

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
 Data File : BF099218.D
 Acq On : 8 Oct 2017 3:51
 Operator : SJ/JU
 Sample : I5530-08 5X
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LB-33(0-0.5)

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	25	rVB3	53322	121843	15.45%	1.389%
2	5.075	505	508	515	rBV	75576	77318	9.81%	0.881%
3	5.481	573	577	587	rVB	509538	496674	62.99%	5.661%
4	6.487	745	748	760	rBV	547806	509024	64.56%	5.802%
5	6.634	769	773	776	rBV	603682	518914	65.81%	5.915%
6	6.863	809	812	816	rBV	812460	645614	81.88%	7.359%
7	7.022	835	839	842	rBV	457200	413442	52.43%	4.713%
8	7.422	904	907	911	rBV	323200	267213	33.89%	3.046%
9	8.145	1027	1030	1034	rBV	971569	788502	100.00%	8.988%
10	9.216	1209	1212	1221	rBV	648052	518068	65.70%	5.905%
11	9.610	1276	1279	1285	rVB	70436	61258	7.77%	0.698%
12	9.763	1302	1305	1310	rBV	45947	36831	4.67%	0.420%
13	9.822	1310	1315	1319	rVB2	8668	10364	1.31%	0.118%
14	9.904	1325	1329	1332	rBV	776030	707548	89.73%	8.065%
15	9.928	1332	1333	1337	rVB2	9879	9652	1.22%	0.110%
16	10.322	1398	1400	1403	rVB	13199	9458	1.20%	0.108%
17	10.451	1418	1422	1427	rVB4	8983	13547	1.72%	0.154%
18	10.686	1459	1462	1469	rVB	216795	194243	24.63%	2.214%
19	10.792	1477	1480	1489	rVB2	14068	20279	2.57%	0.231%
20	11.239	1553	1556	1558	rBV2	12459	11439	1.45%	0.130%
21	11.386	1578	1581	1584	rBV2	715179	639676	81.13%	7.291%
22	11.410	1584	1585	1589	rVV	111810	76596	9.71%	0.873%
23	11.463	1592	1594	1597	rVB	38676	28998	3.68%	0.331%
24	11.622	1617	1621	1624	rBV4	9830	10864	1.38%	0.124%
25	11.892	1663	1667	1669	rBV	29731	30059	3.81%	0.343%
26	11.916	1669	1671	1674	rVV	44895	36415	4.62%	0.415%
27	11.969	1677	1680	1682	rVV	19478	19948	2.53%	0.227%
28	11.998	1682	1685	1688	rVV2	40835	49704	6.30%	0.567%
29	12.022	1688	1689	1693	rVB	23421	16322	2.07%	0.186%
30	12.180	1714	1716	1719	rVV2	15499	13137	1.67%	0.150%
31	12.216	1719	1722	1727	rVB6	15003	19463	2.47%	0.222%
32	12.363	1745	1747	1750	rVB2	16255	12265	1.56%	0.140%
33	12.386	1750	1751	1754	rVB2	15452	10181	1.29%	0.116%
34	12.433	1756	1759	1762	rBV	43210	45167	5.73%	0.515%

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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 >
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35	12.469	1762	1765	1768	rVV3	21991	30686	3.89%	0.350%
36	12.522	1772	1774	1779	rBV5	18295	24628	3.12%	0.281%
37	12.598	1784	1787	1792	rBV	179948	170256	21.59%	1.941%
38	12.645	1792	1795	1796	rBV3	9565	9423	1.20%	0.107%
39	12.698	1801	1804	1807	rVB	16902	15701	1.99%	0.179%
40	12.833	1821	1827	1833	rBV	202018	227324	28.83%	2.591%
41	12.886	1833	1836	1840	rVB2	22185	24647	3.13%	0.281%
42	12.969	1846	1850	1853	rBV	498751	413159	52.40%	4.709%
43	13.157	1876	1882	1885	rBV	44989	59711	7.57%	0.681%
44	13.263	1897	1900	1902	rBV	38117	35959	4.56%	0.410%
45	14.027	2026	2030	2033	rBV	689701	697534	88.46%	7.951%
46	15.445	2268	2271	2276	rVB	82910	104736	13.28%	1.194%
47	15.510	2277	2282	2290	rVB	385998	519247	65.85%	5.919%

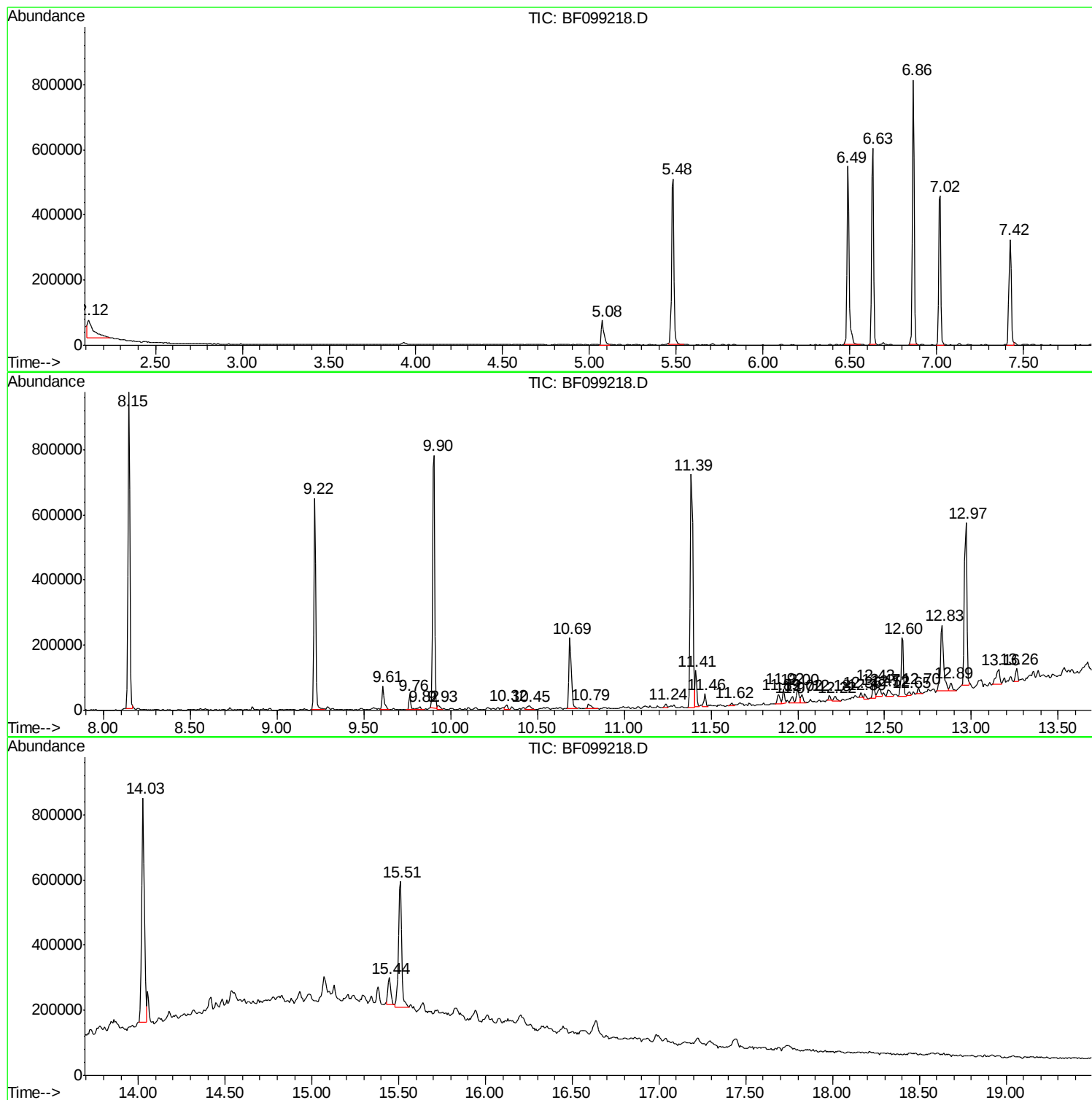
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ClientSampled :
LB-33(0-0.5)

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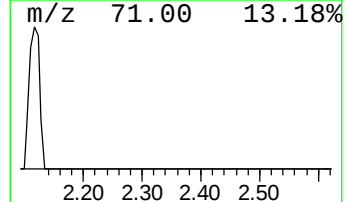
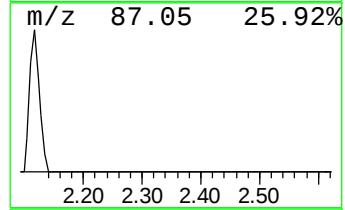
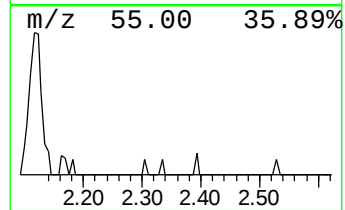
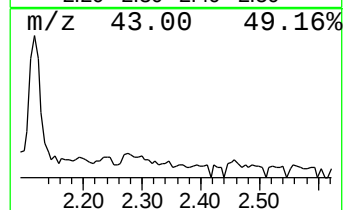
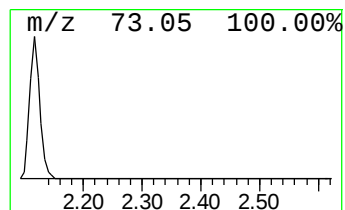
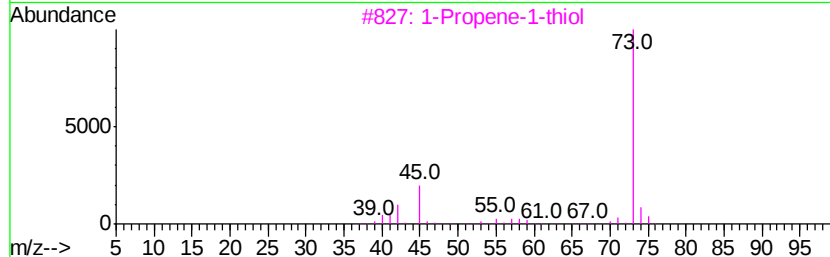
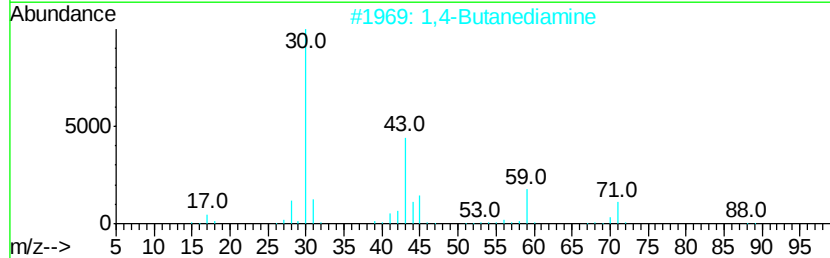
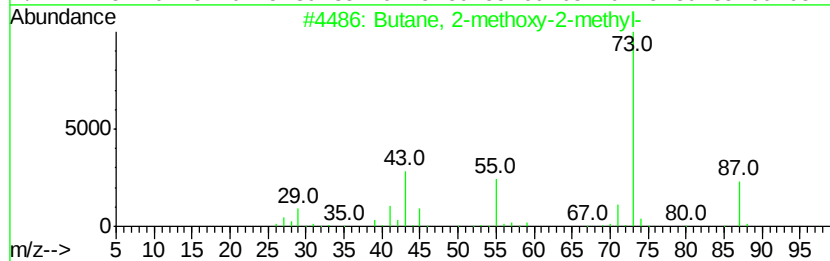
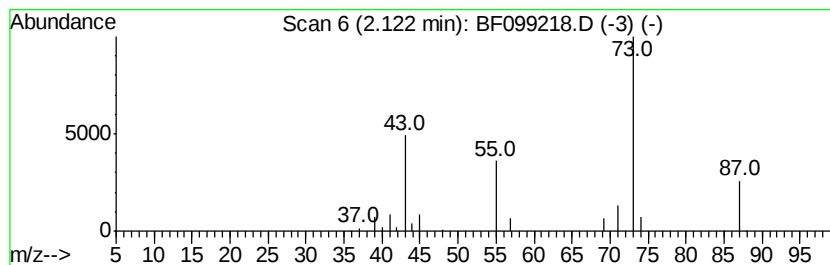
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.77 ng	121843	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	72
2		1,4-Butanediamine	88	C4H12N2	000110-60-1	9
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	5
4		Ethyl formate	74	C3H6O2	000109-94-4	5
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



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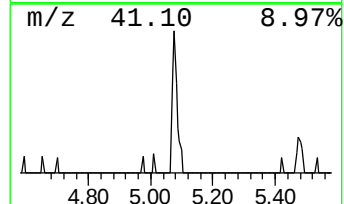
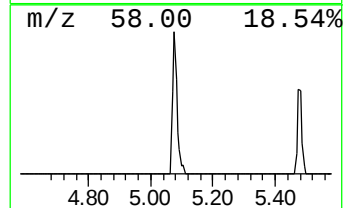
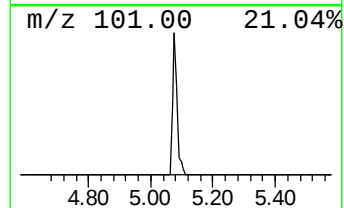
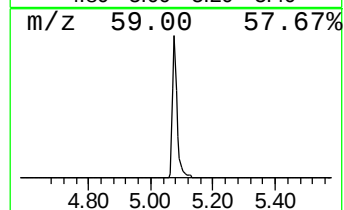
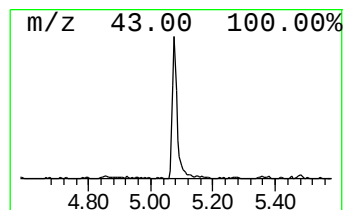
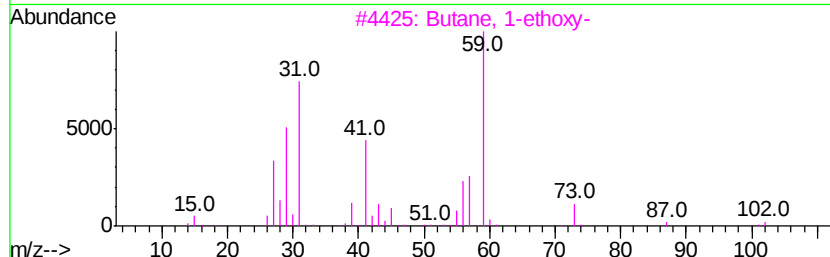
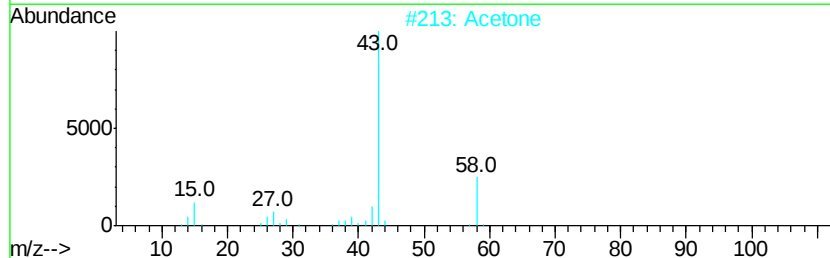
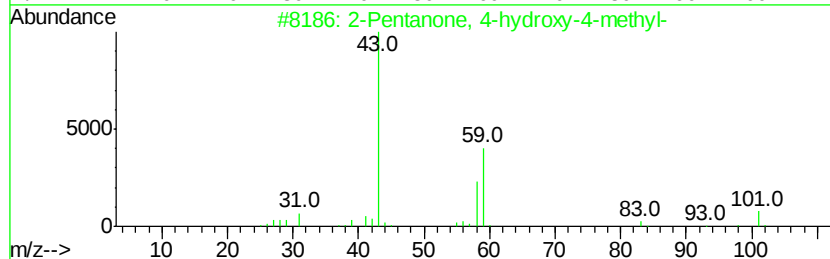
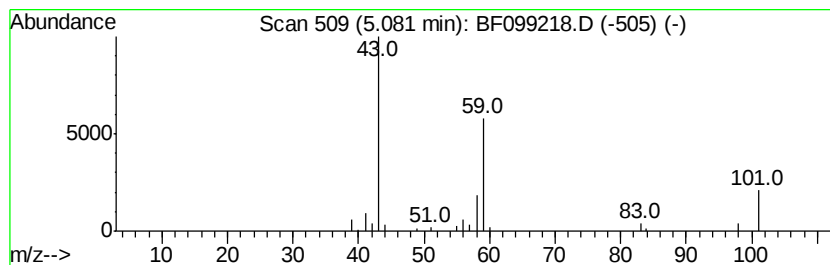
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Peak Number 2 unknown5.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.40 ng	77318	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetone	58	C3H6O	000067-64-1	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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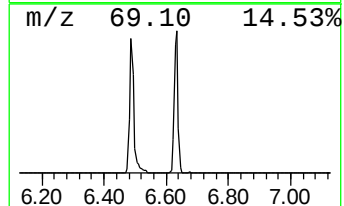
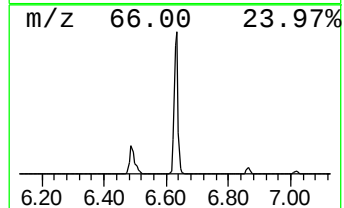
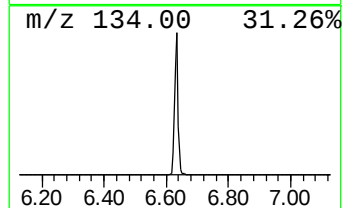
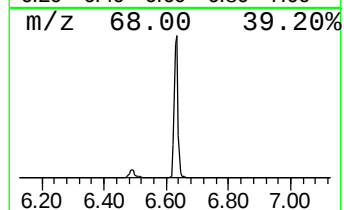
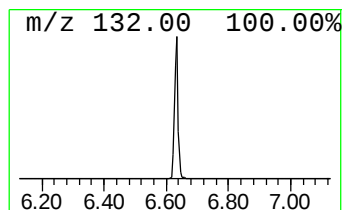
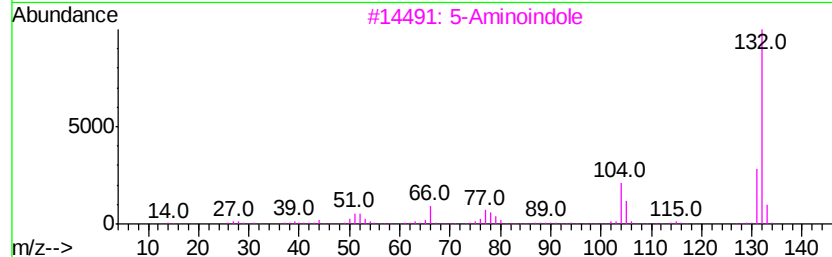
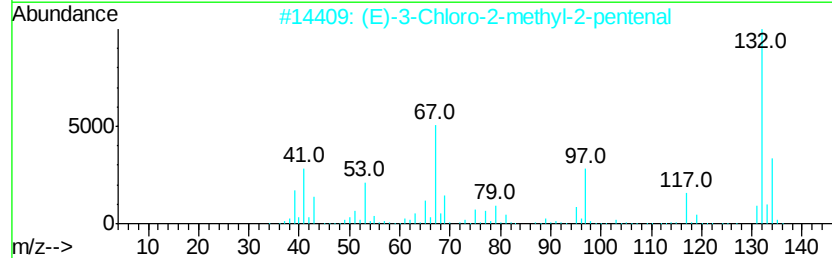
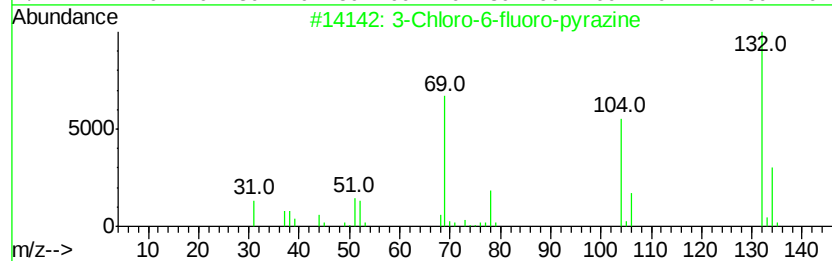
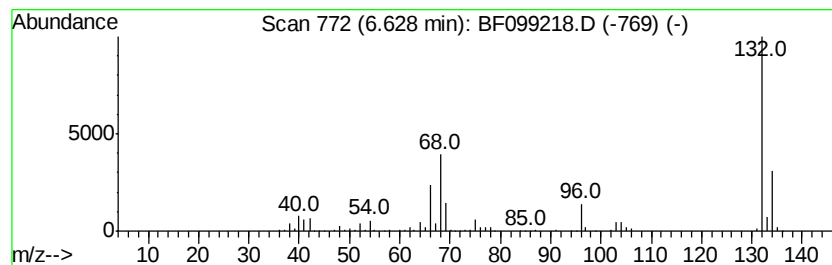
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	16.08 ng	518914	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	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Xenon	132	Xe	007440-63-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	3.8	ng	121843	1	6.86	645614	20.0
unknown5.08	5.08	2.4	ng	77318	1	6.86	645614	20.0
unknown6.63	6.63	16.1	ng	518914	1	6.86	645614	20.0