

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031518\
 Data File : BF103675.D
 Acq On : 15 Mar 2018 18:28
 Operator : JU/SJ
 Sample : J1888-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PT-BN-WP

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-BF031518.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	11	rVB	478328	538849	6.76%	0.342%
2	2.316	34	39	45	rVB	222958	279284	3.50%	0.177%
3	4.116	340	345	351	rVB	376873	448656	5.63%	0.285%
4	5.216	528	532	542	rVB	91103	121527	1.52%	0.077%
5	5.587	589	595	598	rBV	3826299	4213949	52.84%	2.677%
6	6.587	758	765	768	rBV	3700520	4215386	52.85%	2.678%
7	6.734	785	790	794	rBV	3839689	4293104	53.83%	2.727%
8	6.969	826	830	831	rBV	1139257	1200008	15.05%	0.762%
9	6.987	831	833	836	rVB	3348090	2581565	32.37%	1.640%
10	7.128	852	857	858	rBV	3458787	4085525	51.23%	2.595%
11	7.481	913	917	920	rBV	2596790	2283619	28.63%	1.451%
12	7.528	920	925	928	rBV	2676840	2683887	33.65%	1.705%
13	8.251	1043	1048	1049	rBV	1419936	1504740	18.87%	0.956%
14	8.275	1049	1052	1055	rVB	4912492	4621664	57.95%	2.936%
15	8.969	1164	1170	1173	rVB	5518833	6230097	78.12%	3.958%
16	9.057	1181	1185	1189	rBV	200427	161776	2.03%	0.103%
17	9.322	1225	1230	1234	rBV	4535618	4874820	61.12%	3.097%
18	9.728	1292	1299	1303	rBV	2483544	3408942	42.74%	2.166%
19	9.798	1303	1311	1314	rVV	3555309	4236209	53.12%	2.691%
20	9.880	1318	1325	1328	rVV	5863249	7975450	100.00%	5.066%
21	10.010	1342	1347	1349	rBV2	1572293	1515630	19.00%	0.963%
22	10.051	1349	1354	1357	rVB	5468689	6163105	77.28%	3.915%
23	10.192	1372	1378	1380	rBV	2669325	2816815	35.32%	1.789%
24	10.216	1380	1382	1386	rVB	3659746	3433546	43.05%	2.181%
25	10.427	1411	1418	1421	rBV	4394183	4729672	59.30%	3.004%
26	10.557	1433	1440	1444	rBV2	4994460	6251078	78.38%	3.971%
27	10.798	1476	1481	1484	rBV	2837385	2910624	36.49%	1.849%
28	11.498	1596	1600	1602	rBV	1400257	1529575	19.18%	0.972%
29	11.527	1602	1605	1608	rVB	4520299	4781559	59.95%	3.037%
30	12.063	1690	1696	1699	rBV	5265448	6108301	76.59%	3.880%
31	12.727	1802	1809	1812	rBV	5075110	6081398	76.25%	3.863%
32	12.951	1841	1847	1851	rBV	3664766	4045391	50.72%	2.570%
33	13.092	1865	1871	1874	rBV	4532286	4782573	59.97%	3.038%
34	13.568	1947	1952	1955	rBV	5325078	5885130	73.79%	3.738%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.115	2041	2045	2047	rBV	3267887	3084231	38.67%	1.959%
36	14.145	2047	2050	2054	rVV2	3990580	5711397	71.61%	3.628%
37	14.180	2054	2056	2059	rVB	2882054	2359883	29.59%	1.499%
38	15.239	2228	2236	2238	rBV	3056085	5075092	63.63%	3.224%
39	15.268	2238	2241	2259	rVB	2985950	3636557	45.60%	2.310%
40	15.639	2294	2304	2308	rBV	3641159	6717859	84.23%	4.267%
41	15.686	2308	2312	2332	rVB	924968	1210325	15.18%	0.769%
42	17.280	2567	2583	2591	rBV2	2105471	5831970	73.12%	3.705%
43	17.739	2648	2661	2672	rBV	1105737	2799419	35.10%	1.778%

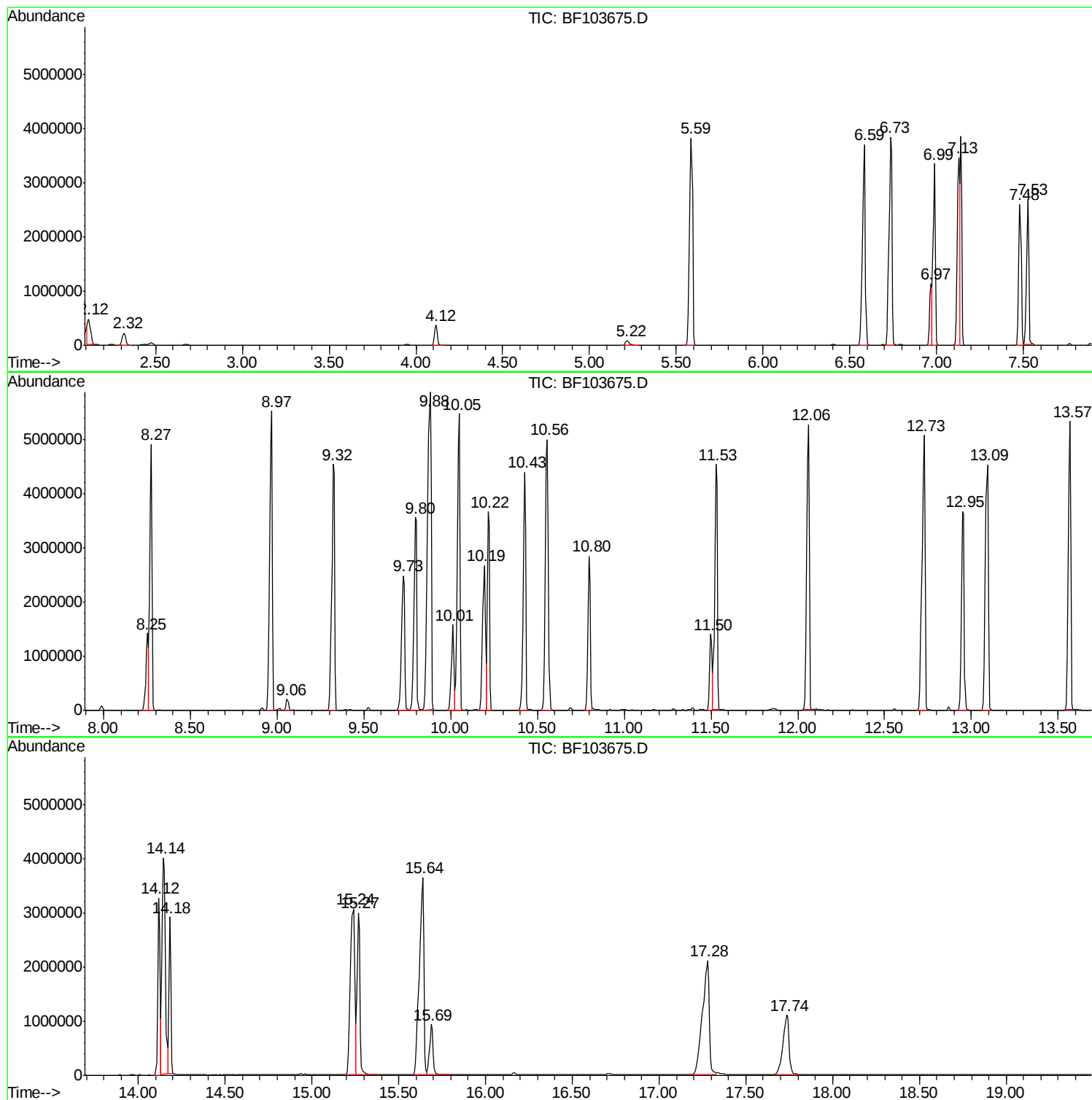
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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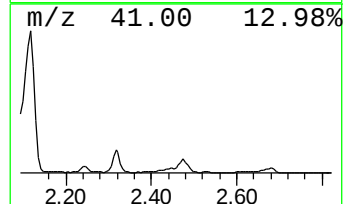
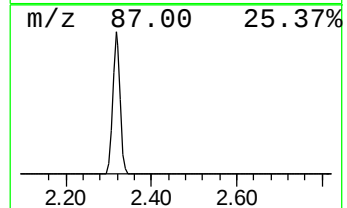
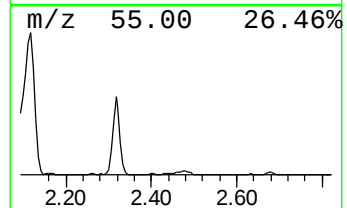
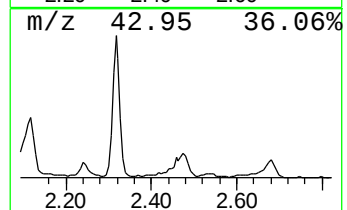
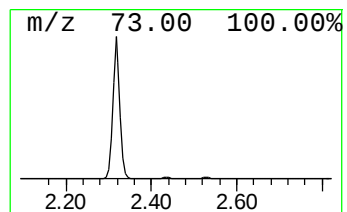
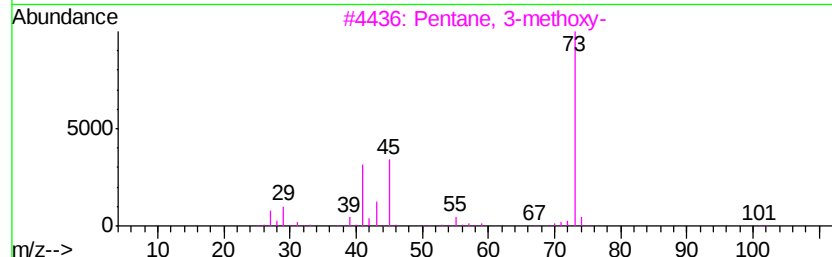
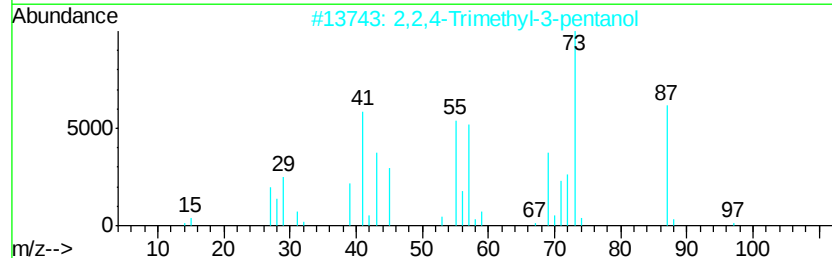
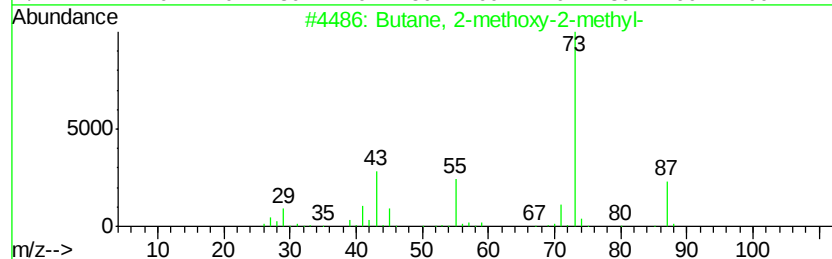
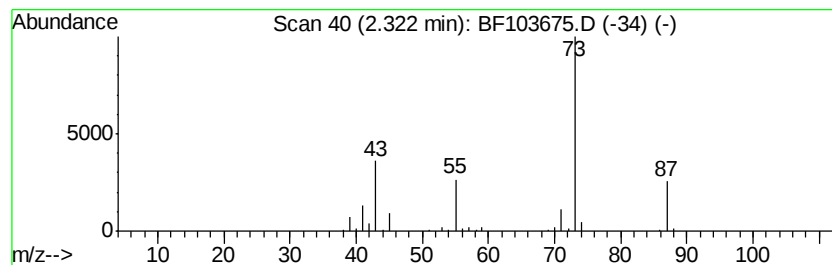
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	4.65 ng	279284	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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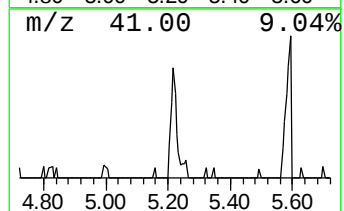
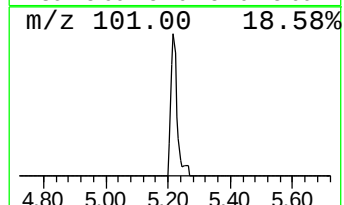
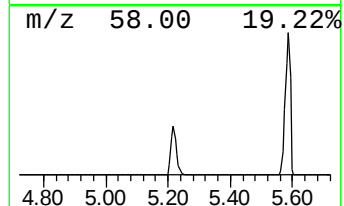
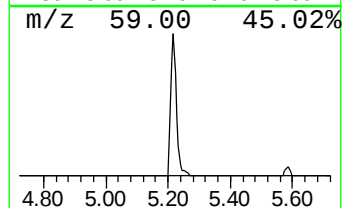
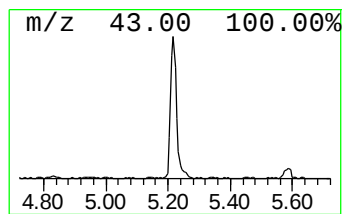
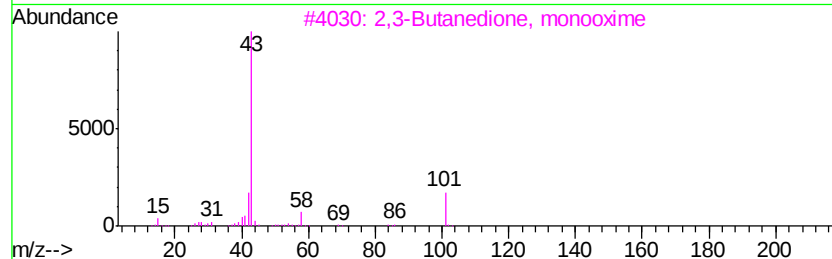
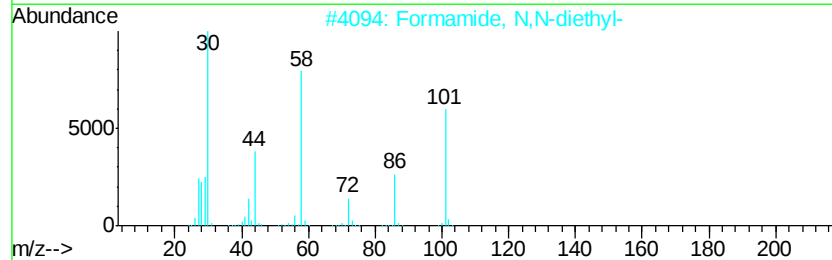
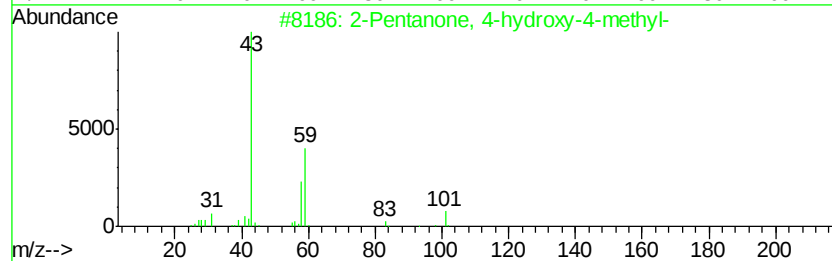
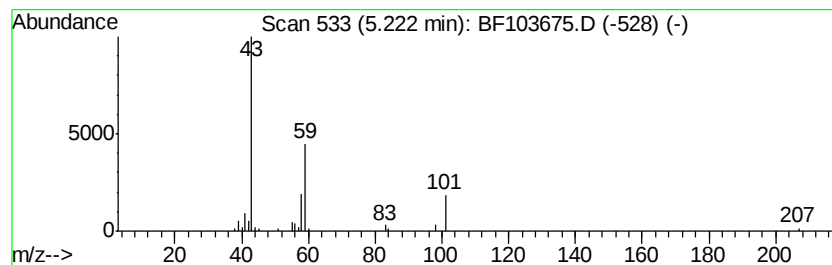
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.03 ng	121527	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		Succindialdehyde	86	C4H6O2	000638-37-9	9



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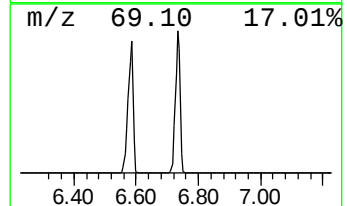
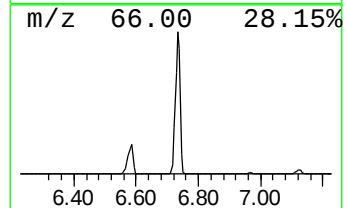
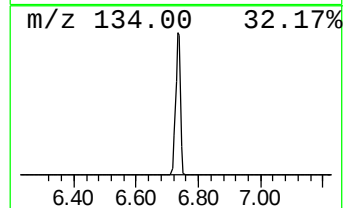
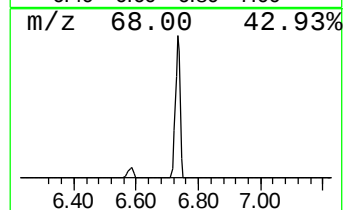
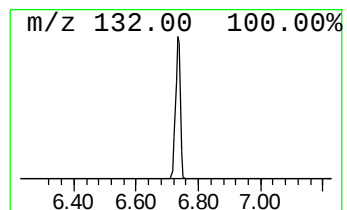
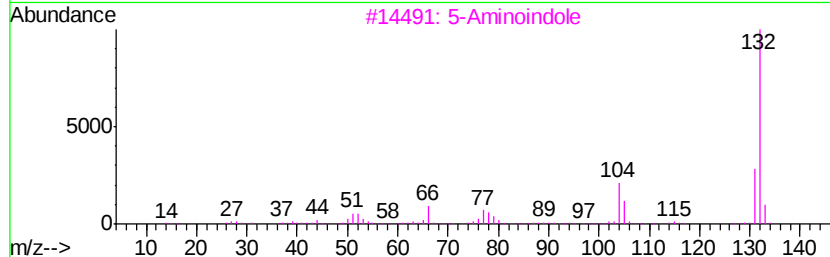
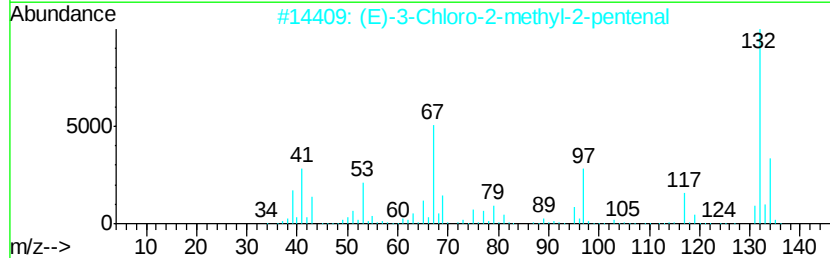
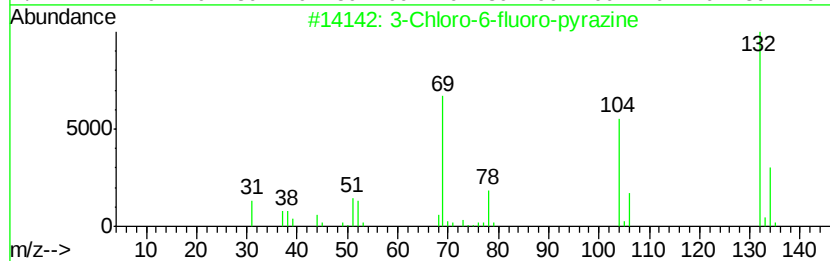
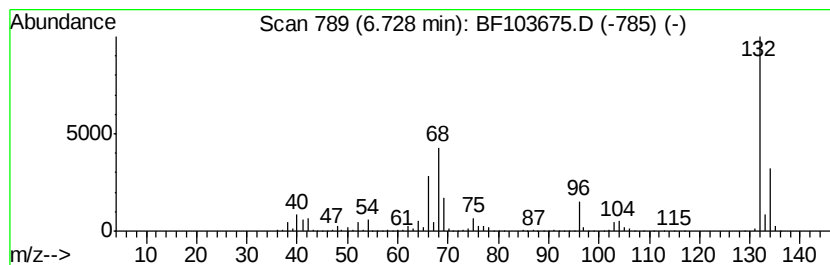
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	71.55 ng	4293100	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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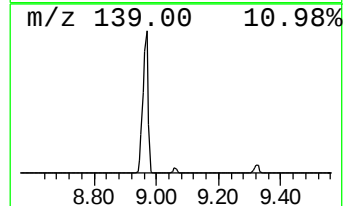
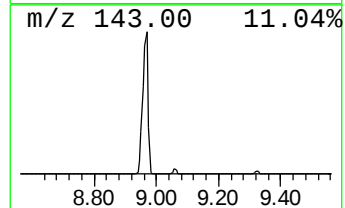
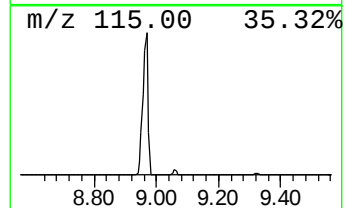
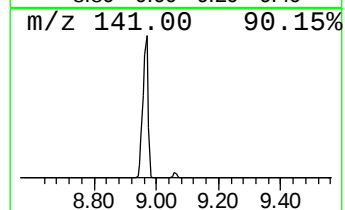
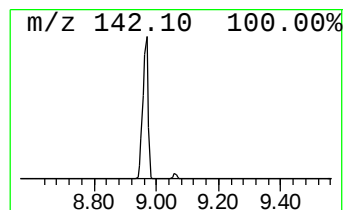
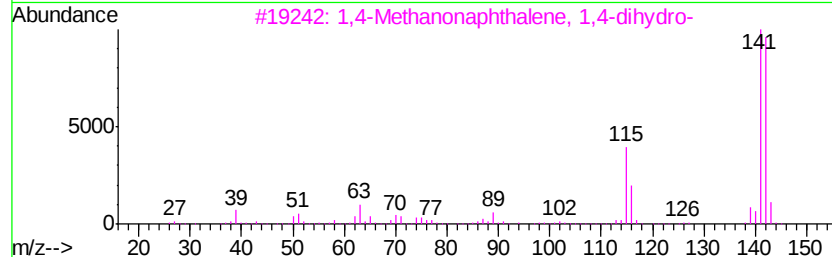
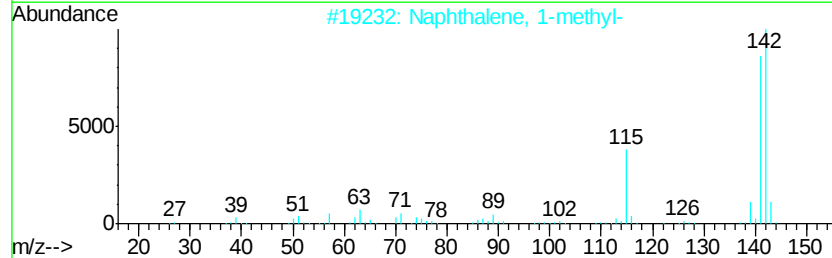
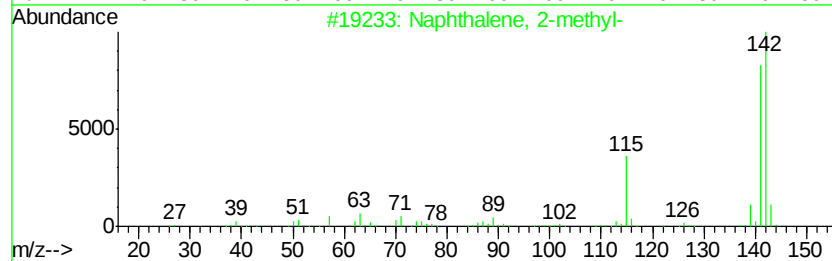
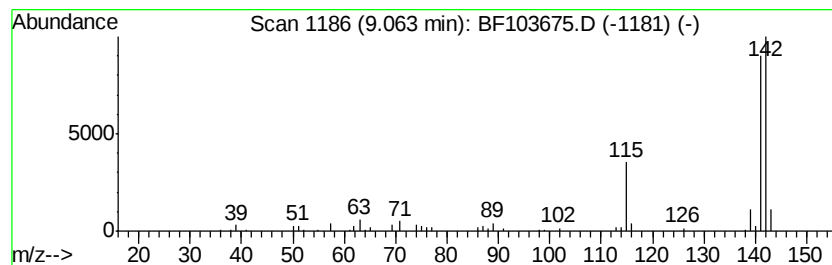
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	2.15 ng	161776	Naphthalene-d8	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.32	4.7	ng	279284	1	6.97	1200010	20.0
2-Pentanone, 4-hy...	5.22	2.0	ng	121527	1	6.97	1200010	20.0
unknown6.73	6.73	71.5	ng	4293100	1	6.97	1200010	20.0
Naphthalene, 1-me...	9.06	2.1	ng	161776	2	8.25	1504740	20.0