

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100517\
 Data File : BF099121.D
 Acq On : 5 Oct 2017 23:34
 Operator : SJ/JU
 Sample : I5585-07 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G68-1.5-3

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	2.140	6	9	16	rVB2	54935	90472	8.38%	0.788%
2	5.075	505	508	515	rBV	94395	98347	9.11%	0.857%
3	5.475	572	576	586	rVB	689002	609371	56.47%	5.308%
4	6.481	744	747	757	rBV	687934	625970	58.01%	5.453%
5	6.628	768	772	776	rBV	825119	650279	60.26%	5.665%
6	6.863	808	812	815	rBV	907021	739159	68.50%	6.439%
7	6.916	817	821	826	rBV	22254	20100	1.86%	0.175%
8	7.016	834	838	842	rBV	602917	496900	46.05%	4.329%
9	7.422	903	907	910	rBV	478222	375325	34.78%	3.269%
10	8.145	1023	1030	1033	rBV	1299449	1030669	95.51%	8.978%
11	9.216	1208	1212	1215	rBV	974225	731079	67.75%	6.368%
12	9.486	1255	1258	1261	rBV	34219	27553	2.55%	0.240%
13	9.610	1276	1279	1282	rBV	73664	56924	5.27%	0.496%
14	9.757	1301	1304	1308	rBV	23196	18951	1.76%	0.165%
15	9.898	1323	1328	1332	rBV	1194377	1079142	100.00%	9.400%
16	10.322	1393	1400	1403	rVB2	17025	16011	1.48%	0.139%
17	10.686	1458	1462	1472	rVB	360529	335880	31.12%	2.926%
18	10.792	1477	1480	1490	rBV	23265	29863	2.77%	0.260%
19	11.239	1552	1556	1559	rBV2	14800	13229	1.23%	0.115%
20	11.386	1577	1581	1584	rBV	1168176	986727	91.44%	8.595%
21	11.410	1584	1585	1588	rVV	54853	28193	2.61%	0.246%
22	11.457	1591	1593	1596	rVB	15705	12779	1.18%	0.111%
23	11.916	1668	1671	1673	rVB	18816	15488	1.44%	0.135%
24	11.998	1681	1685	1687	rBV2	22210	22488	2.08%	0.196%
25	12.433	1756	1759	1762	rBV	15058	14958	1.39%	0.130%
26	12.521	1771	1774	1778	rVB	19766	16607	1.54%	0.145%
27	12.598	1783	1787	1790	rBV	295013	232945	21.59%	2.029%
28	12.827	1823	1826	1829	rVB	191806	147855	13.70%	1.288%
29	12.963	1846	1849	1853	rVB	588716	492428	45.63%	4.290%
30	13.045	1859	1863	1867	rVB4	12901	19493	1.81%	0.170%
31	13.151	1874	1881	1884	rBV3	26657	37868	3.51%	0.330%
32	13.221	1890	1893	1895	rBV	17741	16782	1.56%	0.146%
33	13.257	1895	1899	1903	rVB2	15671	16881	1.56%	0.147%
34	13.439	1927	1930	1933	rBV	31747	29173	2.70%	0.254%

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G68-1.5-3

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	13.663	1965	1968	1972	rBV	20407	18399	1.70%	0.160%
36	13.768	1982	1986	1989	rBV2	21784	23500	2.18%	0.205%
37	13.821	1993	1995	1999	rVV2	15380	23392	2.17%	0.204%
38	13.868	1999	2003	2007	rVB2	23728	29788	2.76%	0.259%
39	14.021	2025	2029	2032	rBV2	759628	764152	70.81%	6.657%
40	14.045	2032	2033	2041	rVB	106277	91086	8.44%	0.793%
41	14.127	2041	2047	2051	rBV3	12092	15982	1.48%	0.139%
42	14.168	2051	2054	2058	rBV2	11627	13300	1.23%	0.116%
43	14.245	2063	2067	2071	rVB2	11148	15657	1.45%	0.136%
44	14.333	2080	2082	2086	rBV2	27804	23629	2.19%	0.206%
45	14.410	2091	2095	2098	rVV2	18479	19126	1.77%	0.167%
46	14.533	2113	2116	2118	rBV2	13709	14587	1.35%	0.127%
47	14.786	2155	2159	2164	rBV7	8507	14561	1.35%	0.127%
48	14.898	2175	2178	2182	rBV4	7803	13159	1.22%	0.115%
49	15.062	2201	2206	2209	rBV	118313	164980	15.29%	1.437%
50	15.168	2221	2224	2228	rBV	25096	27090	2.51%	0.236%
51	15.368	2252	2258	2263	rVB	61499	77739	7.20%	0.677%
52	15.427	2264	2268	2274	rVB	80062	103183	9.56%	0.899%
53	15.498	2274	2280	2284	rBV	531306	667427	61.85%	5.814%
54	15.709	2314	2316	2323	rVB8	7065	12694	1.18%	0.111%
55	15.939	2350	2355	2358	rBV5	14904	21852	2.02%	0.190%
56	16.445	2436	2441	2447	rVB5	11143	18217	1.69%	0.159%
57	16.962	2524	2529	2537	rBV2	37807	74903	6.94%	0.652%
58	17.039	2538	2542	2549	rVB7	10005	21983	2.04%	0.191%
59	17.203	2565	2570	2575	rBV5	7963	15718	1.46%	0.137%
60	17.415	2598	2606	2613	rBV	27236	57647	5.34%	0.502%

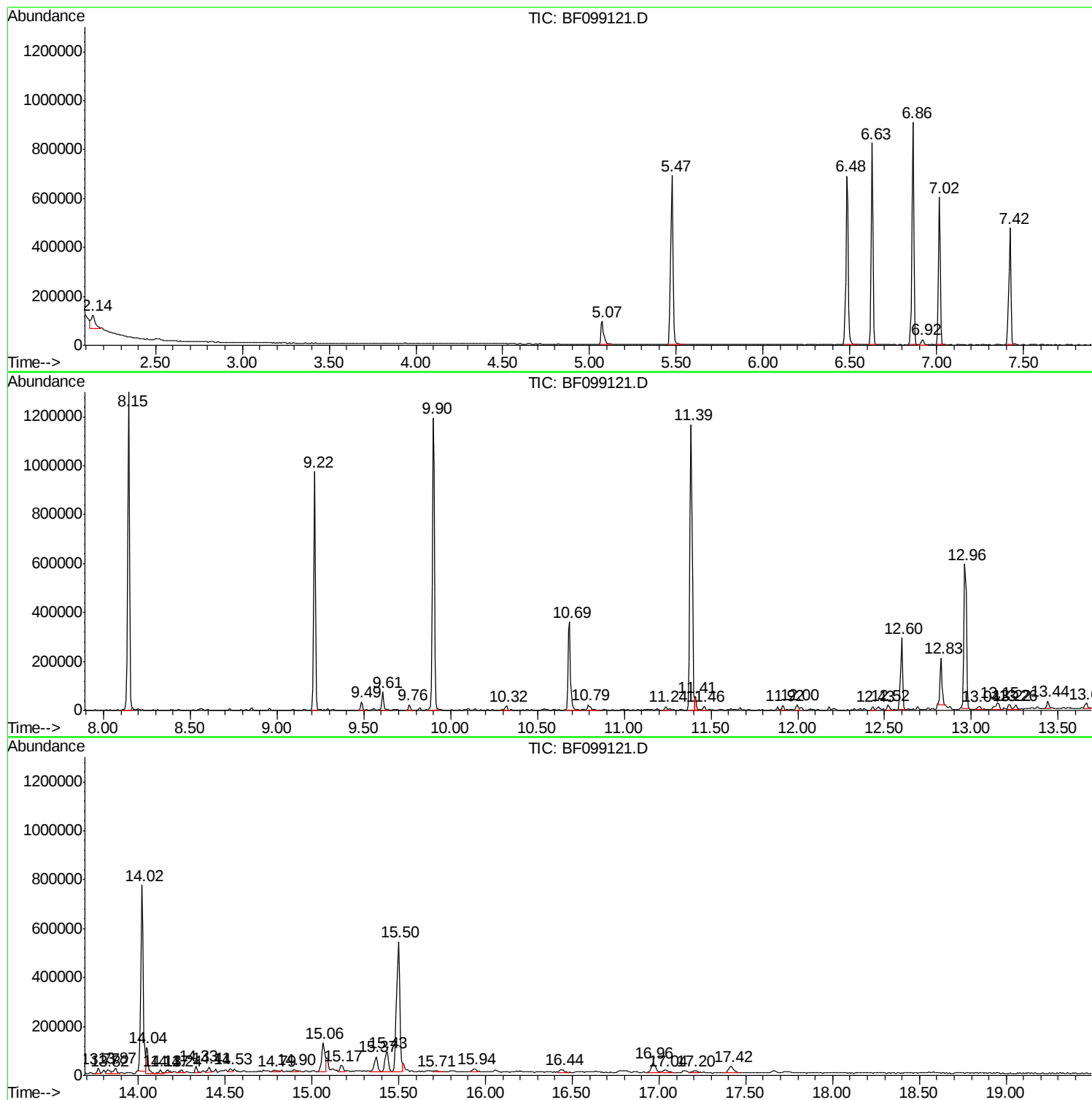
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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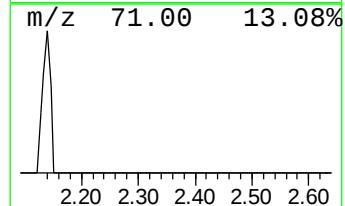
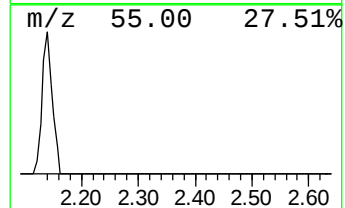
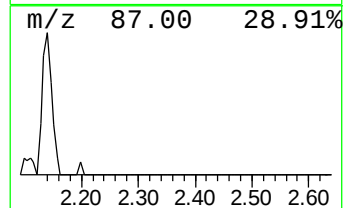
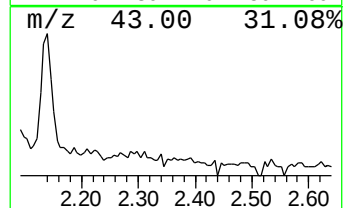
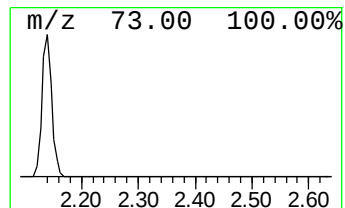
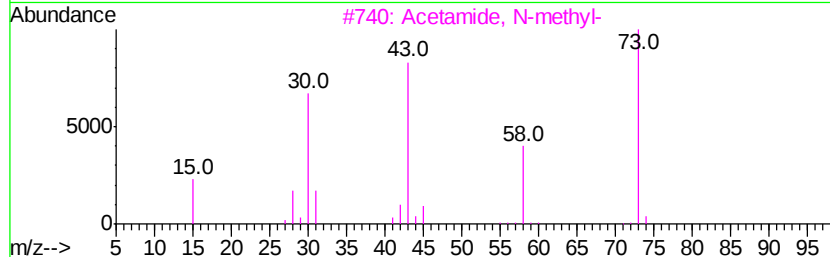
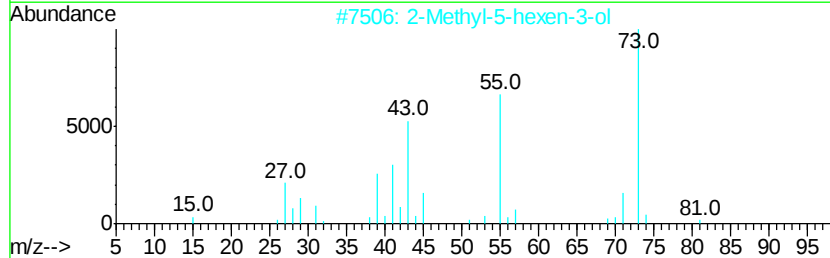
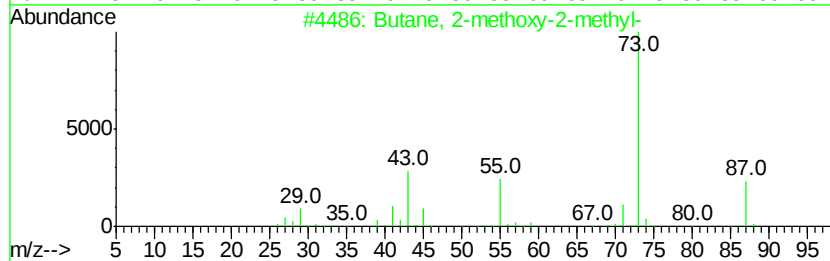
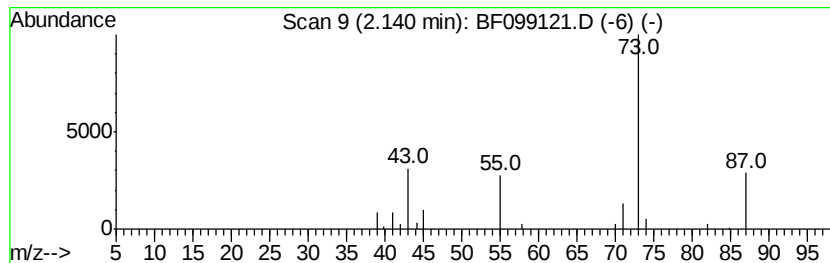
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	2.45 ng	90472	1,4-Dichlorobenzene-d4	6.86

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	9
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	7
4		N-Ethylformamide	73	C3H7NO	000627-45-2	5
5		1,3-Dioxolane	74	C3H6O2	000646-06-0	4



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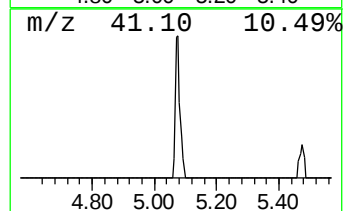
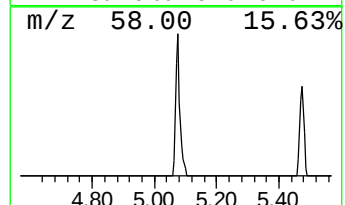
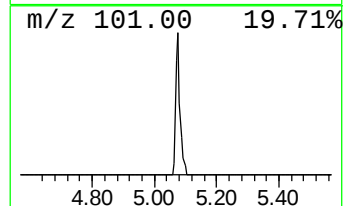
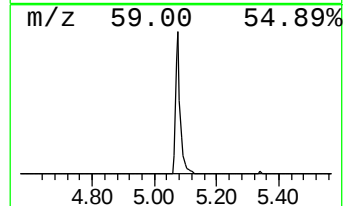
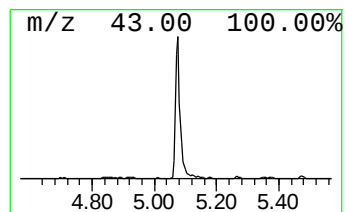
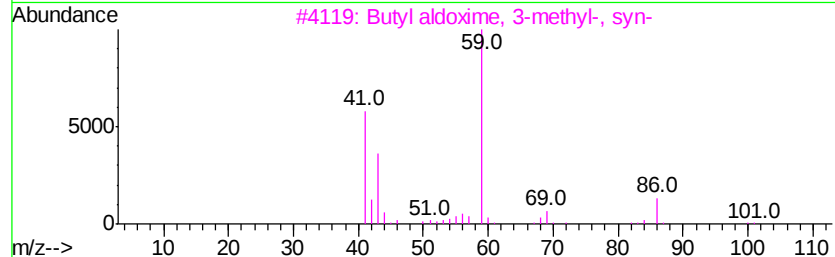
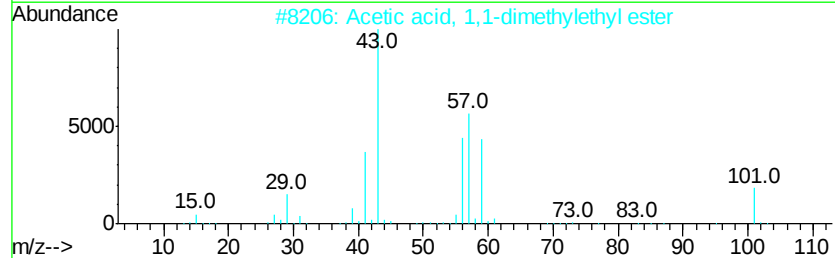
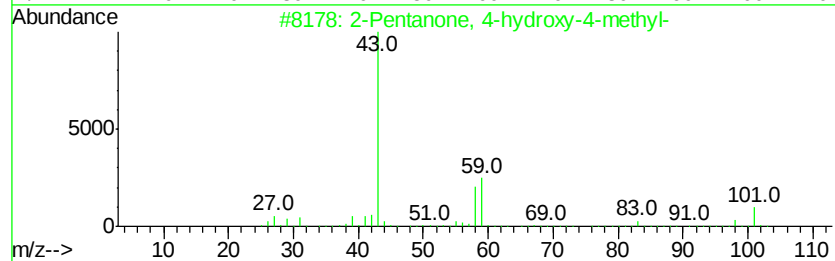
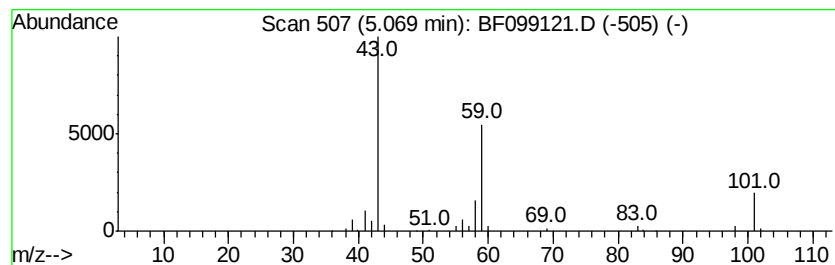
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	2.66 ng	98347	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			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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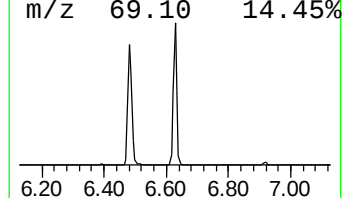
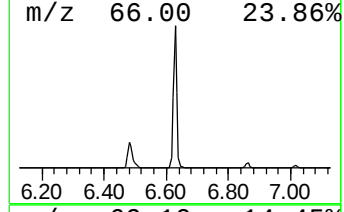
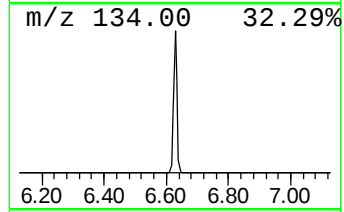
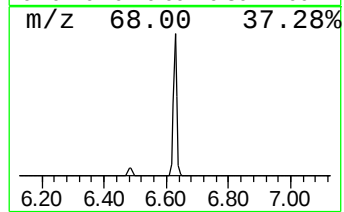
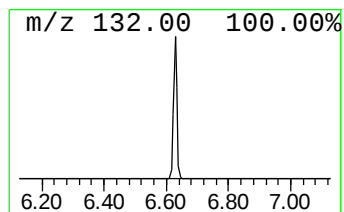
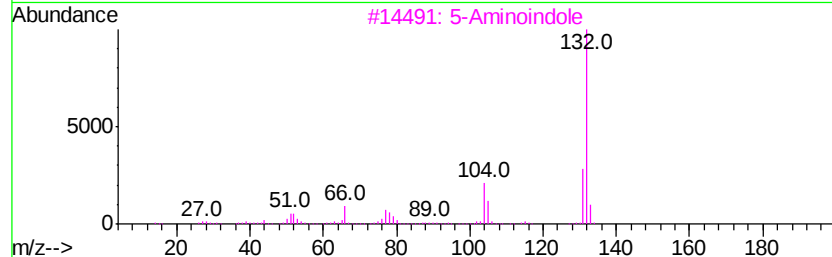
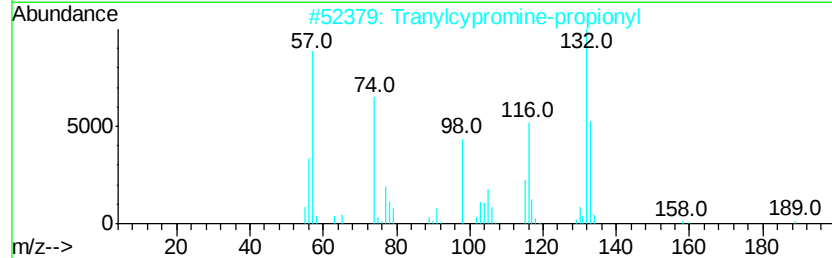
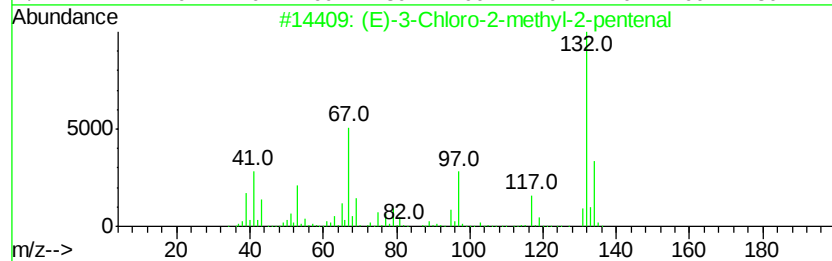
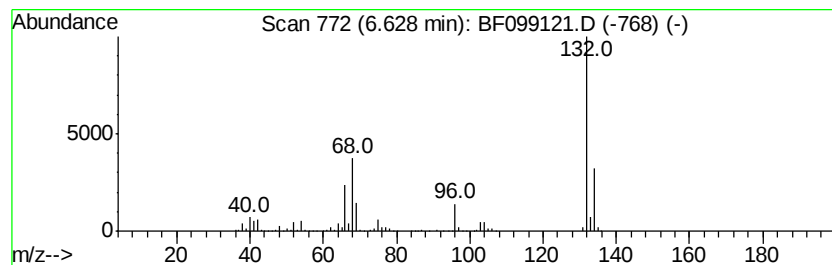
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	17.60 ng	650279	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	



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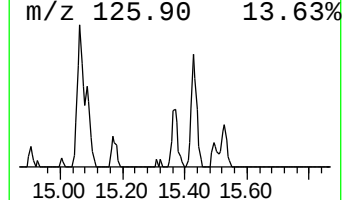
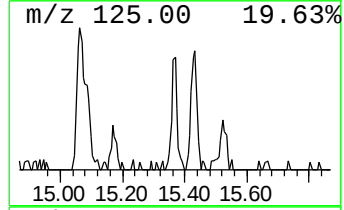
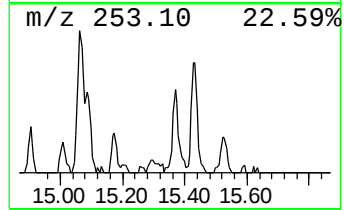
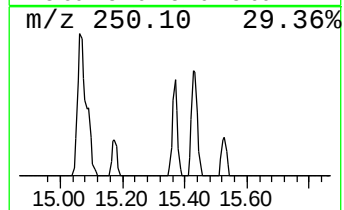
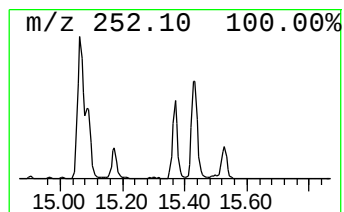
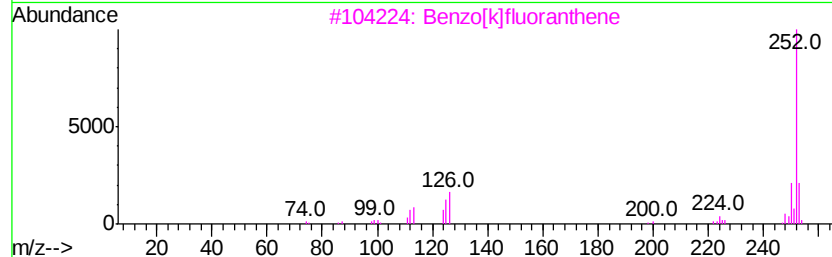
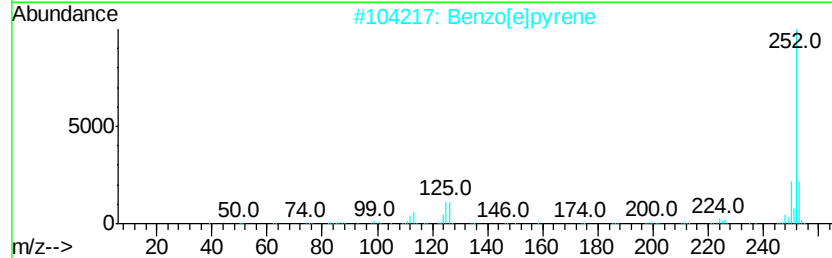
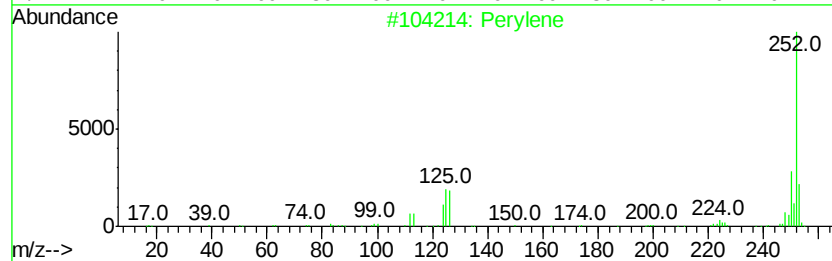
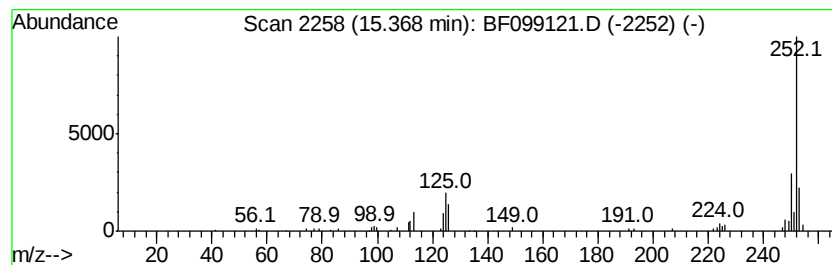
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.33 ng	77739	Perylene-d12	15.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	98
2	Benzo[e]pyrene		252	C20H12	000192-97-2	96
3	Benzo[k]fluoranthene		252	C20H12	000207-08-9	95
4	Benzo[a]pyrene		252	C20H12	000050-32-8	94
5	Benz[e]acephenanthrylene		252	C20H12	000205-99-2	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	2.5	ng	90472	1	6.86	739159	20.0
2-Pentanone, 4-hy...	5.07	2.7	ng	98347	1	6.86	739159	20.0
unknown6.63	6.63	17.6	ng	650279	1	6.86	739159	20.0
Perylene	15.37	2.3	ng	77739	6	15.50	667427	20.0