

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081315\
 Data File : BF080977.D
 Acq On : 13 Aug 2015 12:38
 Operator : UM/IZ
 Sample : PB84980BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84980BL

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-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	186	189	193	rBV	31415	44279	3.09%	0.374%
2	4.921	245	248	254	rBV	717922	977139	68.28%	8.259%
3	5.344	282	285	287	rBV	1387719	1329465	92.90%	11.237%
4	5.756	318	321	323	rBB	38279	34785	2.43%	0.294%
5	6.384	373	376	378	rBV	1327087	1305573	91.23%	11.035%
6	6.510	385	387	390	rBV	1168131	1251239	87.43%	10.576%
7	6.750	406	408	410	rBB	305798	294015	20.54%	2.485%
8	6.899	419	421	424	rBB	758303	889656	62.16%	7.519%
9	7.310	454	457	459	rBV	817897	763453	53.35%	6.453%
10	8.030	518	520	522	rBV	487750	421105	29.42%	3.559%
11	9.105	611	614	617	rBV	1088632	1431147	100.00%	12.096%
12	9.779	670	673	676	rBB	422876	390304	27.27%	3.299%
13	10.568	739	742	744	rBV	658222	656566	45.88%	5.549%
14	11.253	800	802	805	rBV	313251	332240	23.21%	2.808%
15	12.842	938	941	944	rBV	1061534	1092777	76.36%	9.236%
16	13.882	1030	1032	1034	rBV	418428	369582	25.82%	3.124%
17	15.265	1150	1153	1156	rBV	231955	248080	17.33%	2.097%

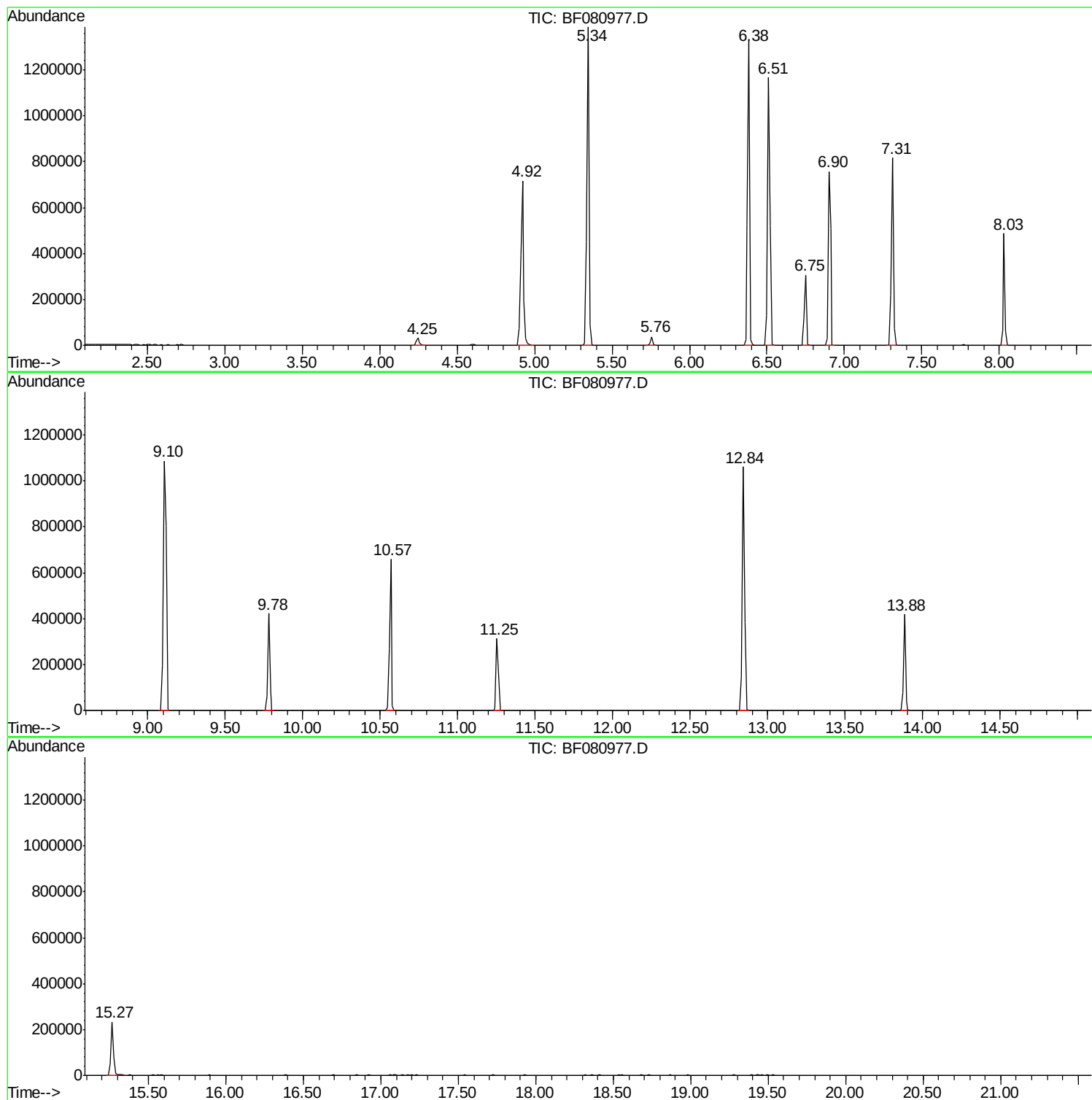
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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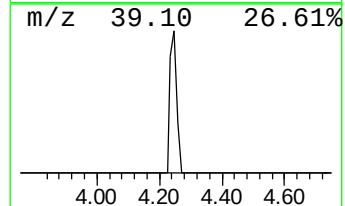
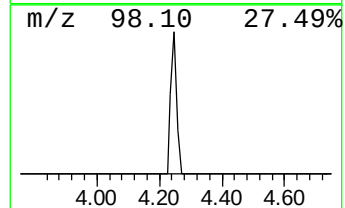
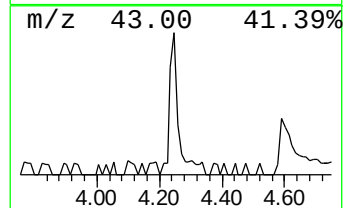
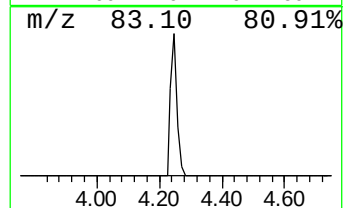
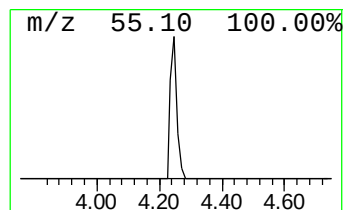
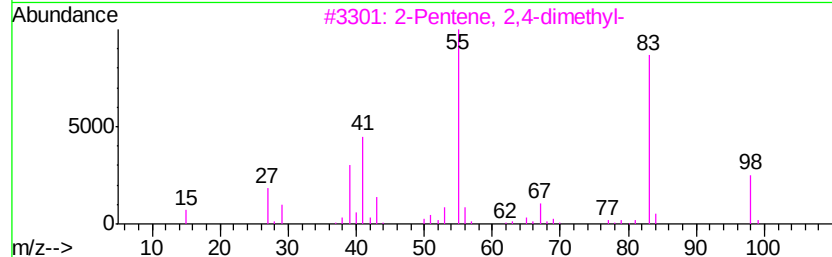
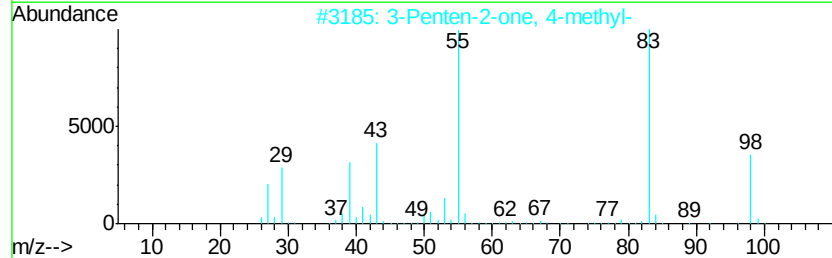
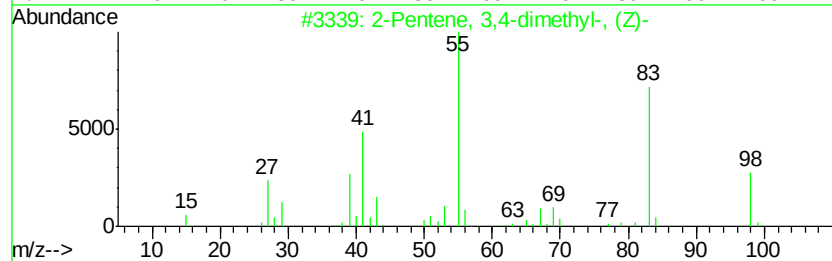
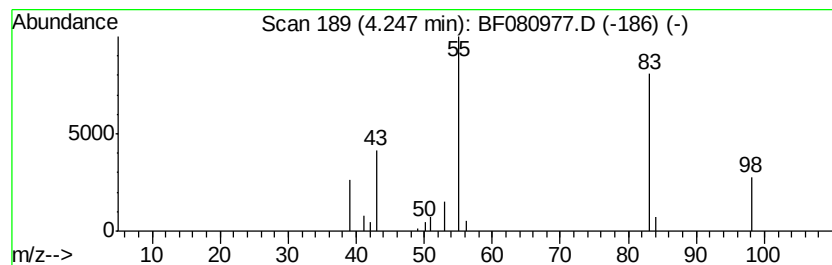
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentene, 3,4-dimethyl-, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	3.01 ng	44279	1,4-Dichlorobenzene-d4	6.75

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



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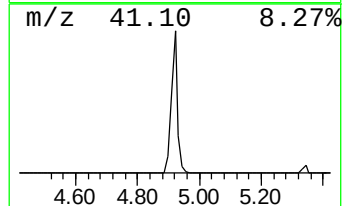
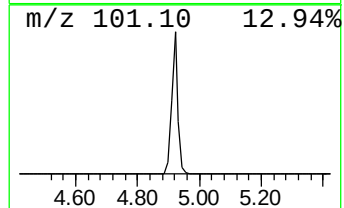
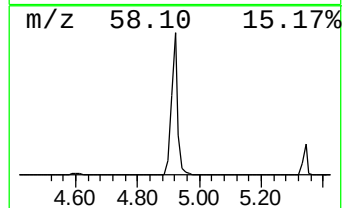
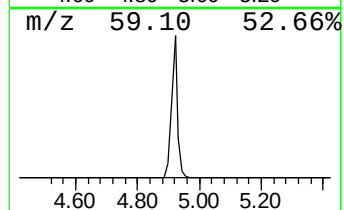
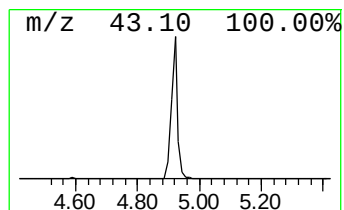
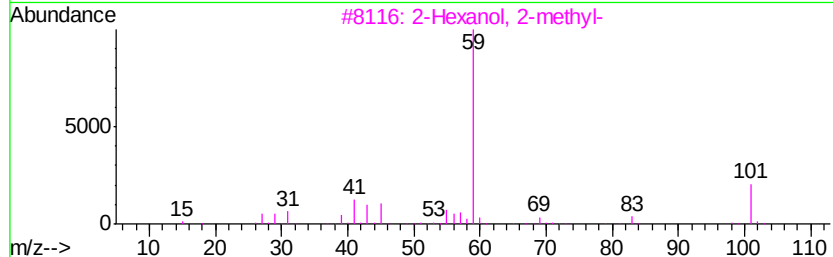
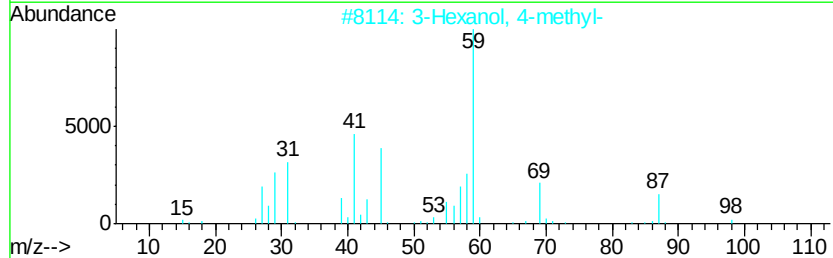
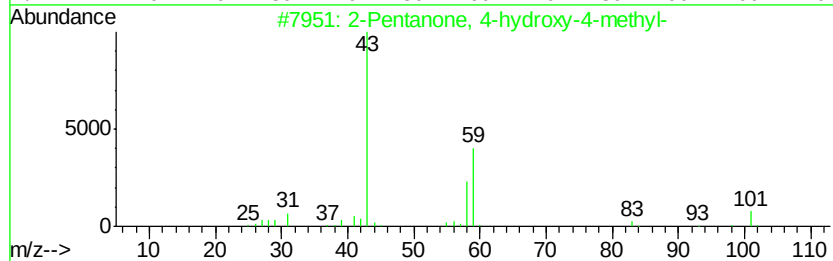
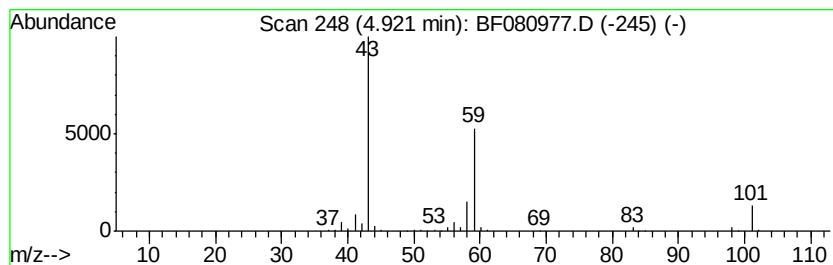
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	66.47 ng	977139	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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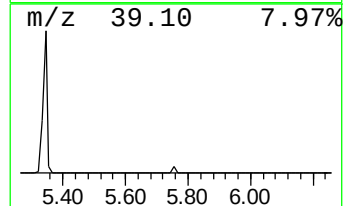
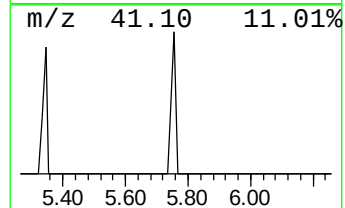
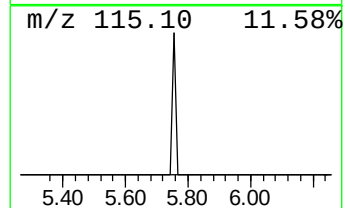
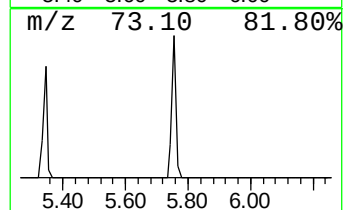
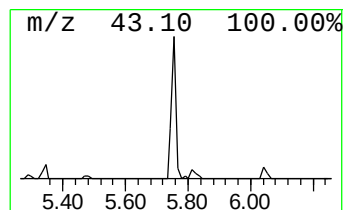
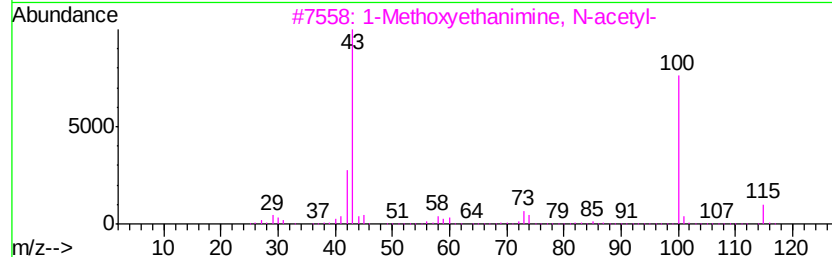
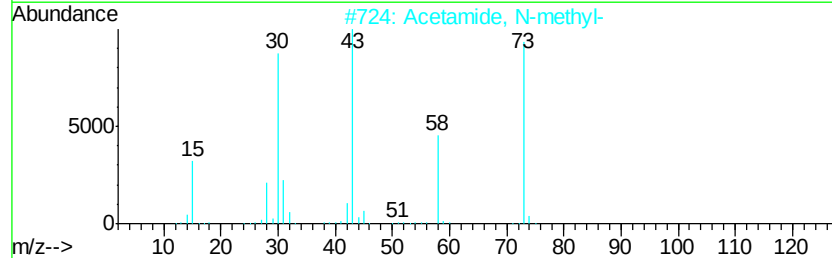
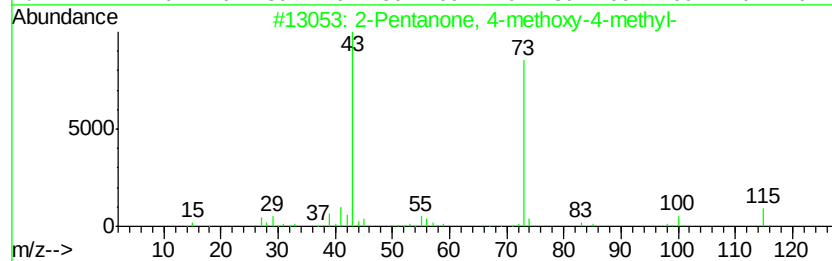
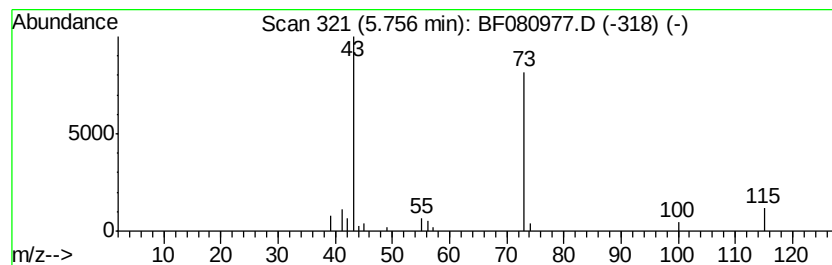
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.76	2.37 ng	34785	1,4-Dichlorobenzene-d4	6.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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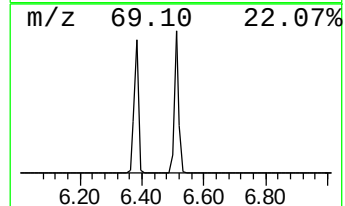
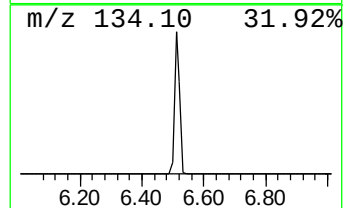
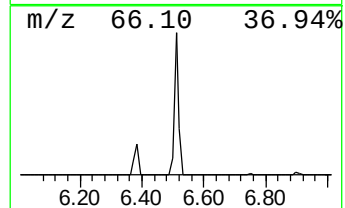
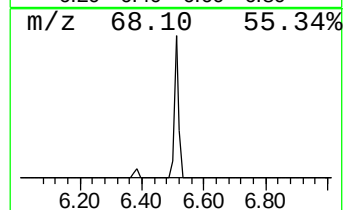
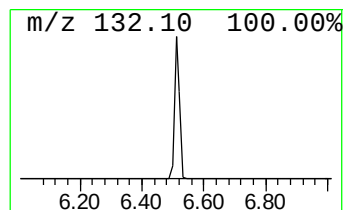
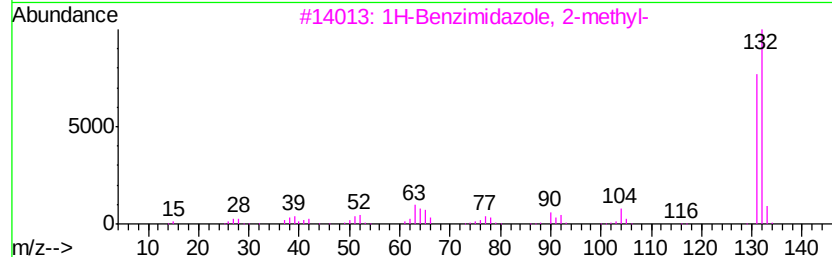
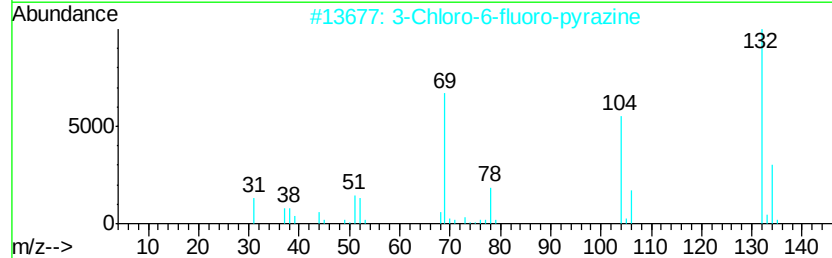
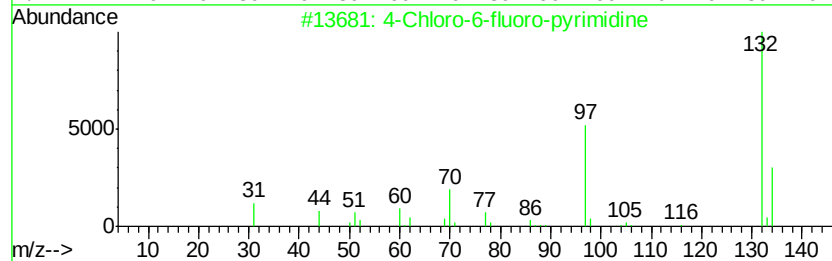
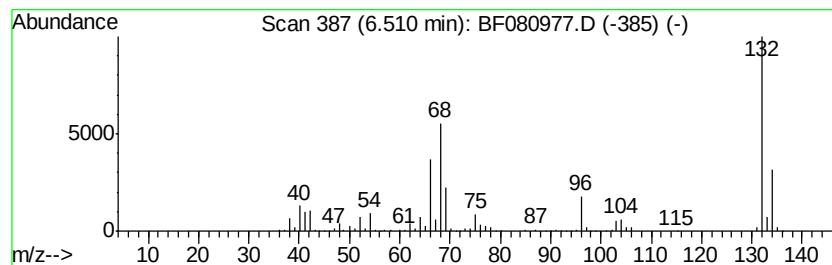
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Peak Number 4 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	85.11 ng	1251240	1,4-Dichlorobenzene-d4	6.75

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	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentene, 3,4-di...	4.25	3.0	ng	44279	1	6.75	294015	20.0
2-Pentanone, 4-hy...	4.92	66.5	ng	977139	1	6.75	294015	20.0
2-Pentanone, 4-me...	5.76	2.4	ng	34785	1	6.75	294015	20.0
unknown6.51	6.51	85.1	ng	1251240	1	6.75	294015	20.0