

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
 Data File : BF104677.D
 Acq On : 20 Apr 2018 16:35
 Operator : JU/SJ
 Sample : J2475-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-01

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-BF040618.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	3.828	292	296	302	rVB	18519	25348	1.18%	0.108%
2	5.010	493	497	506	rVB	68809	88997	4.15%	0.381%
3	5.422	563	567	577	rBV	2136604	1971746	91.94%	8.432%
4	6.445	736	741	759	rVB	1931357	2002565	93.38%	8.564%
5	6.575	759	763	766	rBV	2420466	2041710	95.21%	8.732%
6	6.804	798	802	805	rBV	870771	675102	31.48%	2.887%
7	6.957	824	828	832	rBV	1856127	1666793	77.72%	7.128%
8	7.369	894	898	901	rBV	1424301	1171721	54.64%	5.011%
9	8.086	1017	1020	1026	rBV	997039	812897	37.91%	3.476%
10	8.675	1115	1120	1123	rBV	34373	30361	1.42%	0.130%
11	9.163	1199	1203	1206	rBV	2538877	2144488	100.00%	9.171%
12	9.239	1213	1216	1218	rVB	58438	47228	2.20%	0.202%
13	9.557	1266	1270	1273	rBV	160538	133041	6.20%	0.569%
14	9.704	1292	1295	1298	rBV	30379	26640	1.24%	0.114%
15	9.769	1303	1306	1310	rVB	101481	82856	3.86%	0.354%
16	9.845	1315	1319	1323	rBV	956675	841392	39.24%	3.598%
17	10.045	1351	1353	1357	rVB3	19703	24310	1.13%	0.104%
18	10.086	1357	1360	1364	rBV3	32309	32282	1.51%	0.138%
19	10.239	1384	1386	1388	rBV	24670	25461	1.19%	0.109%
20	10.269	1388	1391	1394	rVB	113641	90028	4.20%	0.385%
21	10.392	1408	1412	1417	rVB4	19867	27740	1.29%	0.119%
22	10.486	1424	1428	1430	rBV2	34856	41811	1.95%	0.179%
23	10.633	1450	1453	1464	rVV	1343009	1213971	56.61%	5.192%
24	10.739	1468	1471	1480	rVB	94844	128010	5.97%	0.547%
25	10.933	1500	1504	1508	rBV6	14602	27435	1.28%	0.117%
26	11.192	1544	1548	1550	rBV2	46330	45647	2.13%	0.195%
27	11.221	1550	1553	1559	rVB3	30277	43285	2.02%	0.185%
28	11.333	1568	1572	1574	rBV	945490	796422	37.14%	3.406%
29	11.357	1574	1576	1582	rVV	279246	236640	11.03%	1.012%
30	11.410	1582	1585	1588	rVB	55058	51042	2.38%	0.218%
31	11.569	1609	1612	1617	rBV	23734	25694	1.20%	0.110%
32	11.616	1617	1620	1624	rVB2	37606	35226	1.64%	0.151%
33	11.833	1654	1657	1659	rBV	44676	41942	1.96%	0.179%
34	11.857	1659	1661	1667	rVB2	92135	103670	4.83%	0.443%

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35	11.945	1673	1676	1679	rBV	65737	76623	3.57%	0.328%
36	11.968	1679	1680	1684	rVB	41175	26106	1.22%	0.112%
37	12.021	1686	1689	1691	rBV2	27165	25493	1.19%	0.109%
38	12.133	1704	1708	1710	rBV2	34248	36128	1.68%	0.155%
39	12.157	1710	1712	1719	rVV2	33493	39289	1.83%	0.168%
40	12.380	1747	1750	1753	rBV	34633	39513	1.84%	0.169%
41	12.416	1753	1756	1759	rVV4	28509	33900	1.58%	0.145%
42	12.468	1763	1765	1771	rVB2	32995	36073	1.68%	0.154%
43	12.545	1775	1778	1782	rBV	521674	426647	19.90%	1.825%
44	12.704	1798	1805	1808	rBV3	18121	40516	1.89%	0.173%
45	12.774	1812	1817	1823	rVV	453657	491774	22.93%	2.103%
46	12.827	1824	1826	1830	rVB2	27107	28815	1.34%	0.123%
47	12.921	1835	1842	1845	rBV	1975751	1863883	86.92%	7.971%
48	12.992	1851	1854	1858	rVB2	31769	41926	1.96%	0.179%
49	13.080	1866	1869	1870	rBV2	29055	30014	1.40%	0.128%
50	13.104	1871	1873	1877	rVB	50505	45700	2.13%	0.195%
51	13.174	1882	1885	1887	rBV	27520	24170	1.13%	0.103%
52	13.210	1888	1891	1894	rVV2	40087	38694	1.80%	0.165%
53	13.333	1909	1912	1915	rBV2	33215	37025	1.73%	0.158%
54	13.615	1957	1960	1963	rVB	51241	52886	2.47%	0.226%
55	13.721	1975	1978	1981	rBV2	48296	64065	2.99%	0.274%
56	13.774	1981	1987	1990	rVV2	187354	270565	12.62%	1.157%
57	13.810	1990	1993	2002	rVB2	257117	357905	16.69%	1.531%
58	13.974	2017	2021	2024	rBV2	742053	872934	40.71%	3.733%
59	14.004	2024	2026	2034	rVB	236301	214697	10.01%	0.918%
60	15.015	2195	2198	2202	rBV	225961	336486	15.69%	1.439%
61	15.321	2246	2250	2256	rVB	124253	162606	7.58%	0.695%
62	15.380	2257	2260	2265	rVB	173581	204951	9.56%	0.876%
63	15.445	2266	2271	2274	rBV	410887	527208	24.58%	2.255%
64	16.892	2513	2517	2525	rBV2	84327	183108	8.54%	0.783%

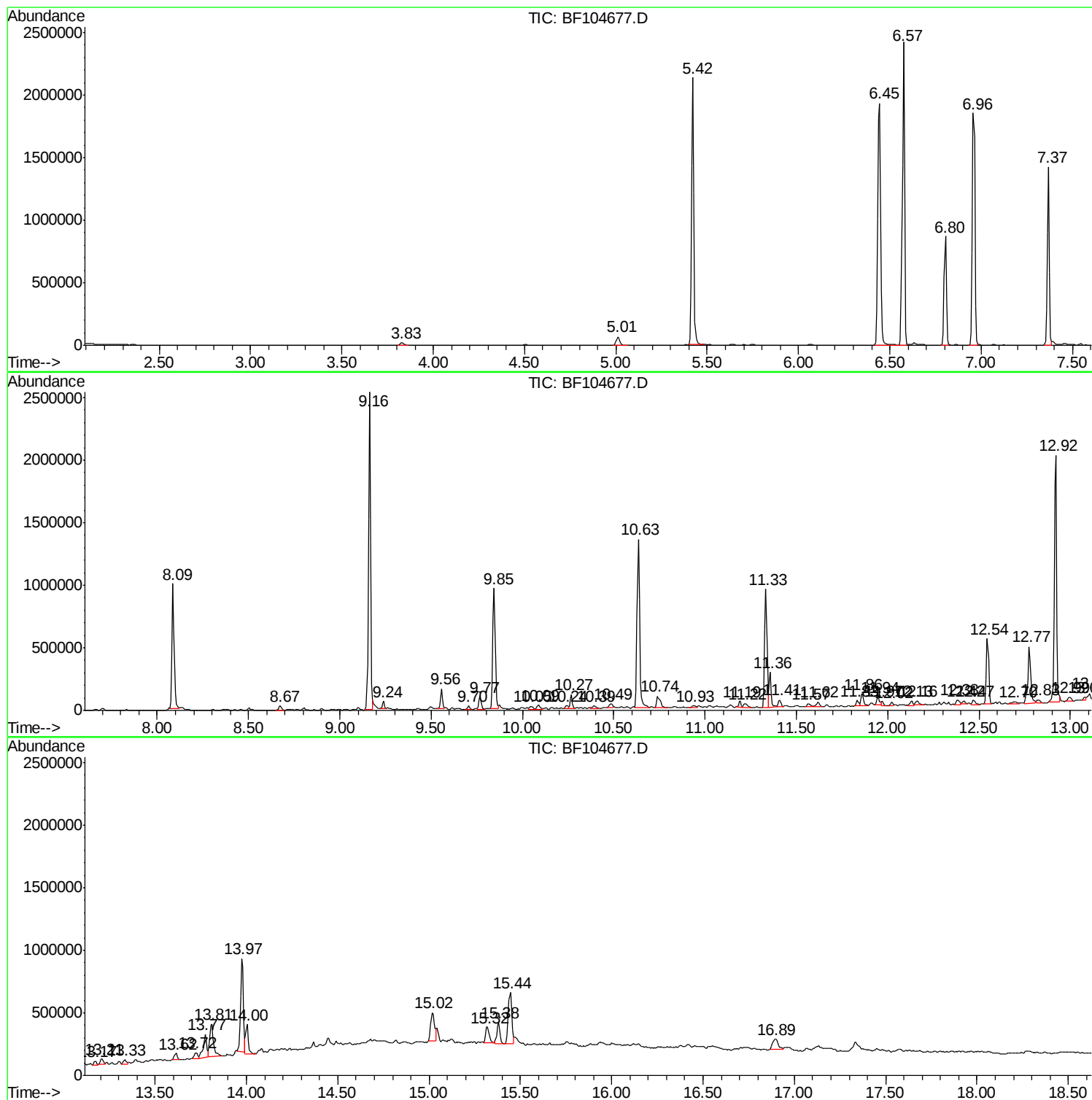
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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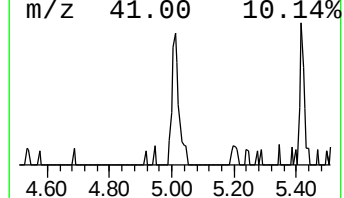
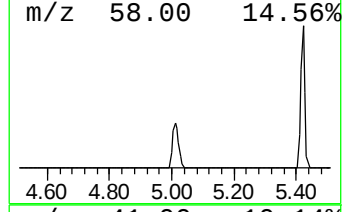
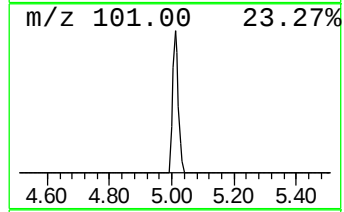
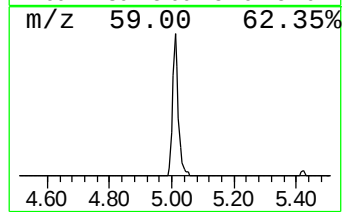
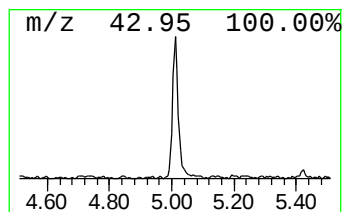
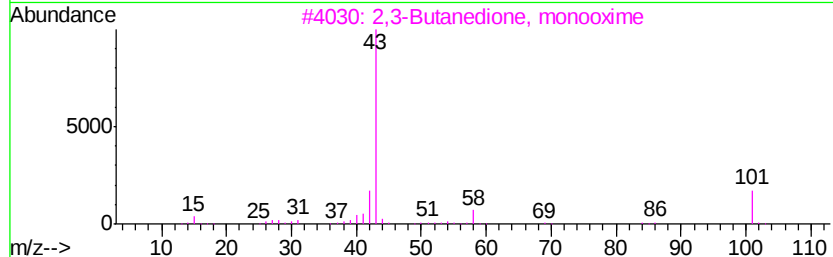
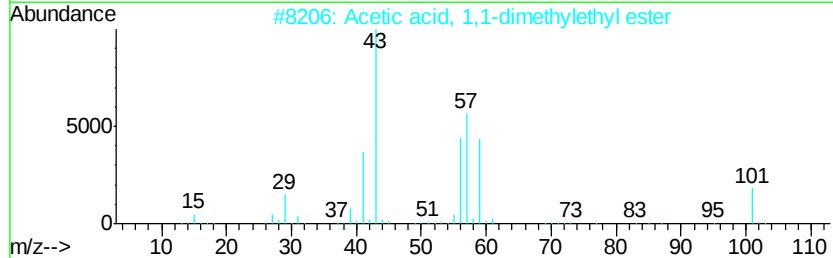
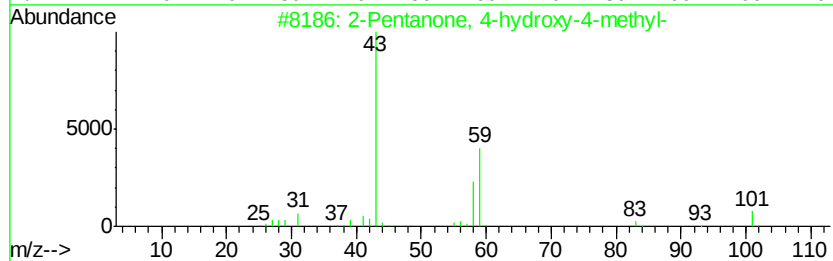
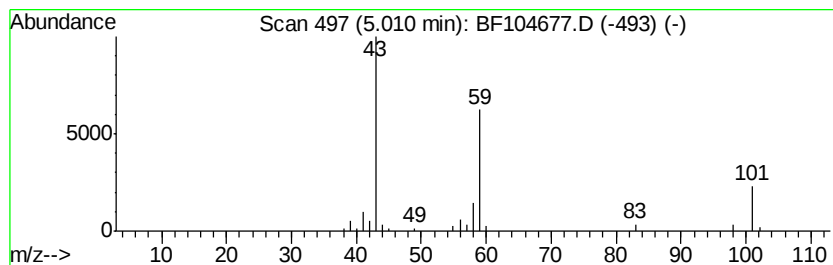
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.64 ng	88997	1,4-Dichlorobenzene-d4	6.80

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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			1,2-Butanediol	90	C4H10O2	000584-03-2	17



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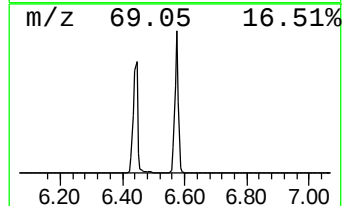
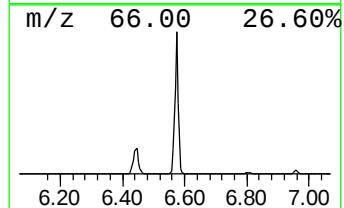
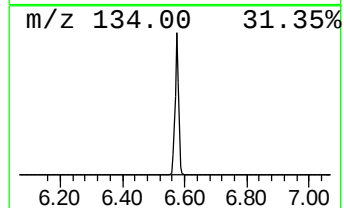
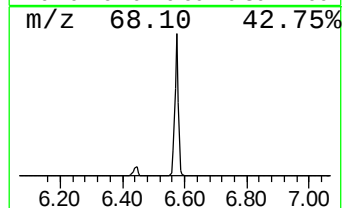
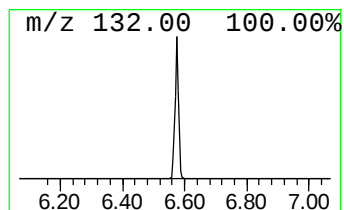
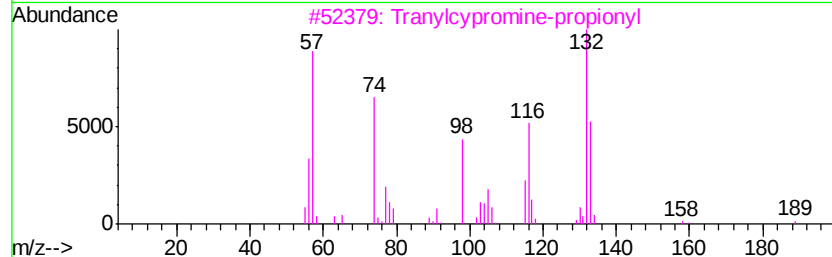
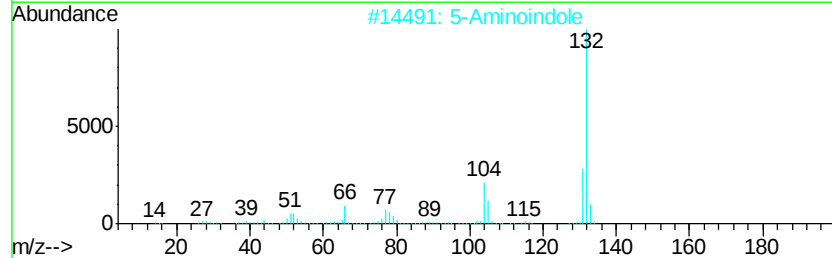
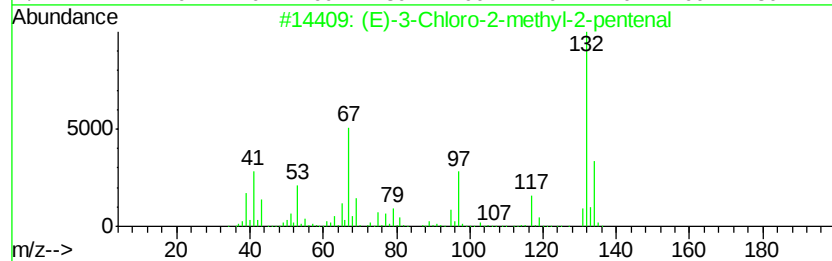
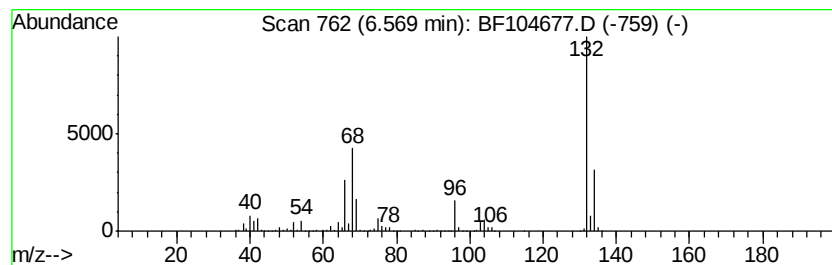
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	60.49 ng	2041710	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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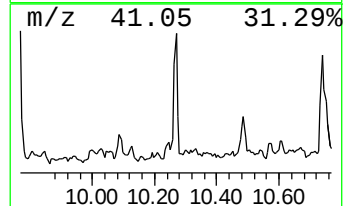
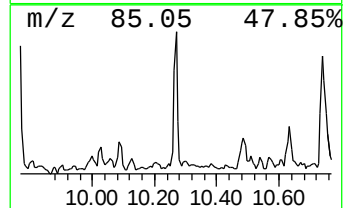
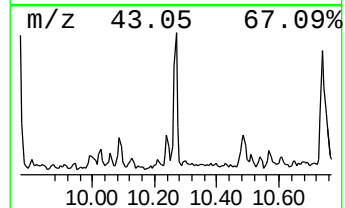
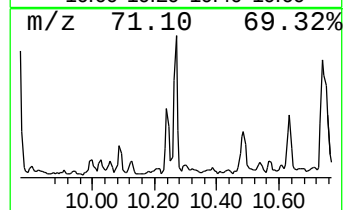
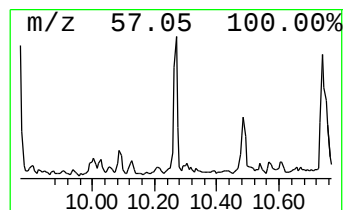
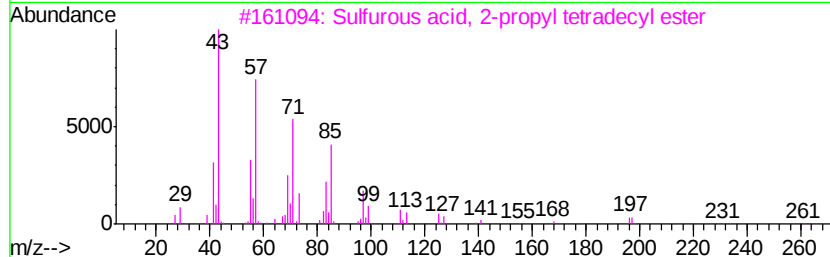
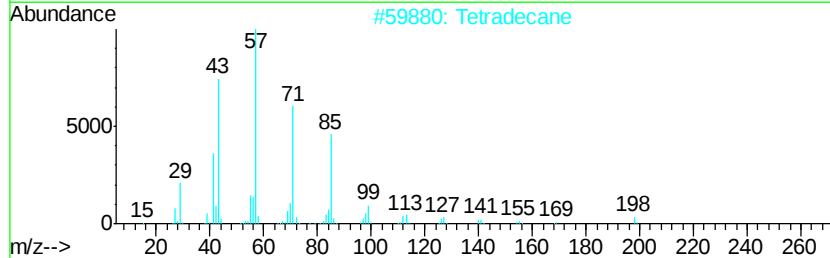
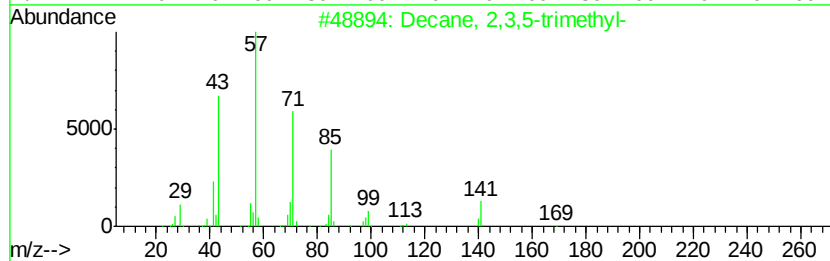
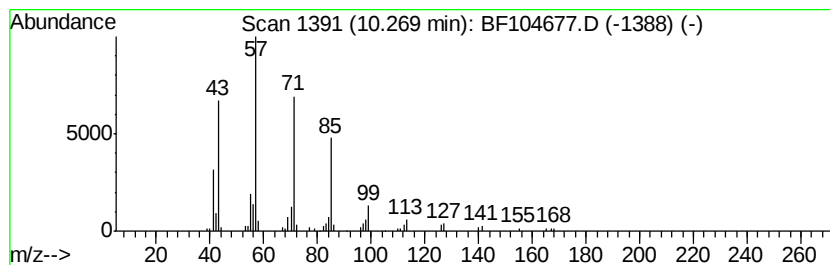
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane, 2,3,5-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.14 ng	90028	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2		Tetradecane	198	C14H30	000629-59-4	87
3		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	86
4		Pentadecane	212	C15H32	000629-62-9	86
5		Hexadecane	226	C16H34	000544-76-3	83



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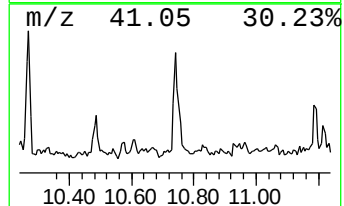
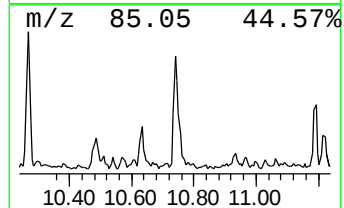
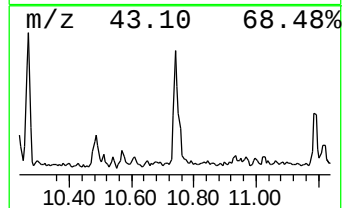
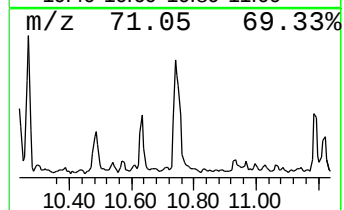
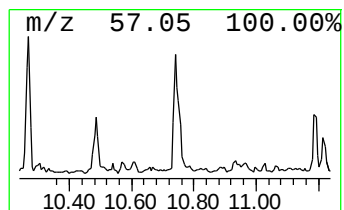
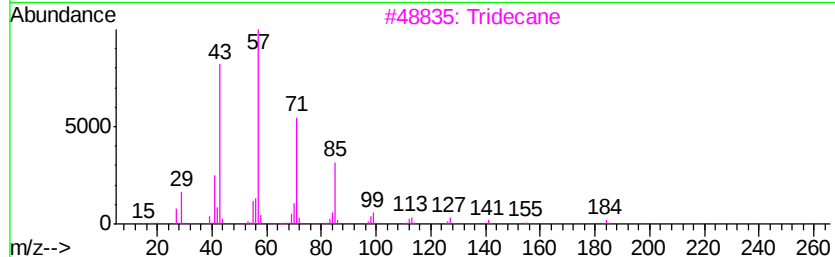
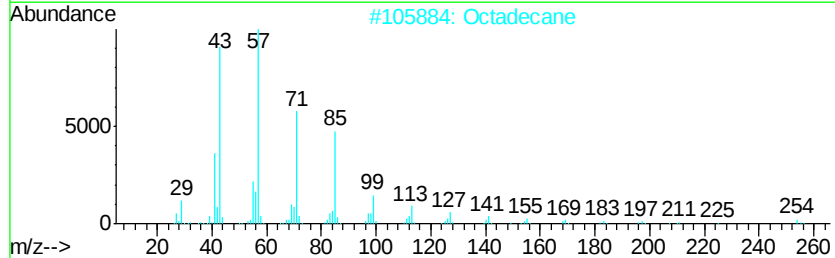
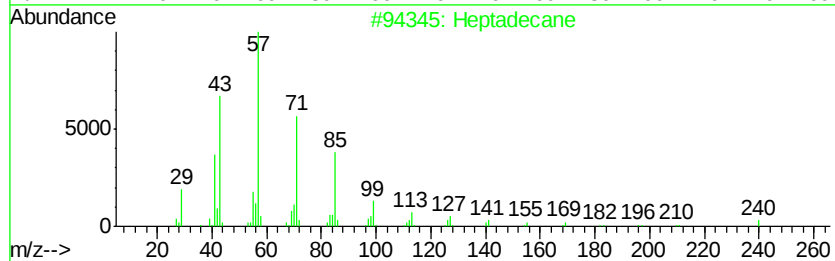
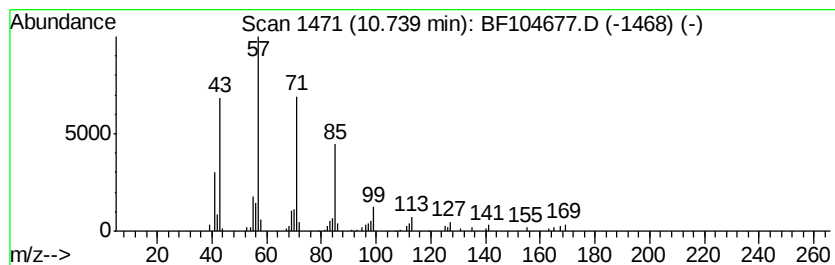
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	3.21 ng	128010	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Octadecane		254	C18H38	000593-45-3	90
3	Tridecane		184	C13H28	000629-50-5	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Tetradecane		198	C14H30	000629-59-4	87



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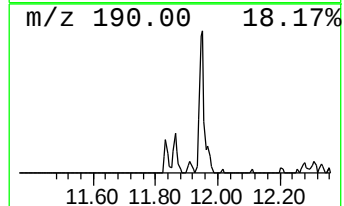
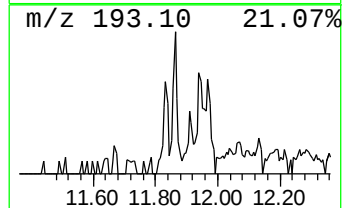
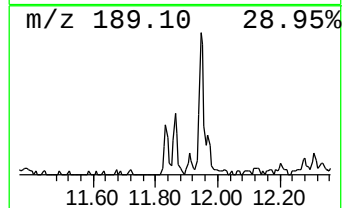
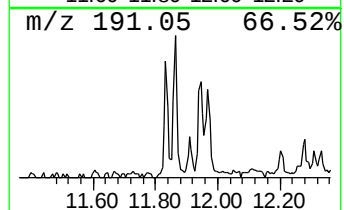
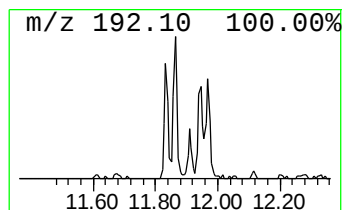
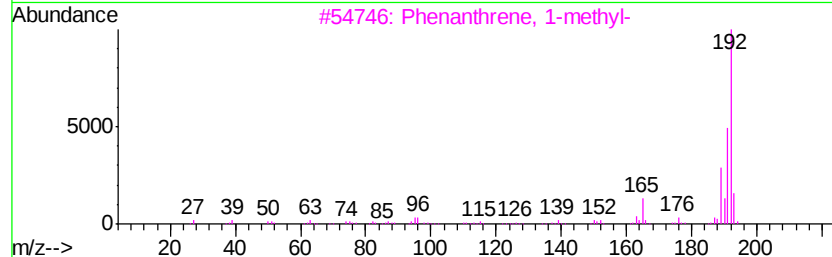
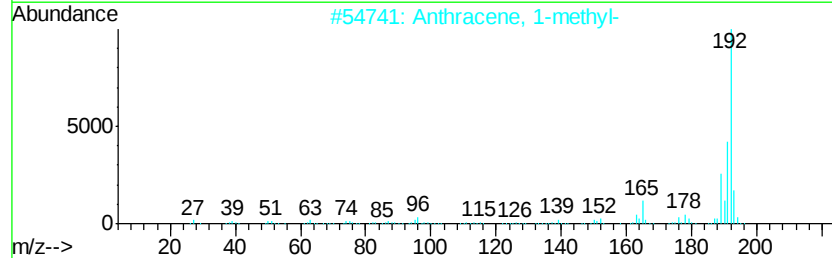
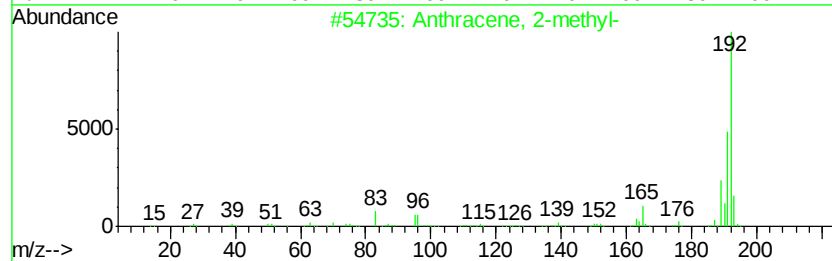
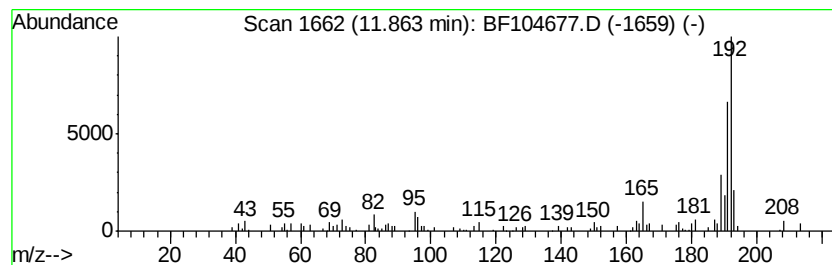
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.60 ng	103670	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60
5		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	60



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
Data File : BF104677.D
Acq On : 20 Apr 2018 16:35
Operator : JU/SJ
Sample : J2475-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-01

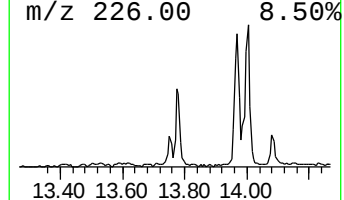
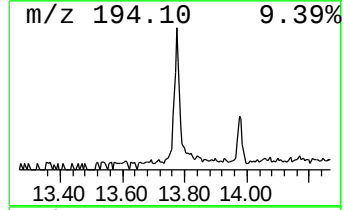
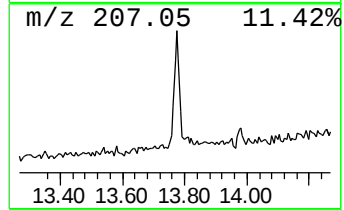
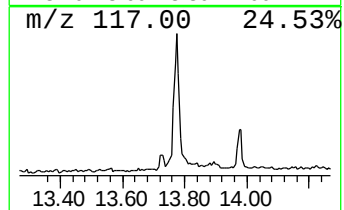
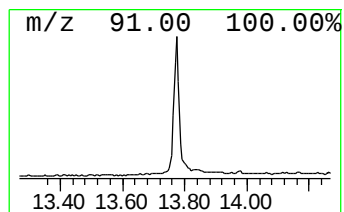
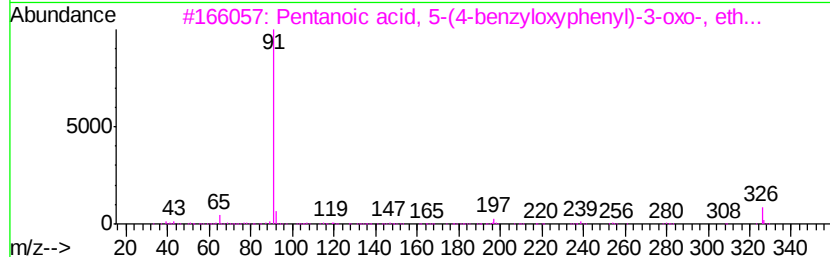
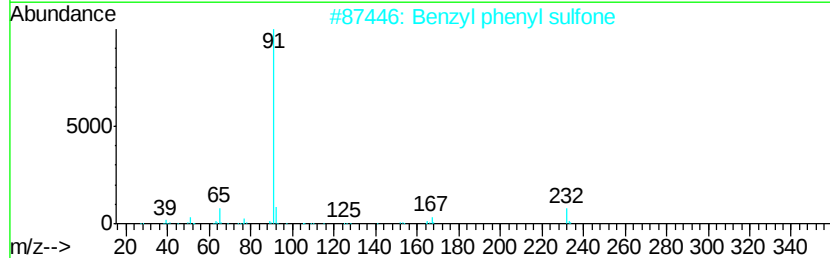
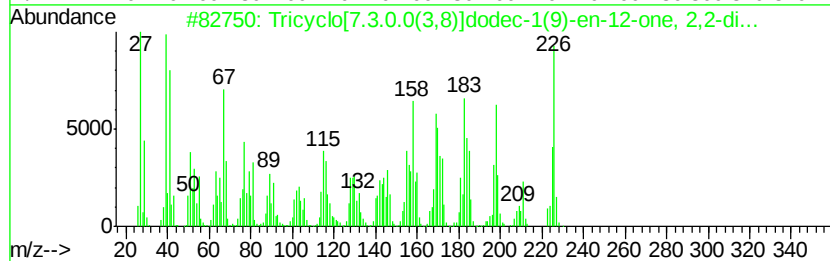
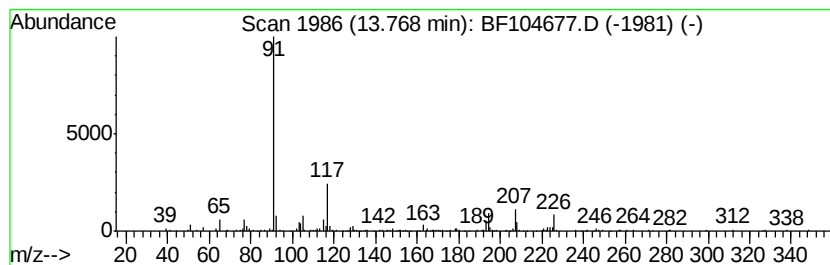
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	6.20 ng	270565	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricyclo[7.3.0.0(3,8)]dodec-1(9)...	226	C14H14N2O	1000160-53-8	18
2		Benzyl phenyl sulfone	232	C13H12O2S	003112-88-7	10
3		Pentanoic acid, 5-(4-benzvloxyvph...	326	C20H22O4	1000266-41-6	10
4		Nordestrel	312	C21H28O2	006533-00-2	10
5		Benzoic acid, 2-(2-phenylethyl)-	226	C15H14O2	004890-85-1	10



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Sample : J2475-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-01

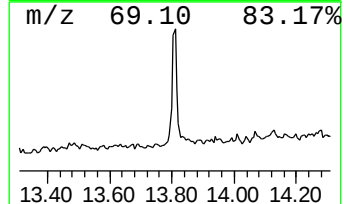
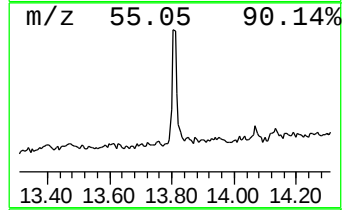
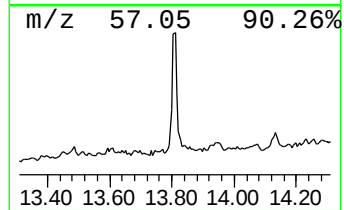
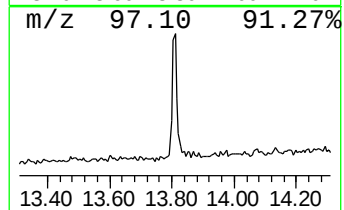
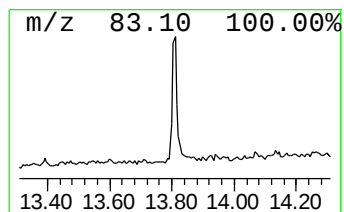
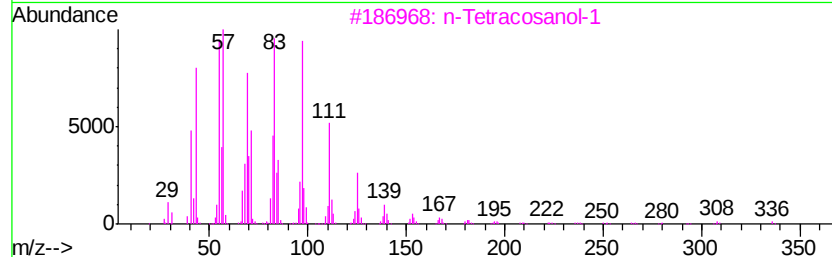
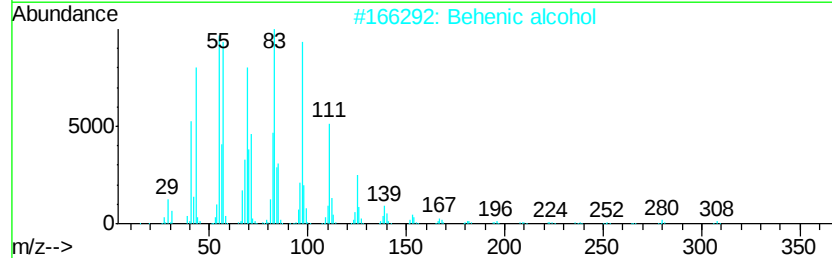
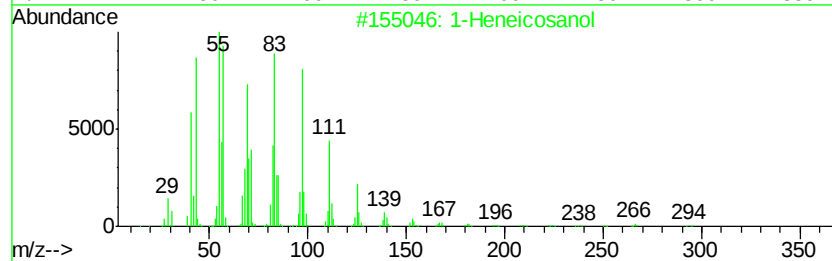
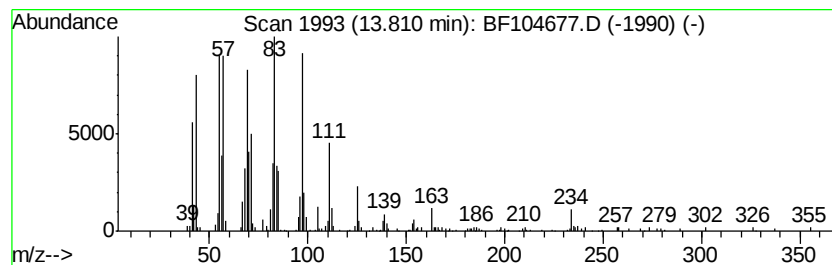
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	8.20 ng	357905	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93



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Sample : J2475-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

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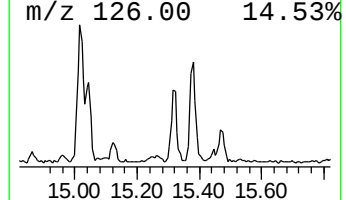
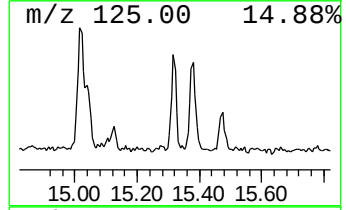
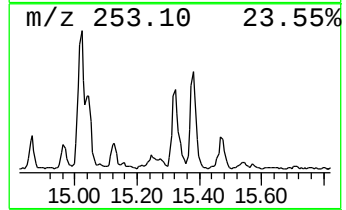
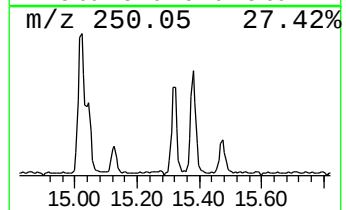
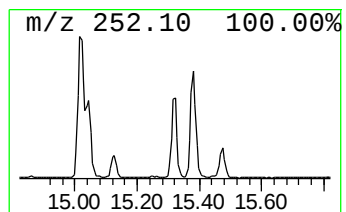
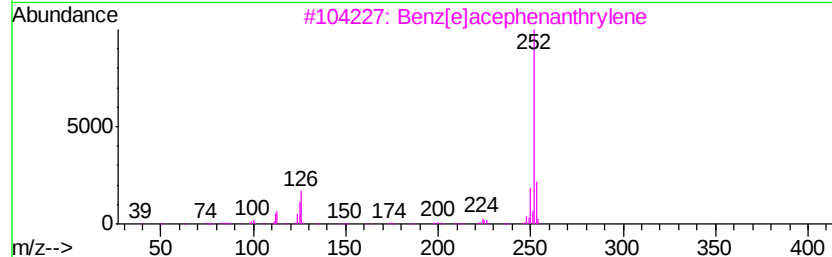
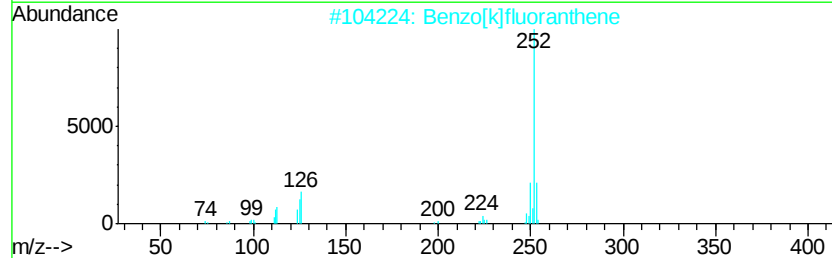
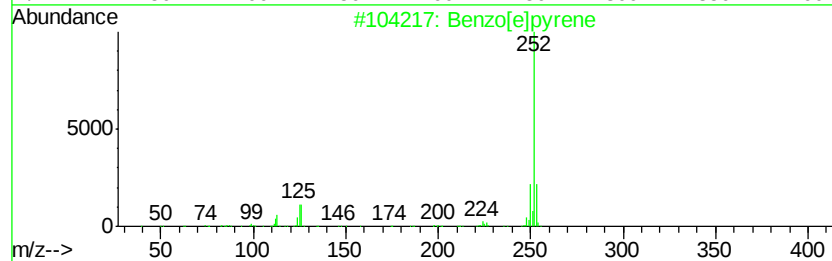
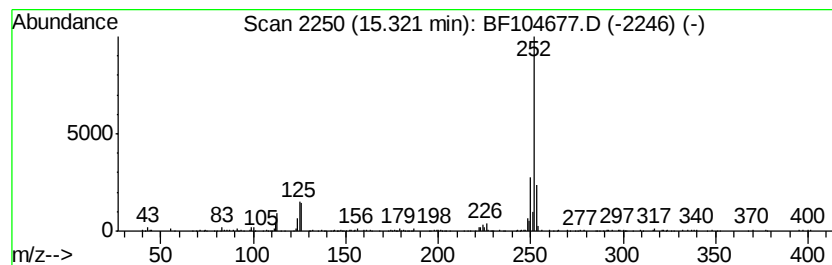
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	6.17 ng	162606	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	97
4		Benzo[a]pyrene	252	C20H12	000050-32-8	96
5		Perylene	252	C20H12	000198-55-0	95



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Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.57	6.57	60.5	ng	2041710	1	6.80	675102	20.0
Decane, 2,3,5-tri...	10.27	2.1	ng	90028	3	9.85	841392	20.0
Heptadecane	10.74	3.2	ng	128010	4	11.33	796422	20.0
Anthracene, 2-met...	11.86	2.6	ng	103670	4	11.33	796422	20.0
unknown13.77	13.77	6.2	ng	270565	5	13.98	872934	20.0
1-Heneicosanol	13.81	8.2	ng	357905	5	13.98	872934	20.0
Benzo[e]pyrene	15.32	6.2	ng	162606	6	15.44	527208	20.0