

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
 Data File : BF086863.D
 Acq On : 10 May 2016 16:50
 Operator : UM/SJ
 Sample : PB90444BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90444BL

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-BF050916.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	4.144	177	180	183	rBV	2532847	4053928	31.38%	8.169%
2	4.887	238	245	247	rBV	4505645	12919023	100.00%	26.033%
3	5.287	278	280	300	rBV	2595945	2654799	20.55%	5.350%
4	5.687	313	315	317	rBV	634421	739941	5.73%	1.491%
5	6.339	369	372	380	rBV	2623349	2782838	21.54%	5.608%
6	6.453	380	382	385	rBV	2877835	2641124	20.44%	5.322%
7	6.681	400	402	413	rVB	1102725	1051665	8.14%	2.119%
8	6.841	413	416	418	rBV	2526432	2997676	23.20%	6.041%
9	7.253	449	452	454	rBV	2467231	2426361	18.78%	4.889%
10	7.973	512	515	517	rBV	1071981	1306624	10.11%	2.633%
11	9.047	606	609	612	rBV	3997228	4111104	31.82%	8.284%
12	9.722	665	668	670	rBV	1452062	1524285	11.80%	3.072%
13	10.510	734	737	739	rBV	1553091	1957368	15.15%	3.944%
14	11.196	795	797	800	rBV	1806572	1583945	12.26%	3.192%
15	12.785	933	936	938	rBV	4302818	4464417	34.56%	8.996%
16	13.825	1024	1027	1029	rBV	1437109	1356390	10.50%	2.733%
17	15.197	1144	1147	1150	rBV	890923	1053366	8.15%	2.123%

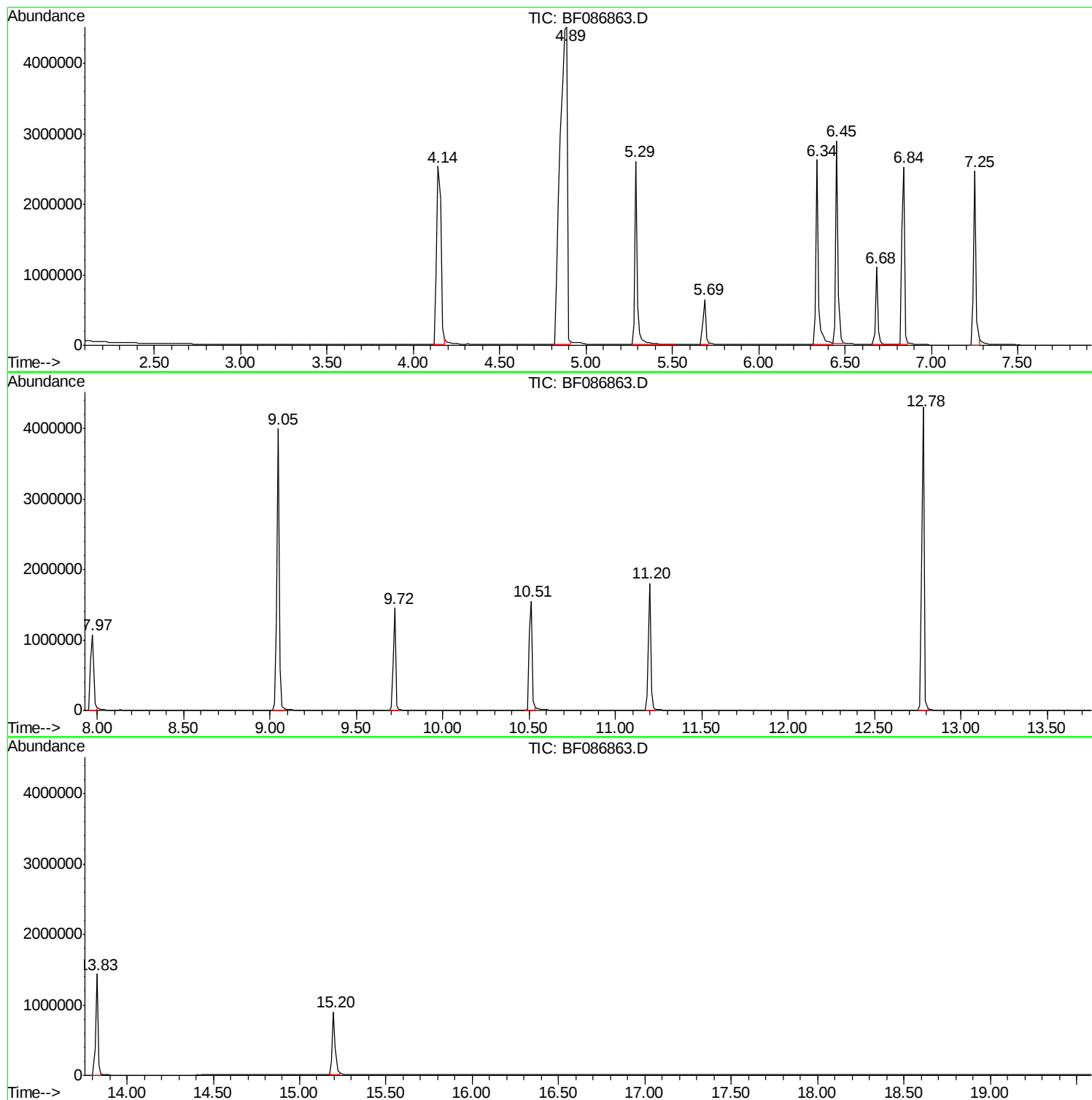
Sum of corrected areas: 49624854

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



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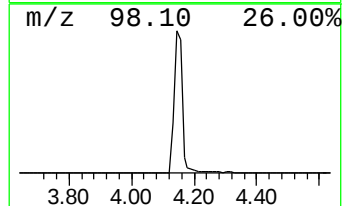
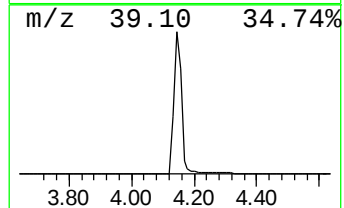
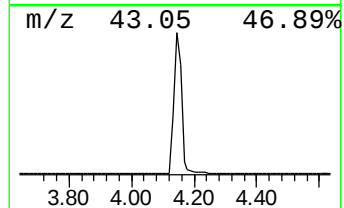
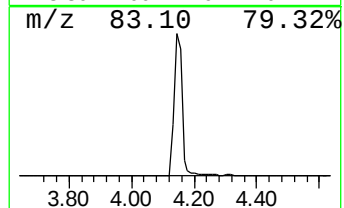
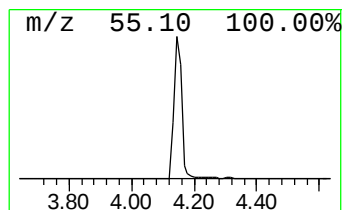
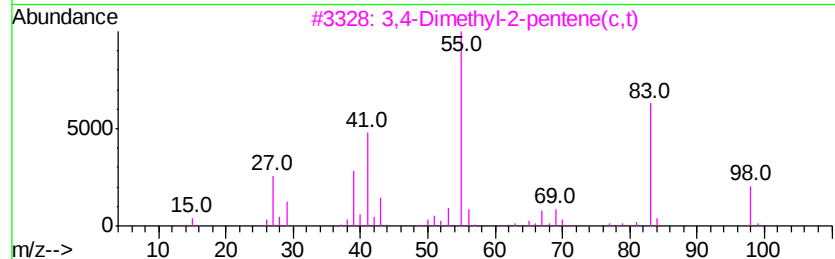
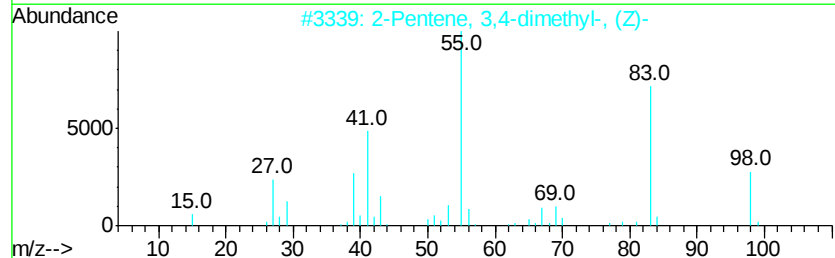
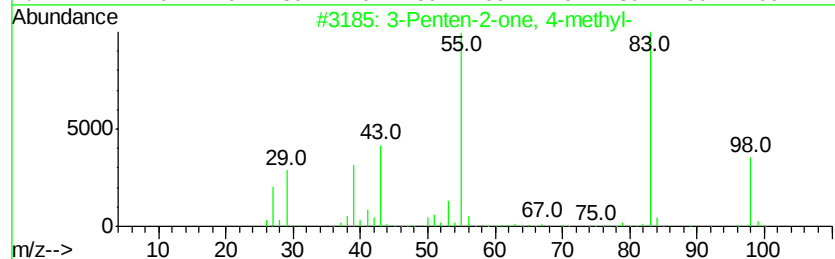
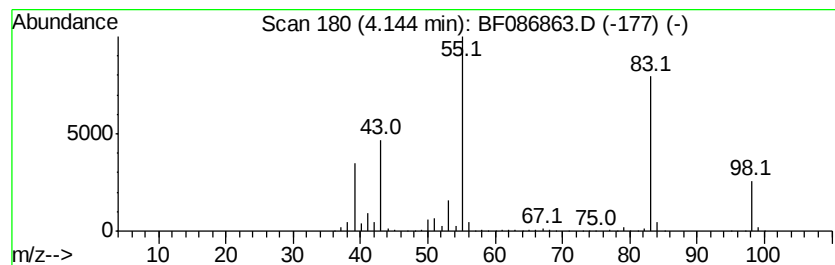
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	77.10 ng	4053930	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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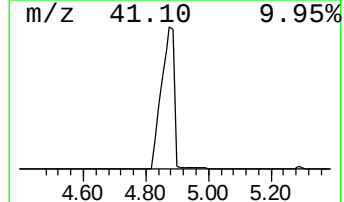
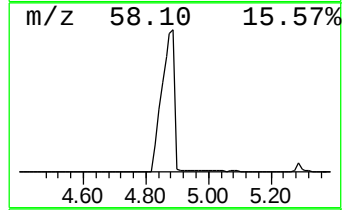
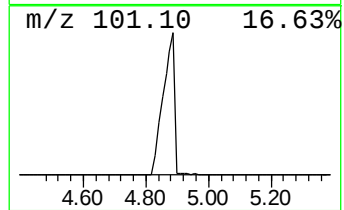
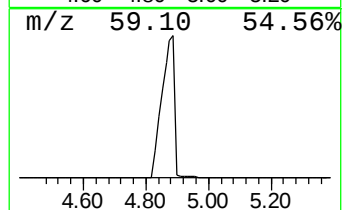
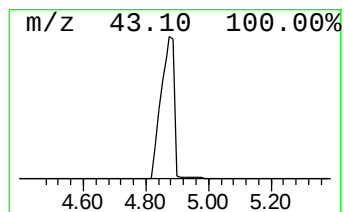
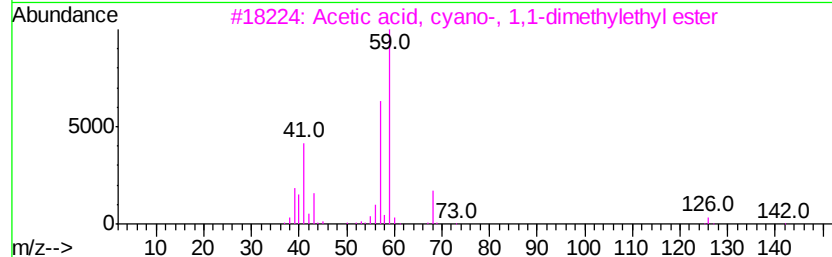
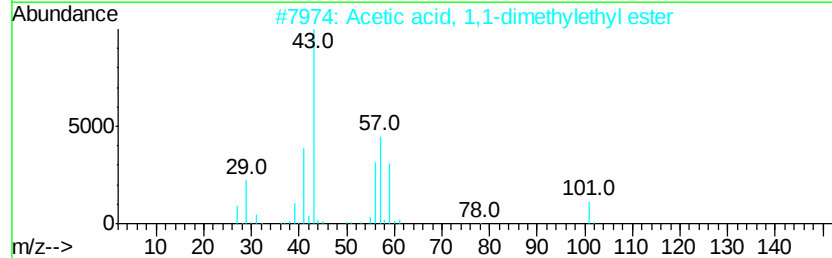
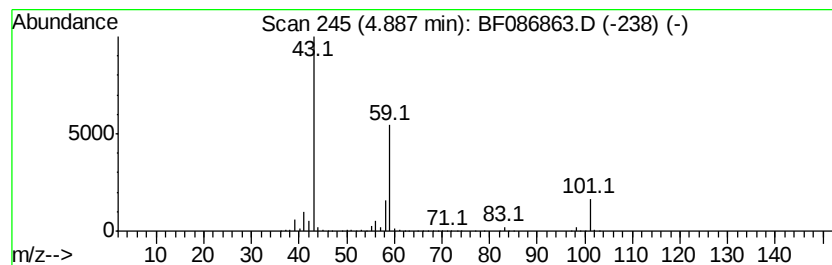
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	245.69 ng	12919000	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Acetone	58	C3H6O	000067-64-1	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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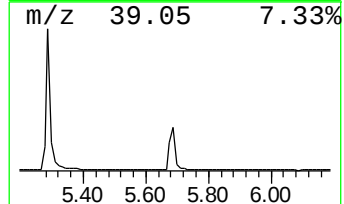
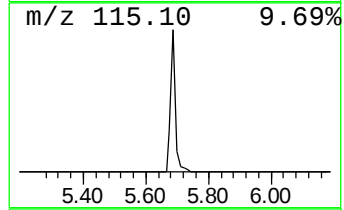
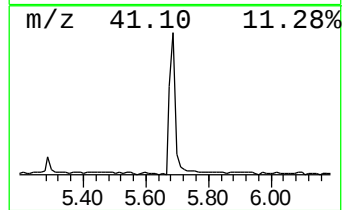
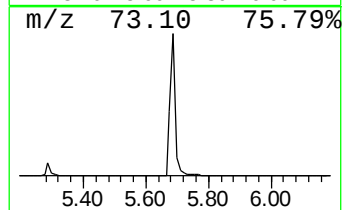
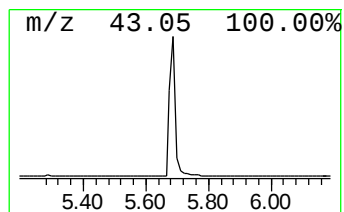
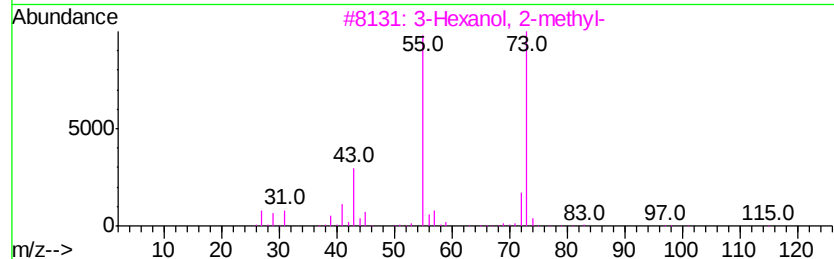
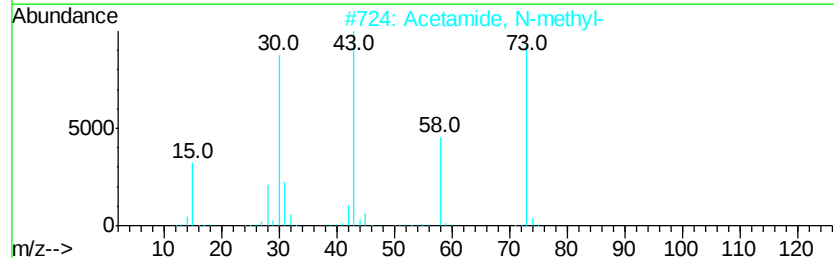
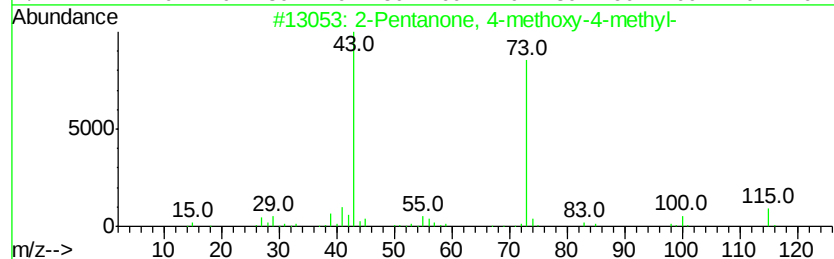
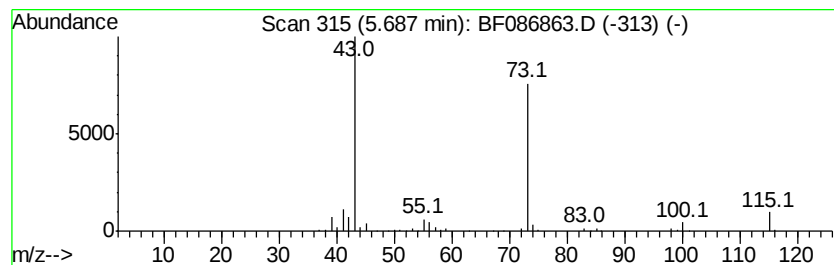
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	14.07 ng	739941	1,4-Dichlorobenzene-d4	6.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		Heptane	100	C7H16	000142-82-5	9



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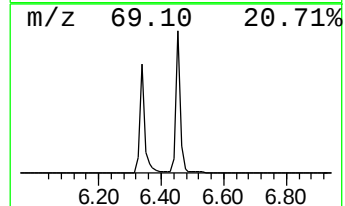
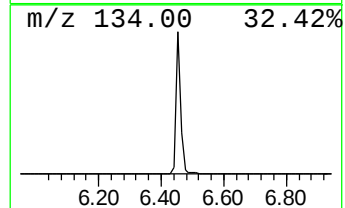
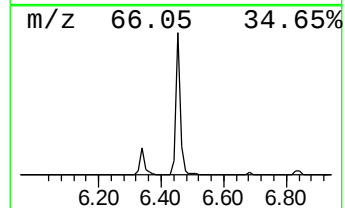
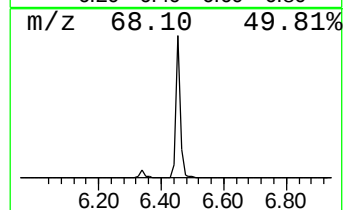
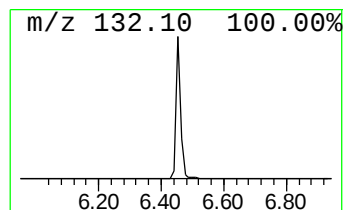
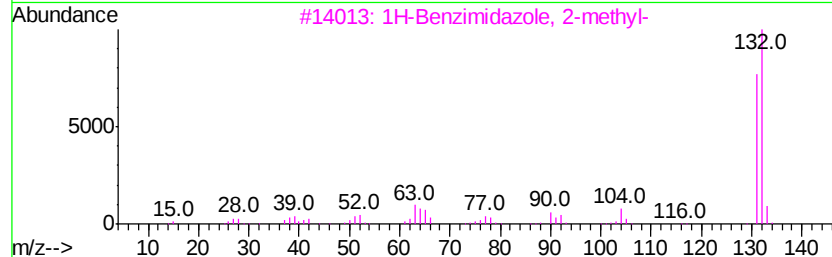
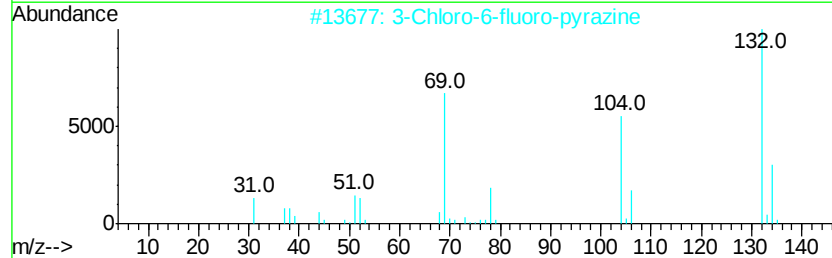
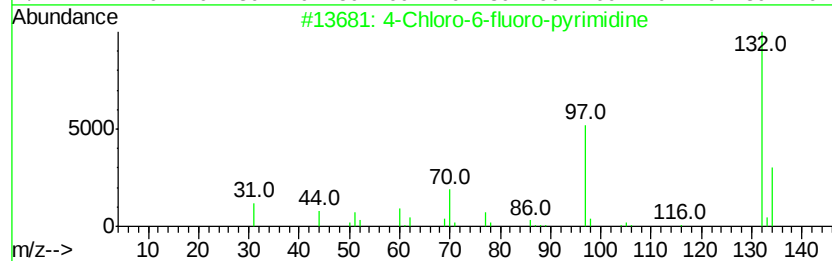
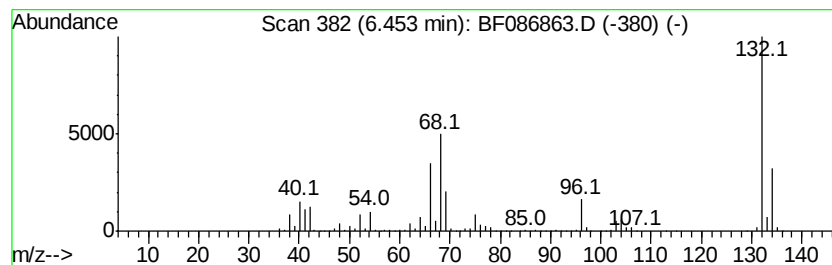
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Peak Number 4 unknown6.45 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	50.23 ng	2641120	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.14	77.1	ng	4053930	1	6.68	1051670	20.0
2-Pentanone, 4-hy...	4.89	245.7	ng	12919000	1	6.68	1051670	20.0
2-Pentanone, 4-me...	5.69	14.1	ng	739941	1	6.68	1051670	20.0
unknown6.45	6.45	50.2	ng	2641120	1	6.68	1051670	20.0