

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080747.D
Acq On : 31 Jul 2015 21:56
Operator : TP/UM
Sample : G3125-15
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

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-BF073015.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	2.178	5	8	10	rBV	39209	73529	2.22%	0.236%
2	4.407	201	203	208	rBV	130200	180990	5.47%	0.581%
3	5.047	256	259	262	rBV	1825403	2824071	85.35%	9.071%
4	5.458	292	295	297	rBV	3283037	3308791	100.00%	10.628%
5	5.859	328	330	333	rVB	98211	108748	3.29%	0.349%
6	6.476	381	384	386	rBV	3012111	2998521	90.62%	9.631%
7	6.613	394	396	399	rBV	2611843	2945082	89.01%	9.460%
8	6.853	415	417	419	rBV	1003534	873397	26.40%	2.805%
9	7.001	428	430	433	rVB	1738472	2288702	69.17%	7.351%
10	7.413	463	466	468	rBV	2196888	2256787	68.21%	7.249%
11	7.493	468	473	479	rVB	37364	55555	1.68%	0.178%
12	8.133	526	529	531	rBV	1231871	1079520	32.63%	3.467%
13	9.207	620	623	626	rBV	3126954	3135480	94.76%	10.071%
14	9.607	655	658	660	rBV	675863	771585	23.32%	2.478%
15	9.882	680	682	685	rVB	1123566	1083177	32.74%	3.479%
16	10.328	717	721	722	rVB2	28828	48950	1.48%	0.157%
17	10.670	748	751	753	rBV	1972530	2042326	61.72%	6.560%
18	10.796	758	762	765	rVB2	55923	94237	2.85%	0.303%
19	11.242	799	801	802	rBV	62800	50517	1.53%	0.162%
20	11.368	809	812	814	rBV	1042913	1087590	32.87%	3.493%
21	11.665	836	838	841	rBV	48631	43923	1.33%	0.141%
22	11.893	856	858	867	rBV	73198	105326	3.18%	0.338%
23	12.945	948	950	953	rBV	2291943	2424741	73.28%	7.788%
24	13.985	1039	1041	1044	rBV	502273	676666	20.45%	2.173%
25	15.402	1162	1165	1168	rBV	412779	575101	17.38%	1.847%

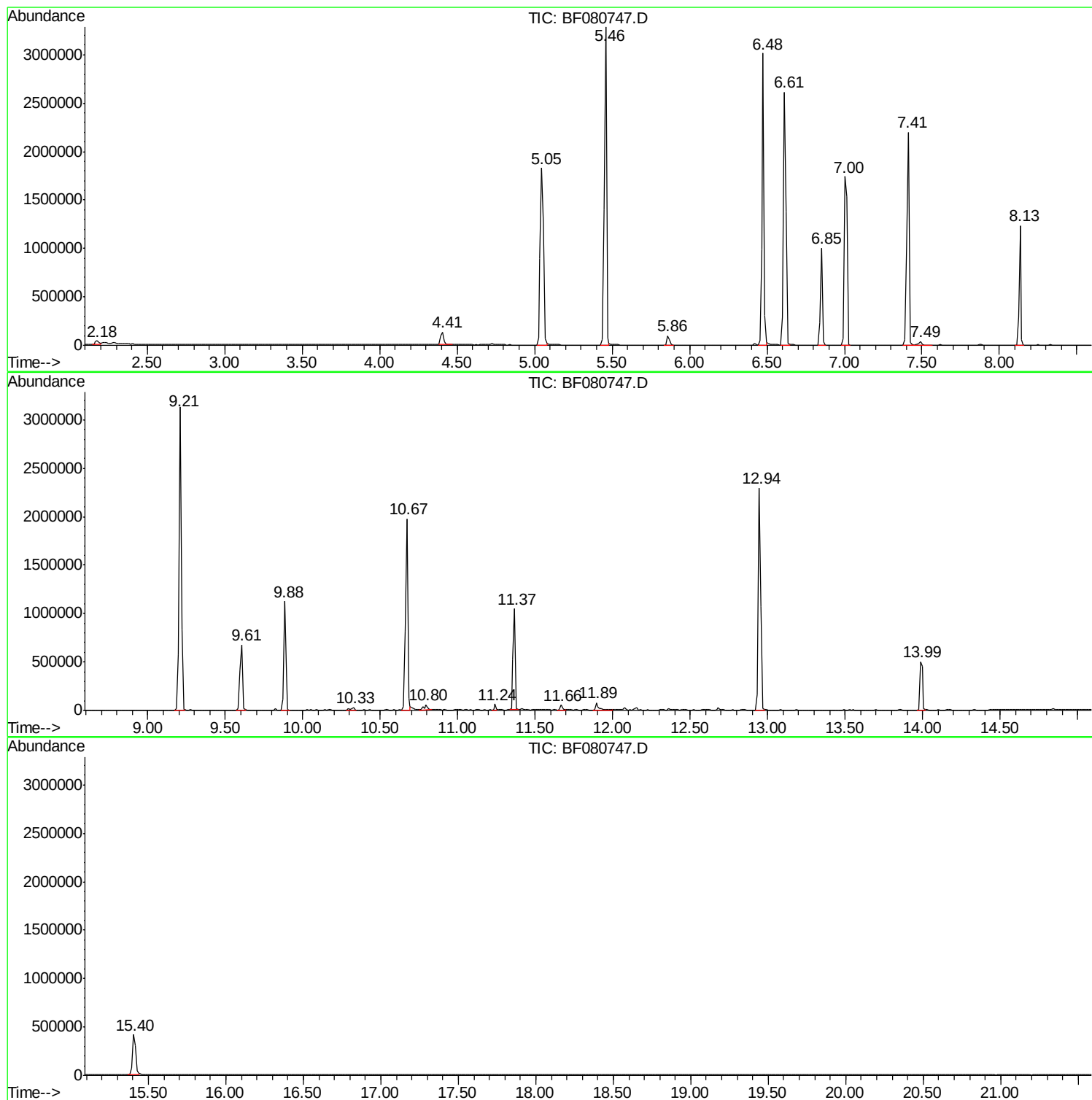
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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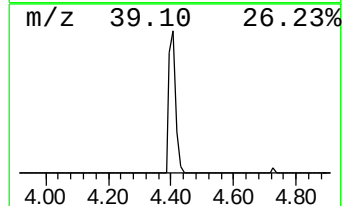
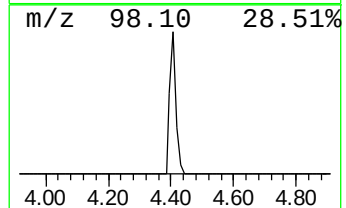
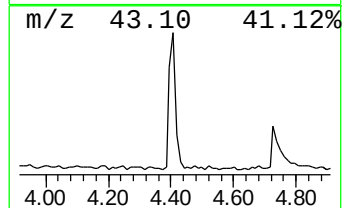
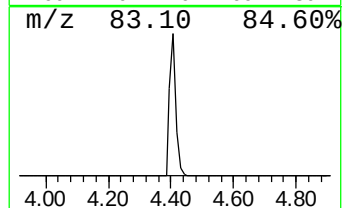
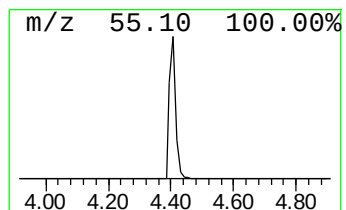
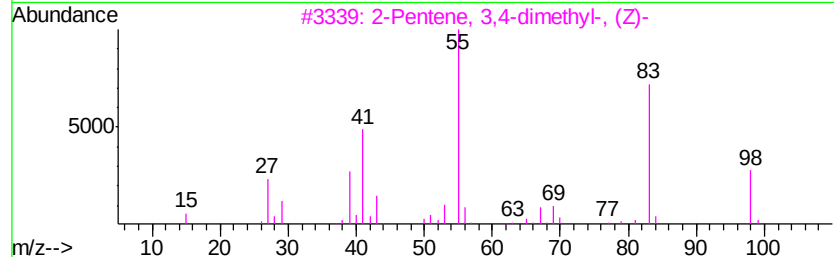
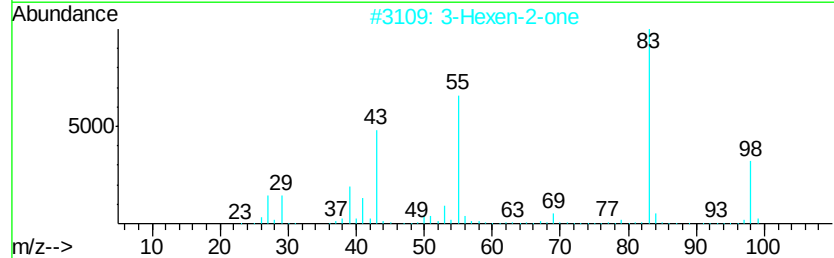
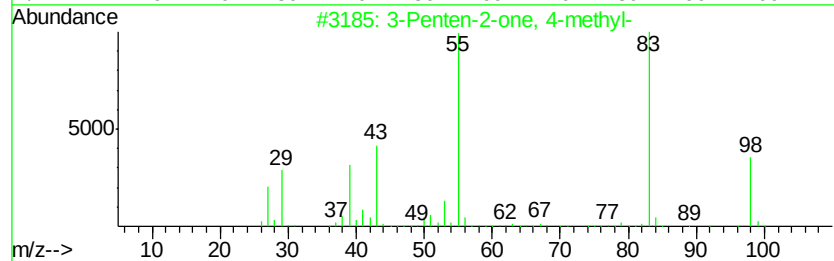
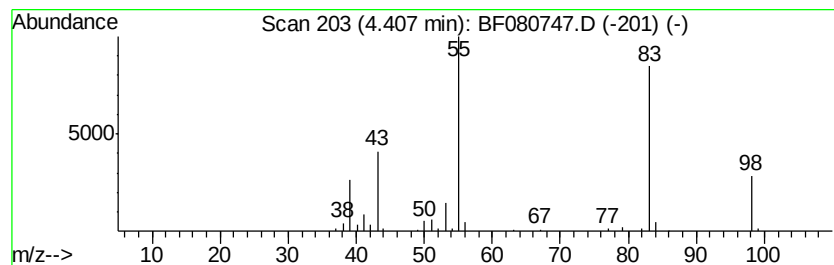
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	4.14 ng	180990	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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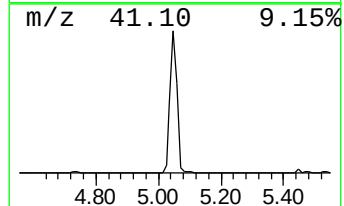
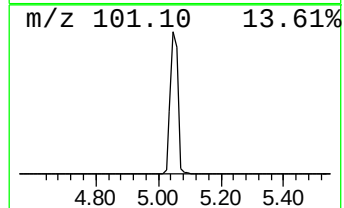
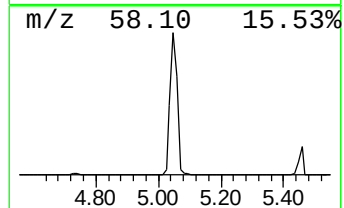
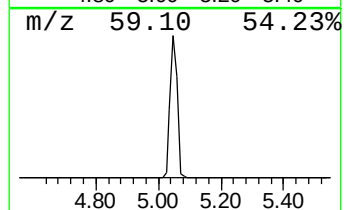
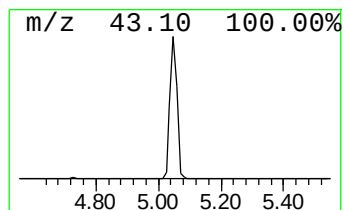
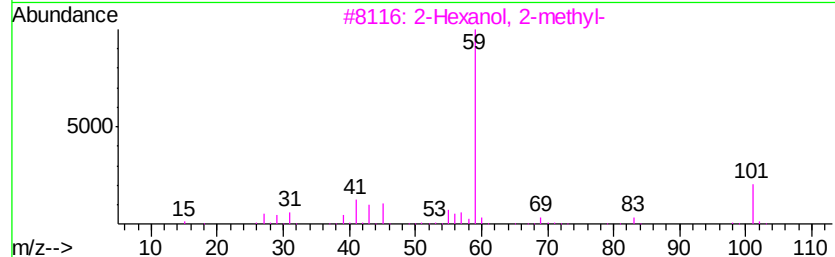
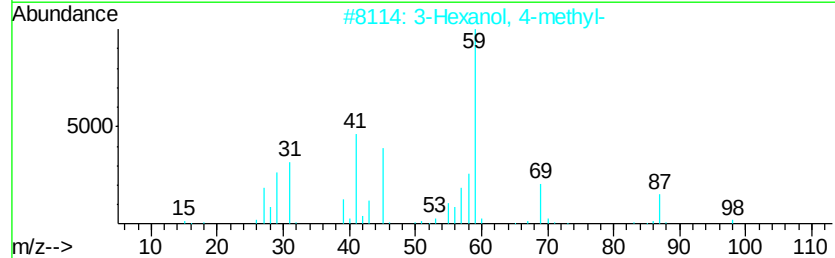
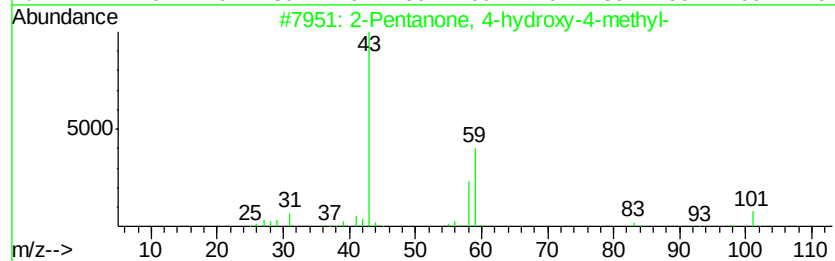
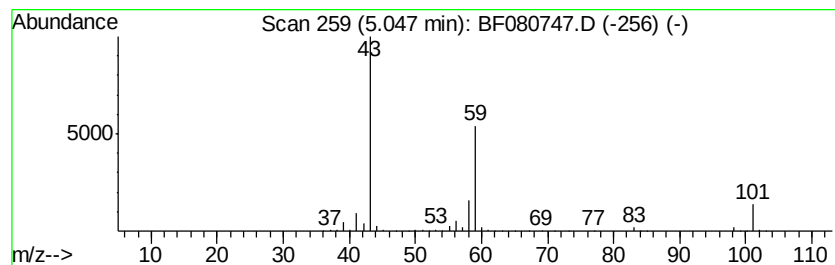
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.05	64.67 ng	2824070	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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Instrument :
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ClientSampleId :

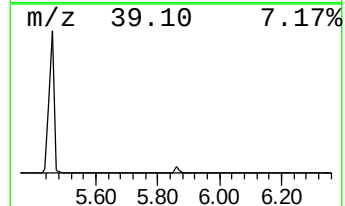
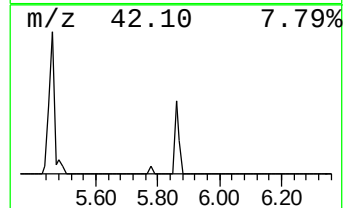
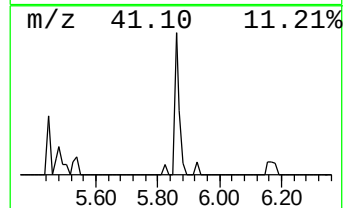
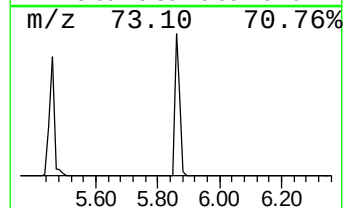
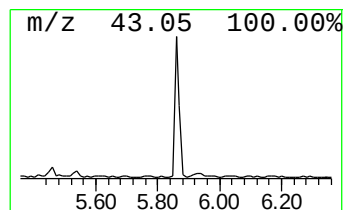
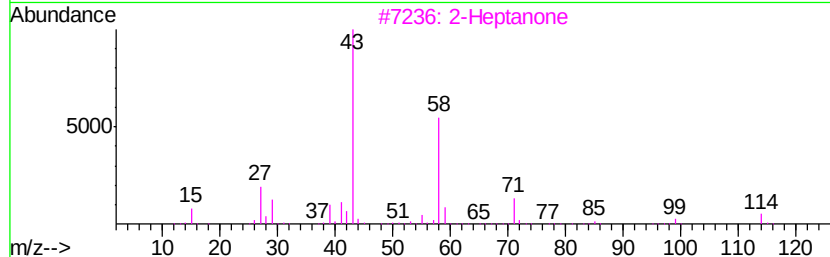
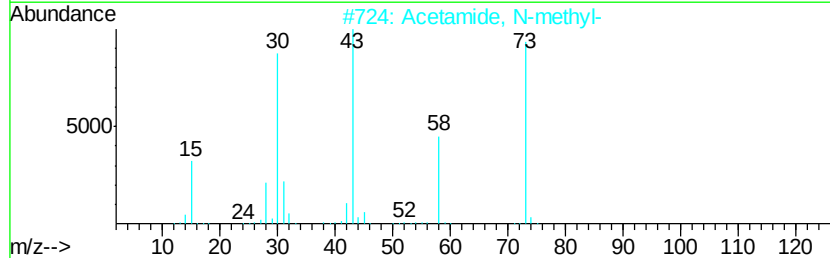
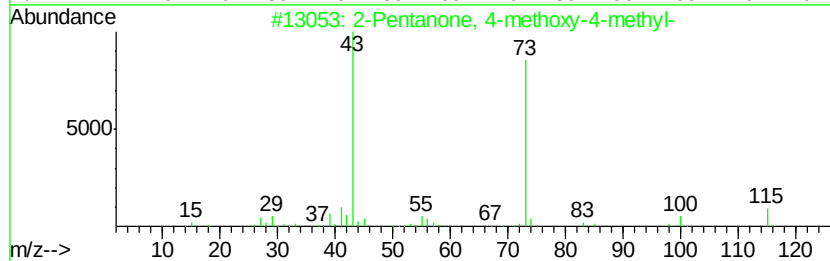
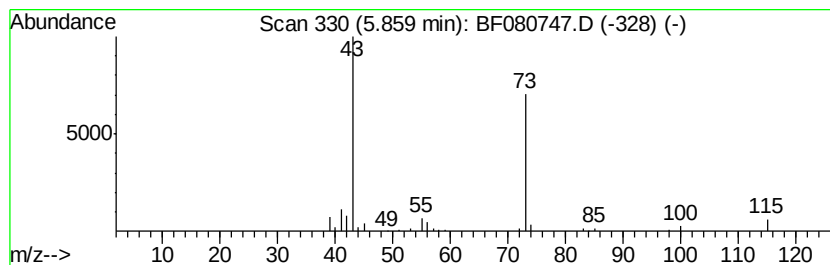
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.49 ng	108748	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
3		2-Heptanone	114	C7H14O	000110-43-0	23
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	10



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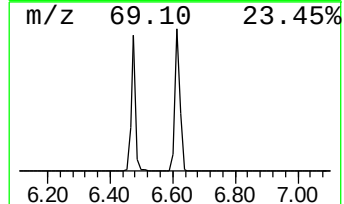
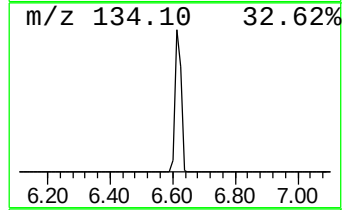
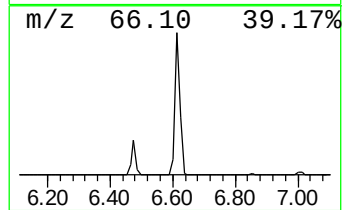
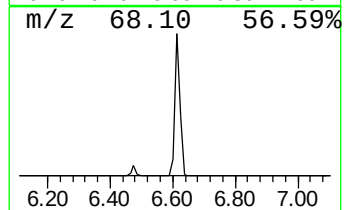
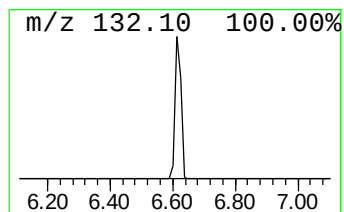
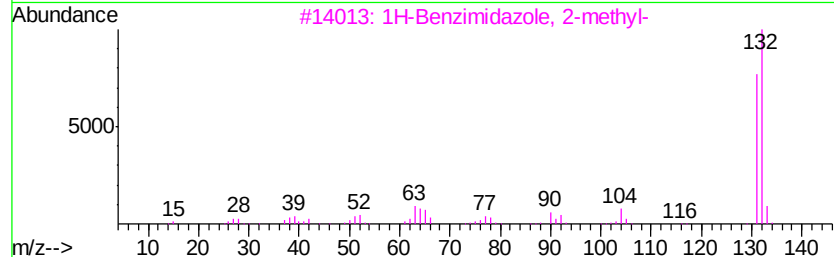
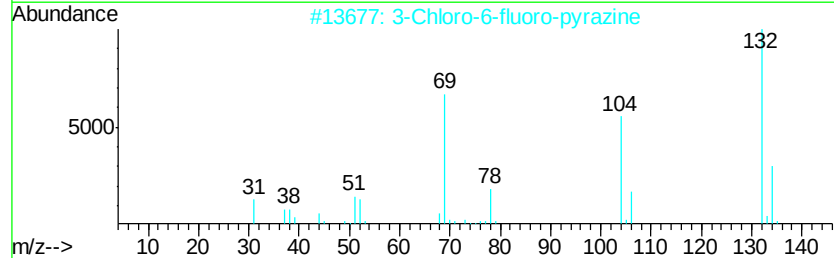
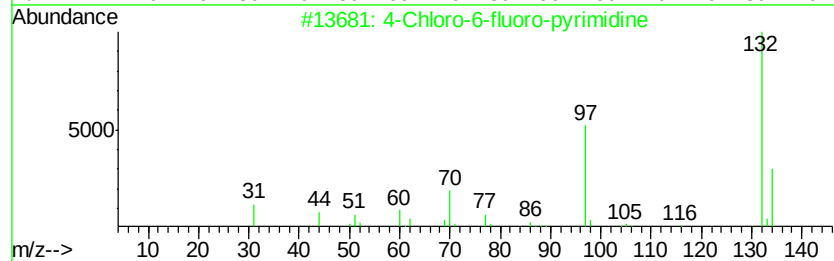
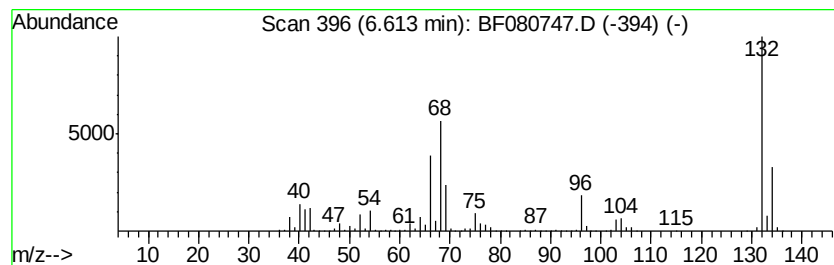
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	67.44 ng	2945080	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	4.1 ng		180990	1	6.85	873397	20.0
2-Pentanone, 4-hy...	5.05	64.7 ng		2824070	1	6.85	873397	20.0
unknown5.86	5.86	2.5 ng		108748	1	6.85	873397	20.0
unknown6.61	6.61	67.4 ng		2945080	1	6.85	873397	20.0