

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
 Data File : BF095081.D
 Acq On : 11 May 2017 15:48
 Operator : SJ/MA
 Sample : PB98841BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98841BL

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-BF050217.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	2.890	158	162	176	rBV	45445	91967	2.08%	0.353%
2	4.066	356	362	382	rBV	903563	1638659	37.07%	6.283%
3	5.048	514	529	532	rBV	1535745	4420974	100.00%	16.951%
4	5.666	630	634	667	rBV	697121	1455980	32.93%	5.583%
5	6.213	722	727	736	rBV	261408	349629	7.91%	1.341%
6	7.248	899	903	919	rBV	745568	1378836	31.19%	5.287%
7	7.372	919	924	938	rVB	1090299	1740683	39.37%	6.674%
8	7.707	977	981	995	rVB	406339	511716	11.57%	1.962%
9	7.942	1016	1021	1033	rBV	1641767	1947222	44.05%	7.466%
10	8.607	1129	1134	1160	rBV	1031648	1504786	34.04%	5.770%
11	9.725	1320	1324	1344	rBV	437858	717768	16.24%	2.752%
12	11.501	1620	1626	1642	rBV	2358423	3114625	70.45%	11.942%
13	12.554	1800	1805	1825	rBV2	473109	825463	18.67%	3.165%
14	13.848	2021	2025	2044	rBV	565370	966041	21.85%	3.704%
15	14.960	2209	2214	2232	rBV	507744	853479	19.31%	3.272%
16	15.630	2322	2328	2334	rBV	42180	49095	1.11%	0.188%
17	15.930	2372	2379	2391	rBV	33292	48299	1.09%	0.185%
18	17.283	2603	2609	2613	rBV	2377089	3044043	68.85%	11.672%
19	18.630	2833	2838	2855	rBV	548633	834038	18.87%	3.198%
20	20.294	3117	3121	3133	rBV	385202	587112	13.28%	2.251%

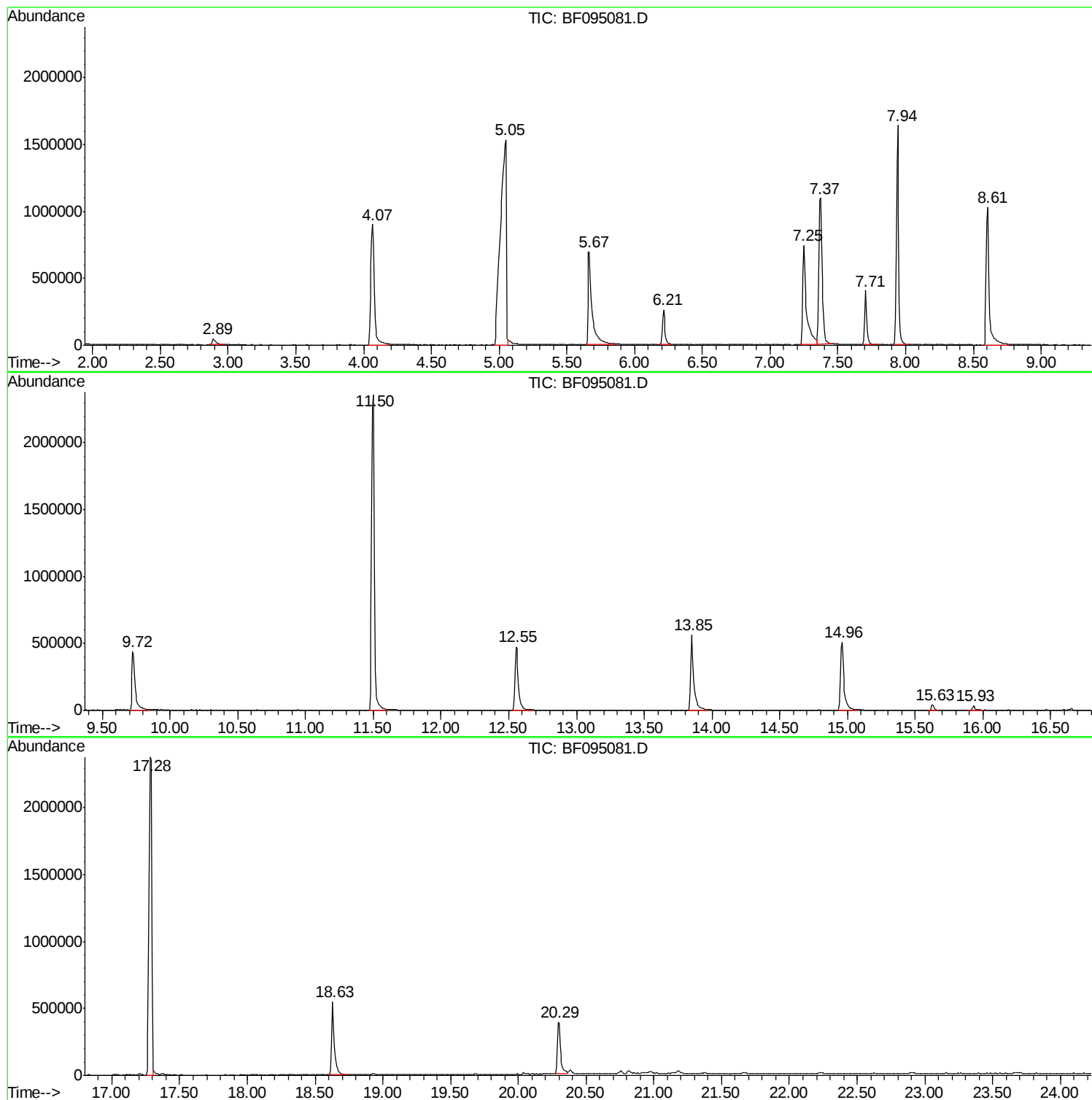
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB98841BL

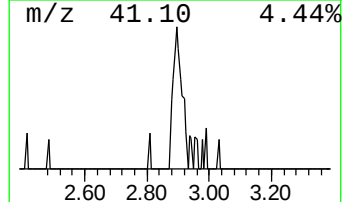
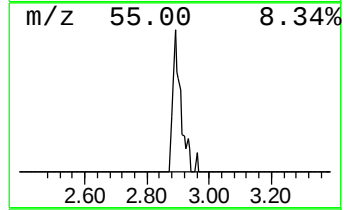
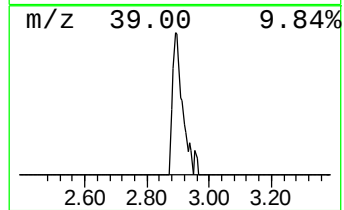
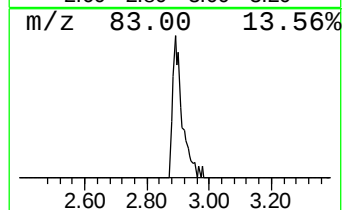
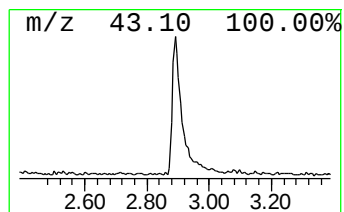
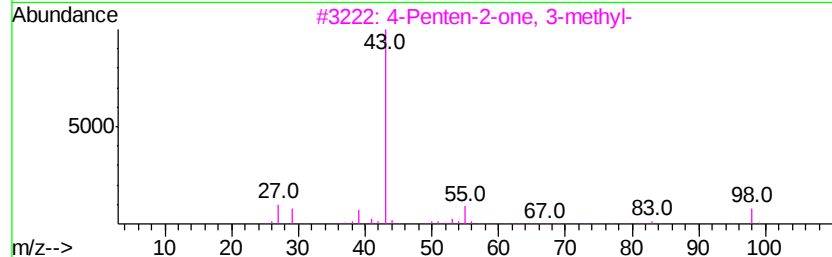
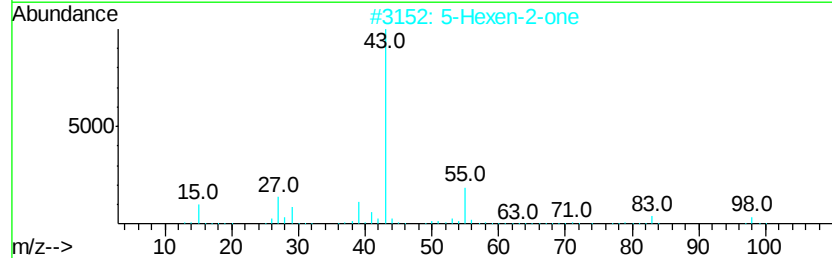
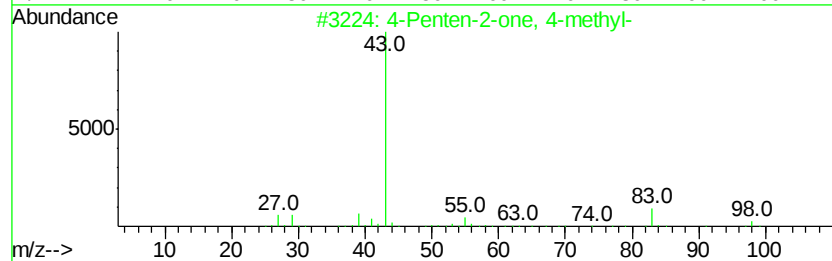
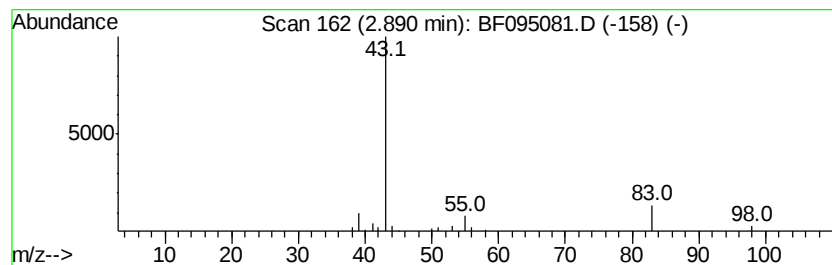
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	3.59 ng	91967	1,4-Dichlorobenzene-d4	7.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			5-Hexen-2-one	98	C6H10O	000109-49-9	64
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	53
4			2H-Pyran, 3,4-dihydro-6-methyl-	98	C6H10O	016015-11-5	9
5			4-Hexen-2-one	98	C6H10O	025659-22-7	9



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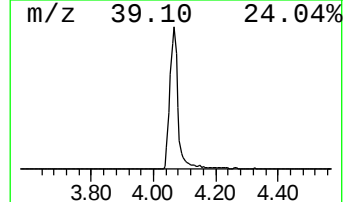
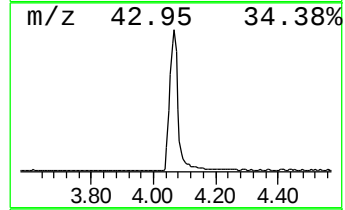
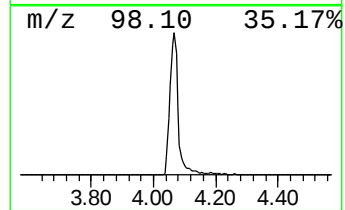
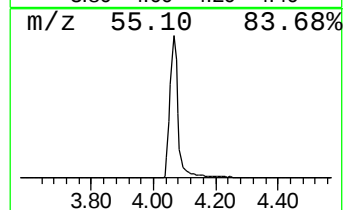
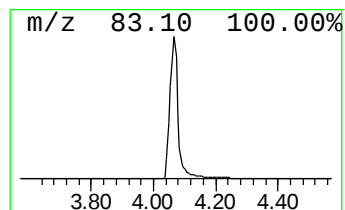
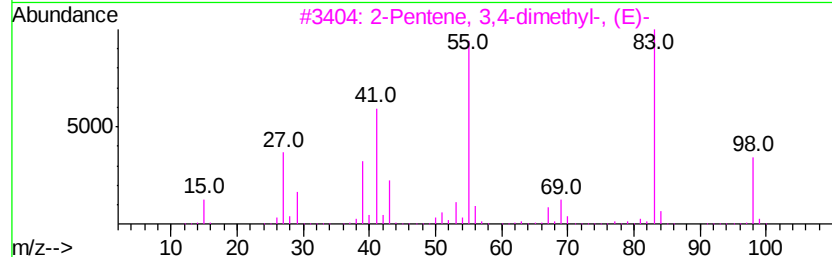
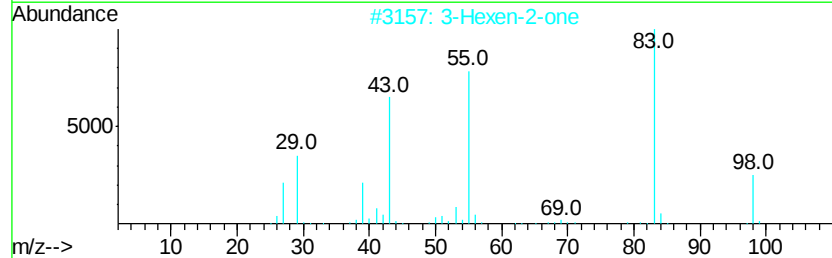
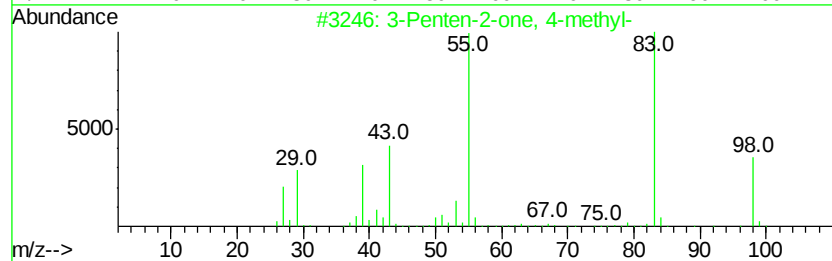
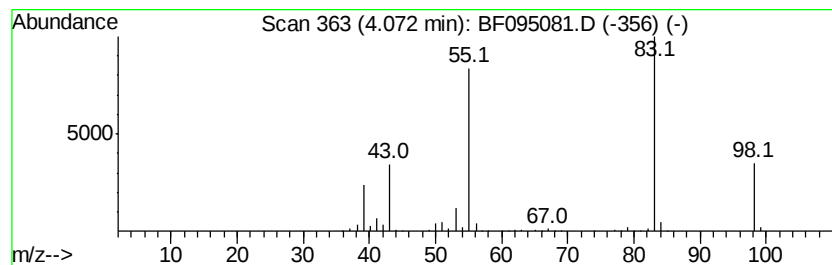
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	64.05 ng	1638660	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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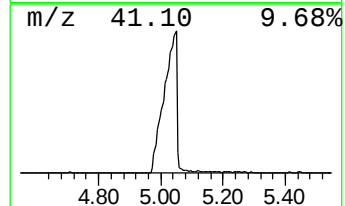
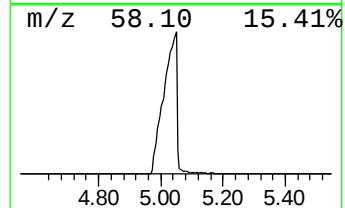
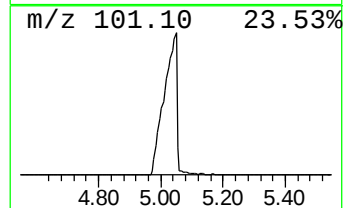
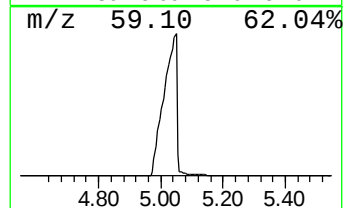
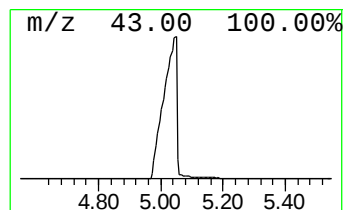
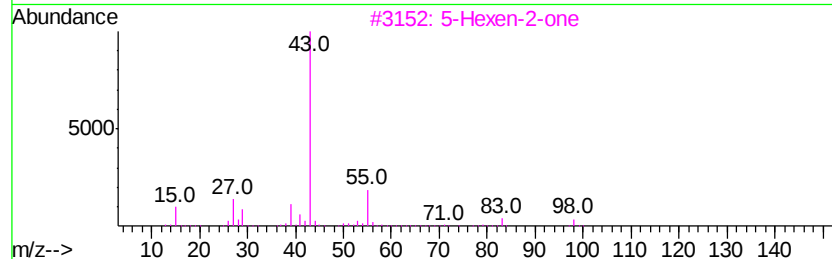
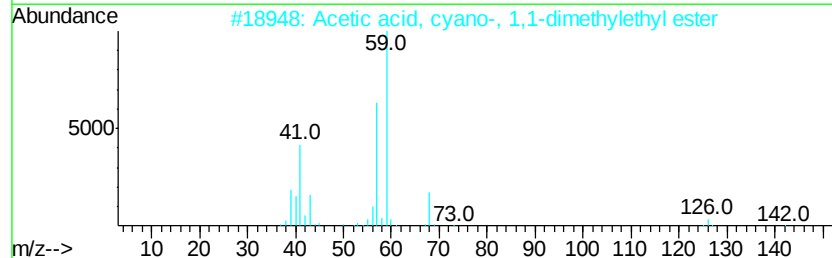
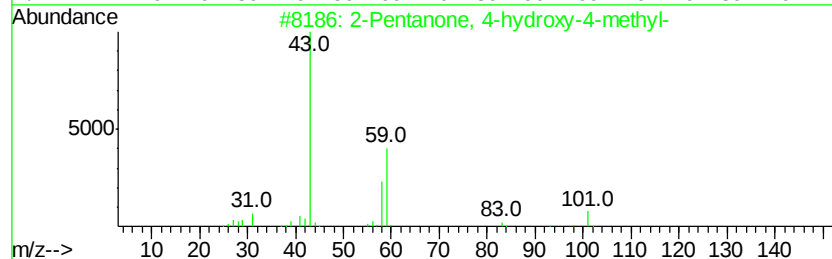
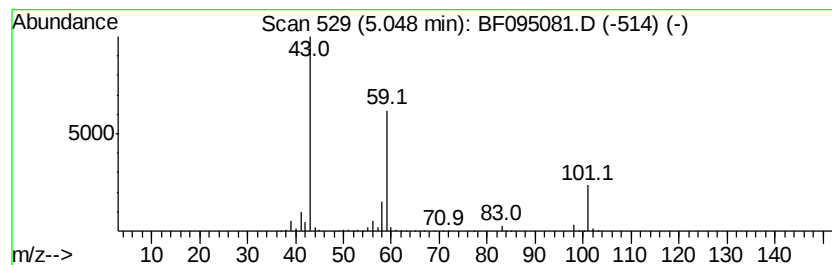
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	172.79 ng	4420970	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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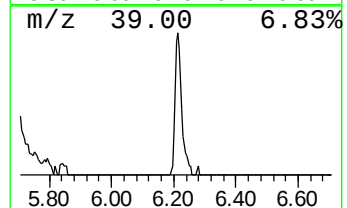
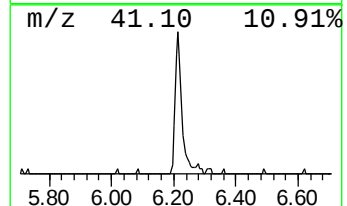
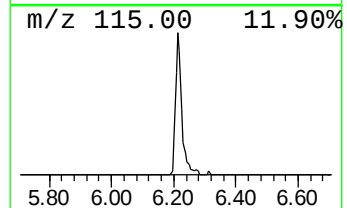
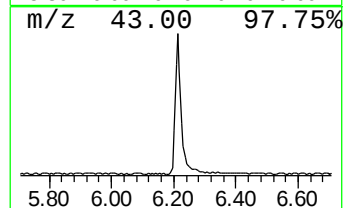
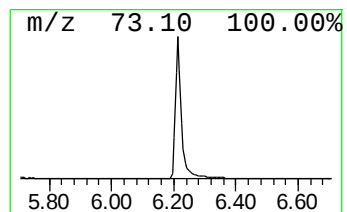
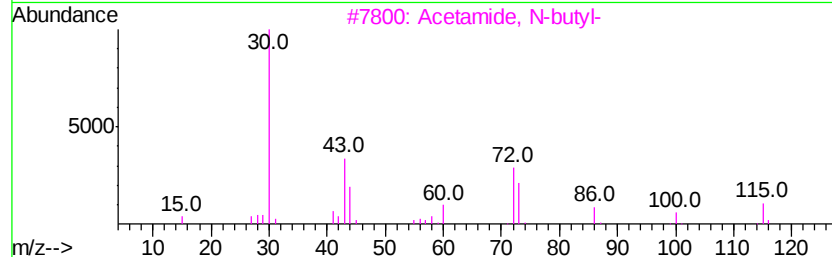
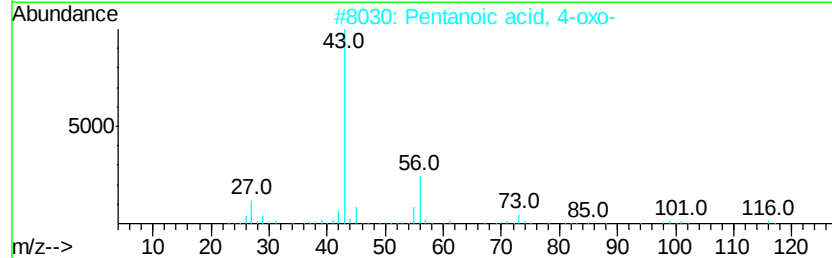
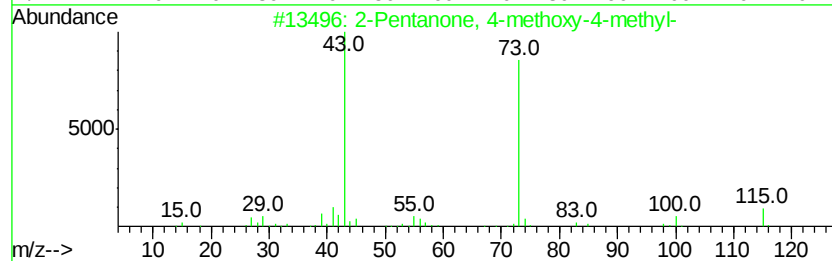
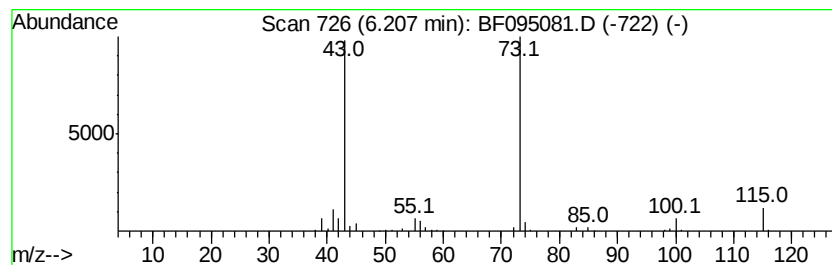
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	13.67 ng	349629	1,4-Dichlorobenzene-d4	7.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78	
2	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	12	
3	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9	



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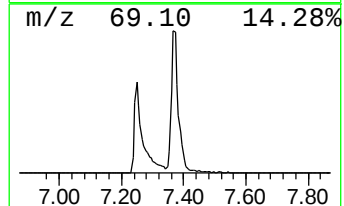
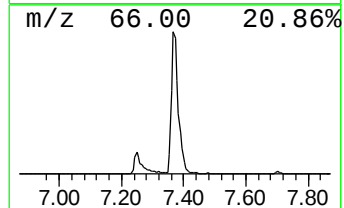
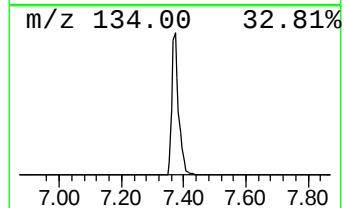
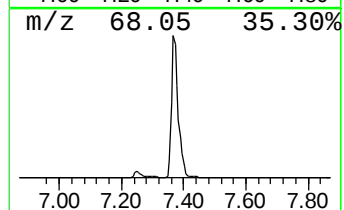
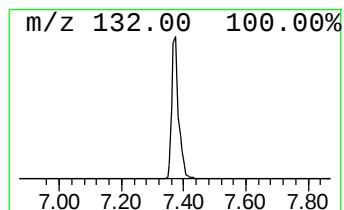
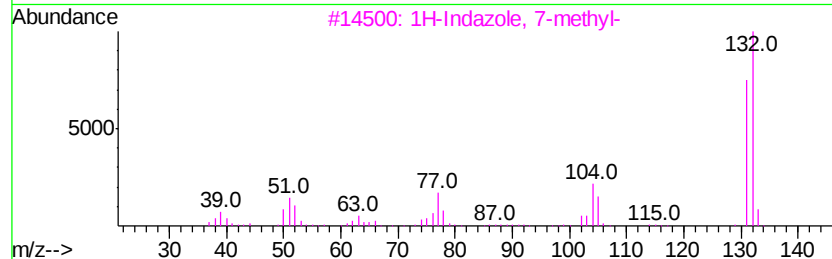
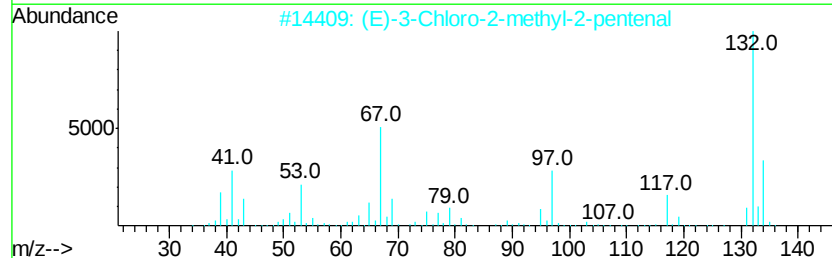
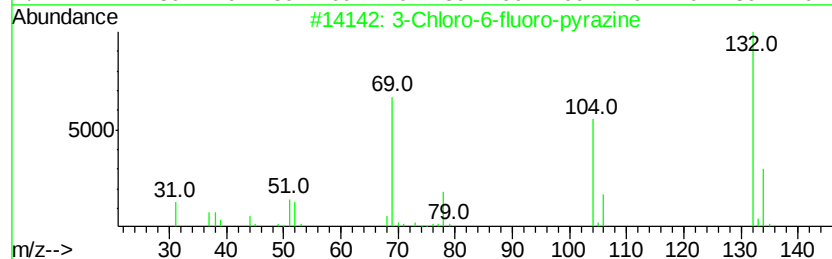
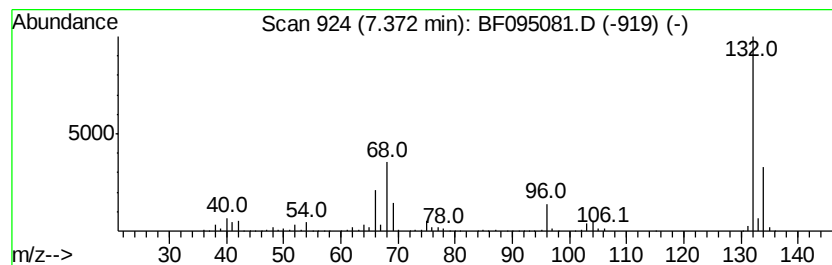
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	68.03 ng	1740680	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Xenon	132	Xe	007440-63-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	2.89	3.6	ng	91967	1	7.71	511716	20.0
3-Penten-2-one, 4...	4.07	64.0	ng	1638660	1	7.71	511716	20.0
2-Pentanone, 4-hy...	5.05	172.8	ng	4420970	1	7.71	511716	20.0
2-Pentanone, 4-me...	6.21	13.7	ng	349629	1	7.71	511716	20.0
unknown7.37	7.37	68.0	ng	1740680	1	7.71	511716	20.0