

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102017\
 Data File : BF099704.D
 Acq On : 20 Oct 2017 16:47
 Operator : SJ/JU
 Sample : I5929-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-2-COMP

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	5.040	499	502	522	rBV	244072	396013	15.66%	1.607%
2	5.446	566	571	589	rBV	2088935	2250700	89.02%	9.131%
3	6.457	739	743	761	rBV	1911202	2381625	94.20%	9.662%
4	6.587	761	765	769	rVV	2409642	2333587	92.30%	9.467%
5	6.651	773	776	790	rVB	145808	159481	6.31%	0.647%
6	6.810	800	803	813	rVB	638042	574369	22.72%	2.330%
7	6.969	826	830	833	rBV	2100383	1869574	73.95%	7.585%
8	7.381	896	900	903	rBV	1435621	1424787	56.36%	5.780%
9	8.092	1018	1021	1028	rBV	929028	772425	30.55%	3.134%
10	9.169	1199	1204	1207	rBV	2812840	2528216	100.00%	10.257%
11	9.563	1264	1271	1275	rVB	51509	55736	2.20%	0.226%
12	9.710	1292	1296	1300	rBV2	23537	31064	1.23%	0.126%
13	9.845	1313	1319	1322	rBV	901436	772434	30.55%	3.134%
14	9.881	1322	1325	1328	rVB	104937	94552	3.74%	0.384%
15	10.051	1352	1354	1358	rVB	59756	54747	2.17%	0.222%
16	10.245	1384	1387	1389	rBV3	38080	39183	1.55%	0.159%
17	10.392	1409	1412	1417	rVB	171118	157235	6.22%	0.638%
18	10.551	1437	1439	1443	rVB	36095	26869	1.06%	0.109%
19	10.639	1450	1454	1458	rBV	1271830	1178785	46.63%	4.782%
20	10.751	1469	1473	1476	rBV2	73092	79364	3.14%	0.322%
21	11.186	1544	1547	1549	rBV2	32076	34609	1.37%	0.140%
22	11.233	1553	1555	1559	rVB	39269	32476	1.28%	0.132%
23	11.333	1569	1572	1574	rBV	685291	610261	24.14%	2.476%
24	11.357	1574	1576	1580	rVB	466578	405223	16.03%	1.644%
25	11.410	1582	1585	1588	rBV	90703	78895	3.12%	0.320%
26	11.839	1655	1658	1659	rBV	46924	43485	1.72%	0.176%
27	11.869	1661	1663	1665	rVB	65228	51150	2.02%	0.208%
28	11.916	1668	1671	1673	rVB	30622	27150	1.07%	0.110%
29	11.951	1674	1677	1679	rBV	181570	157987	6.25%	0.641%
30	12.133	1705	1708	1713	rVB	38873	39483	1.56%	0.160%
31	12.551	1775	1779	1782	rBV	947265	787169	31.14%	3.194%
32	12.580	1782	1784	1788	rVB2	43537	38478	1.52%	0.156%
33	12.704	1802	1805	1807	rVB2	34654	29444	1.16%	0.119%
34	12.763	1812	1815	1816	rVV2	143636	145250	5.75%	0.589%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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35	12.780	1816	1818	1824	rVV	698748	567031	22.43%	2.300%
36	12.827	1824	1826	1831	rVB2	27894	28155	1.11%	0.114%
37	12.916	1836	1841	1845	rBV	1727158	1657299	65.55%	6.724%
38	12.992	1851	1854	1861	rBV3	32557	54570	2.16%	0.221%
39	13.110	1866	1874	1877	rBV	105990	140223	5.55%	0.569%
40	13.174	1882	1885	1888	rBV	84559	74861	2.96%	0.304%
41	13.216	1888	1892	1898	rVB3	34241	53556	2.12%	0.217%
42	13.339	1910	1913	1919	rBV3	20736	29736	1.18%	0.121%
43	13.727	1976	1979	1981	rBV	29245	28675	1.13%	0.116%
44	13.751	1981	1983	1985	rVV	41590	47816	1.89%	0.194%
45	13.798	1989	1991	1996	rVV2	88182	115098	4.55%	0.467%
46	13.851	1998	2000	2003	rVB	40231	36004	1.42%	0.146%
47	13.939	2012	2015	2017	rBV	30687	32814	1.30%	0.133%
48	13.980	2017	2022	2025	rVV2	664890	783724	31.00%	3.180%
49	14.004	2025	2026	2030	rVB	160518	100327	3.97%	0.407%
50	14.086	2037	2040	2043	rBV2	23706	28215	1.12%	0.114%
51	15.016	2194	2198	2201	rBV	90489	129190	5.11%	0.524%
52	15.045	2201	2203	2208	rVB2	70765	75077	2.97%	0.305%
53	15.316	2246	2249	2254	rVB	50862	56716	2.24%	0.230%
54	15.380	2256	2260	2263	rVV	56047	61745	2.44%	0.250%
55	15.439	2263	2270	2275	rVV2	440722	564998	22.35%	2.292%
56	15.839	2334	2338	2342	rVB	36828	49731	1.97%	0.202%
57	16.327	2416	2421	2428	rBV2	30110	54040	2.14%	0.219%
58	16.910	2513	2520	2529	rVB4	51576	103808	4.11%	0.421%
59	17.362	2591	2597	2601	rBV4	12898	27366	1.08%	0.111%
60	17.580	2628	2634	2641	rBV5	20271	51241	2.03%	0.208%
61	19.456	2946	2953	2955	rBV8	15408	35015	1.38%	0.142%

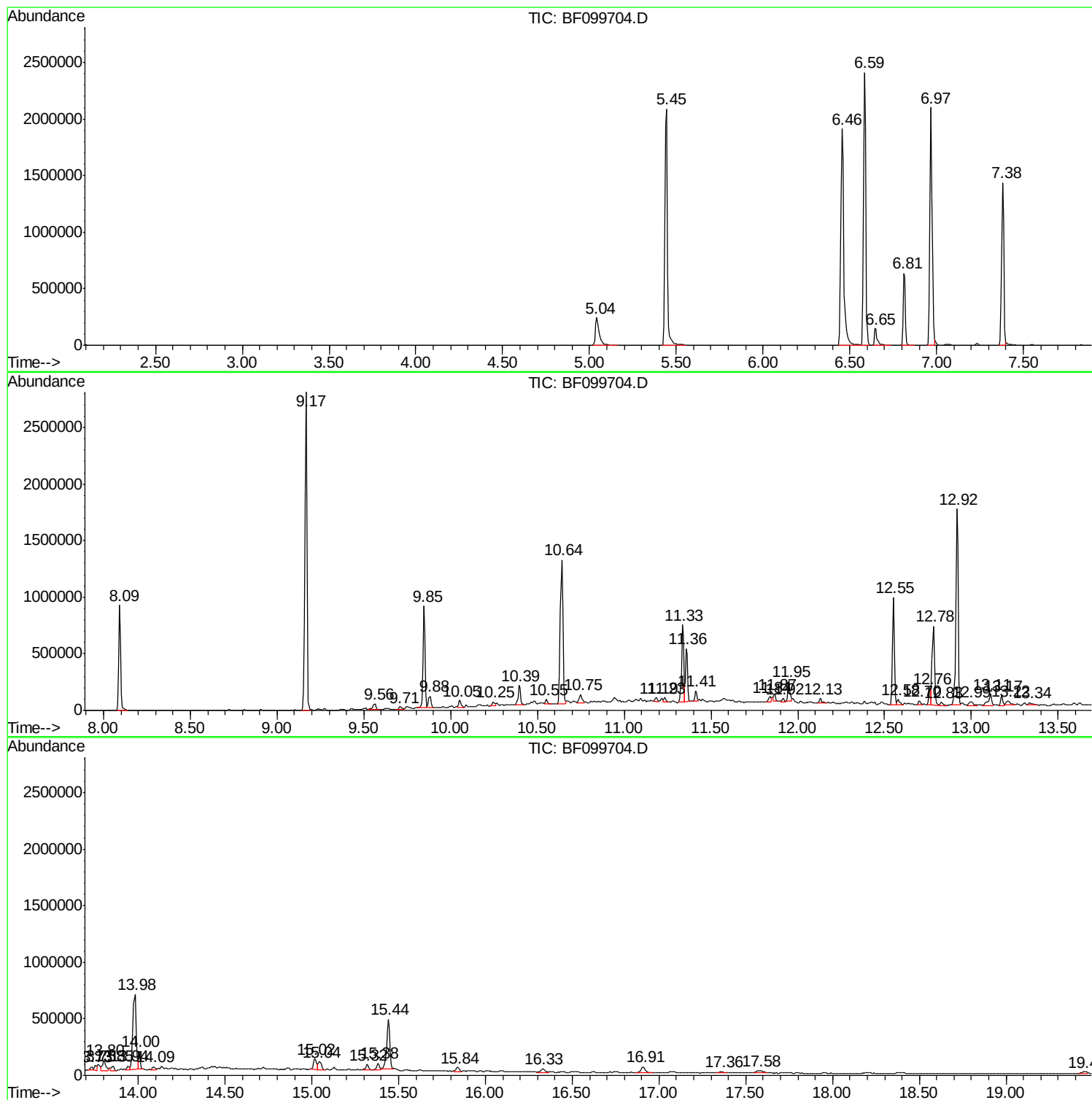
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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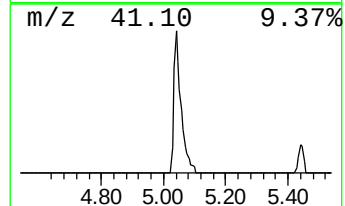
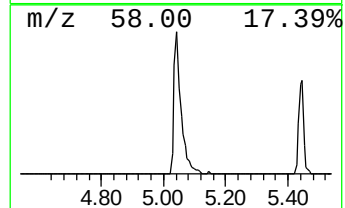
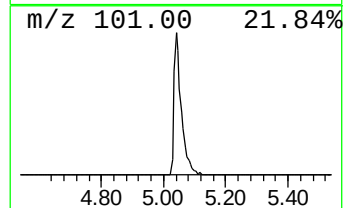
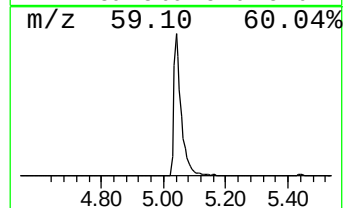
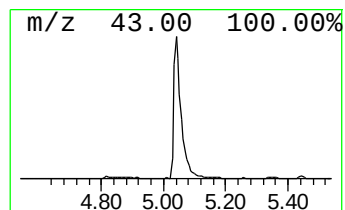
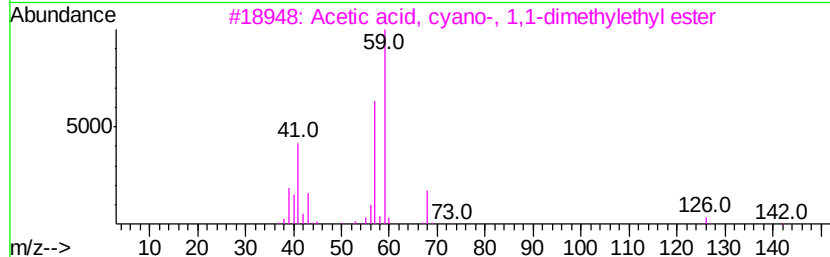
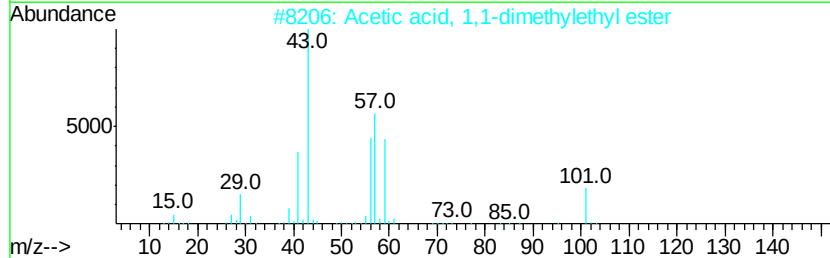
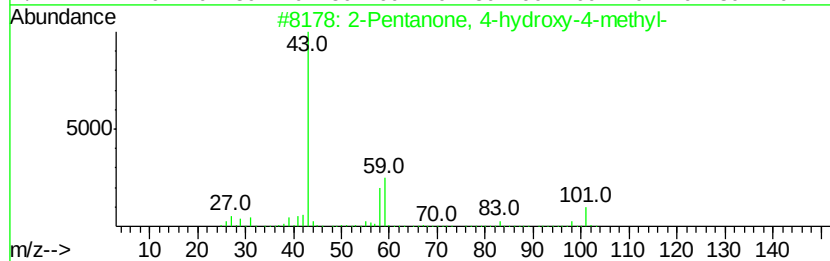
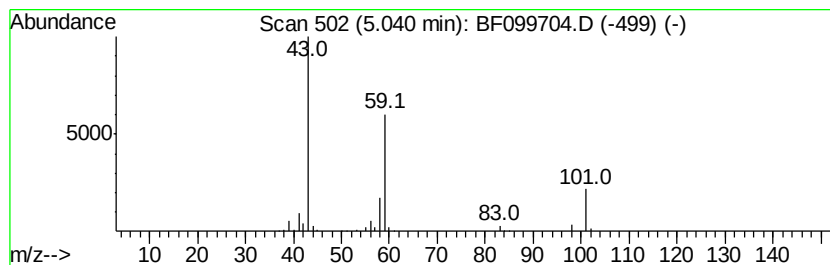
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	13.79 ng	396013	1,4-Dichlorobenzene-d4	6.81

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			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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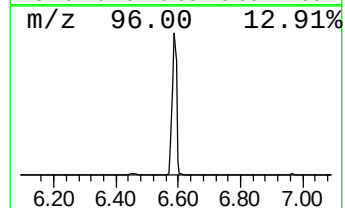
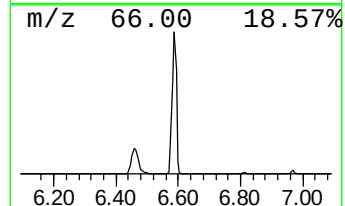
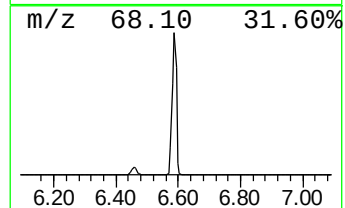
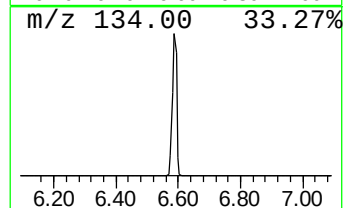
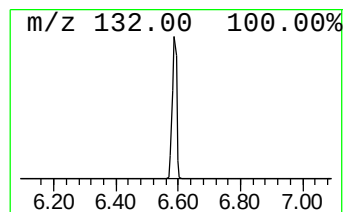
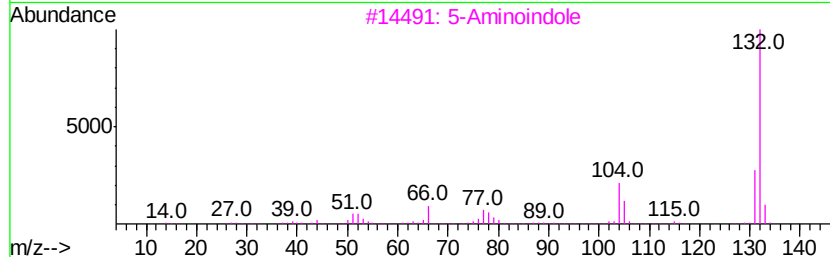
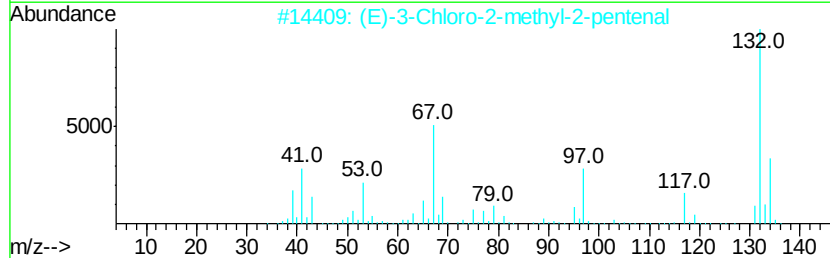
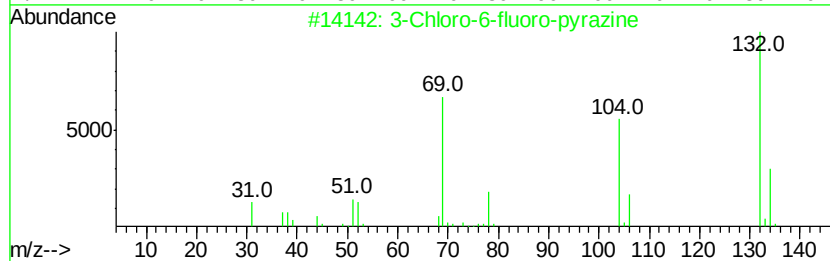
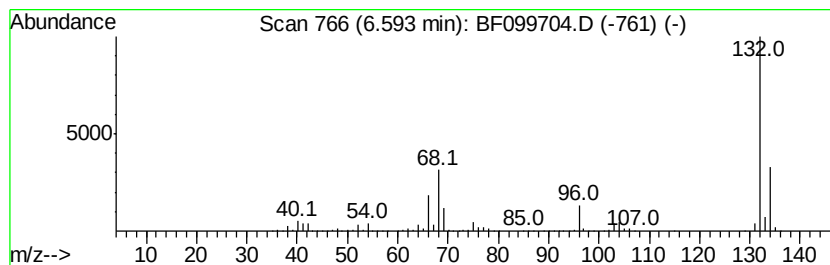
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	81.26 ng	2333590	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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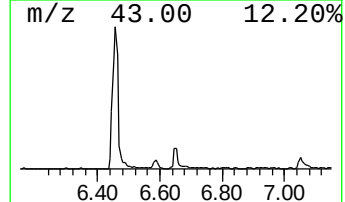
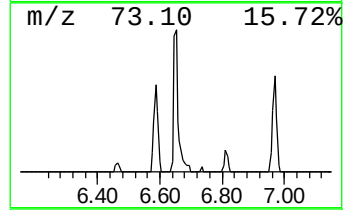
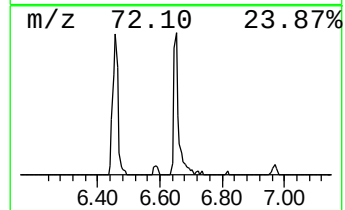
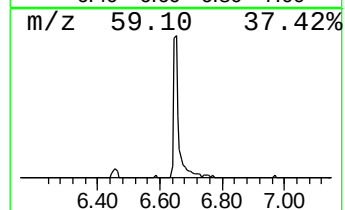
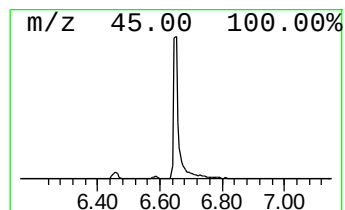
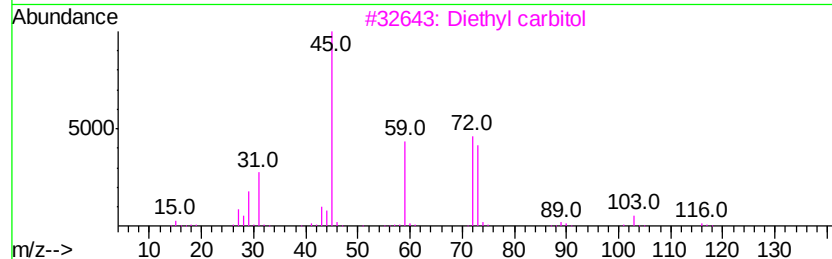
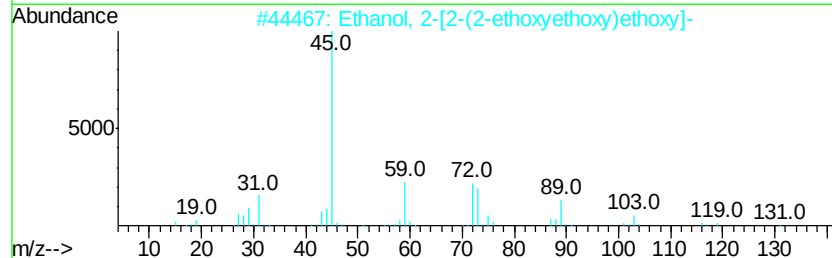
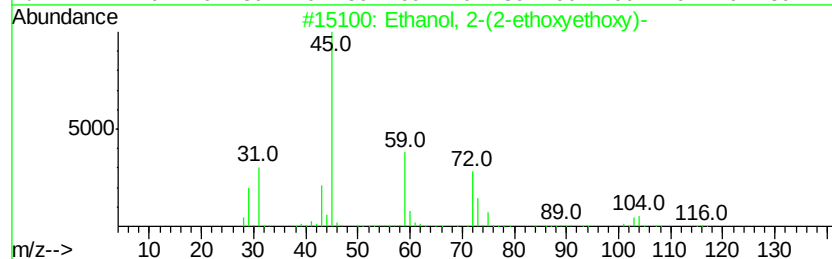
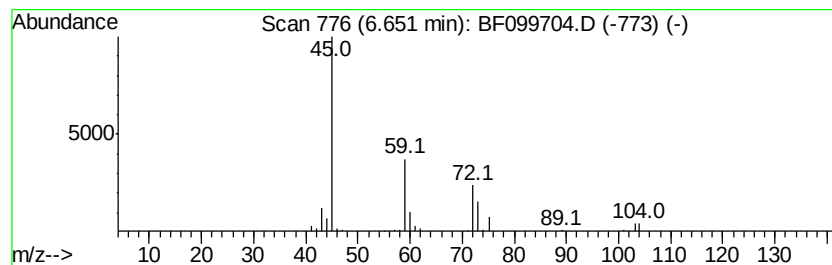
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.65	5.55 ng	159481	1,4-Dichlorobenzene-d4	6.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
3	Diethyl carbitol	162	C8H18O3	000112-36-7	56
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



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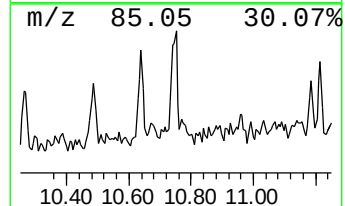
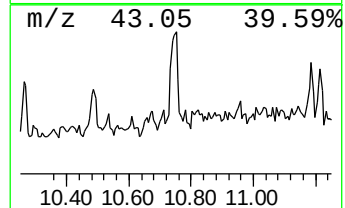
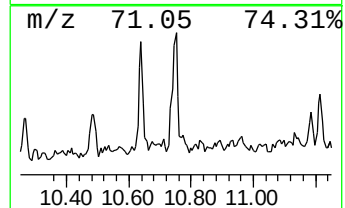
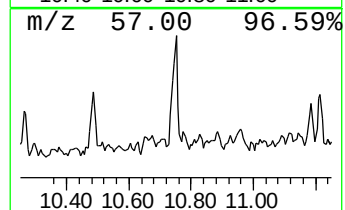
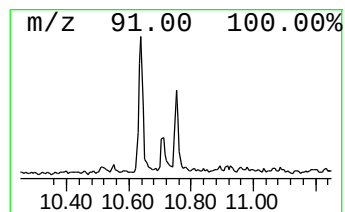
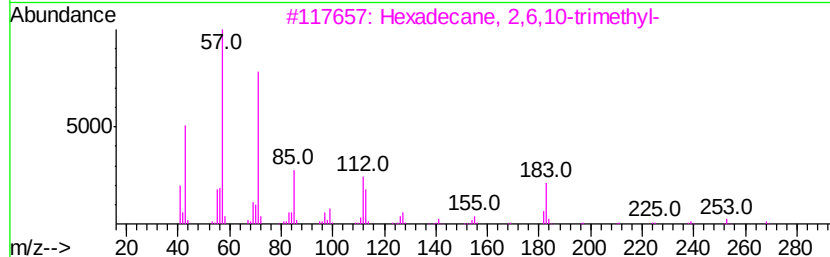
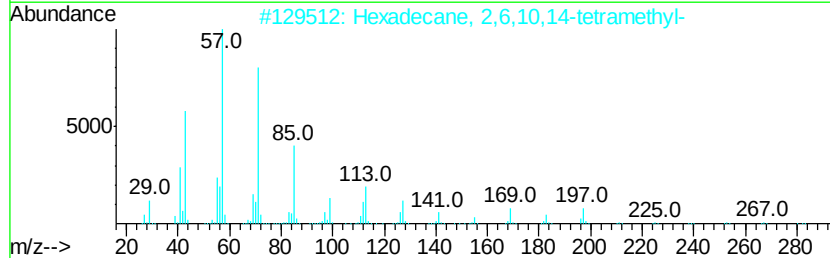
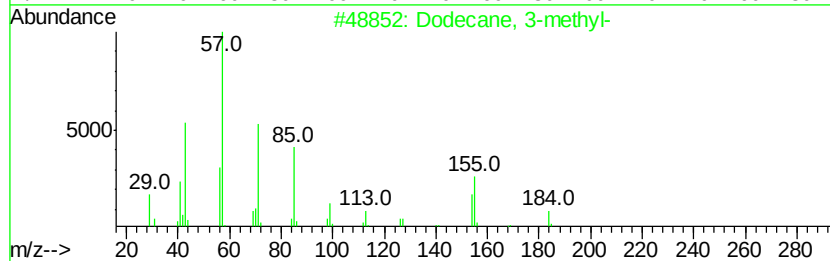
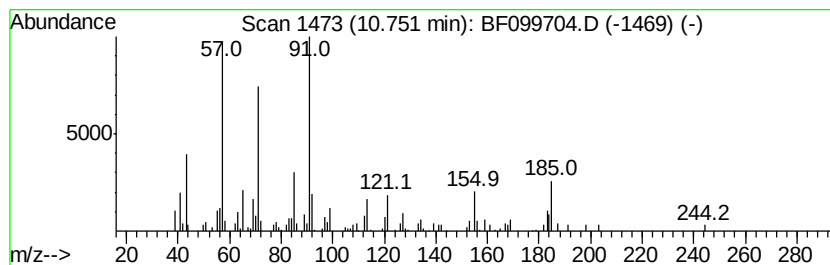
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.75	2.60 ng	79364	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 3-methyl-	184	C13H28	017312-57-1	50
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	49
3	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	47
4	Tetradecane	198	C14H30	000629-59-4	46
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43



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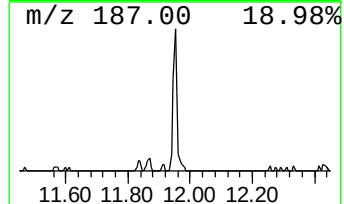
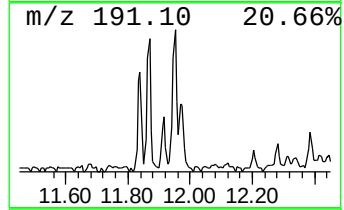
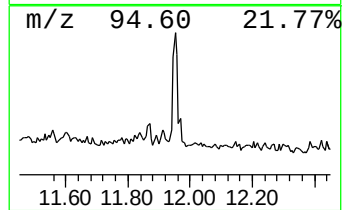
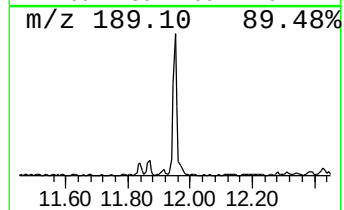
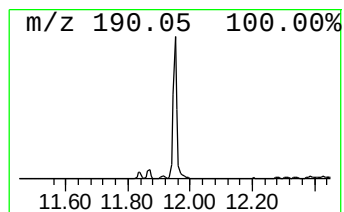
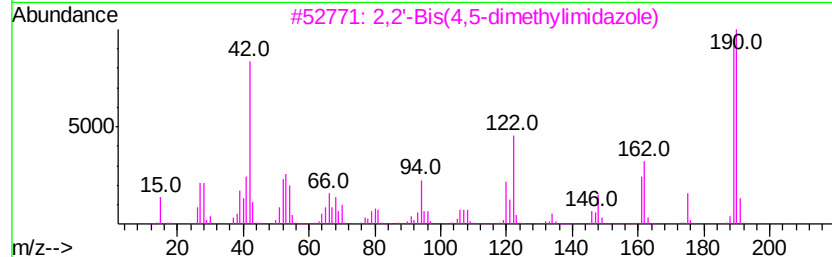
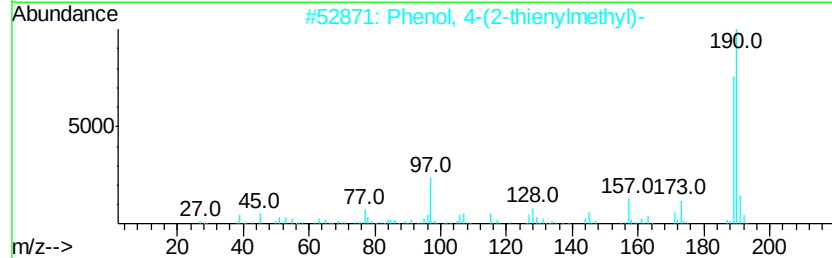
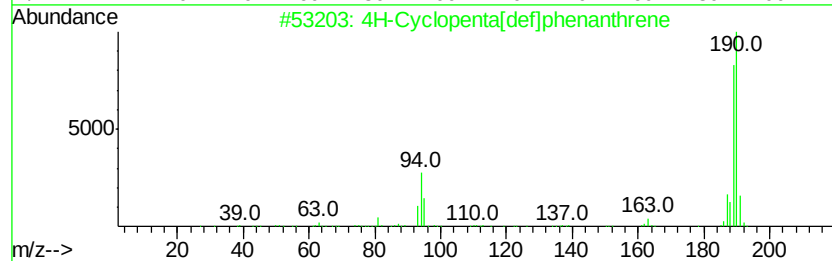
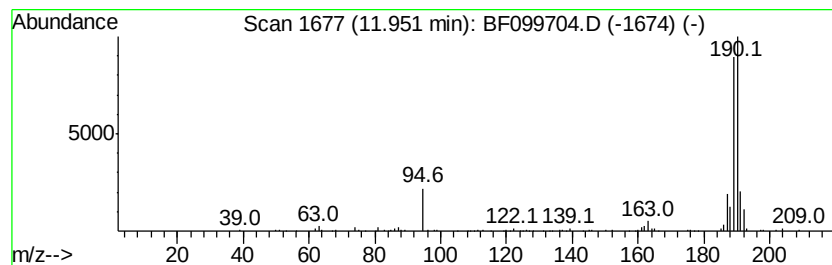
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ClientSampleId :
TP-1-2-COMP

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 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	5.18 ng	157987	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	72
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	Hydrazinecarboxaldehyde, 2-[3-(m...	190	C4H6N4OS2	038362-25-3	22
5	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102017\
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Acq On : 20 Oct 2017 16:47
Operator : SJ/JU
Sample : I5929-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

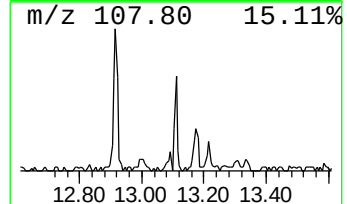
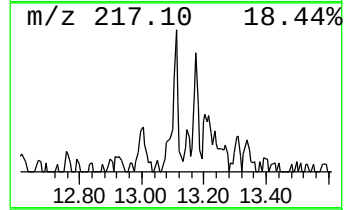
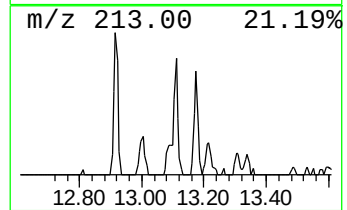
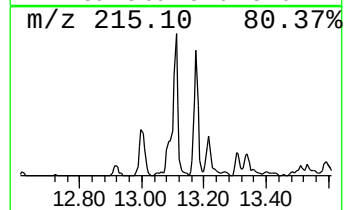
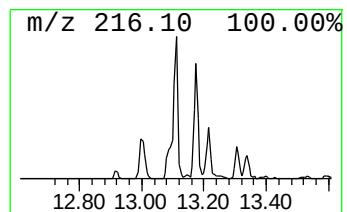
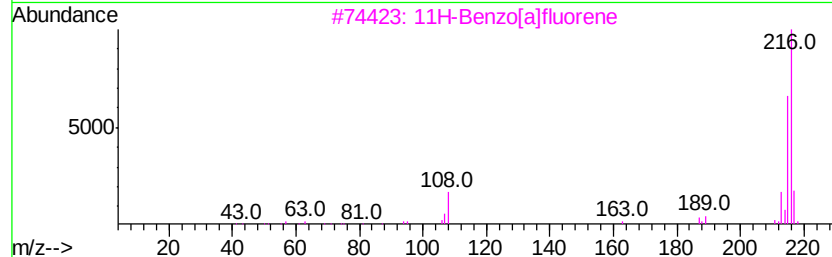
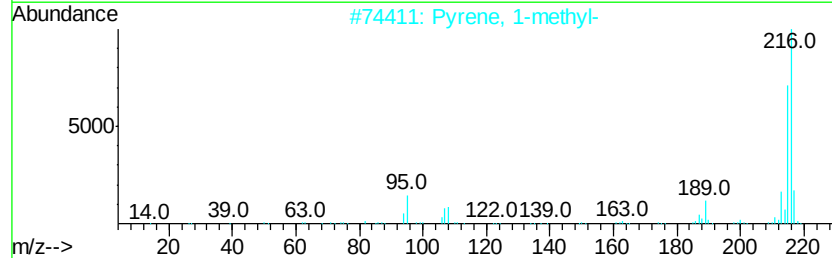
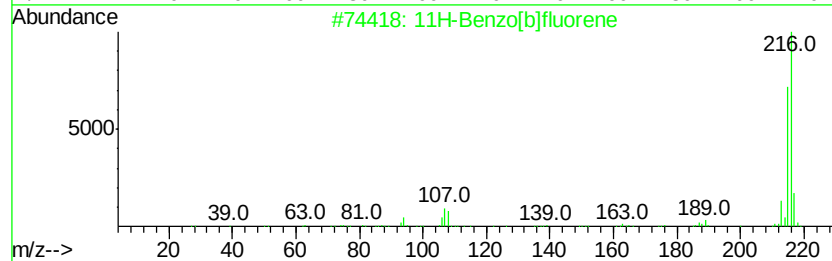
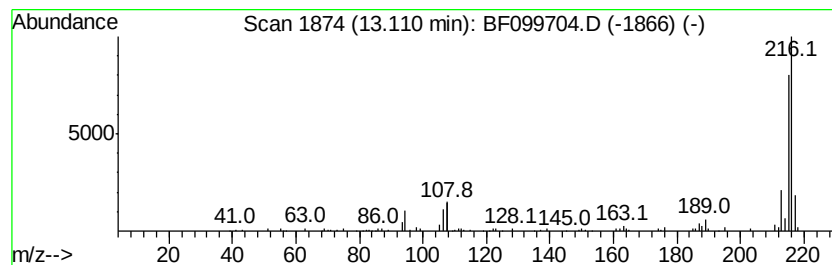
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ClientSampleId :
TP-1-2-COMP

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 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.11	3.58 ng	140223	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102017\
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Sample : I5929-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1-2-COMP

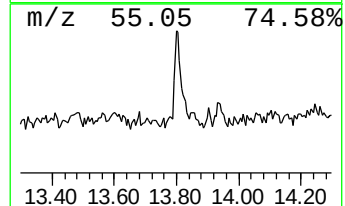
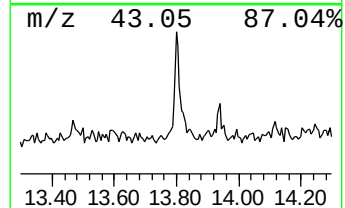
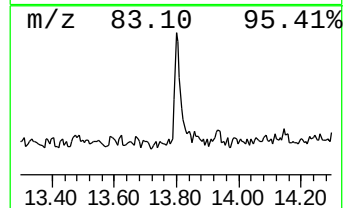
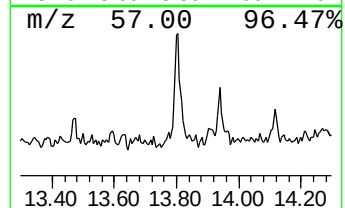
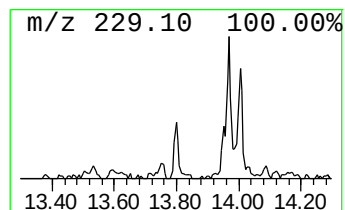
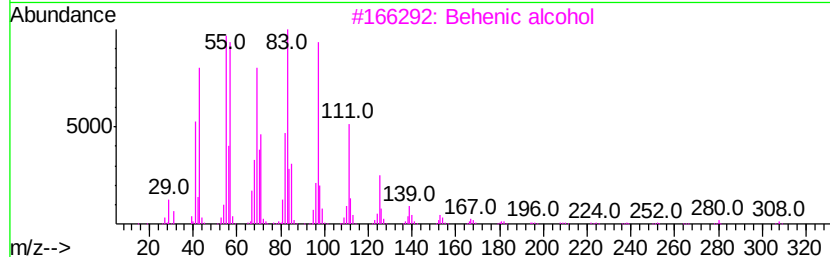
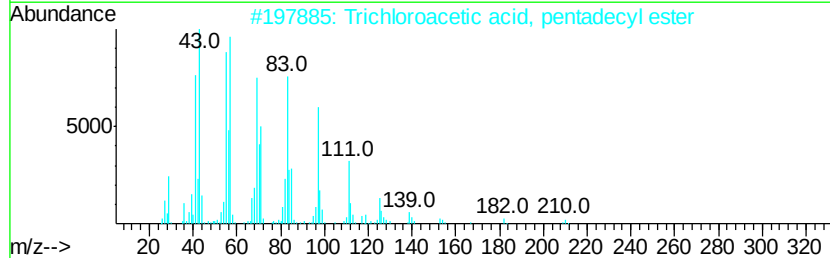
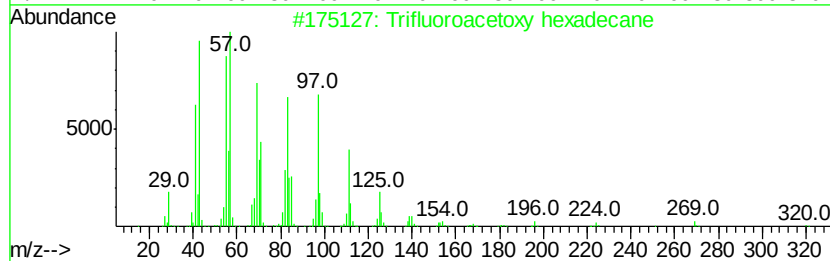
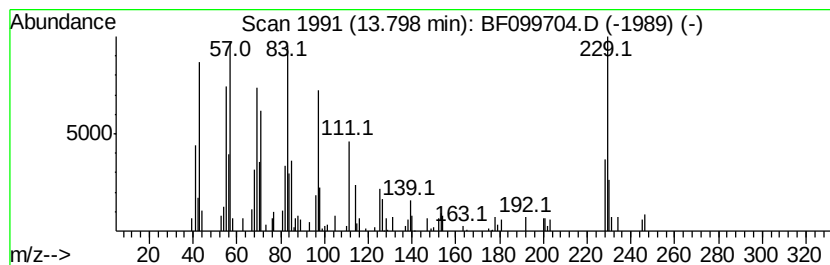
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.94 ng	115098	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	64
3		Behenic alcohol	326	C22H46O	000661-19-8	64
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
5		1-Heptacosanol	396	C27H56O	002004-39-9	64



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Sample : I5929-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

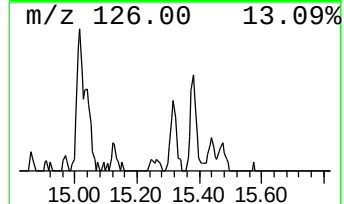
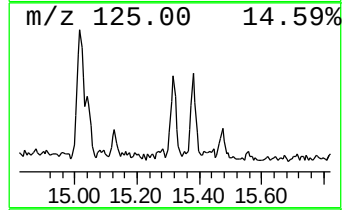
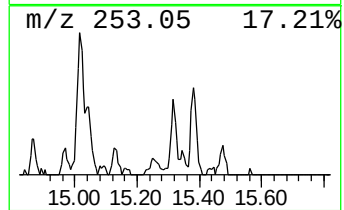
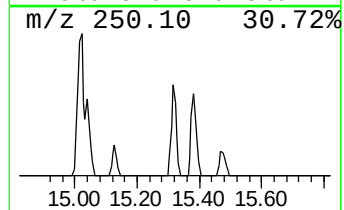
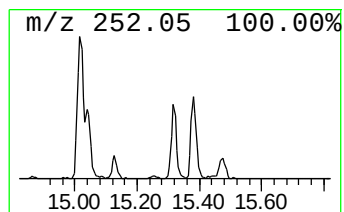
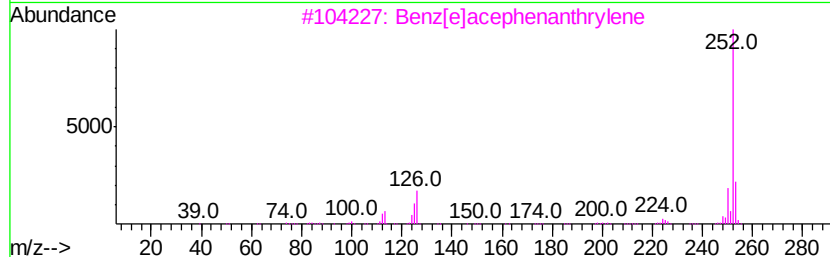
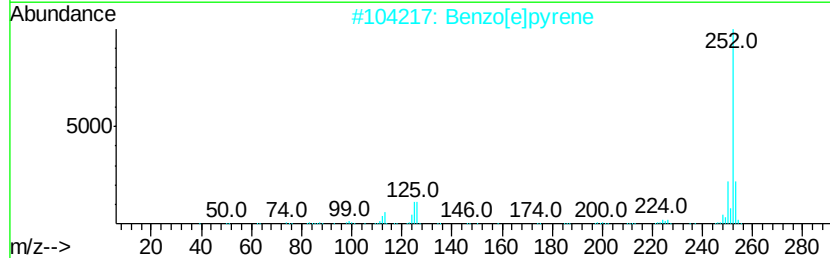
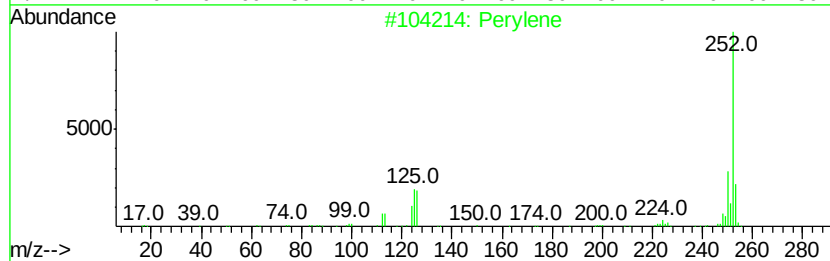
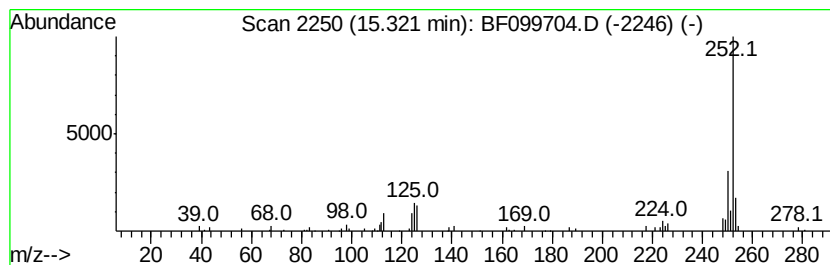
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.01 ng	56716	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	97
2		Benzo[el]pyrene	252	C20H12	000192-97-2	96
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
4		Benzo[a]pyrene	252	C20H12	000050-32-8	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102017\
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Sample : I5929-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	13.8	ng	396013	1	6.81	574369	20.0
unknown6.59	6.59	81.3	ng	2333590	1	6.81	574369	20.0
Ethanol, 2-(2-eth...	6.65	5.5	ng	159481	1	6.81	574369	20.0
Dodecane, 3-methyl-	10.75	2.6	ng	79364	4	11.33	610261	20.0
4H-Cyclopenta[def...	11.95	5.2	ng	157987	4	11.33	610261	20.0
11H-Benzo[b]fluorene	13.11	3.6	ng	140223	5	13.98	783724	20.0
Trifluoroacetoxy ...	13.80	2.9	ng	115098	5	13.98	783724	20.0
Perylene	15.32	2.0	ng	56716	6	15.44	564998	20.0