

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081315\
 Data File : BF080996.D
 Acq On : 14 Aug 2015 00:50
 Operator : UM/IZ
 Sample : PB84967BL
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84967BL

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-BF080715.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	4.247	187	189	192	rBB	24532	29178	2.43%	0.343%
2	4.921	245	248	251	rBV	451109	726200	60.44%	8.525%
3	5.344	283	285	288	rBV	772381	873160	72.67%	10.250%
4	5.756	319	321	323	rBB	38449	30893	2.57%	0.363%
5	6.384	373	376	379	rBV	760810	745718	62.06%	8.754%
6	6.522	385	388	390	rBV	792506	1076306	89.57%	12.635%
7	6.750	406	408	410	rBB	255884	212327	17.67%	2.492%
8	6.910	419	422	424	rBB	550569	665036	55.35%	7.807%
9	7.310	455	457	460	rBV	516700	568253	47.29%	6.671%
10	8.030	518	520	523	rBB	249296	229160	19.07%	2.690%
11	9.116	612	615	617	rBV	1037433	1201588	100.00%	14.105%
12	9.779	671	673	676	rBB	249691	247867	20.63%	2.910%
13	10.568	739	742	744	rBV	602286	569187	47.37%	6.682%
14	11.253	800	802	805	rBV	198684	266218	22.16%	3.125%
15	12.842	939	941	944	rBV	716438	726622	60.47%	8.530%
16	13.882	1030	1032	1035	rBV	258740	217833	18.13%	2.557%
17	15.265	1151	1153	1156	rBV	94482	133120	11.08%	1.563%

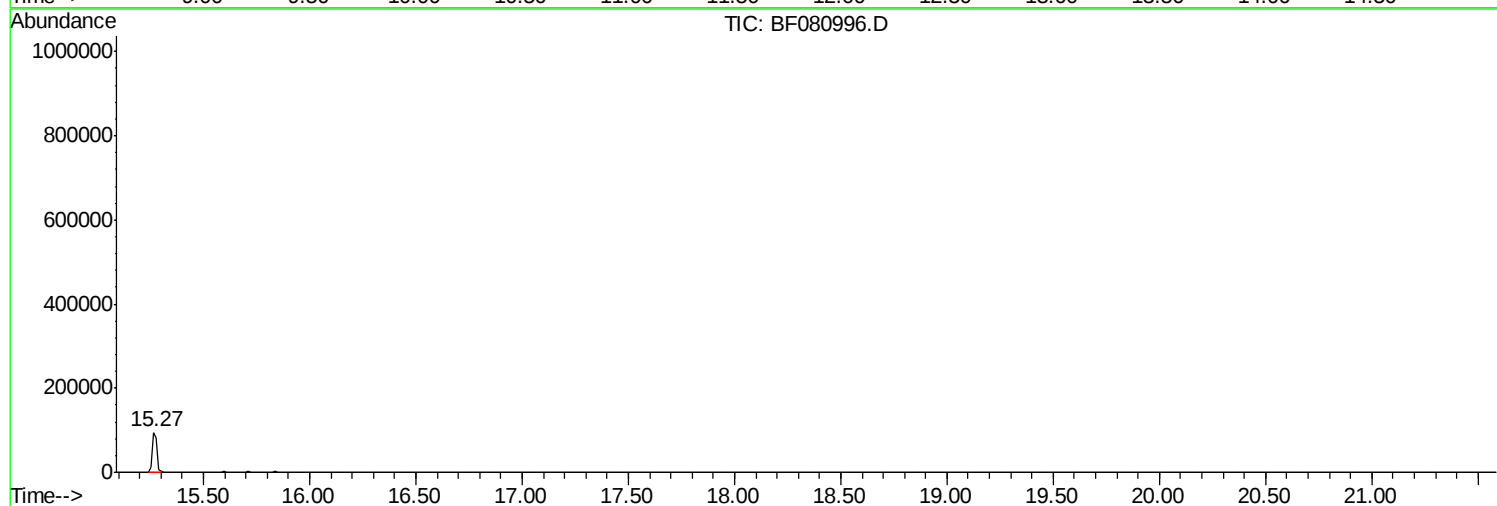
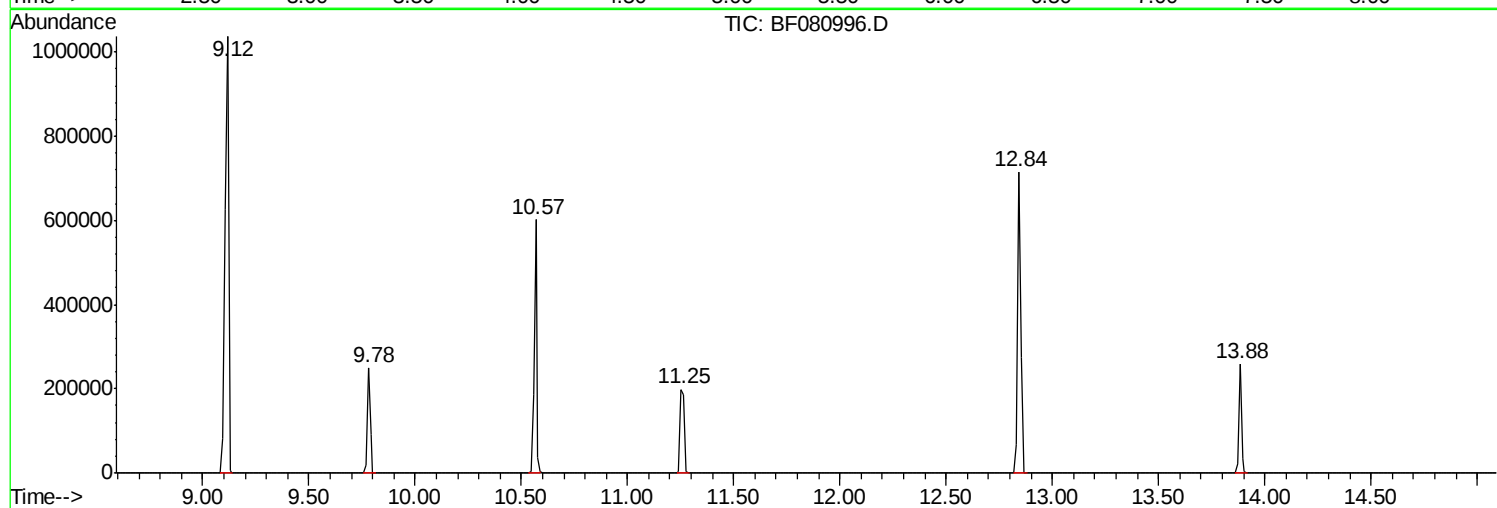
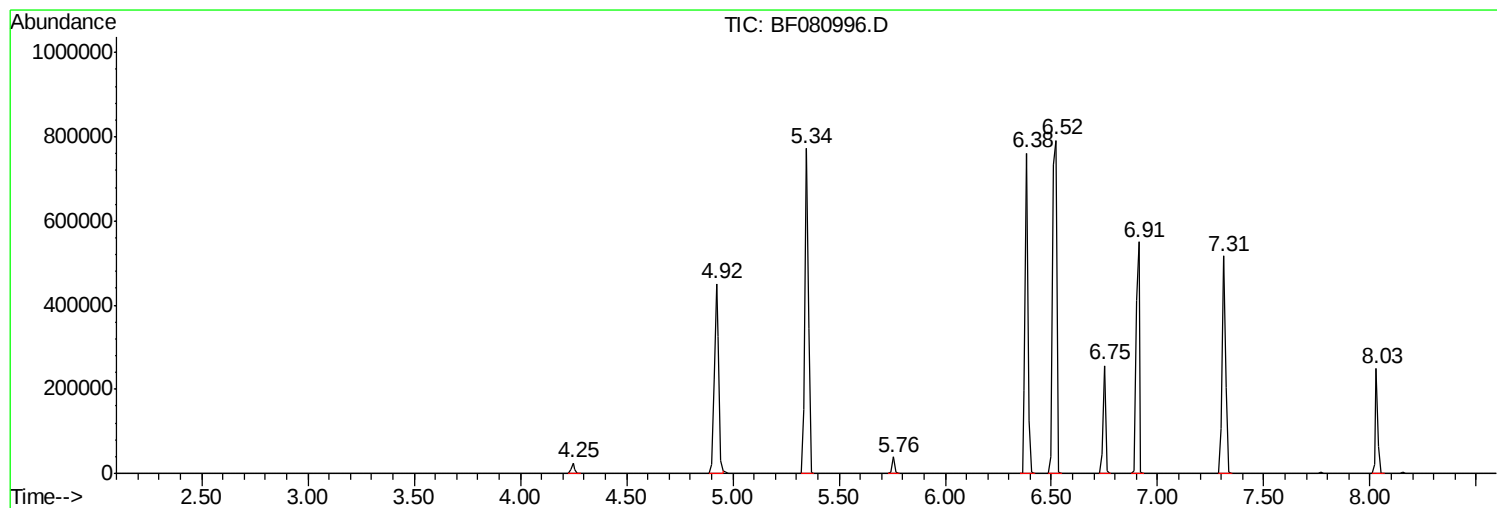
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB84967BL

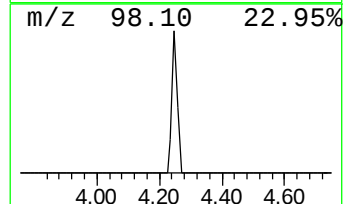
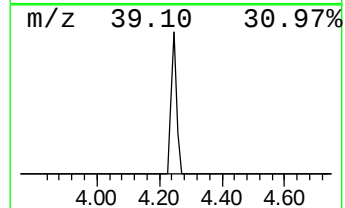
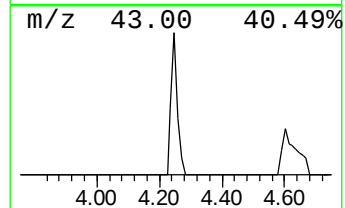
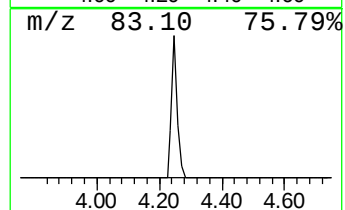
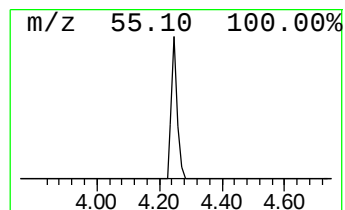
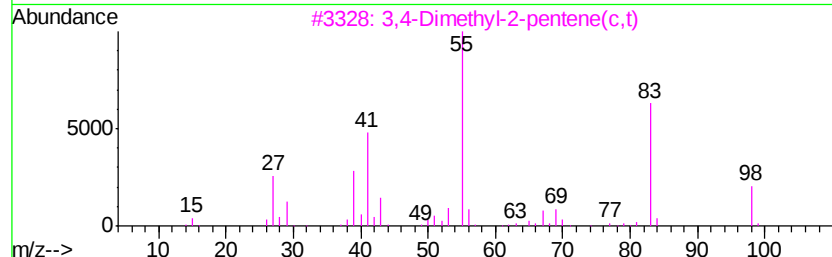
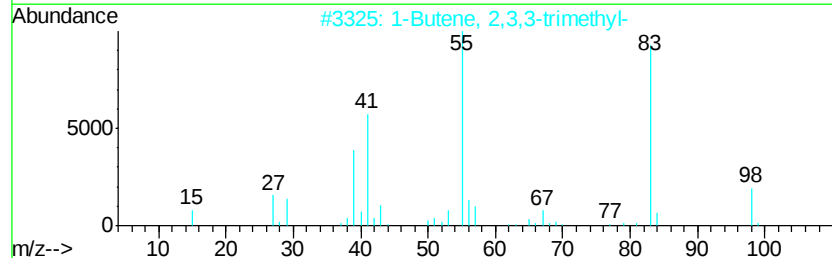
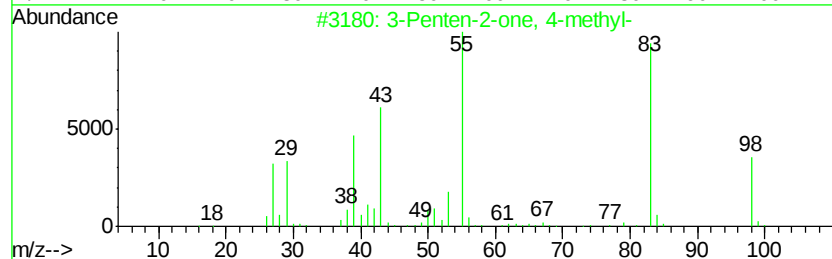
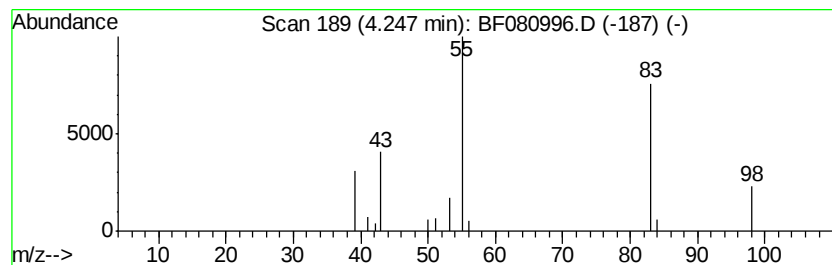
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	2.75 ng	29178	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	86
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	72
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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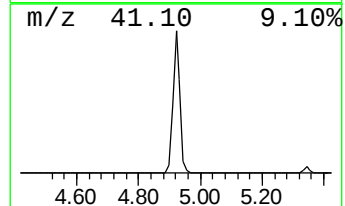
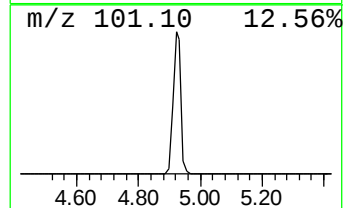
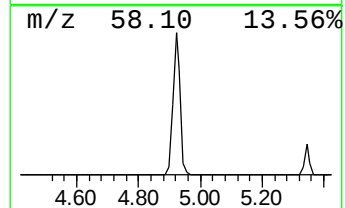
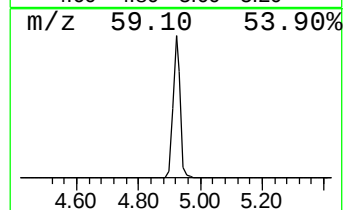
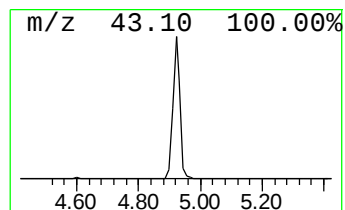
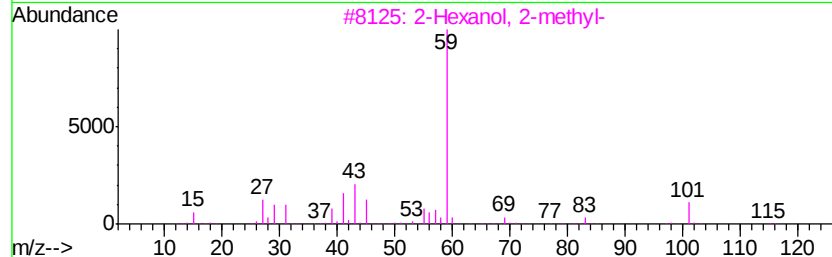
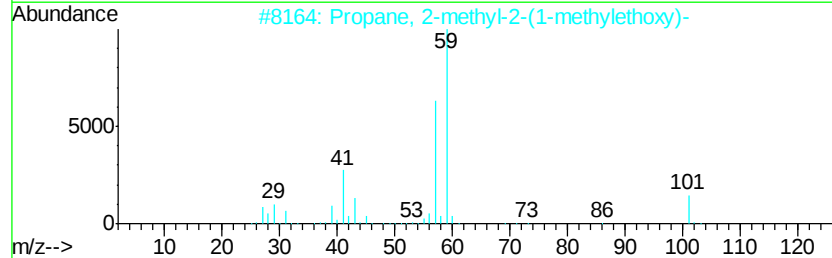
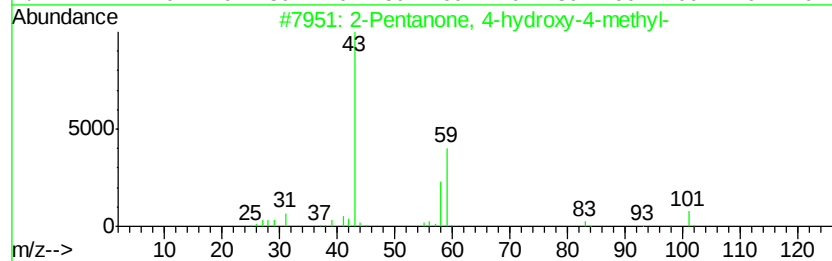
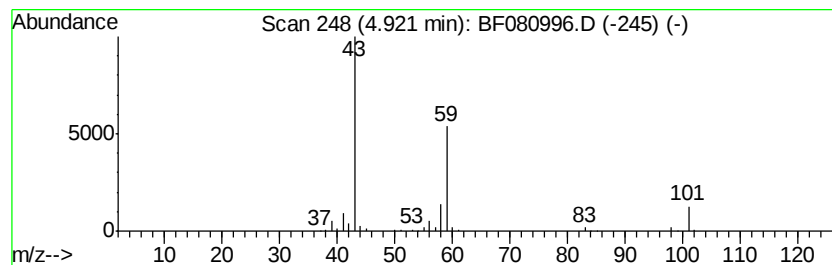
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	68.40 ng	726200	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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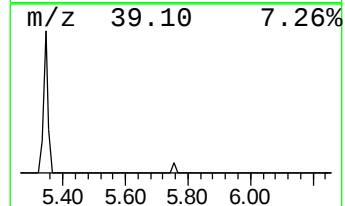
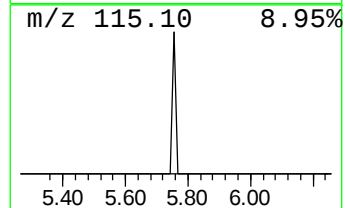
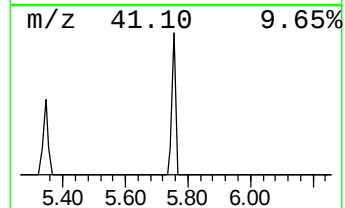
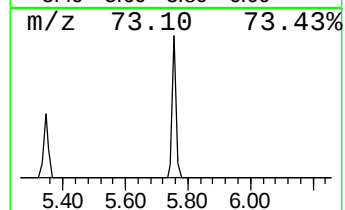
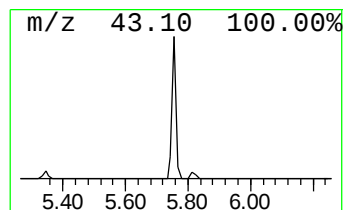
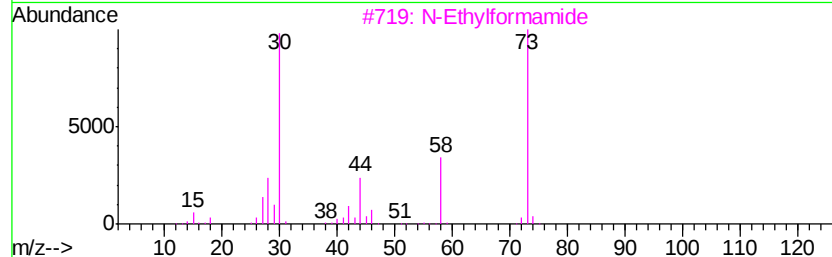
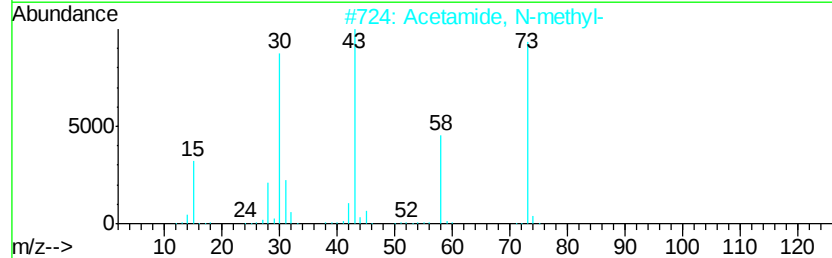
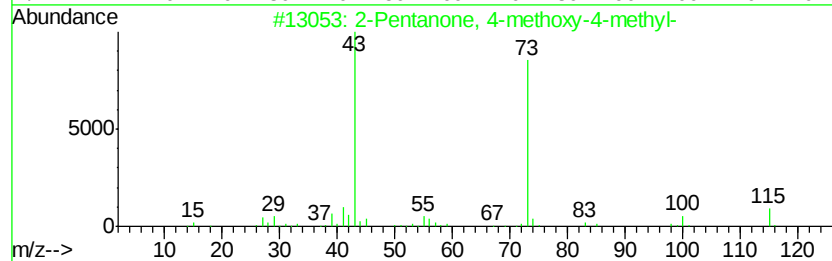
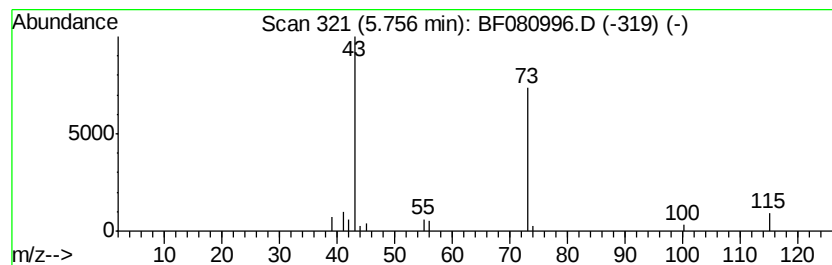
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.76	2.91 ng	30893	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	7
4		Guanidine, methyl-	73	C2H7N3	000471-29-4	7
5		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	5



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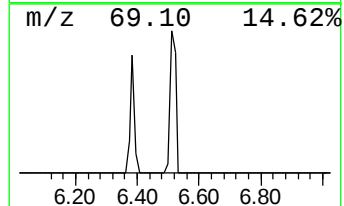
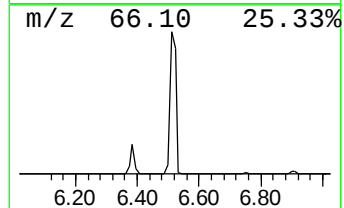
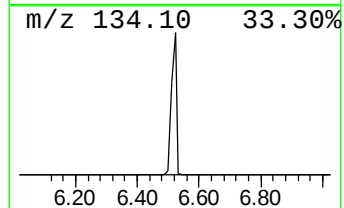
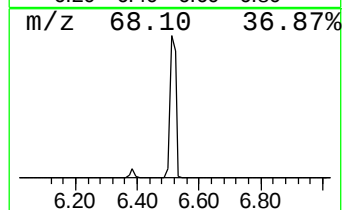
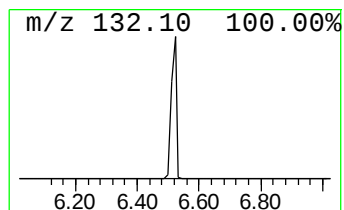
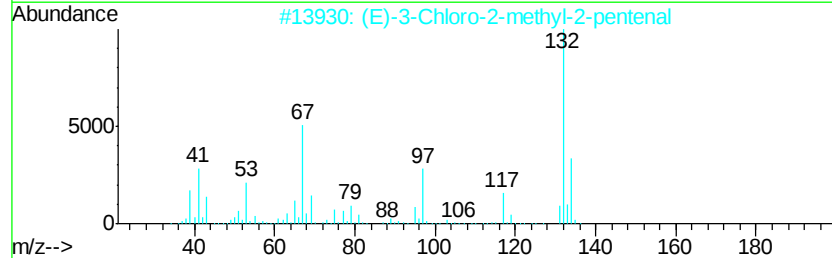
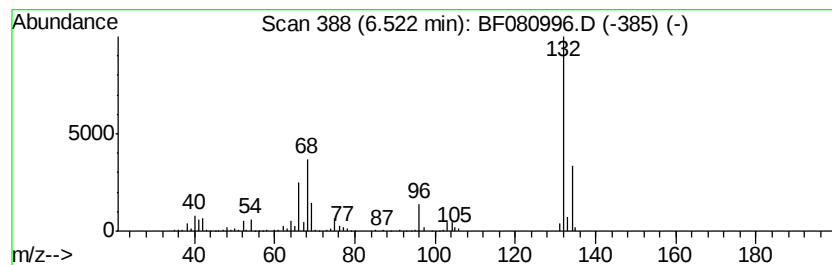
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	101.38 ng	1076310	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
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
3-Penten-2-one, 4...	4.25	2.8	ng	29178	1	6.75	212327	20.0
2-Pentanone, 4-hy...	4.92	68.4	ng	726200	1	6.75	212327	20.0
2-Pentanone, 4-me...	5.76	2.9	ng	30893	1	6.75	212327	20.0
unknown6.52	6.52	101.4	ng	1076310	1	6.75	212327	20.0