

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
 Data File : BF100937.D
 Acq On : 28 Nov 2017 16:46
 Operator : SJ/JU
 Sample : I6579-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HAR-5-E(0-1)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	505	509	522	rBV	162649	210166	14.78%	1.531%
2	5.481	572	577	580	rBV	1353109	1286843	90.48%	9.375%
3	6.493	743	749	761	rBV	1258379	1350471	94.96%	9.838%
4	6.628	768	772	775	rBV	1536319	1378472	96.93%	10.042%
5	6.857	808	811	815	rBV	468385	369652	25.99%	2.693%
6	7.016	834	838	841	rBV	1241561	1037630	72.96%	7.559%
7	7.422	902	907	910	rBV	914073	814671	57.28%	5.935%
8	8.140	1025	1029	1032	rBV	587654	459448	32.31%	3.347%
9	8.692	1119	1123	1127	rBV	89831	68555	4.82%	0.499%
10	9.216	1207	1212	1215	rBV	1687625	1422188	100.00%	10.361%
11	9.604	1275	1278	1285	rBB	65842	49508	3.48%	0.361%
12	9.892	1324	1327	1331	rBV2	534900	462344	32.51%	3.368%
13	10.604	1444	1448	1452	rBV	346556	280007	19.69%	2.040%
14	10.681	1458	1461	1473	rBV	767373	734656	51.66%	5.352%
15	11.380	1577	1580	1582	rBV	480256	383595	26.97%	2.794%
16	11.404	1582	1584	1587	rVB	103762	75062	5.28%	0.547%
17	11.880	1659	1665	1666	rBV2	19711	19332	1.36%	0.141%
18	11.898	1666	1668	1673	rVB2	29983	43079	3.03%	0.314%
19	11.992	1680	1684	1686	rBV2	27725	29615	2.08%	0.216%
20	12.427	1754	1758	1762	rBV2	21306	30607	2.15%	0.223%
21	12.592	1781	1786	1790	rBV	201757	170604	12.00%	1.243%
22	12.822	1819	1825	1831	rBV	182629	195061	13.72%	1.421%
23	12.869	1831	1833	1839	rVB2	11953	16619	1.17%	0.121%
24	12.963	1845	1849	1852	rBV	1143202	981197	68.99%	7.148%
25	13.039	1857	1862	1866	rBV4	18227	31442	2.21%	0.229%
26	13.151	1874	1881	1884	rBV2	31453	50441	3.55%	0.367%
27	13.251	1895	1898	1902	rBV2	26499	31842	2.24%	0.232%
28	13.657	1965	1967	1972	rVB	24498	25537	1.80%	0.186%
29	13.769	1982	1986	1989	rBV3	21021	32337	2.27%	0.236%
30	13.857	1997	2001	2010	rVB3	45579	82659	5.81%	0.602%
31	14.021	2021	2029	2031	rBV2	472254	540180	37.98%	3.935%
32	14.045	2031	2033	2041	rVB	122364	115507	8.12%	0.841%
33	14.404	2091	2094	2097	rBV	32176	32701	2.30%	0.238%
34	14.527	2113	2115	2117	rBV3	19634	18593	1.31%	0.135%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.063	2202	2206	2209	rBV	95297	145412	10.22%	1.059%
36	15.363	2254	2257	2262	rVB	53030	64771	4.55%	0.472%
37	15.427	2264	2268	2274	rBV	102981	140760	9.90%	1.025%
38	15.492	2274	2279	2284	rBV	310575	419124	29.47%	3.053%
39	15.933	2351	2354	2356	rBV4	17516	21693	1.53%	0.158%
40	16.968	2525	2530	2535	rVB2	31814	64418	4.53%	0.469%
41	17.415	2601	2606	2614	rBV	19698	40031	2.81%	0.292%

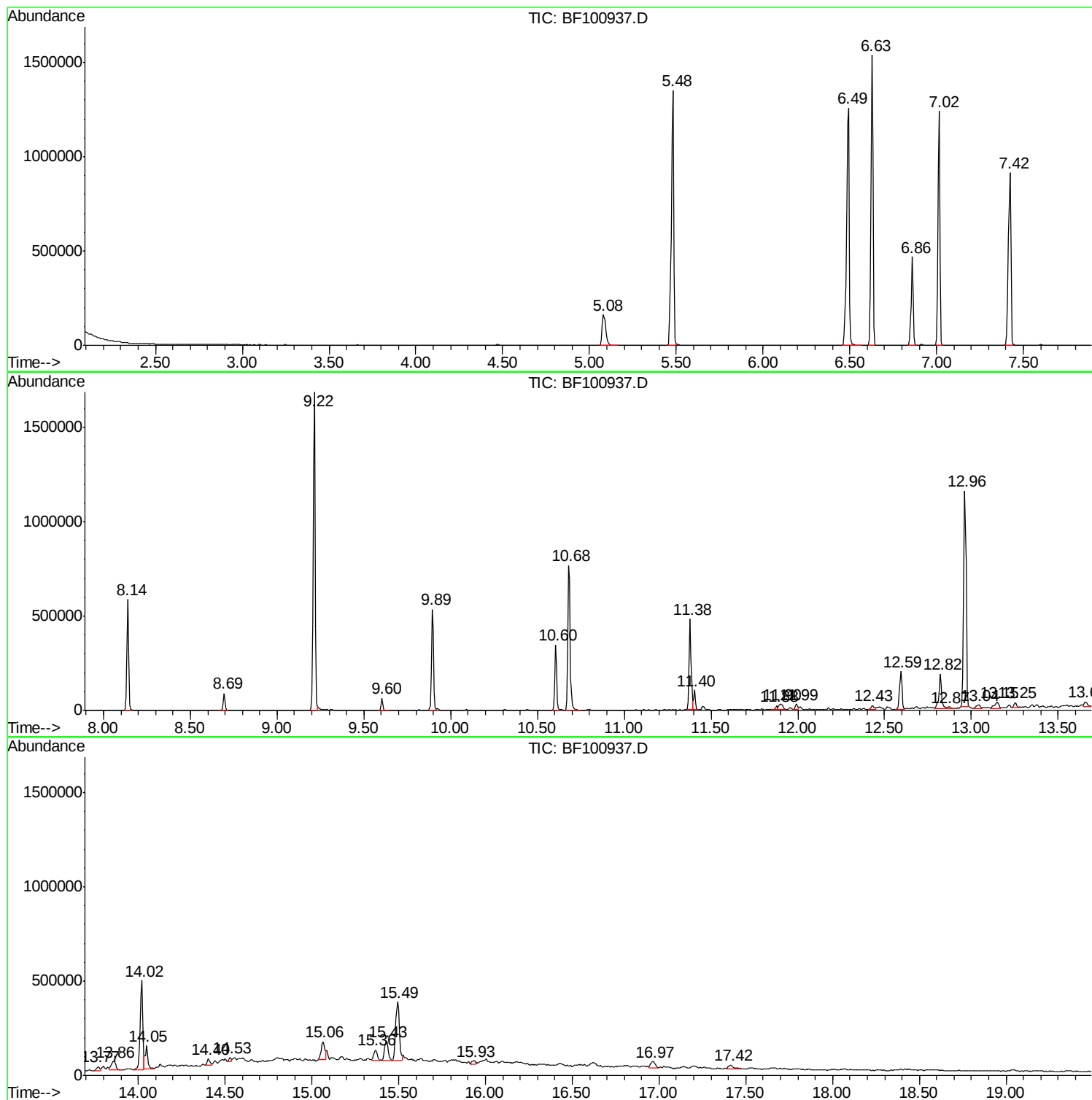
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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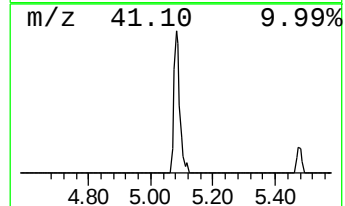
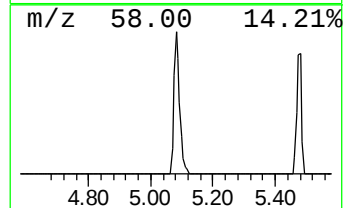
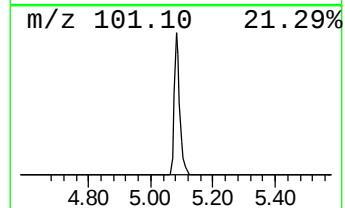
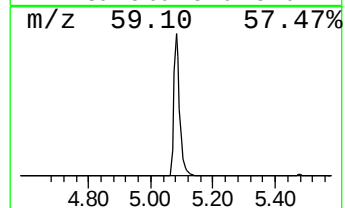
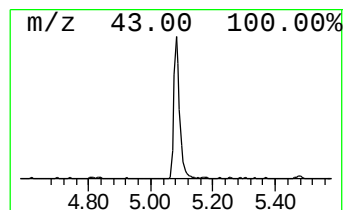
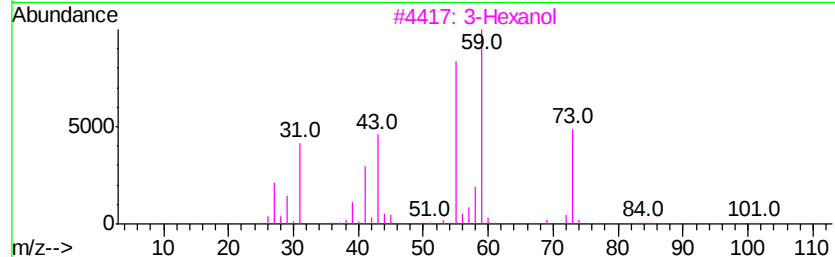
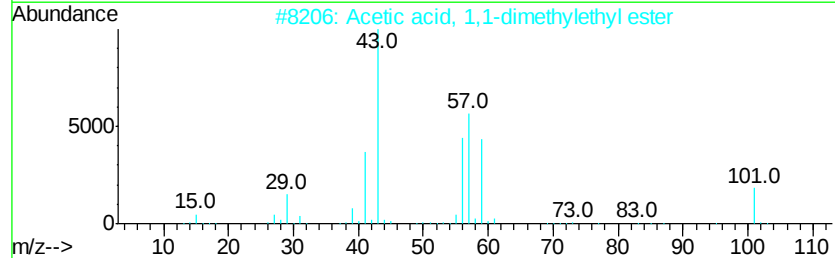
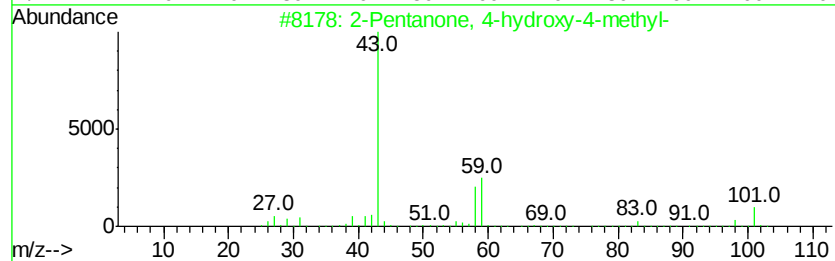
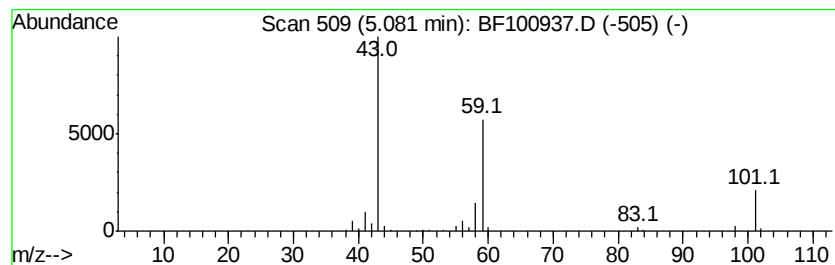
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	11.37 ng	210166	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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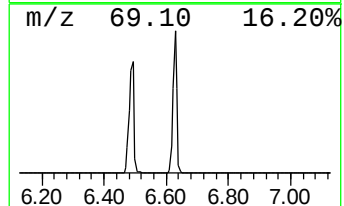
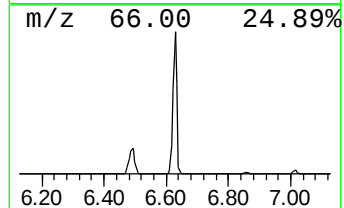
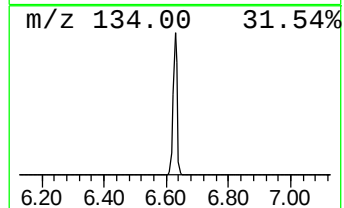
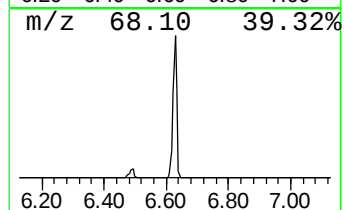
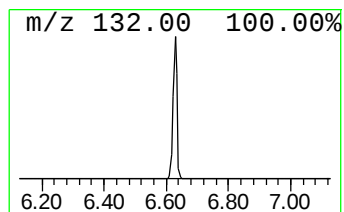
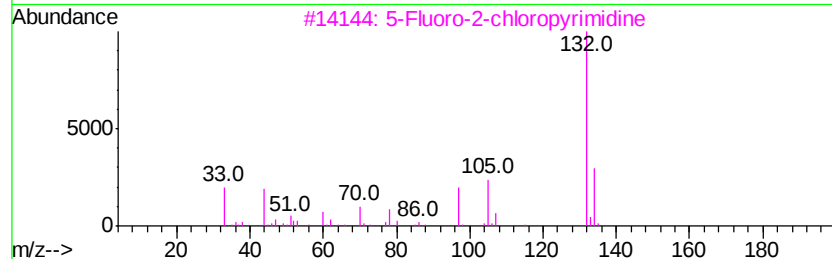
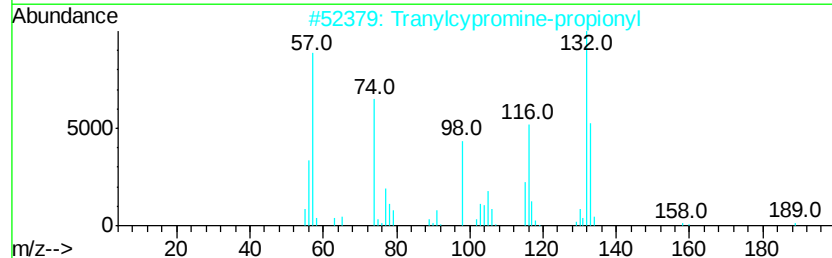
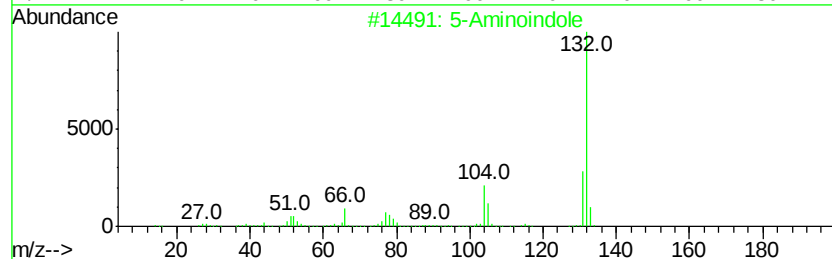
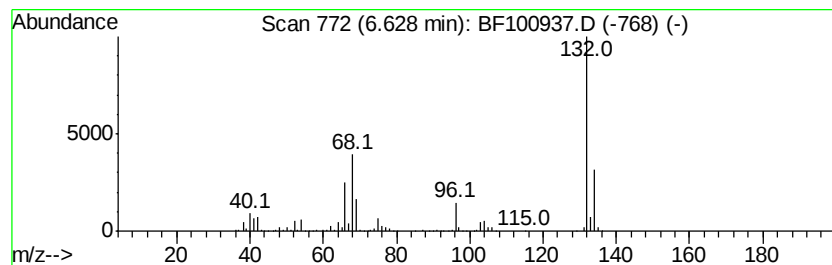
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	74.58 ng	1378470	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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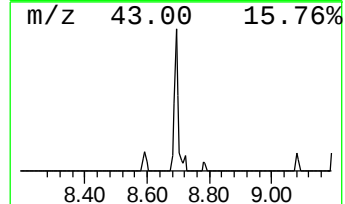
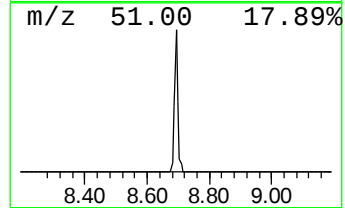
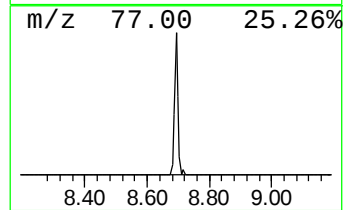
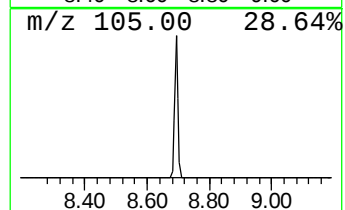
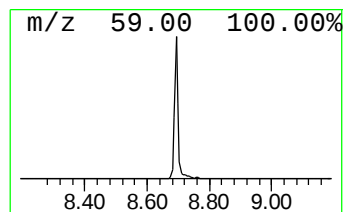
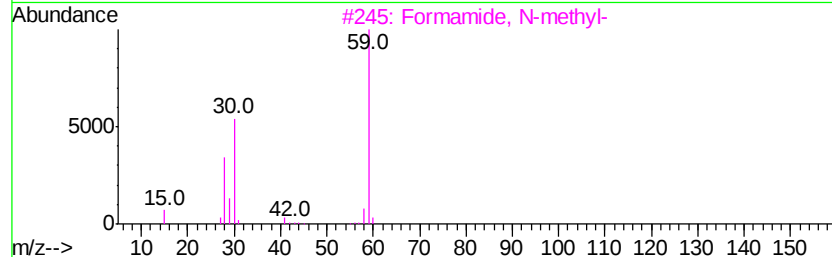
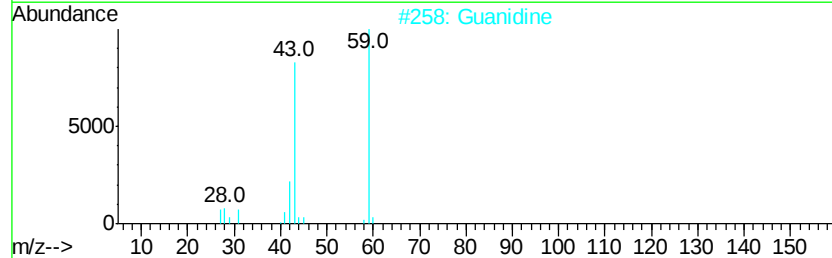
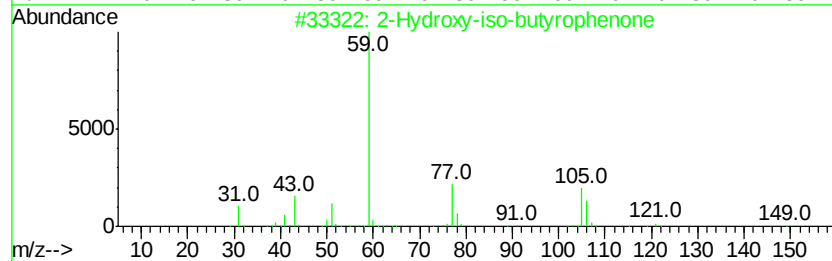
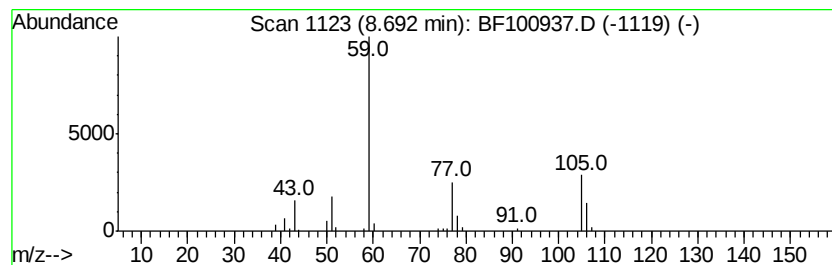
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.98 ng	68555	Napthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2		Guanidine	59	CH5N3	000113-00-8	7
3		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
4		Acetamide	59	C2H5NO	000060-35-5	5
5		Propane, 2-methoxy-	74	C4H10O	000598-53-8	4



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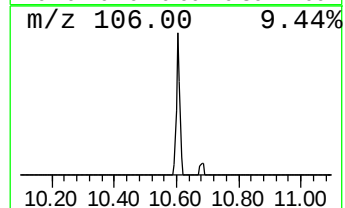
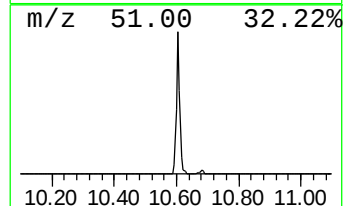
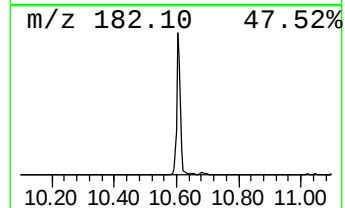
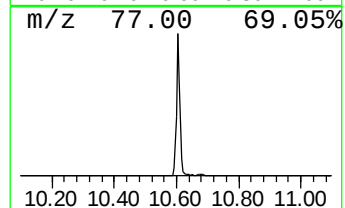
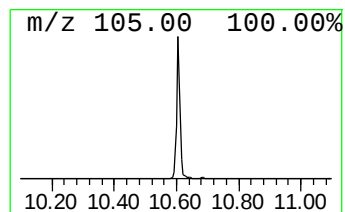
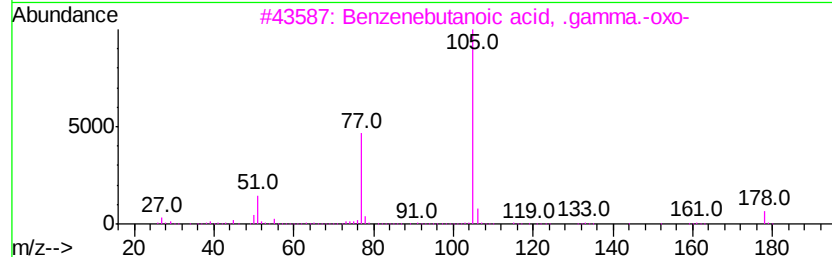
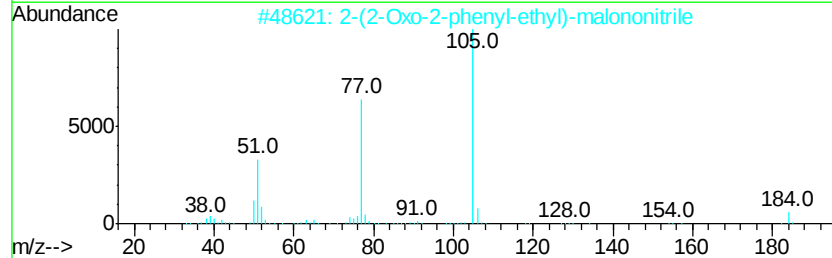
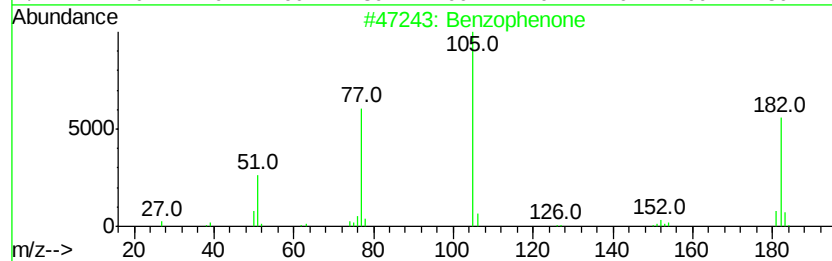
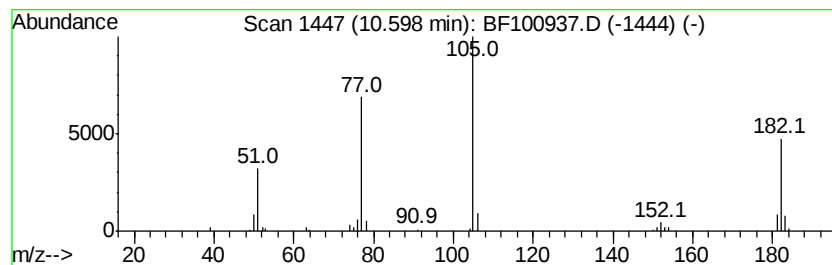
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	12.11 ng	280007	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		2-(2-Oxo-2-phenyl-ethyl)-malononitrile	184	C11H8N2O	1000296-76-9	47
3		Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5		Vinyl benzoate	148	C9H8O2	000769-78-8	47



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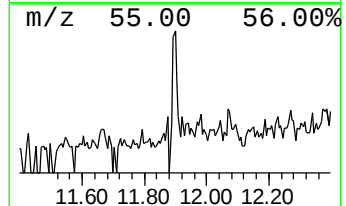
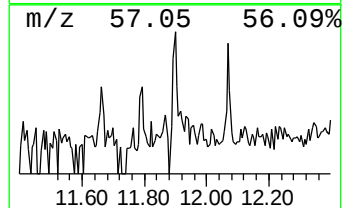
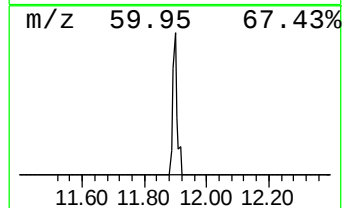
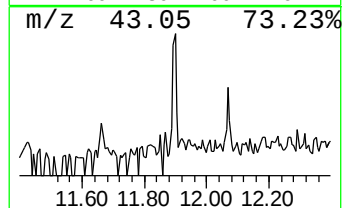
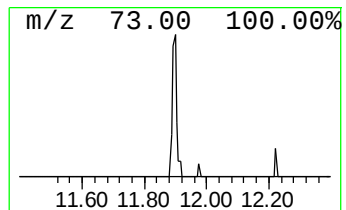
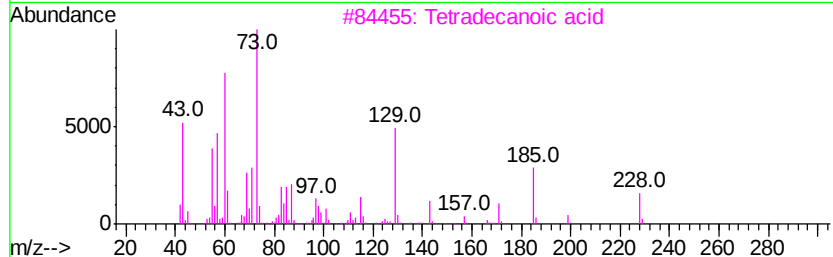
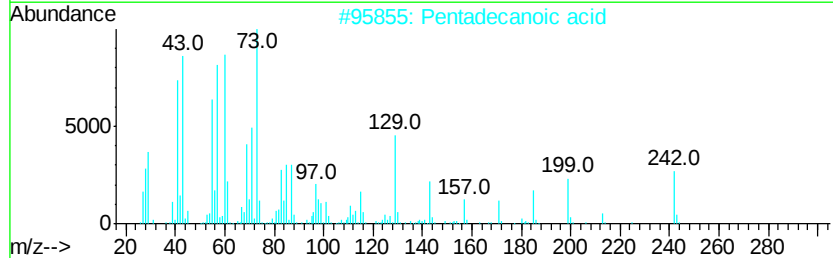
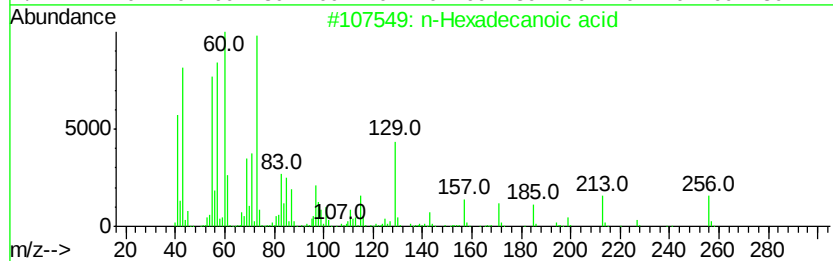
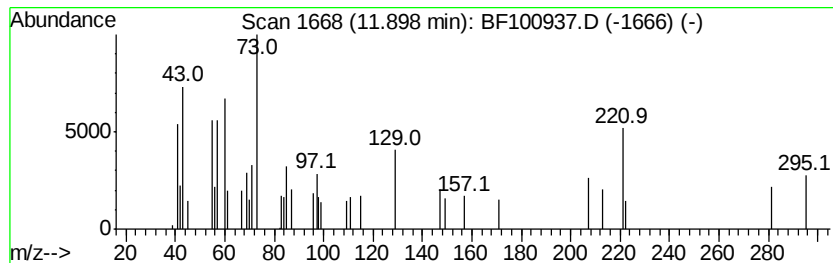
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown11.90 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.25 ng	43079	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	30
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	25
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	25
4		Tridecanoic acid	214	C13H26O2	000638-53-9	22
5		Dodecanoic acid	200	C12H24O2	000143-07-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100937.D
Acq On : 28 Nov 2017 16:46
Operator : SJ/JU
Sample : I6579-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(0-1)

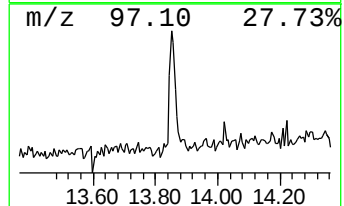
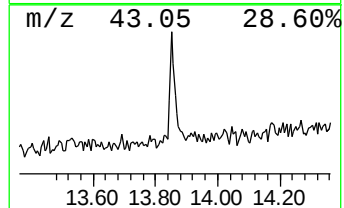
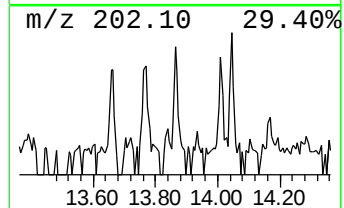
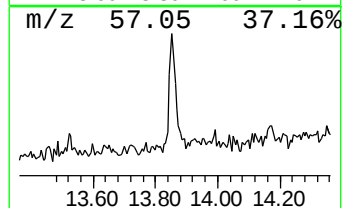
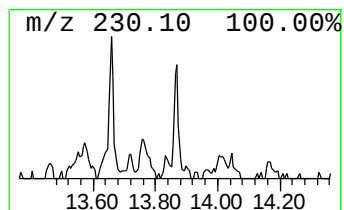
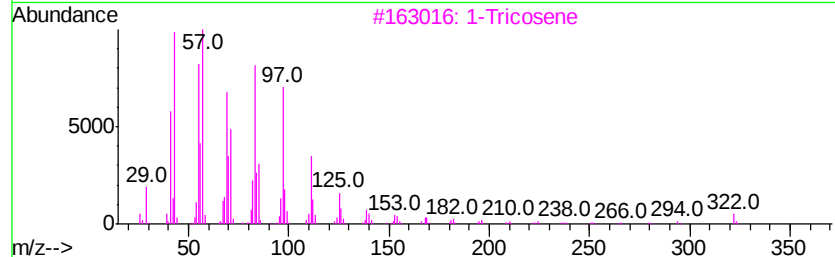
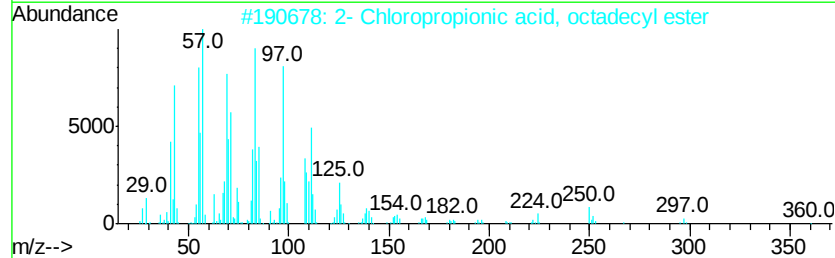
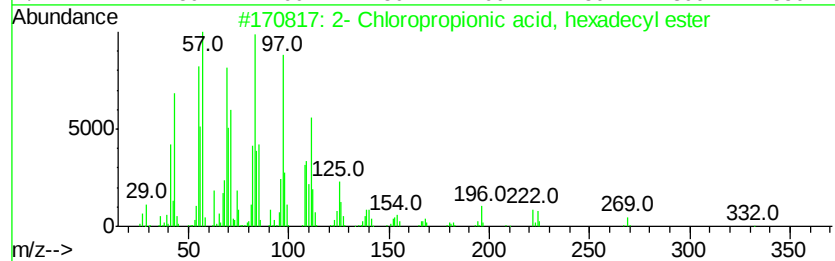
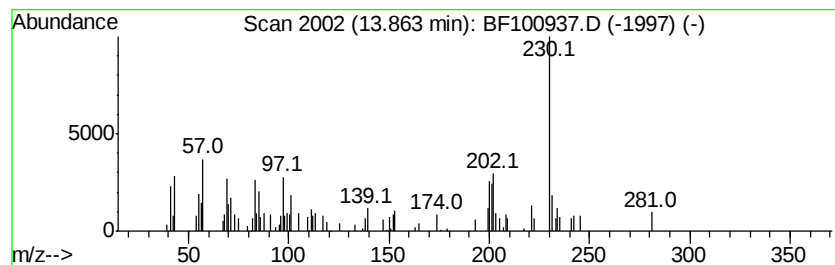
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2- Chloropropionic acid, he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.06 ng	82659	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	70
2	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	70
3	1-	Tricosene	322	C23H46	018835-32-0	70
4	Carbonic acid, hexadecyl 2,2,2-t...		416	C19H35Cl3O3	1000314-56-2	64
5	Behenic alcohol		326	C22H46O	000661-19-8	64



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(0-1)

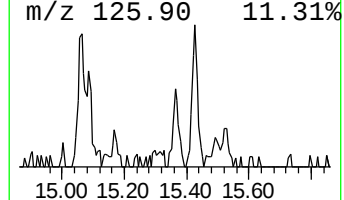
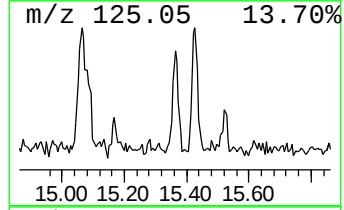
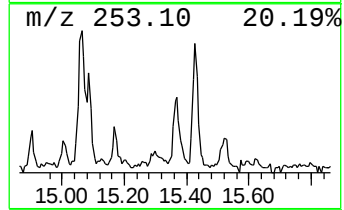
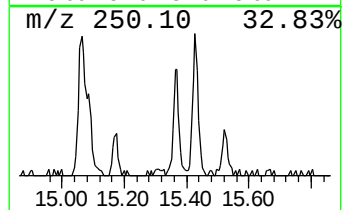
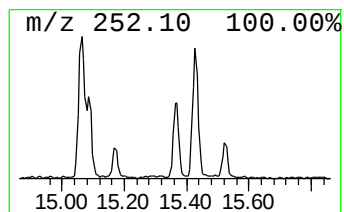
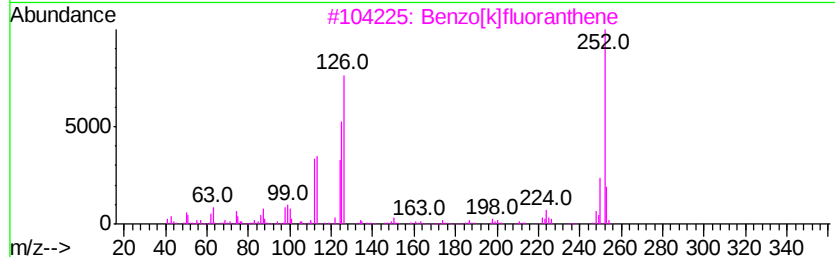
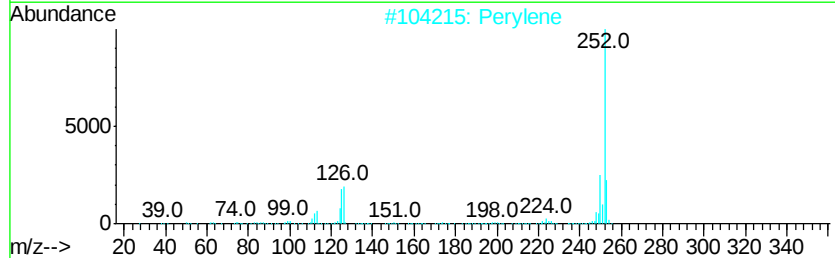
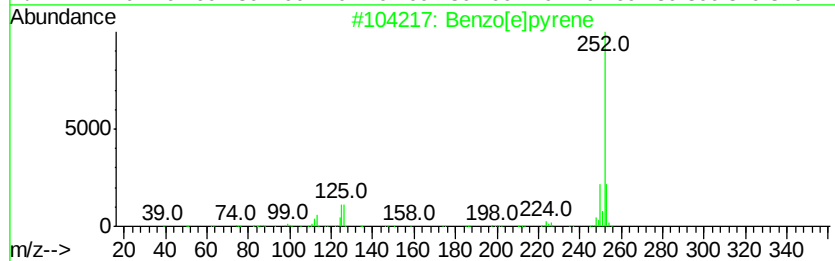
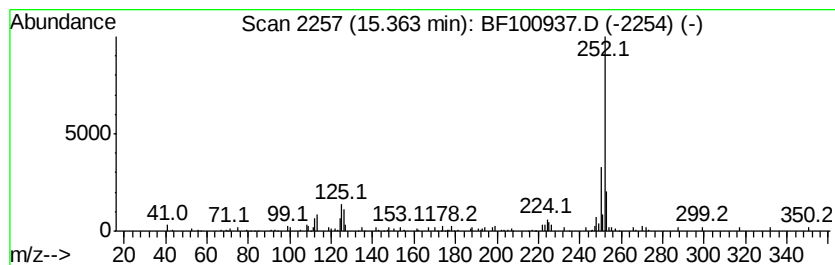
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	3.09 ng	64771	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Perylene	252	C20H12	000198-55-0	94
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	89
5		Benzo[a]pyrene	252	C20H12	000050-32-8	81



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(0-1)

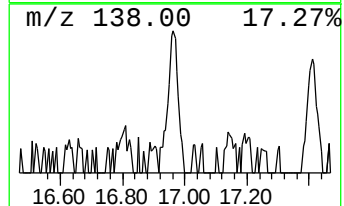
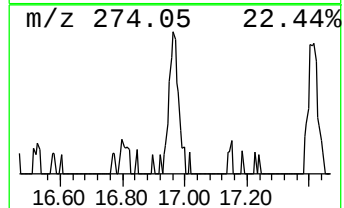
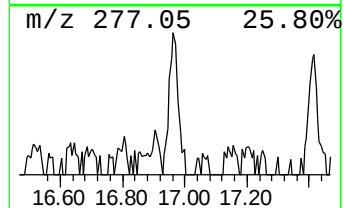
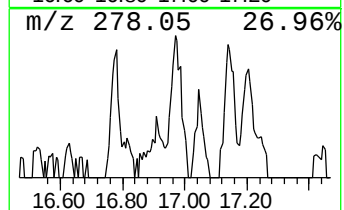
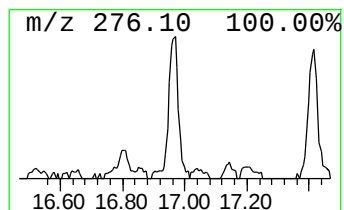
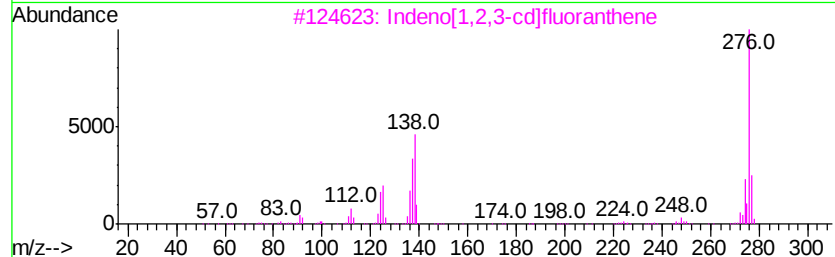
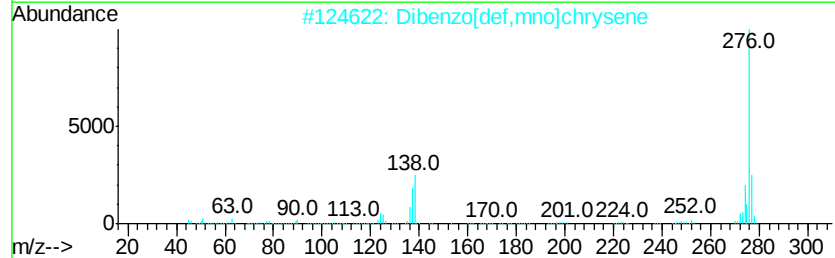
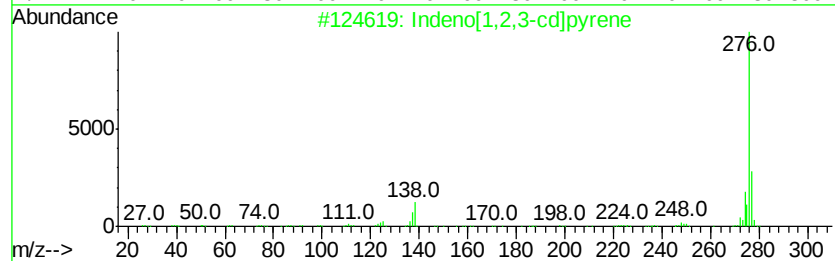
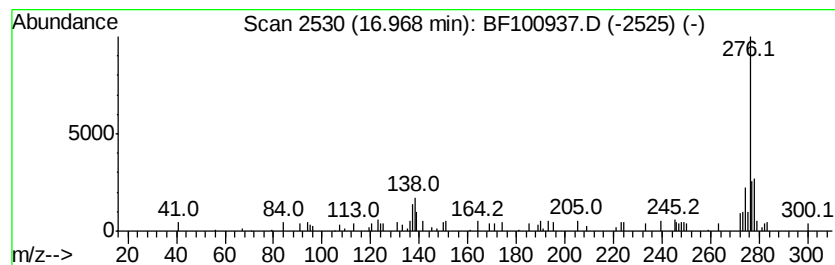
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Indeno[1,2,3-cd]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	3.07 ng	64418	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
2		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	70
3		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	53
4		Phenol, 2-(4-chlorophenyl)iminom...	276	C13H9ClN2O3	1000262-90-3	52
5		Benzo[ghi]perylene	276	C22H12	000191-24-2	50



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(0-1)

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	11.4	ng	210166	1	6.86	369652	20.0
unknown6.63	6.63	74.6	ng	1378470	1	6.86	369652	20.0
2-Hydroxy-iso-but...	8.69	3.0	ng	68555	2	8.14	459448	20.0
Benzophenone	10.60	12.1	ng	280007	3	9.89	462344	20.0
unknown11.90	11.90	2.3	ng	43079	4	11.38	383595	20.0
2- Chloropropioni...	13.86	3.1	ng	82659	5	14.02	540180	20.0
Benzo[e]pyrene	15.36	3.1	ng	64771	6	15.49	419124	20.0
Indeno[1,2,3-cd]p...	16.97	3.1	ng	64418	6	15.49	419124	20.0