

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
 Data File : BF087660.D
 Acq On : 4 Jun 2016 12:13
 Operator : UM/SJ
 Sample : PB91075BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91075BL

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-BF060416.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	1.770	14	16	26	rVB2	603418	1639778	47.87%	5.391%
2	1.895	26	27	51	rVB	1723212	3425211	100.00%	11.260%
3	2.193	51	53	69	rVB	53044	152289	4.45%	0.501%
4	4.410	245	247	250	rBV	596954	650839	19.00%	2.140%
5	5.061	300	304	307	rBV	1404068	2059869	60.14%	6.772%
6	5.461	336	339	341	rBV	1890053	1874205	54.72%	6.161%
7	5.873	372	375	377	rBV	100245	110085	3.21%	0.362%
8	6.479	425	428	430	rBV	1792904	1678263	49.00%	5.517%
9	6.627	438	441	443	rBV	1452858	1938691	56.60%	6.373%
10	6.856	459	461	464	rVB	800518	698703	20.40%	2.297%
11	7.016	472	475	477	rBV	2394276	2158844	63.03%	7.097%
12	7.416	507	510	513	rBV	1258423	1683591	49.15%	5.535%
13	8.147	571	574	576	rBV	784435	943735	27.55%	3.102%
14	9.222	665	668	671	rBV	2841248	2996775	87.49%	9.852%
15	9.896	724	727	730	rVB	1114415	1059766	30.94%	3.484%
16	10.685	793	796	798	rBV	1208681	1297717	37.89%	4.266%
17	11.382	854	857	859	rBV	1144252	1104377	32.24%	3.631%
18	12.971	993	996	998	rBV	3049668	3090170	90.22%	10.159%
19	14.011	1084	1087	1089	rBV	1104538	977403	28.54%	3.213%
20	15.440	1209	1212	1215	rBV	648423	746046	21.78%	2.453%
21	15.805	1241	1244	1249	rBV	22606	39815	1.16%	0.131%
22	16.377	1291	1294	1299	rVB	21630	46227	1.35%	0.152%
23	17.074	1351	1355	1366	rVB	17996	46488	1.36%	0.153%

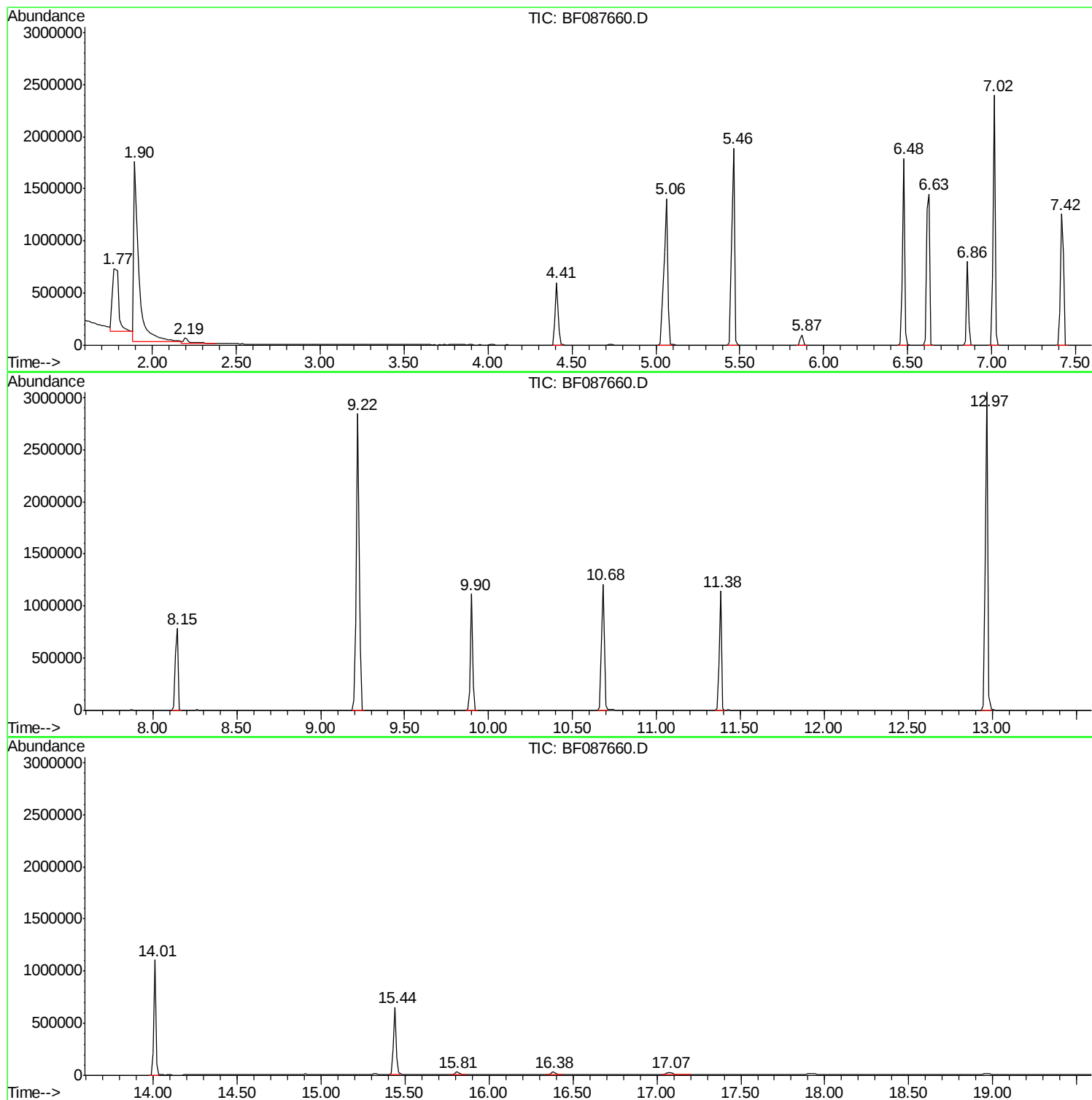
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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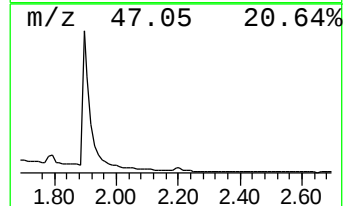
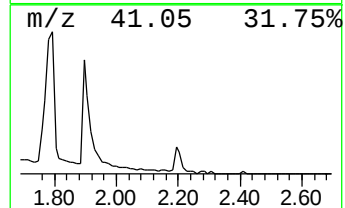
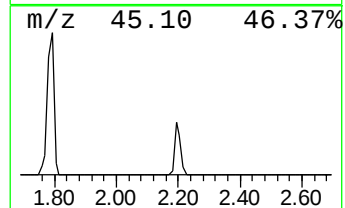
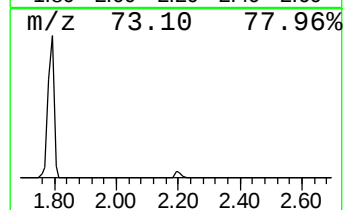
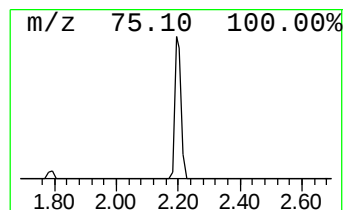
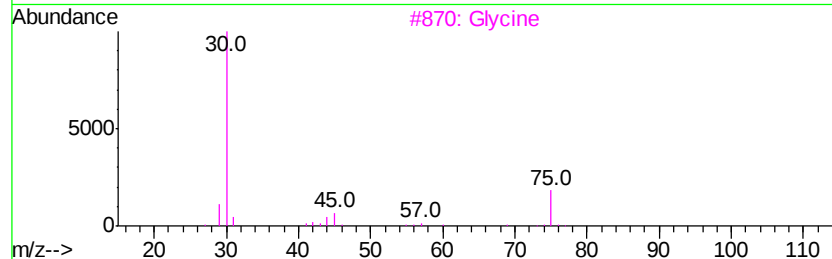
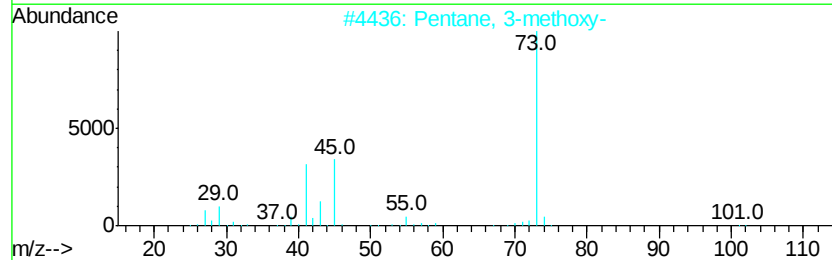
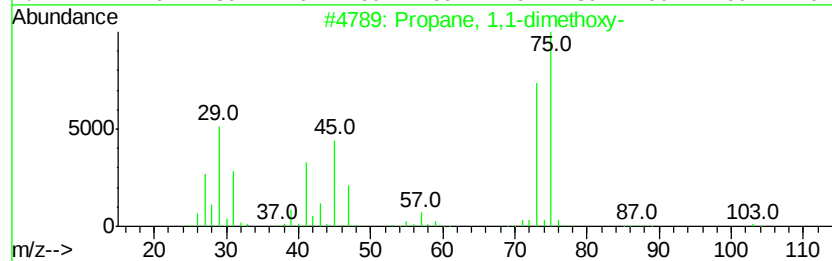
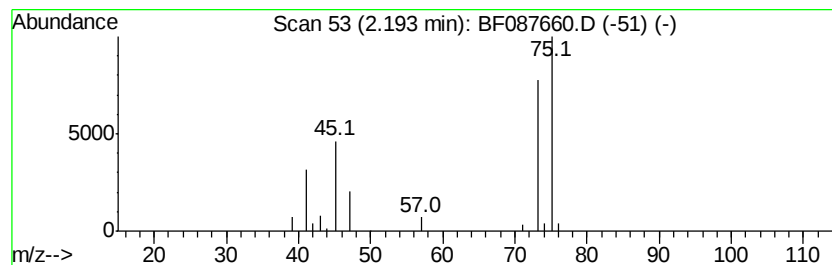
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	4.36 ng	152289	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-			104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-			102	C6H14O	036839-67-5	9
3	Glycine			75	C2H5NO2	000056-40-6	7
4	1,3-Dioxolane			74	C3H6O2	000646-06-0	4
5	Methane, nitroso-			45	CH3NO	000865-40-7	4



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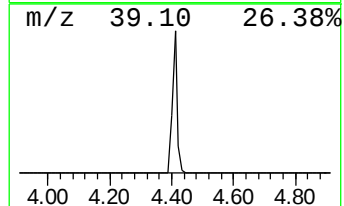
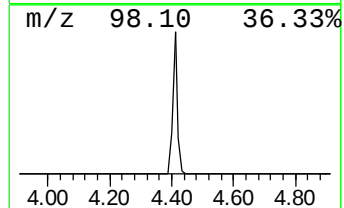
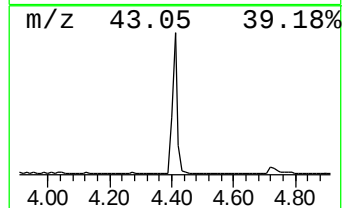
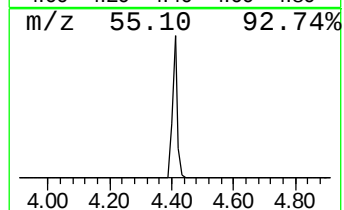
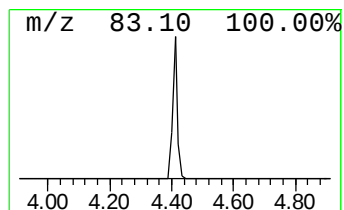
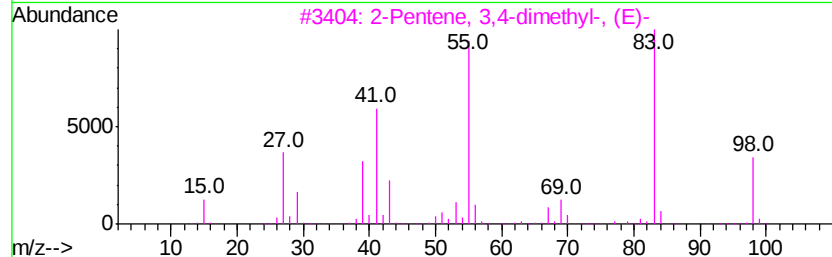
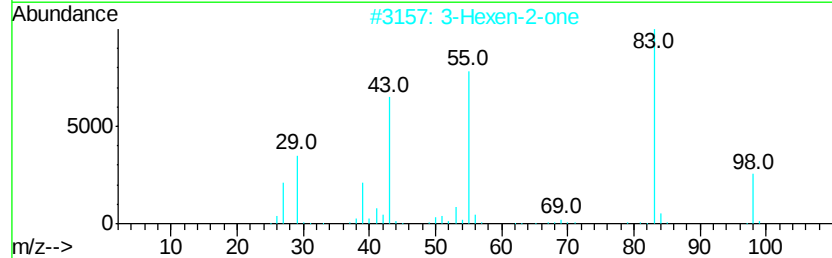
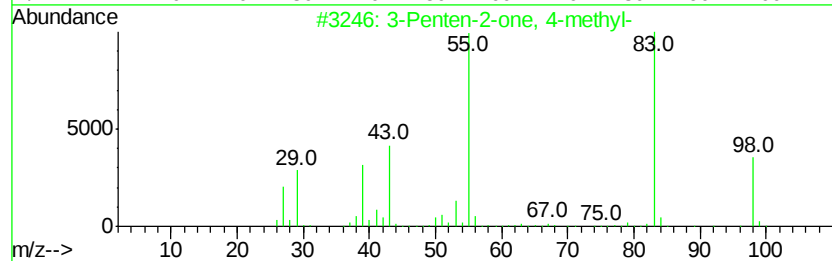
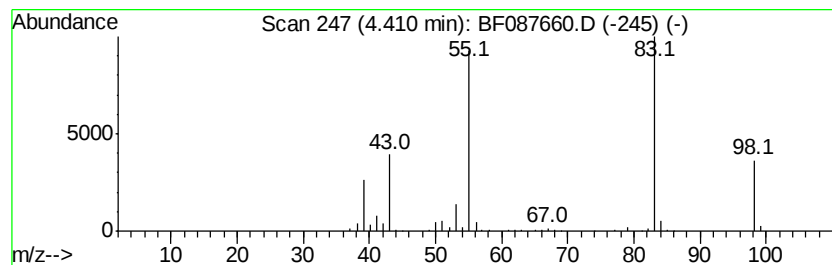
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	18.63 ng	650839	1,4-Dichlorobenzene-d4	6.86

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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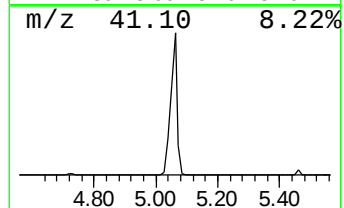
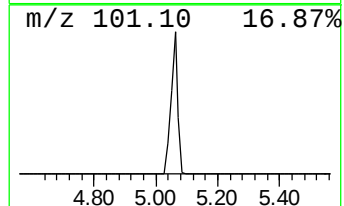
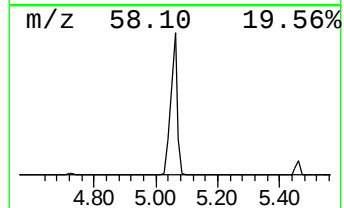
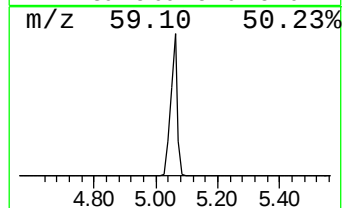
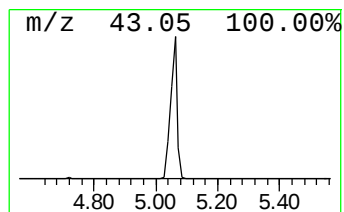
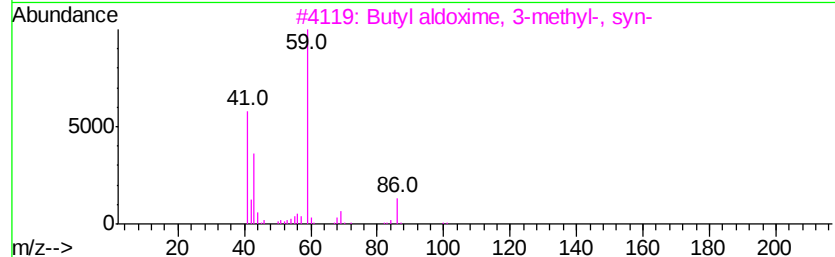
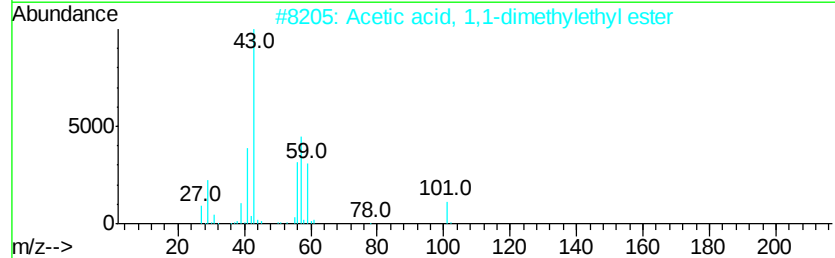
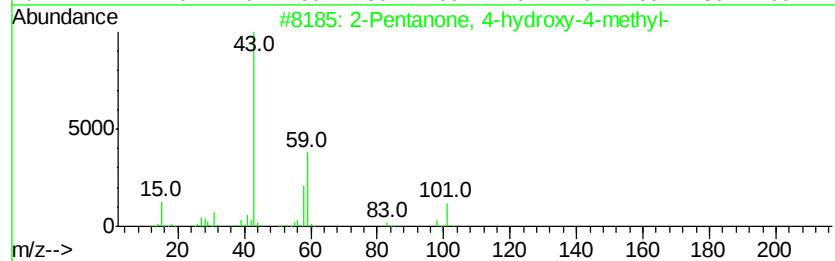
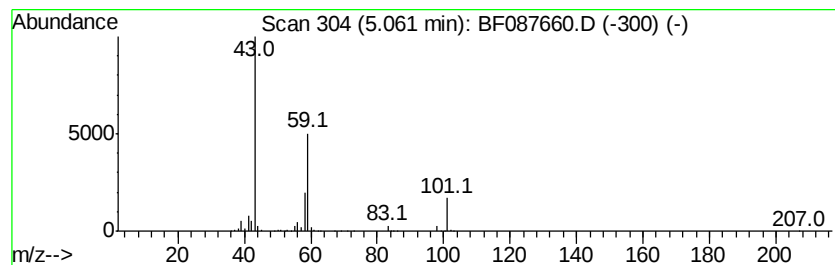
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	58.96 ng	2059870	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO		005780-40-5	17
4	Acetone	58	C3H6O		000067-64-1	16
5	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	12



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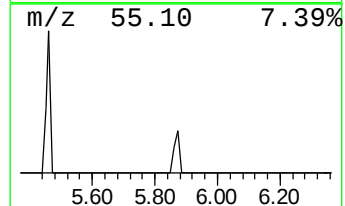
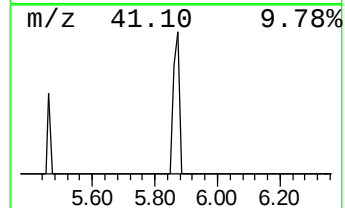
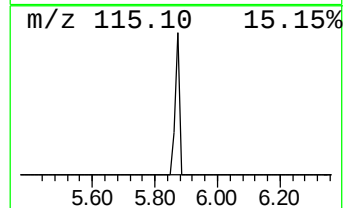
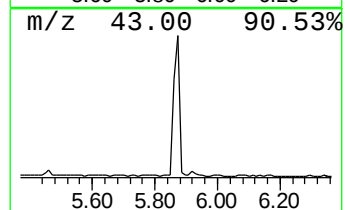
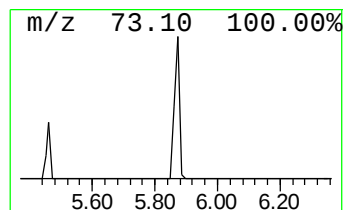
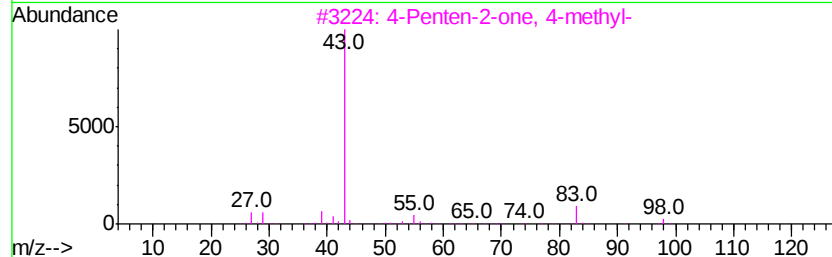
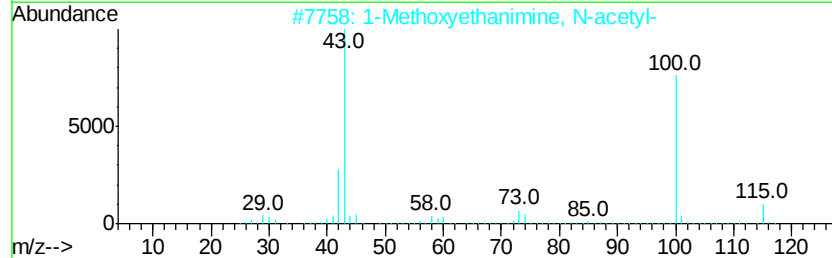
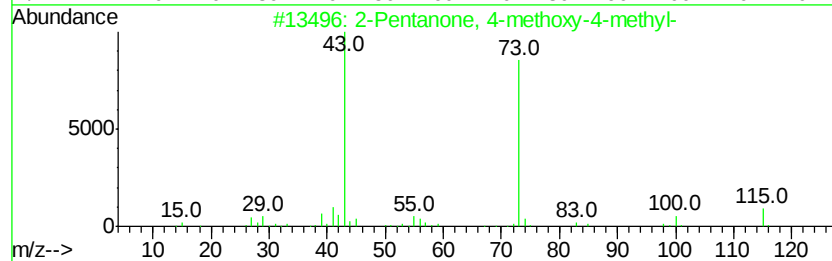
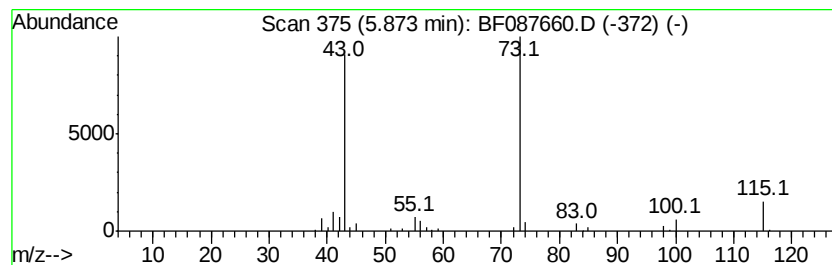
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	3.15 ng	110085	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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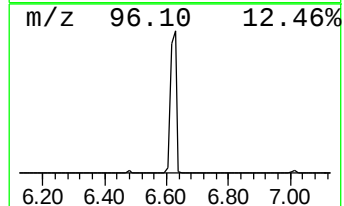
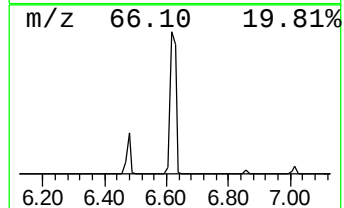
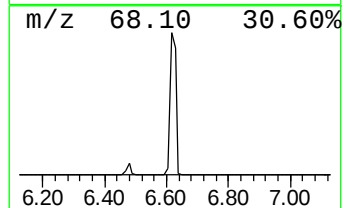
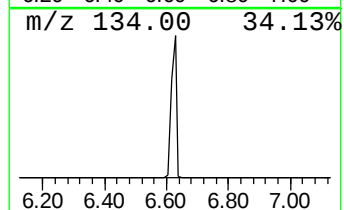
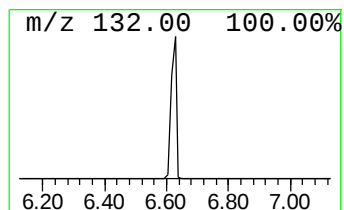
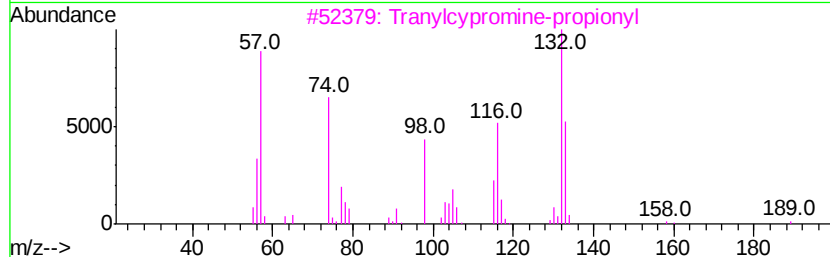
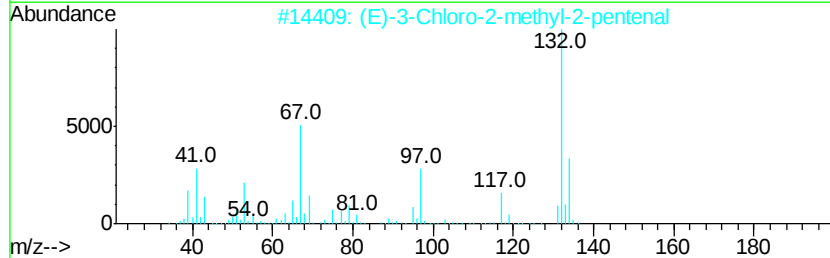
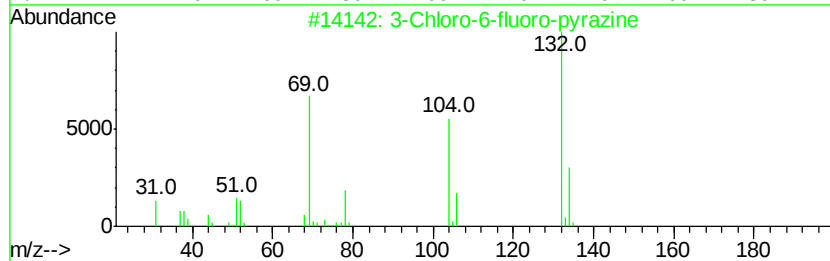
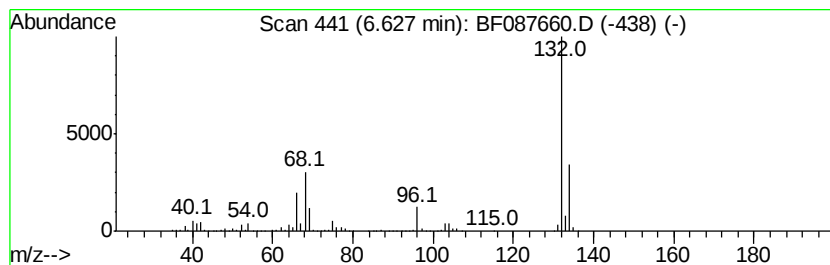
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Peak Number 7 unknown6.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	55.49 ng	1938690	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.19	4.4	ng	152289	1	6.86	698703	20.0
3-Penten-2-one, 4...	4.41	18.6	ng	650839	1	6.86	698703	20.0
2-Pentanone, 4-hy...	5.06	59.0	ng	2059870	1	6.86	698703	20.0
2-Pentanone, 4-me...	5.87	3.1	ng	110085	1	6.86	698703	20.0
unknown6.63	6.63	55.5	ng	1938690	1	6.86	698703	20.0