

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
 Data File : BF087663.D
 Acq On : 4 Jun 2016 13:43
 Operator : UM/SJ
 Sample : PB91062BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91062BL

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	1.804	13	19	21	rVB	4084432	7995286	100.00%	20.667%
2	1.895	26	27	51	rVB	1654530	3482833	43.56%	9.003%
3	2.193	51	53	76	rVB	92297	233118	2.92%	0.603%
4	5.061	301	304	309	rBV	190770	266347	3.33%	0.688%
5	5.461	336	339	341	rBV	2524413	2687135	33.61%	6.946%
6	6.490	425	429	431	rBV	2104775	3070575	38.40%	7.937%
7	6.627	438	441	443	rBV	2765715	3003290	37.56%	7.763%
8	6.856	459	461	464	rBV	804790	686347	8.58%	1.774%
9	7.016	472	475	477	rBV	2554481	2319014	29.00%	5.994%
10	7.416	507	510	513	rBV	1274508	1860079	23.26%	4.808%
11	8.147	571	574	576	rBV	802694	934487	11.69%	2.415%
12	9.222	665	668	671	rBV	2811209	3242529	40.56%	8.381%
13	9.896	724	727	730	rVB	1056631	1007613	12.60%	2.605%
14	10.685	793	796	798	rBV	1957029	1970865	24.65%	5.094%
15	11.382	854	857	859	rBV	1103401	1070134	13.38%	2.766%
16	12.971	993	996	998	rBV	3161937	3186690	39.86%	8.237%
17	14.011	1084	1087	1089	rBV	1070654	958037	11.98%	2.476%
18	15.440	1209	1212	1215	rBV	615427	712728	8.91%	1.842%

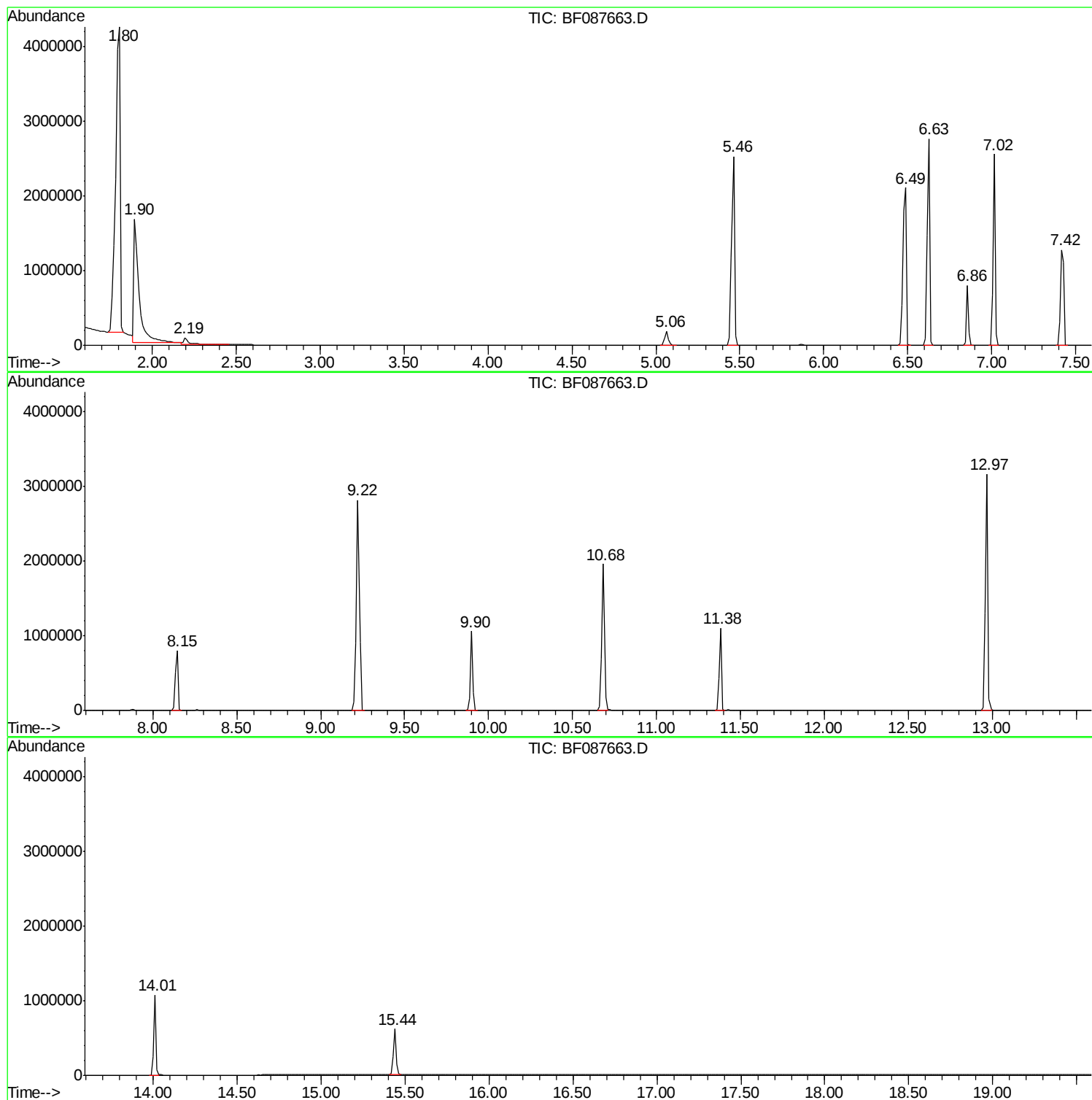
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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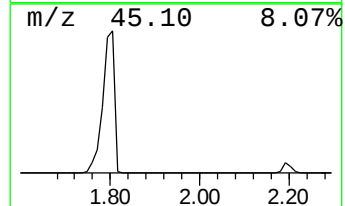
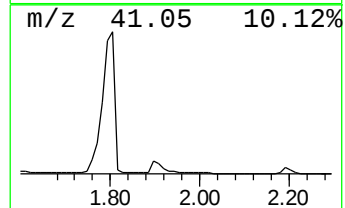
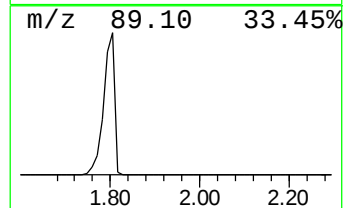
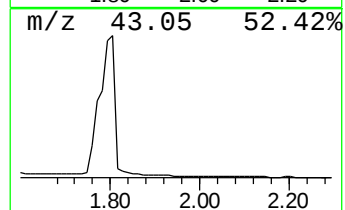
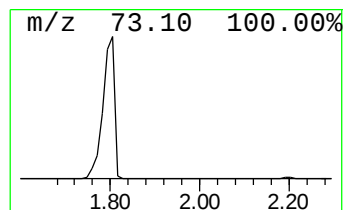
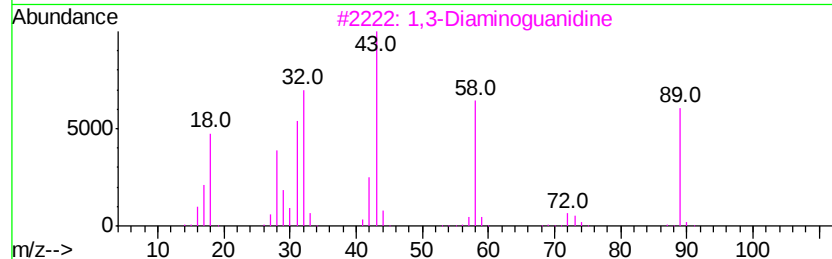
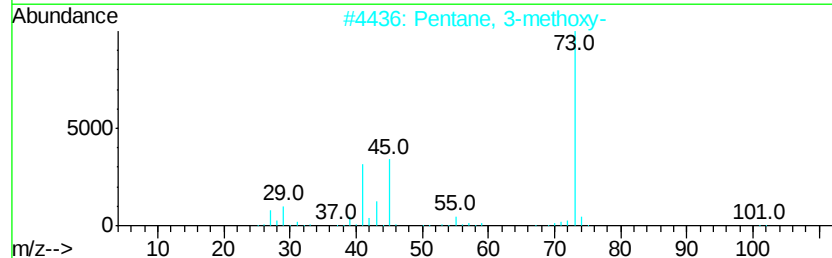
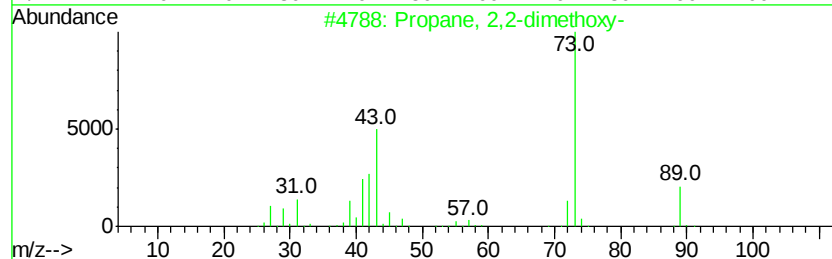
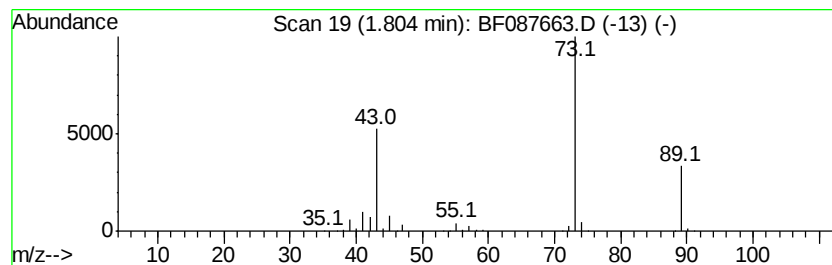
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.80	232.98 ng	7995290	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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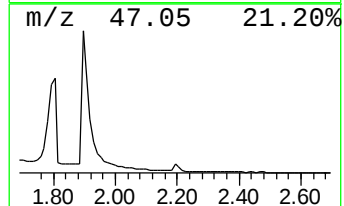
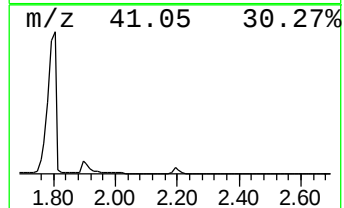
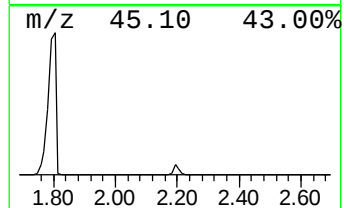
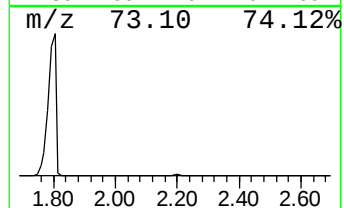
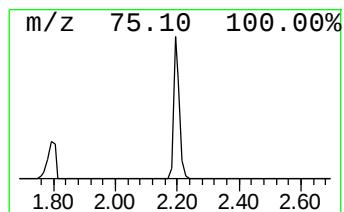
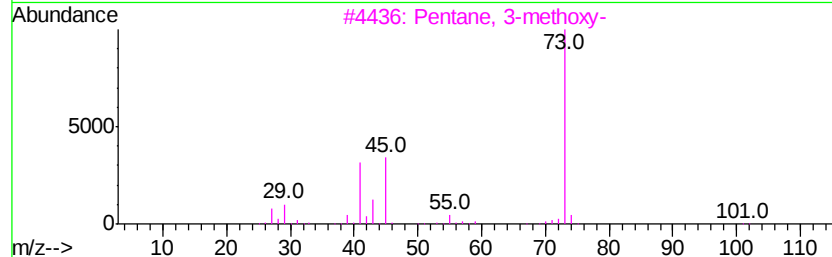
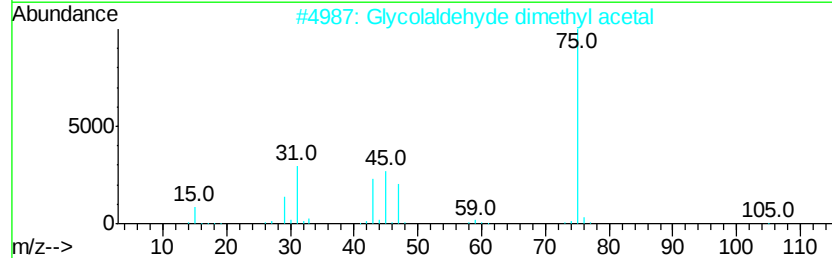
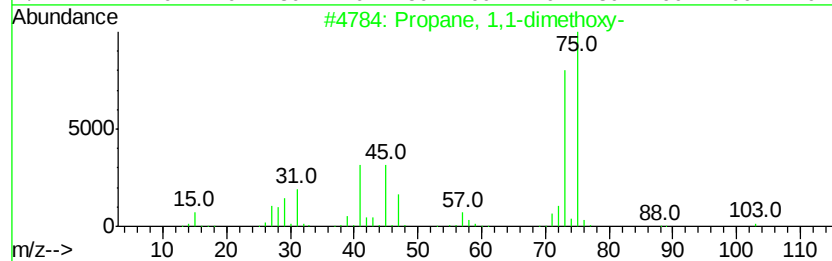
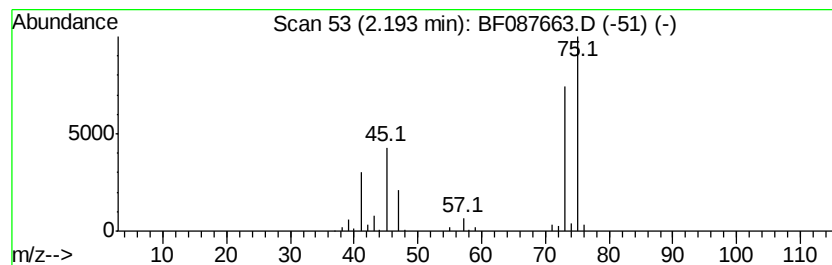
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Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	6.79 ng	233118	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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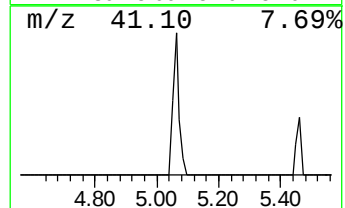
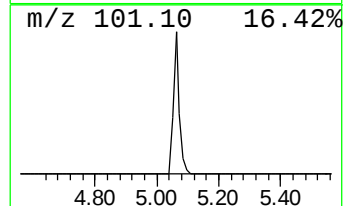
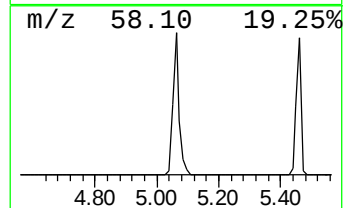
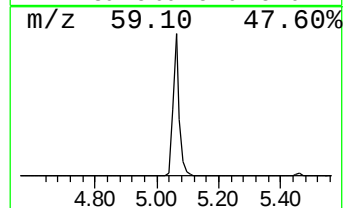
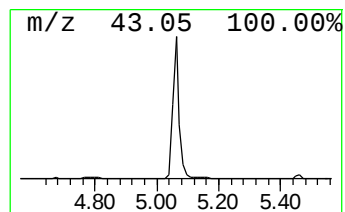
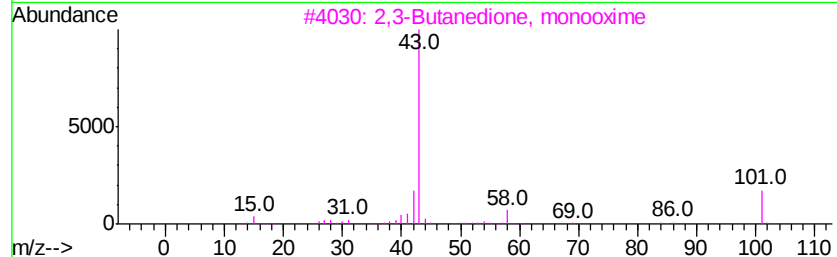
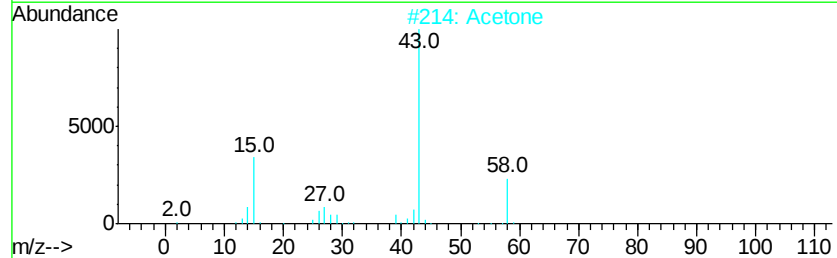
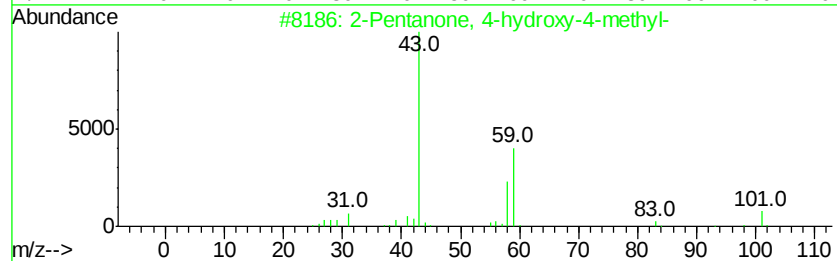
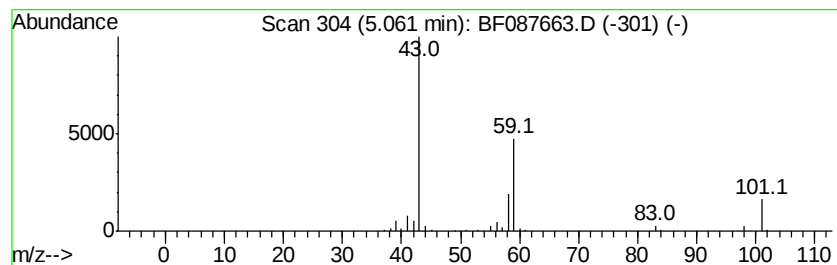
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	7.76 ng	266347	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	72
2		Acetone	58	C3H6O	000067-64-1	16
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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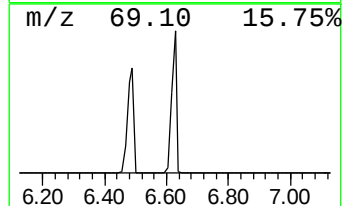
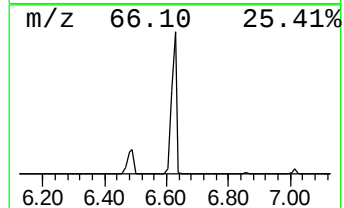
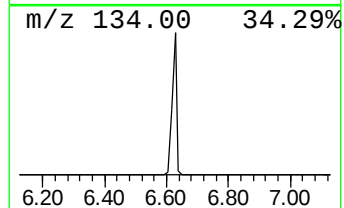
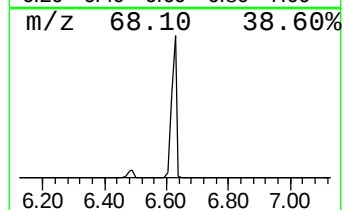
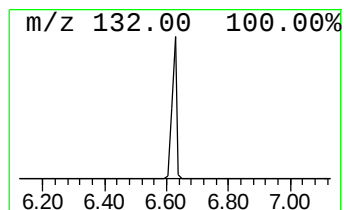
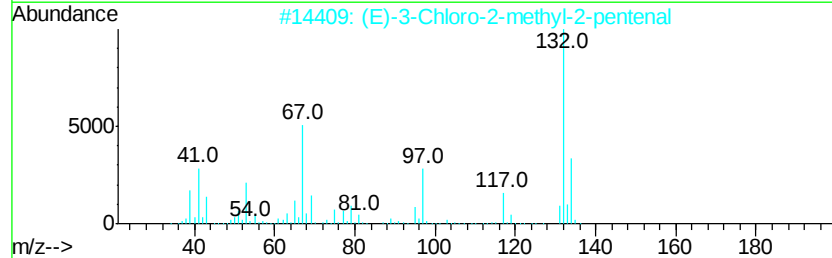
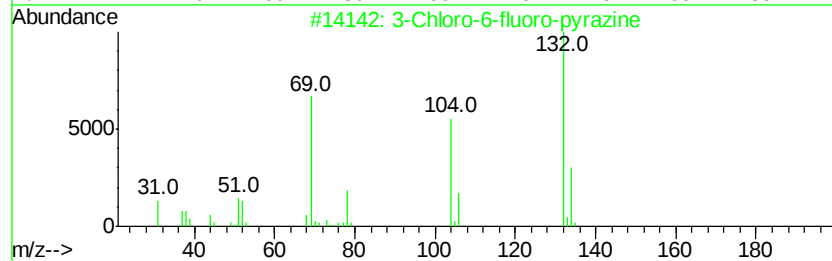
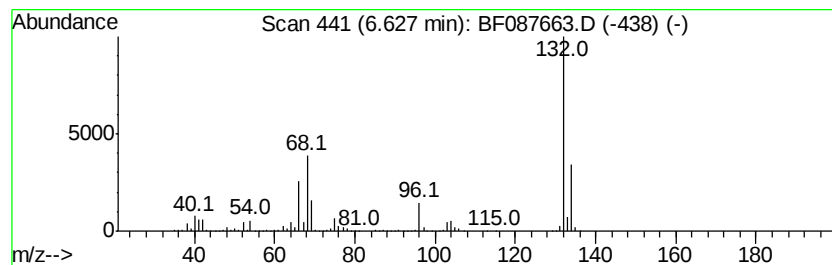
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Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	87.52 ng	3003290	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.80	233.0	ng	7995290	1	6.86	686347	20.0
Propane, 1,1-dime...	2.19	6.8	ng	233118	1	6.86	686347	20.0
2-Pentanone, 4-hy...	5.06	7.8	ng	266347	1	6.86	686347	20.0
unknown6.63	6.63	87.5	ng	3003290	1	6.86	686347	20.0