

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
 Data File : BF099090.D
 Acq On : 5 Oct 2017 2:08
 Operator : SJ/JU
 Sample : I5585-09 5X
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G69-0-1.5

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	2.116	3	5	28	rVB4	47951	135082	15.93%	1.507%
2	5.069	504	507	518	rBV	83418	79624	9.39%	0.889%
3	5.475	572	576	584	rBV	536757	493358	58.20%	5.505%
4	6.486	744	748	755	rBV	528279	494755	58.36%	5.521%
5	6.628	769	772	776	rBV	663994	528237	62.31%	5.894%
6	6.863	808	812	816	rVB	808068	634838	74.89%	7.084%
7	7.016	834	838	842	rBV	478135	408099	48.14%	4.554%
8	7.422	903	907	910	rBV	392176	300782	35.48%	3.356%
9	8.145	1026	1030	1033	rBV	1094692	839306	99.01%	9.366%
10	9.216	1209	1212	1215	rBV	776716	584122	68.90%	6.518%
11	9.610	1276	1279	1282	rBV	77149	56137	6.62%	0.626%
12	9.898	1325	1328	1332	rVB	918755	847737	100.00%	9.460%
13	10.322	1398	1400	1403	rVB	16479	11591	1.37%	0.129%
14	10.686	1459	1462	1467	rVB	305989	245908	29.01%	2.744%
15	10.798	1478	1481	1486	rBV	17092	23965	2.83%	0.267%
16	11.239	1553	1556	1559	rBV2	12868	11982	1.41%	0.134%
17	11.386	1577	1581	1584	rBV	930893	763342	90.04%	8.518%
18	11.410	1584	1585	1588	rVV	99072	54214	6.40%	0.605%
19	11.463	1592	1594	1597	rVB	29498	21505	2.54%	0.240%
20	11.668	1625	1629	1634	rVB4	10383	12562	1.48%	0.140%
21	11.886	1662	1666	1668	rBV	11976	10541	1.24%	0.118%
22	11.916	1668	1671	1674	rVB	17164	15178	1.79%	0.169%
23	11.945	1674	1676	1681	rVB3	14901	18183	2.14%	0.203%
24	11.998	1681	1685	1687	rBV2	18058	18350	2.16%	0.205%
25	12.433	1755	1759	1762	rBV2	10005	14921	1.76%	0.167%
26	12.598	1783	1787	1791	rBV	169926	136997	16.16%	1.529%
27	12.827	1823	1826	1828	rVV	120540	90778	10.71%	1.013%
28	12.851	1828	1830	1833	rVB	26004	21868	2.58%	0.244%
29	12.963	1846	1849	1853	rBV	415162	367592	43.36%	4.102%
30	13.039	1859	1862	1866	rBV5	10523	16082	1.90%	0.179%
31	13.133	1874	1878	1879	rBV4	9256	11780	1.39%	0.131%
32	13.151	1879	1881	1884	rVB	19666	18955	2.24%	0.212%
33	13.192	1884	1888	1891	rBV5	10395	11107	1.31%	0.124%
34	13.386	1918	1921	1923	rBV4	9399	12648	1.49%	0.141%

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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	13.445	1928	1931	1934	rBV2	29351	29348	3.46%	0.327%
36	13.662	1965	1968	1972	rVB2	14458	16006	1.89%	0.179%
37	13.992	2022	2024	2025	rBV2	18118	13043	1.54%	0.146%
38	14.027	2025	2030	2032	rVV	580307	616269	72.70%	6.877%
39	14.051	2032	2034	2038	rVB	63884	59219	6.99%	0.661%
40	15.062	2203	2206	2210	rBV	81275	123325	14.55%	1.376%
41	15.368	2256	2258	2265	rVB	52688	75760	8.94%	0.845%
42	15.433	2265	2269	2275	rBV	67925	102435	12.08%	1.143%
43	15.498	2275	2280	2290	rBV	442591	614015	72.43%	6.852%

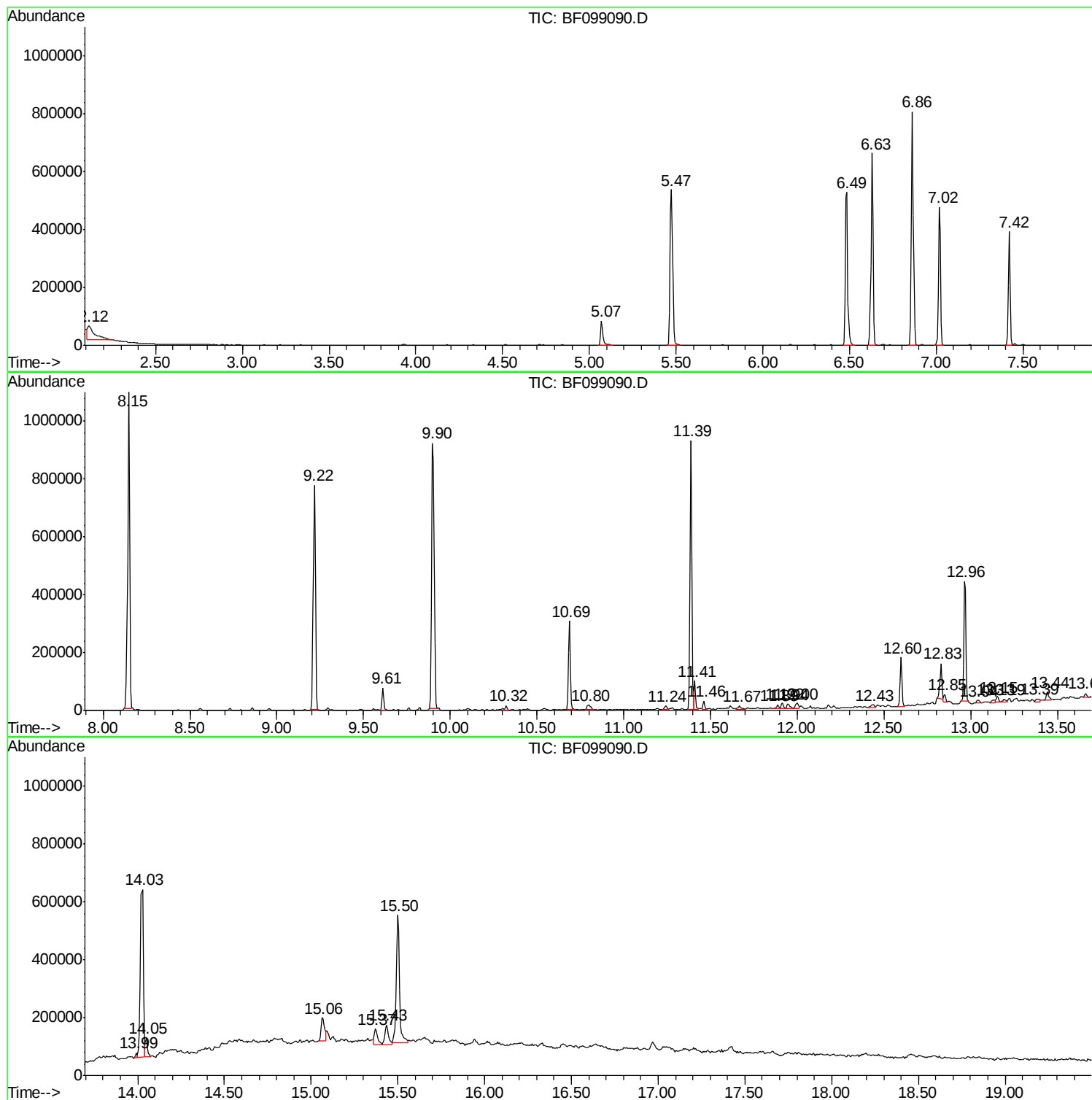
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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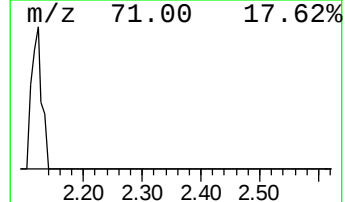
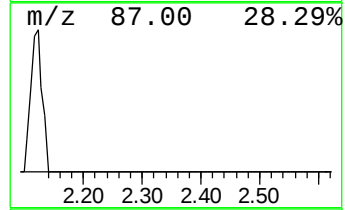
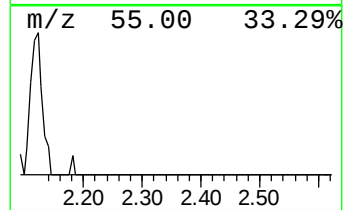
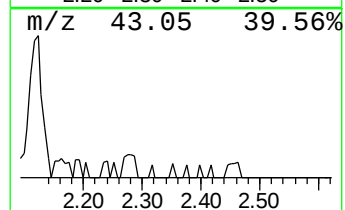
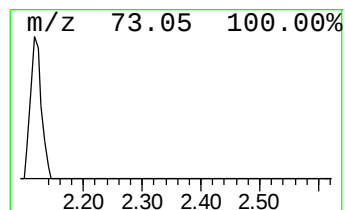
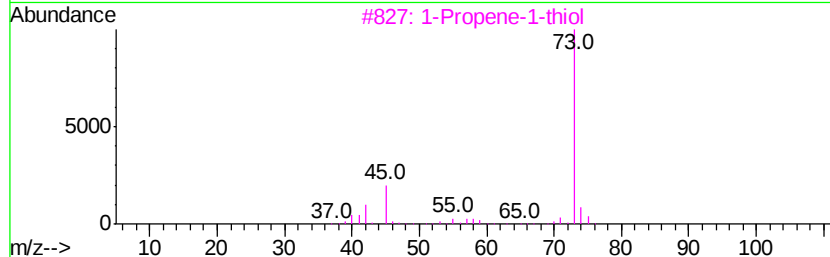
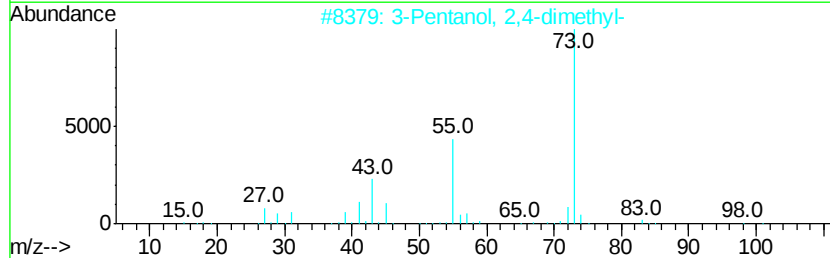
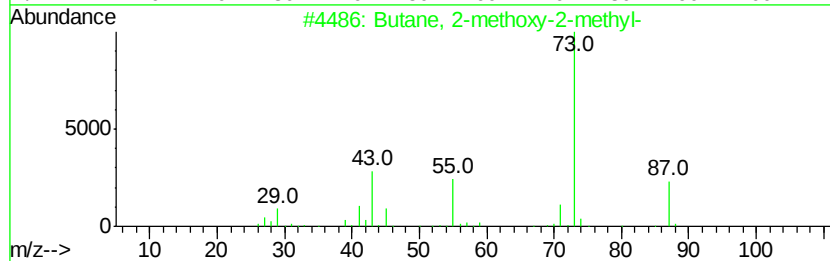
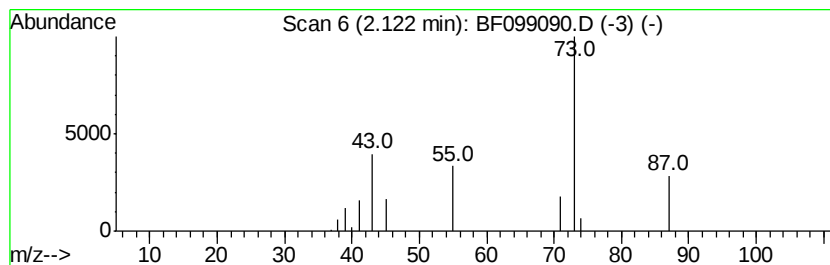
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	4.26 ng	135082	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	5
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5
5			1-Pentanamine	87	C5H13N	000110-58-7	4



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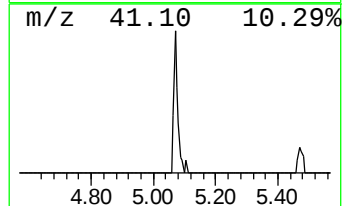
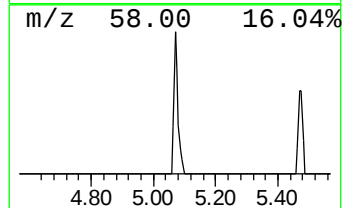
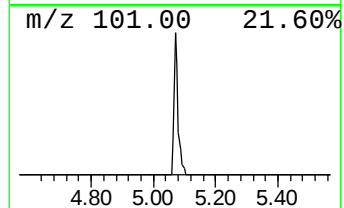
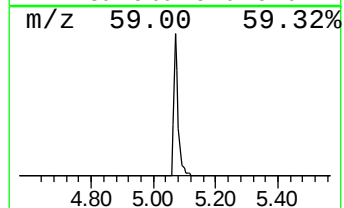
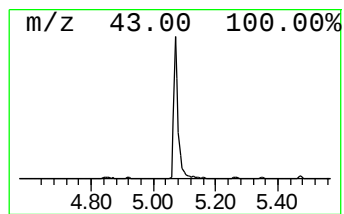
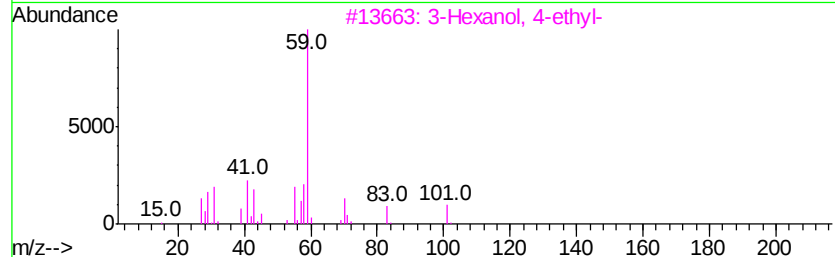
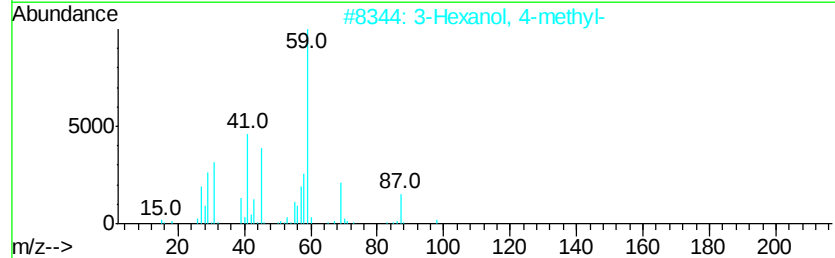
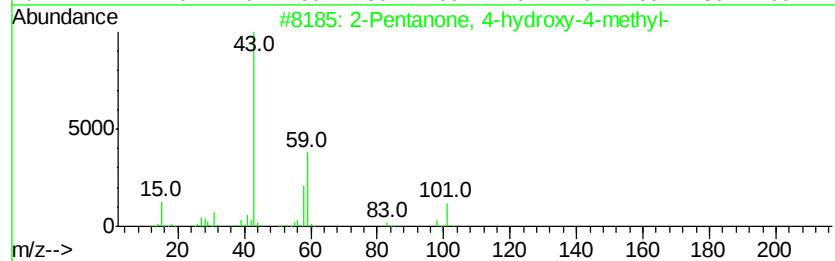
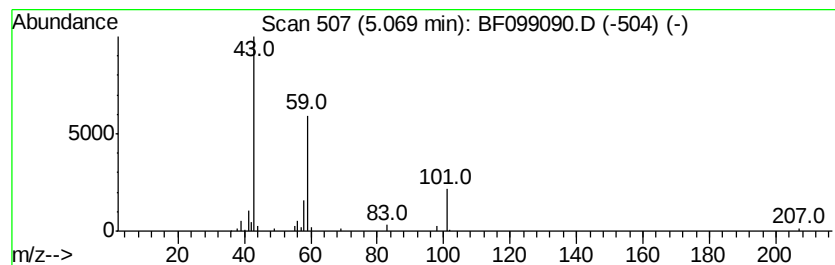
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	2.51 ng	79624	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	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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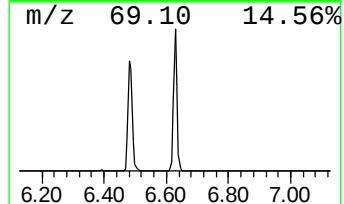
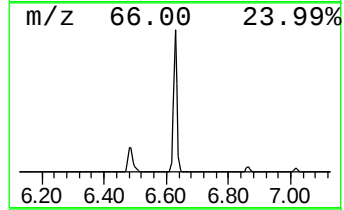
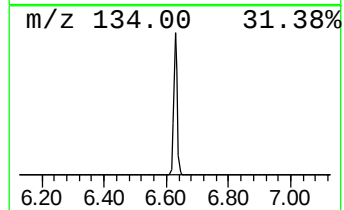
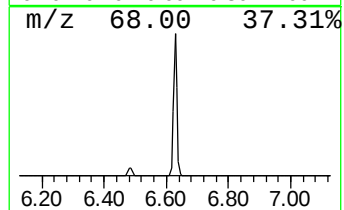
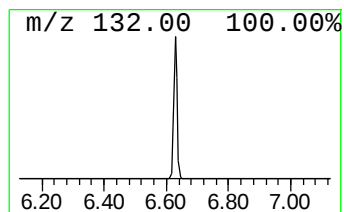
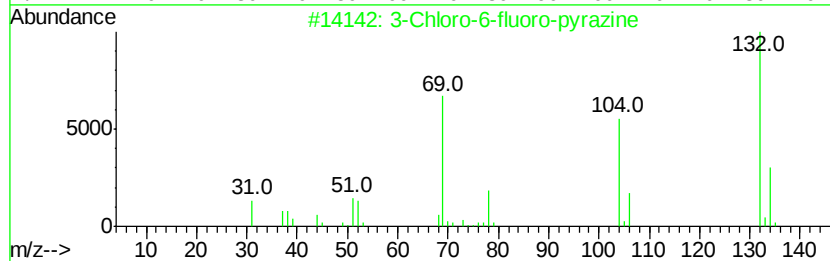
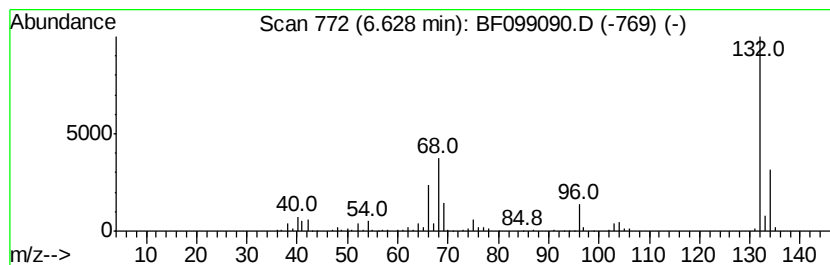
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	16.64 ng	528237	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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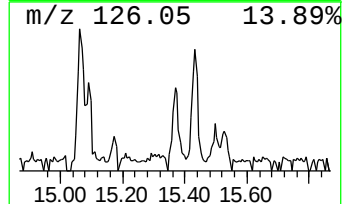
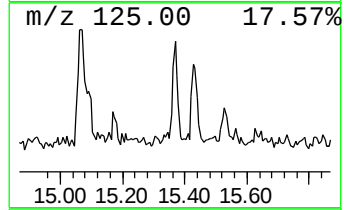
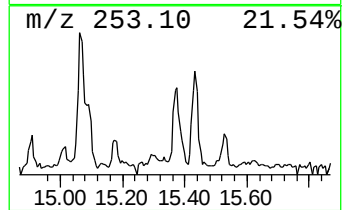
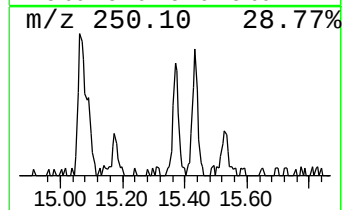
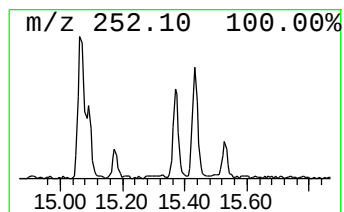
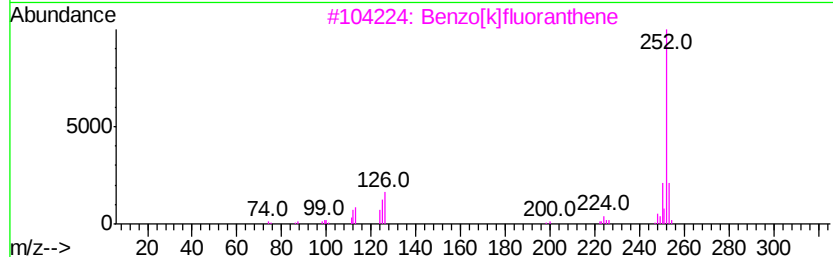
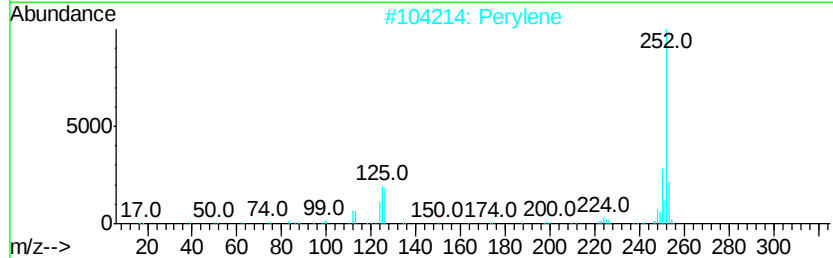
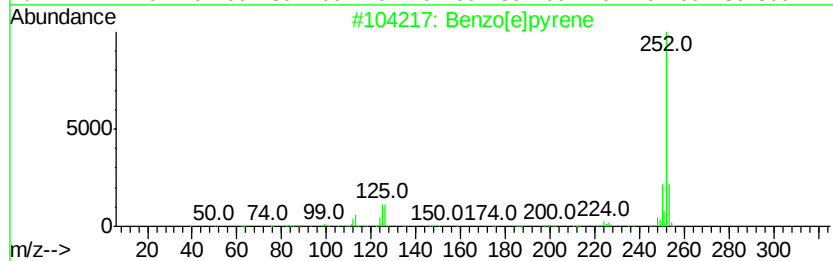
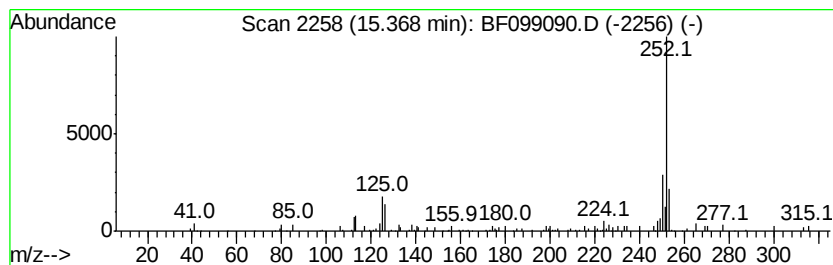
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.47 ng	75760	Perylene-d12	15.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	87
2		Perylene	252	C20H12	000198-55-0	81
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	81
5		Benzo[a]pyrene	252	C20H12	000050-32-8	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	4.3	ng	135082	1	6.86	634838	20.0
2-Pentanone, 4-hy...	5.07	2.5	ng	79624	1	6.86	634838	20.0
unknown6.63	6.63	16.6	ng	528237	1	6.86	634838	20.0
Benzo[e]pyrene	15.37	2.5	ng	75760	6	15.50	614015	20.0