

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
 Data File : BF080767.D
 Acq On : 1 Aug 2015 8:12
 Operator : TP/UM
 Sample : G3121-10
 Misc :
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NCQ-077CS-1(0-19FTBGS)

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-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	2.258	13	15	17	rVB	8348299	11368824	100.00%	21.107%
2	4.418	202	204	209	rBV	186382	251828	2.22%	0.468%
3	5.070	257	261	270	rBV	2591044	3827004	33.66%	7.105%
4	5.470	293	296	298	rBV	4074593	4360934	38.36%	8.096%
5	5.870	328	331	333	rBV	210682	187889	1.65%	0.349%
6	6.487	381	385	387	rBV	3073731	4149847	36.50%	7.705%
7	6.624	394	397	399	rBV	4269437	4630960	40.73%	8.598%
8	6.853	414	417	419	rBV	1064679	890109	7.83%	1.653%
9	7.013	428	431	433	rVB	3047018	3352152	29.49%	6.224%
10	7.413	463	466	468	rBV	2884340	2888351	25.41%	5.362%
11	8.133	526	529	531	rBV	1238407	1103917	9.71%	2.050%
12	9.207	620	623	626	rBV	4061138	4820451	42.40%	8.950%
13	9.882	680	682	685	rVB	1166155	1121644	9.87%	2.082%
14	10.671	748	751	753	rBV	3270227	3295379	28.99%	6.118%
15	11.368	809	812	814	rBV	974921	1131905	9.96%	2.101%
16	12.956	948	951	953	rBV	4081390	5027026	44.22%	9.333%
17	13.985	1039	1041	1044	rBV	593109	786888	6.92%	1.461%
18	15.402	1162	1165	1168	rBV	451857	667344	5.87%	1.239%

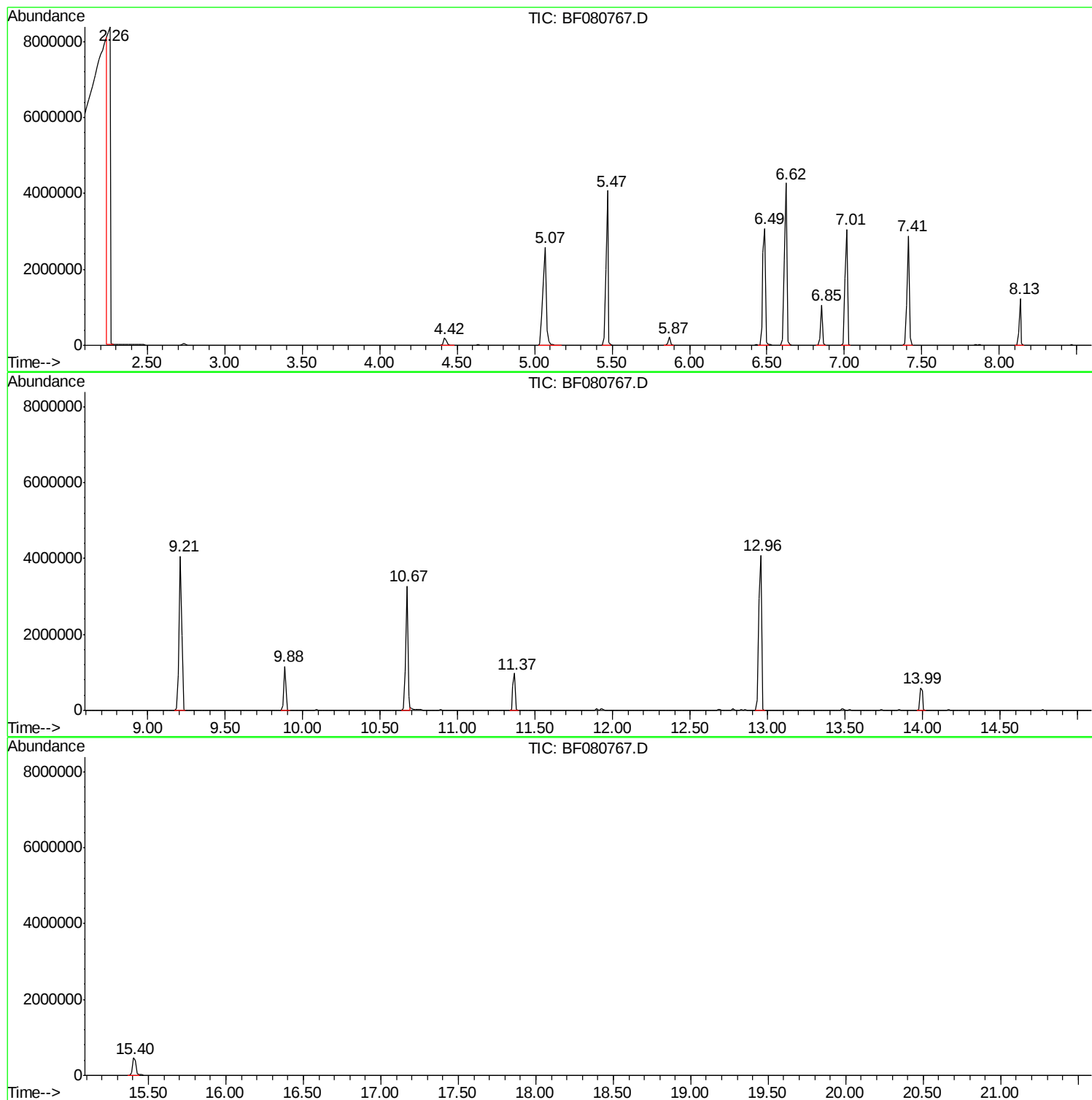
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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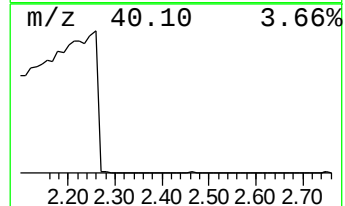
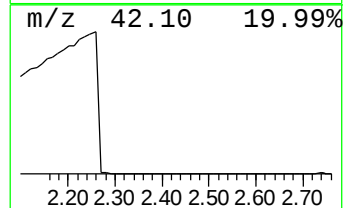
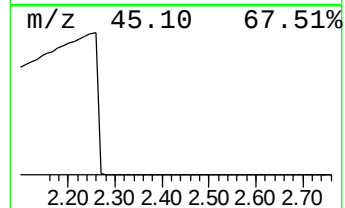
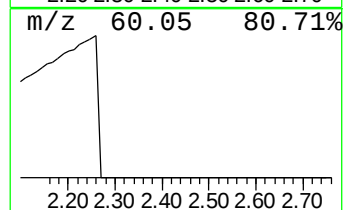
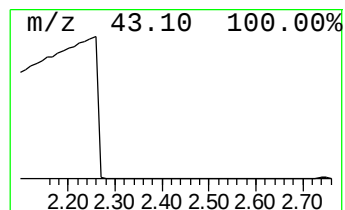
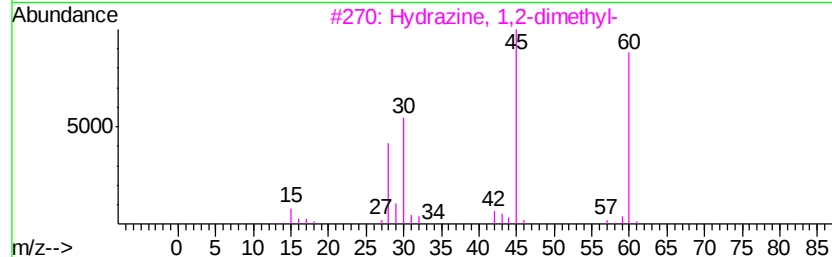
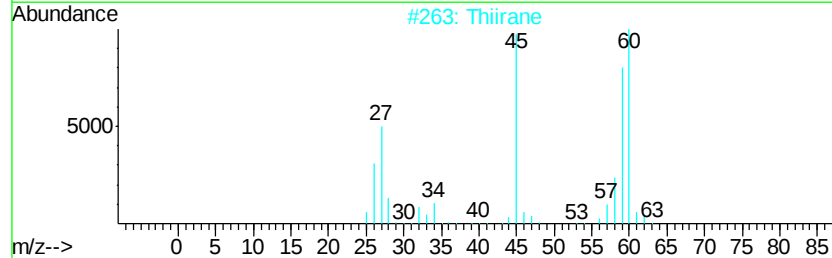
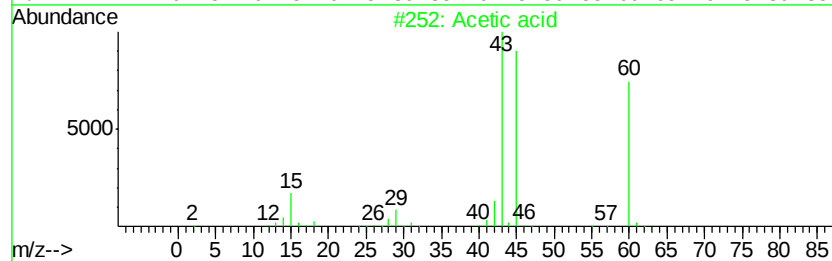
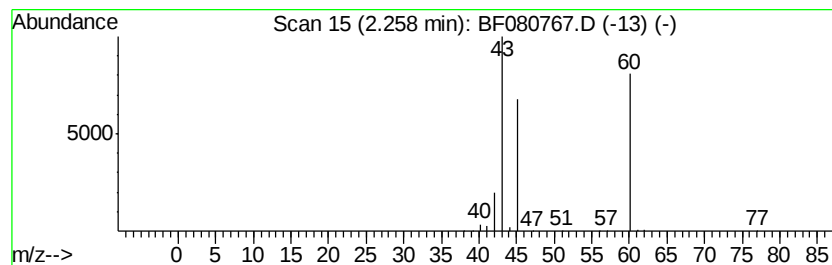
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	255.45 ng	11368800	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	72
2		Thiirane	60	C2H4S	000420-12-2	9
3		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	7
4		Formic acid hydrazide	60	CH4N2O	000624-84-0	4
5		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	4



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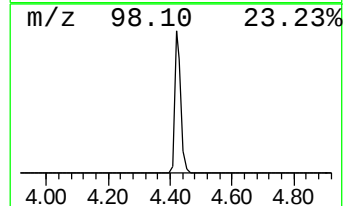
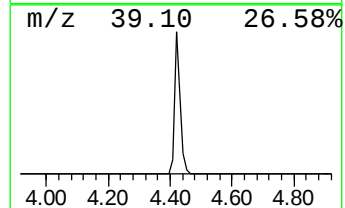
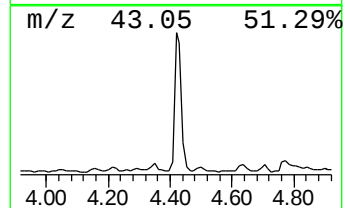
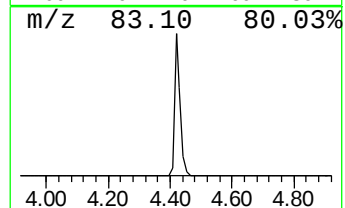
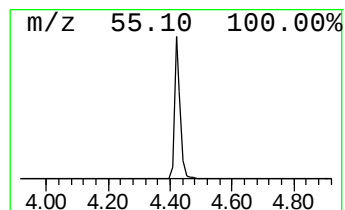
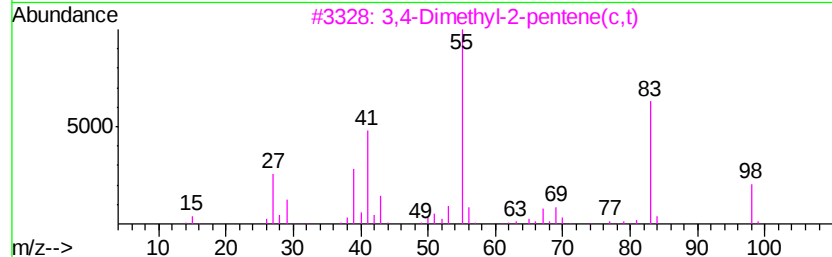
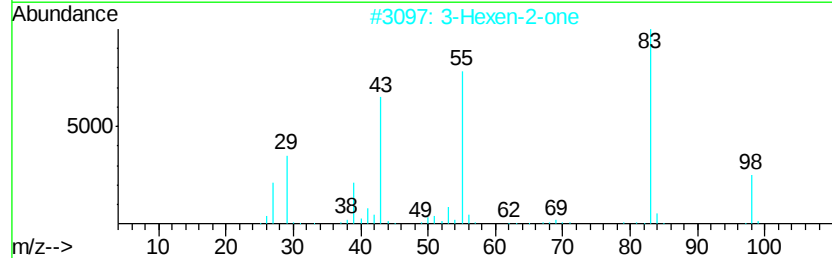
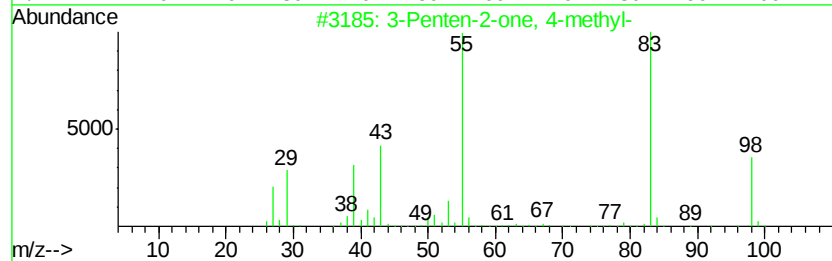
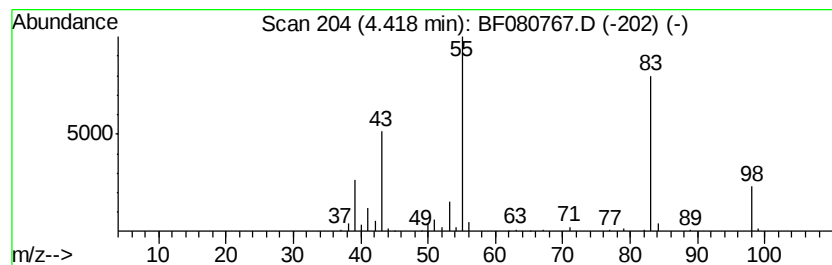
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	5.66 ng	251828	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	90
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64



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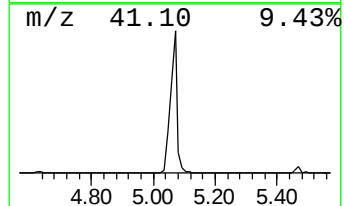
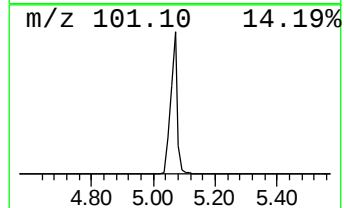
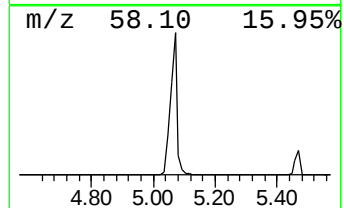
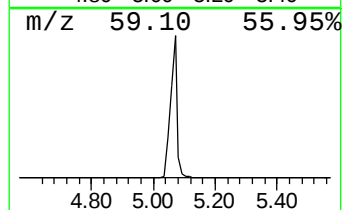
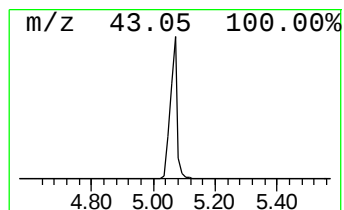
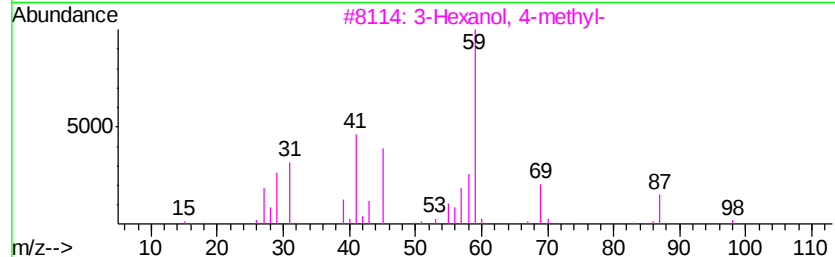
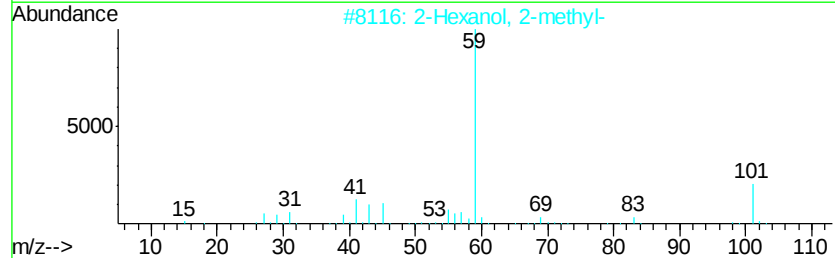
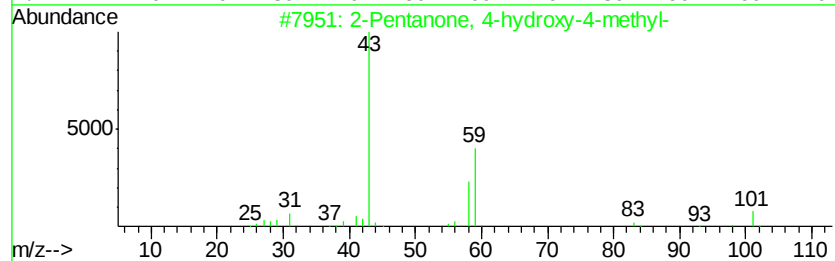
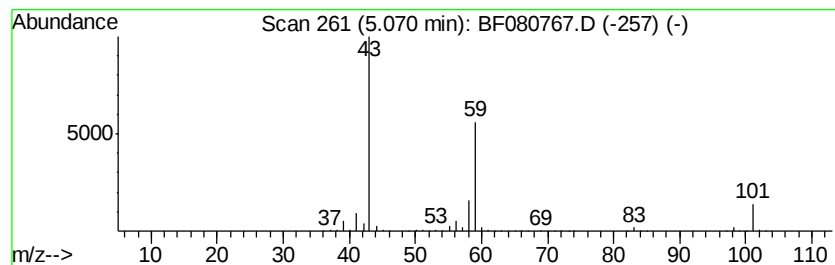
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.07	85.99 ng	3827000	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	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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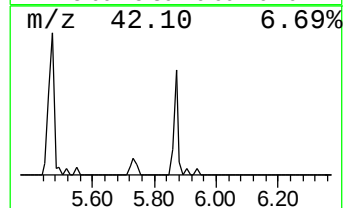
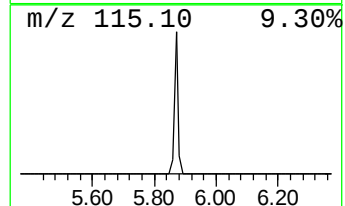
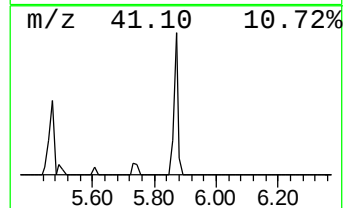
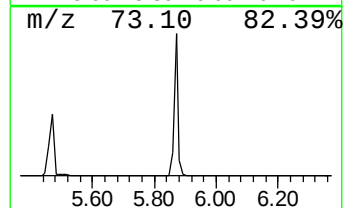
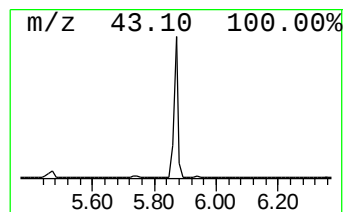
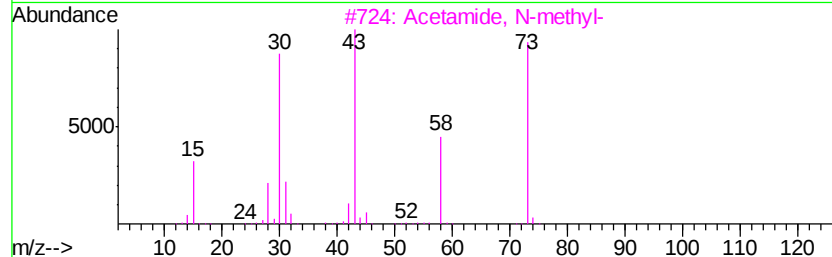
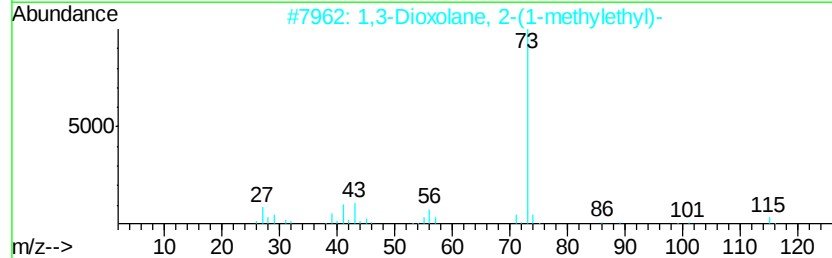
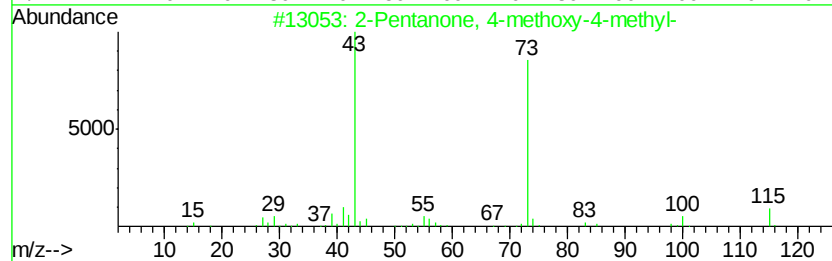
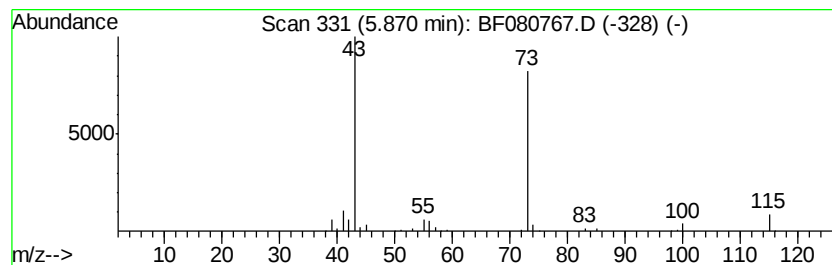
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	4.22 ng	187889	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		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	23
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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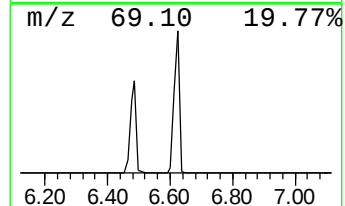
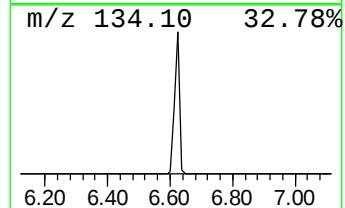
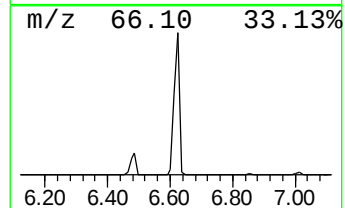
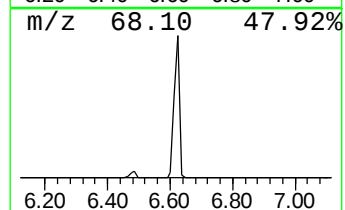
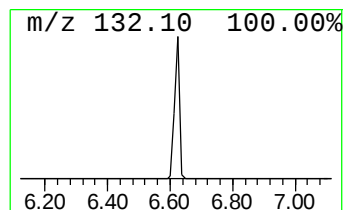
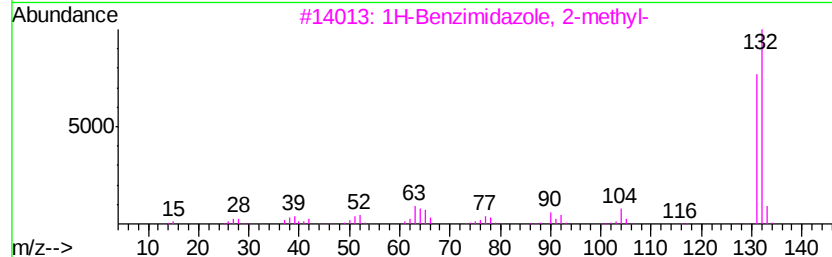
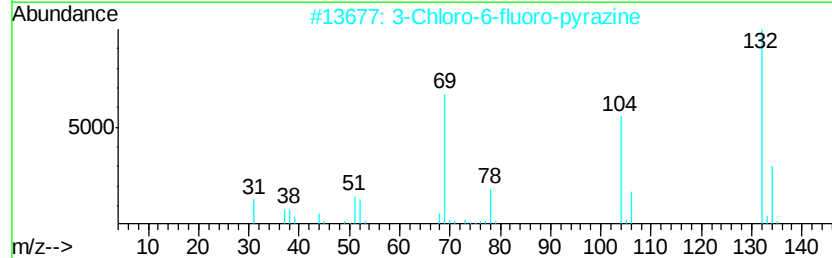
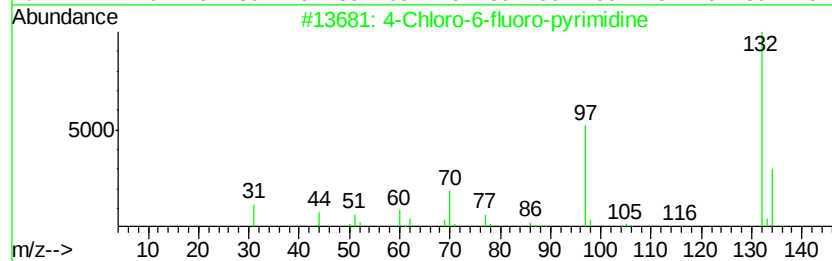
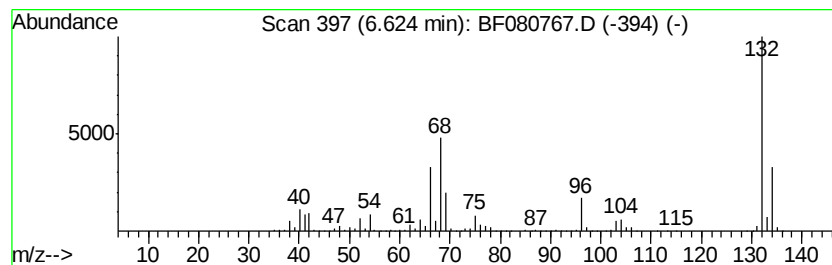
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	104.05 ng	4630960	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	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	2.26	255.4	ng	11368800	1	6.85	890109	20.0
3-Penten-2-one, 4...	4.42	5.7	ng	251828	1	6.85	890109	20.0
2-Pentanone, 4-hy...	5.07	86.0	ng	3827000	1	6.85	890109	20.0
2-Pentanone, 4-me...	5.87	4.2	ng	187889	1	6.85	890109	20.0
unknown6.62	6.62	104.1	ng	4630960	1	6.85	890109	20.0