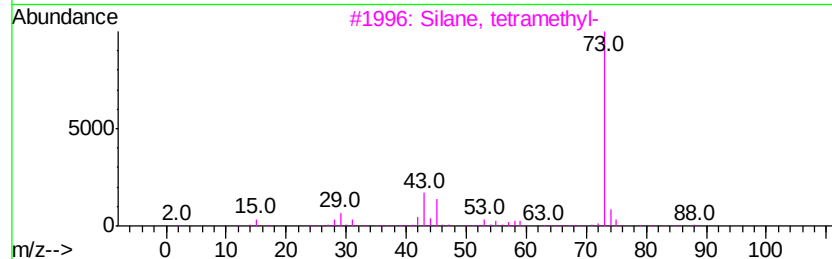
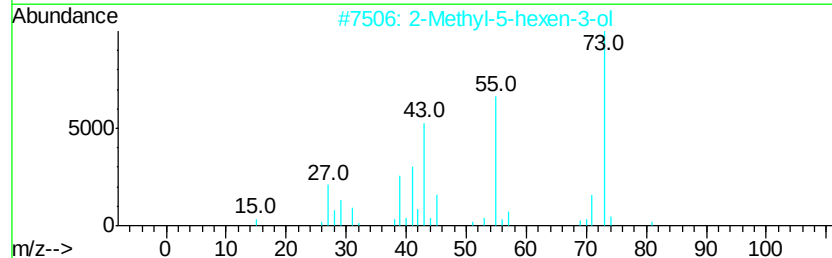
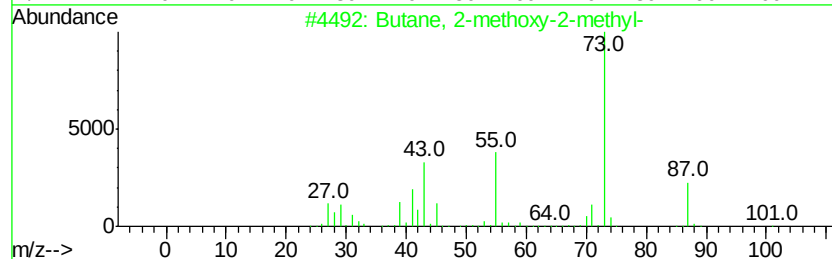
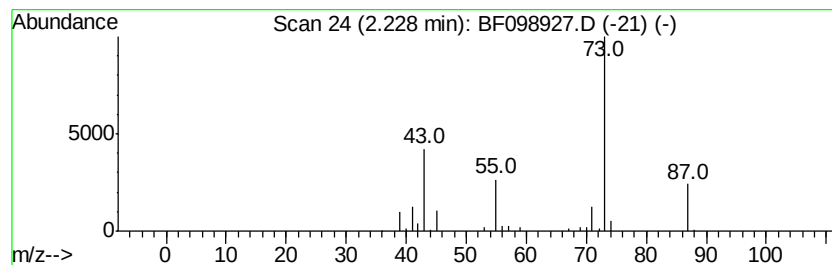
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	4.71 ng	211670	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12



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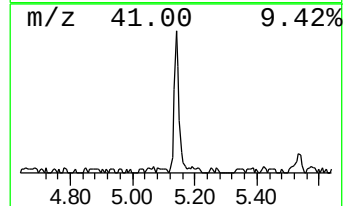
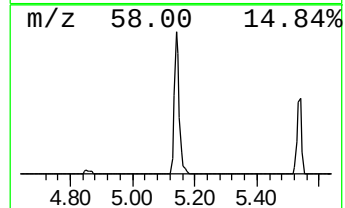
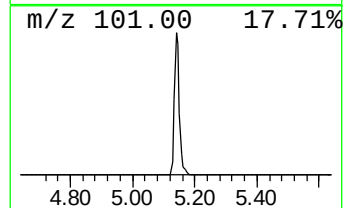
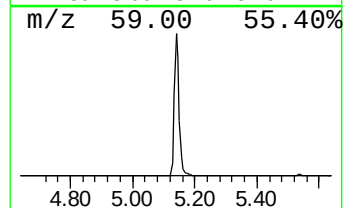
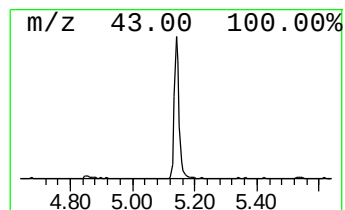
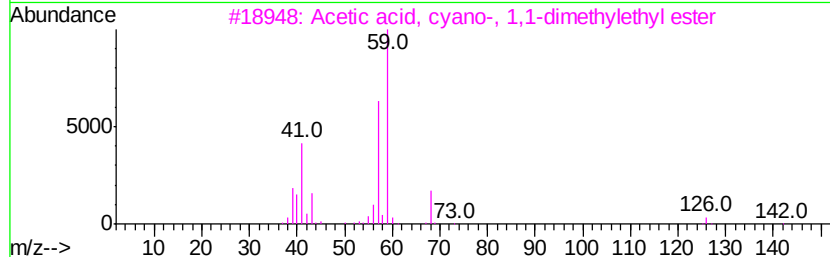
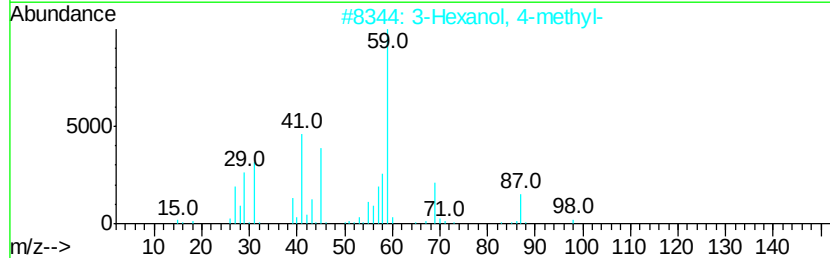
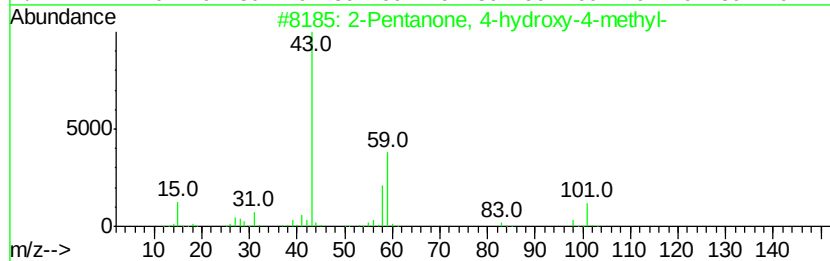
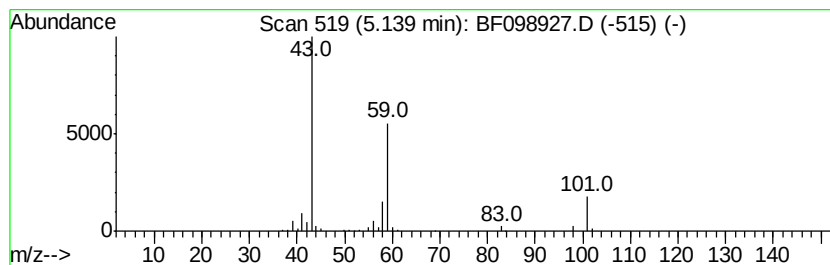
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	8.01 ng	359915	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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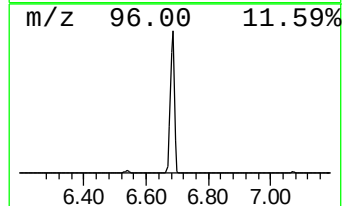
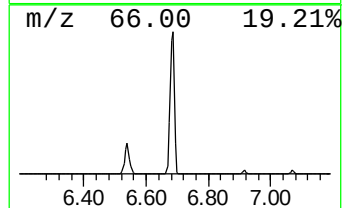
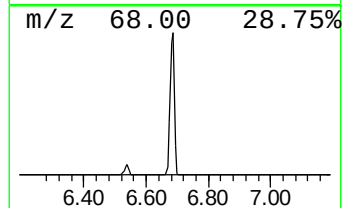
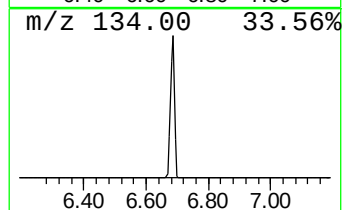
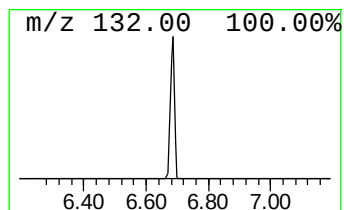
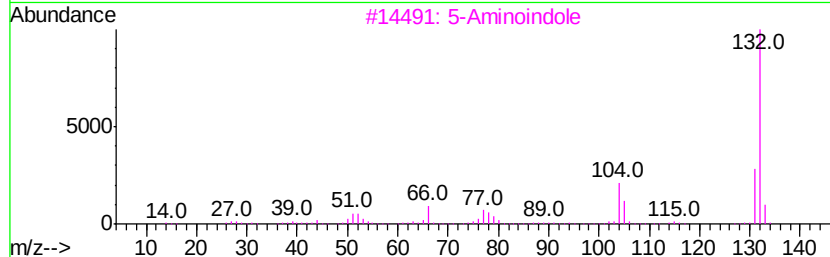
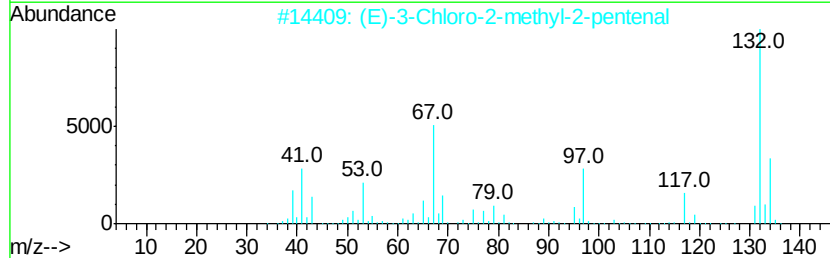
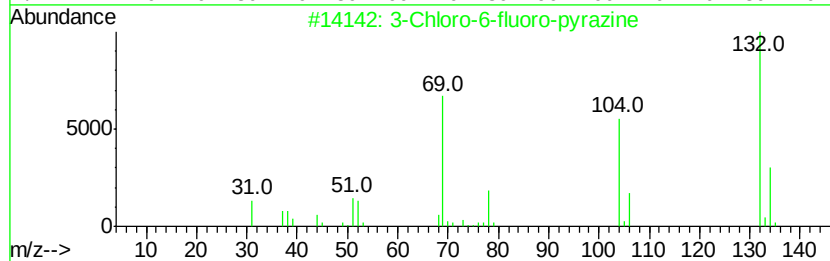
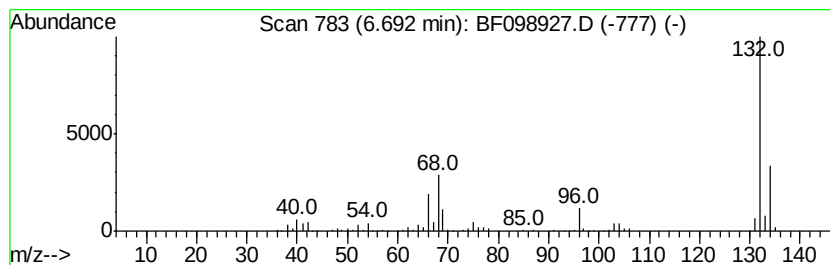
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	38.35 ng	1723920	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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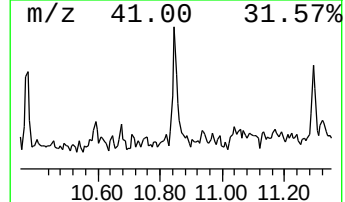
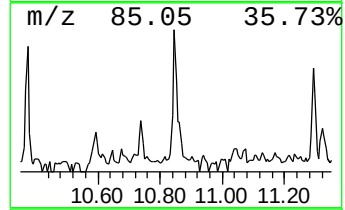
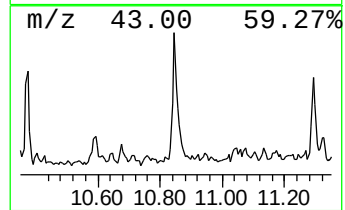
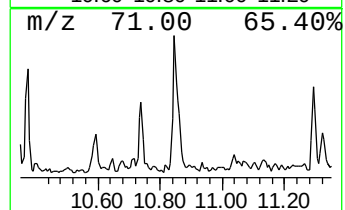
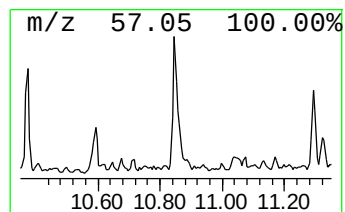
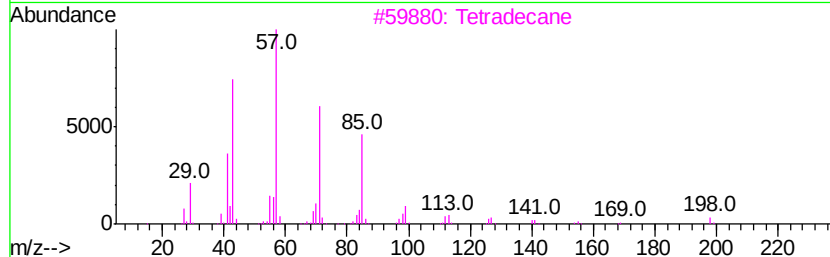
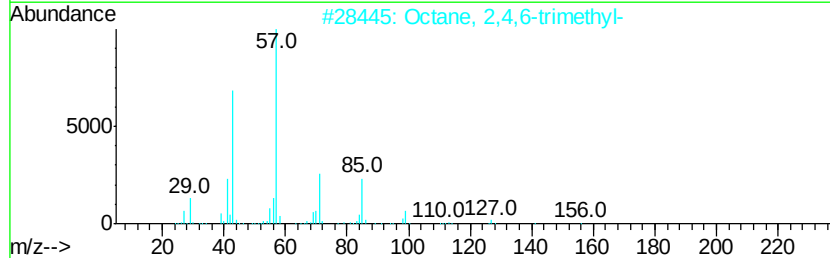
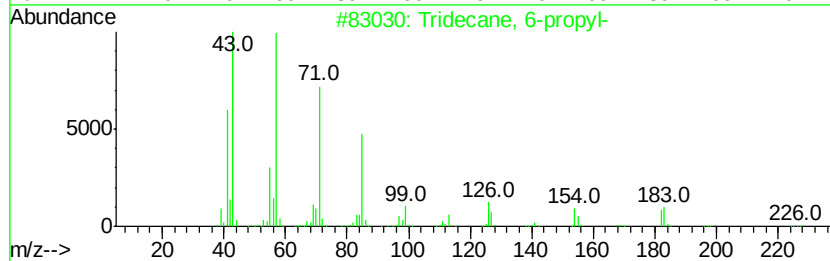
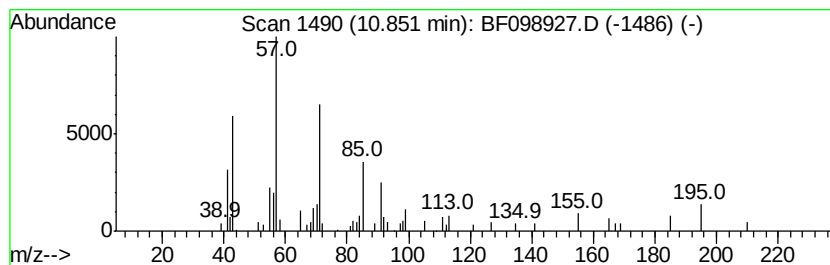
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane, 6-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.85	2.46 ng	102736	Phenanthrene-d10	11.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-propyl-	226	C16H34	055045-10-8	59
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	58
3	Tetradecane	198	C14H30	000629-59-4	58
4	Eicosane	282	C20H42	000112-95-8	53
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	53



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DUP-3-092617

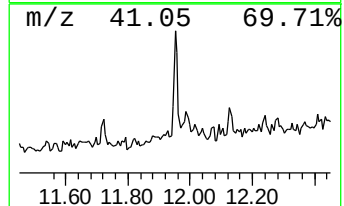
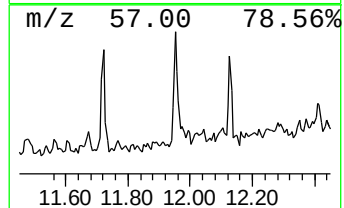
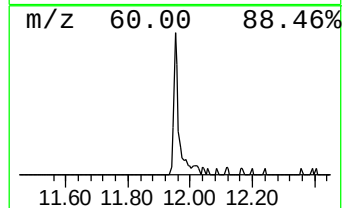
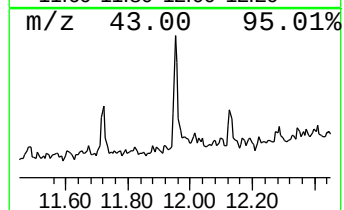
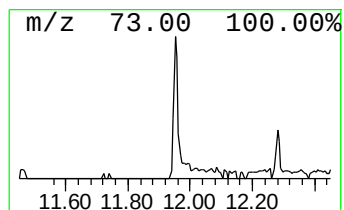
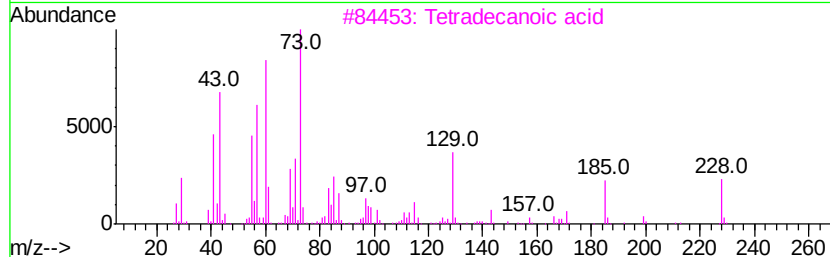
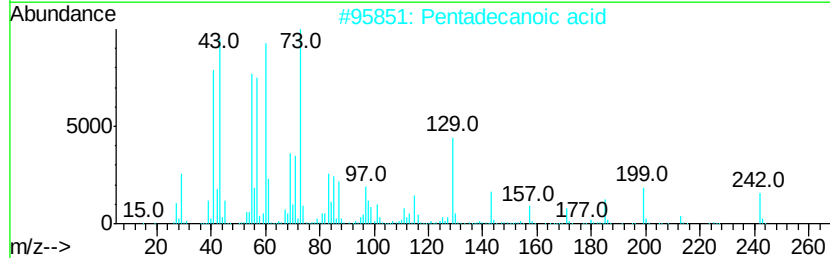
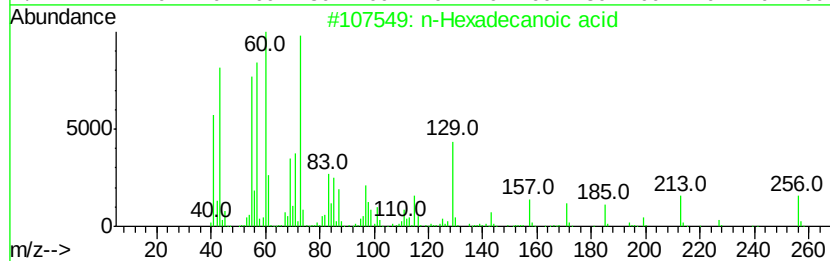
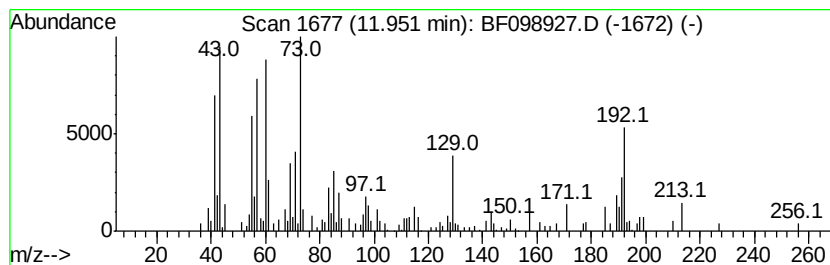
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.95	3.73 ng	155750	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098927.D
Acq On : 29 Sep 2017 00:48
Operator : SJ/JU
Sample : I5457-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

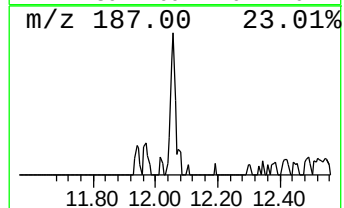
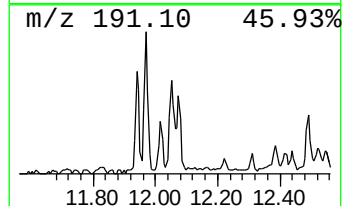
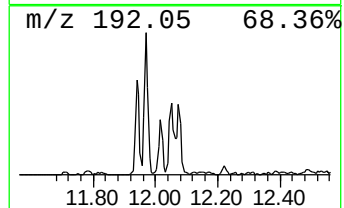
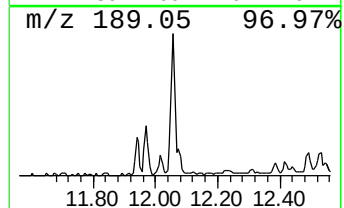
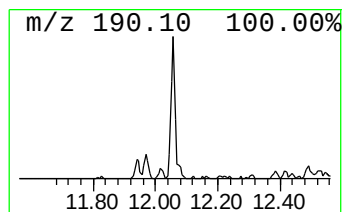
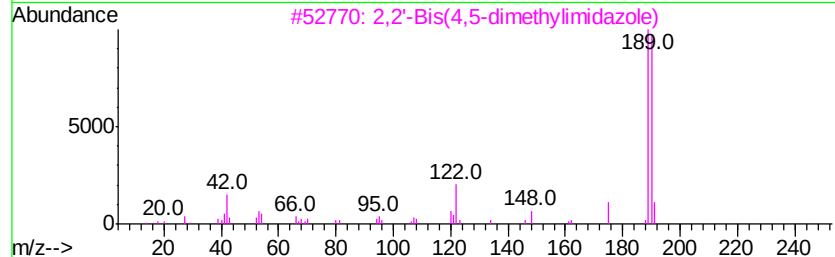
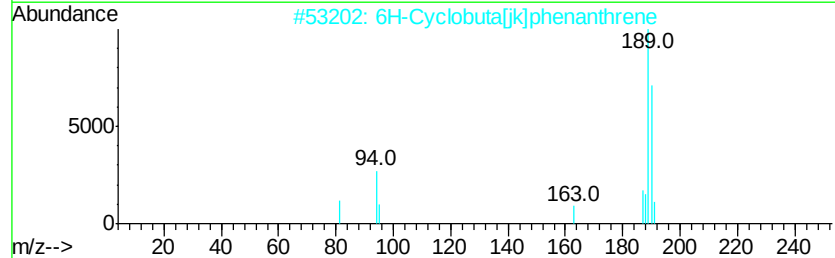
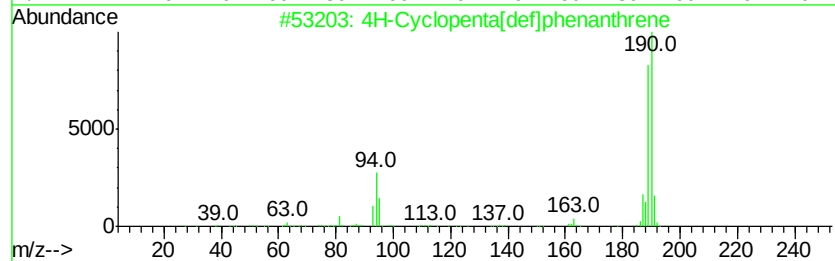
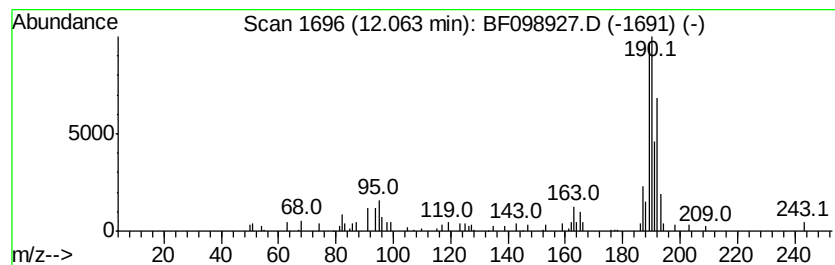
Instrument :
BNA_F
ClientSampleId :
DUP-3-092617

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.06	2.94 ng	122925	Phenanthrene-d10	11.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	40
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098927.D
Acq On : 29 Sep 2017 00:48
Operator : SJ/JU
Sample : I5457-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-3-092617

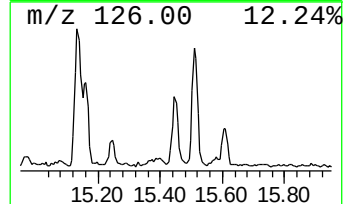
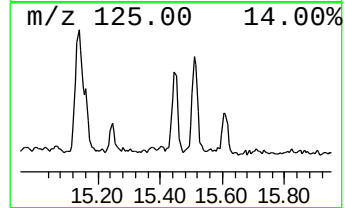
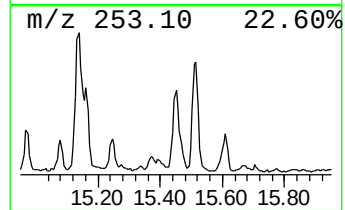
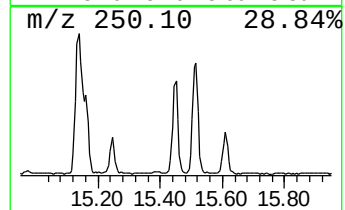
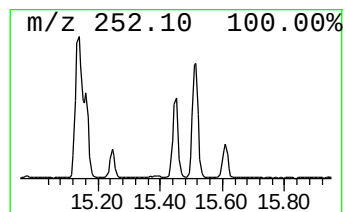
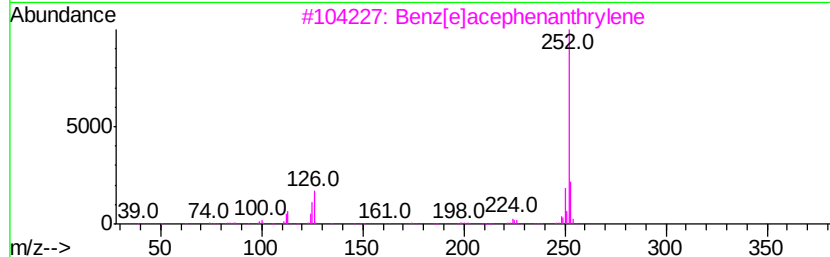
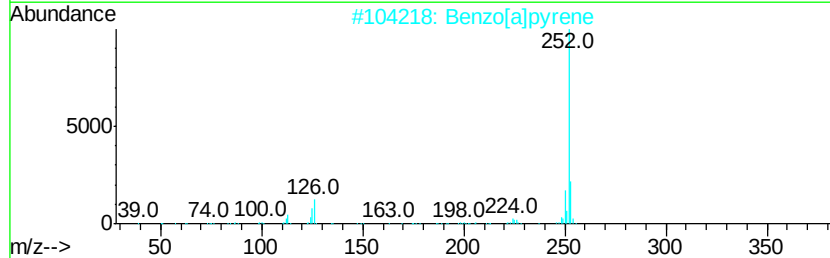
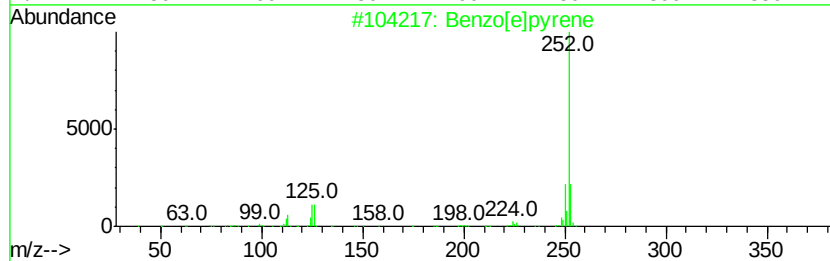
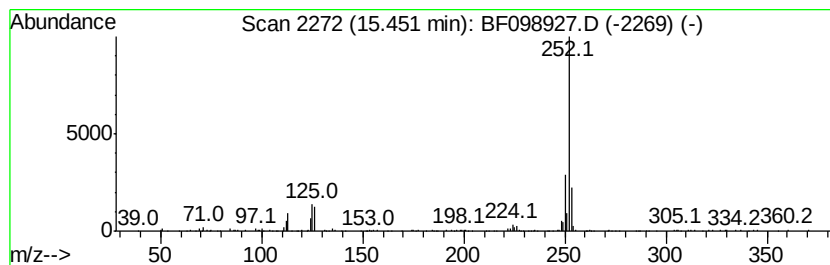
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	7.66 ng	243895	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[a]pyrene	252	C20H12	000050-32-8	96
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4		Perylene	252	C20H12	000198-55-0	93
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
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Acq On : 29 Sep 2017 00:48
Operator : SJ/JU
Sample : I5457-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-3-092617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.23	4.7	ng	211670	1	6.92	898995	20.0
2-Pentanone, 4-hy...	5.14	8.0	ng	359915	1	6.92	898995	20.0
unknown6.69	6.69	38.4	ng	1723920	1	6.92	898995	20.0
Tridecane, 6-propyl-	10.85	2.5	ng	102736	4	11.44	835709	20.0
n-Hexadecanoic acid	11.95	3.7	ng	155750	4	11.44	835709	20.0
4H-Cyclopenta[def...	12.06	2.9	ng	122925	4	11.44	835709	20.0
Benzo[e]pyrene	15.45	7.7	ng	243895	6	15.58	637052	20.0