

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072415\
 Data File : BF080637.D
 Acq On : 24 Jul 2015 20:50
 Operator : TP/UM
 Sample : PB84652BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84652BL

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-BF072415.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	4.441	204	206	211	rVB	36752	55861	3.63%	0.435%
2	5.093	260	263	265	rBV	478398	620110	40.28%	4.828%
3	5.504	297	299	302	rBV	1232652	1227078	79.71%	9.554%
4	5.927	335	336	339	rBV	46564	44783	2.91%	0.349%
5	6.544	387	390	392	rBV	1357108	1302322	84.60%	10.140%
6	6.693	400	403	405	rBV	1400095	1317756	85.60%	10.260%
7	6.933	422	424	426	rVB	367024	350045	22.74%	2.725%
8	7.082	435	437	439	rBV	946751	964704	62.67%	7.511%
9	7.493	470	473	475	rBV	737421	769317	49.97%	5.990%
10	8.213	534	536	539	rBV	387628	417882	27.15%	3.254%
11	9.288	628	630	633	rBV	1048627	1373959	89.25%	10.698%
12	9.973	688	690	692	rBV	634665	508122	33.01%	3.956%
13	10.762	756	759	761	rBV2	630590	865986	56.25%	6.743%
14	11.459	818	820	822	rBV	641557	513010	33.32%	3.994%
15	13.071	958	961	963	rBV	1212007	1539423	100.00%	11.986%
16	14.202	1058	1060	1063	rBV	546161	502841	32.66%	3.915%
17	15.814	1198	1201	1204	rBV	393727	470288	30.55%	3.662%

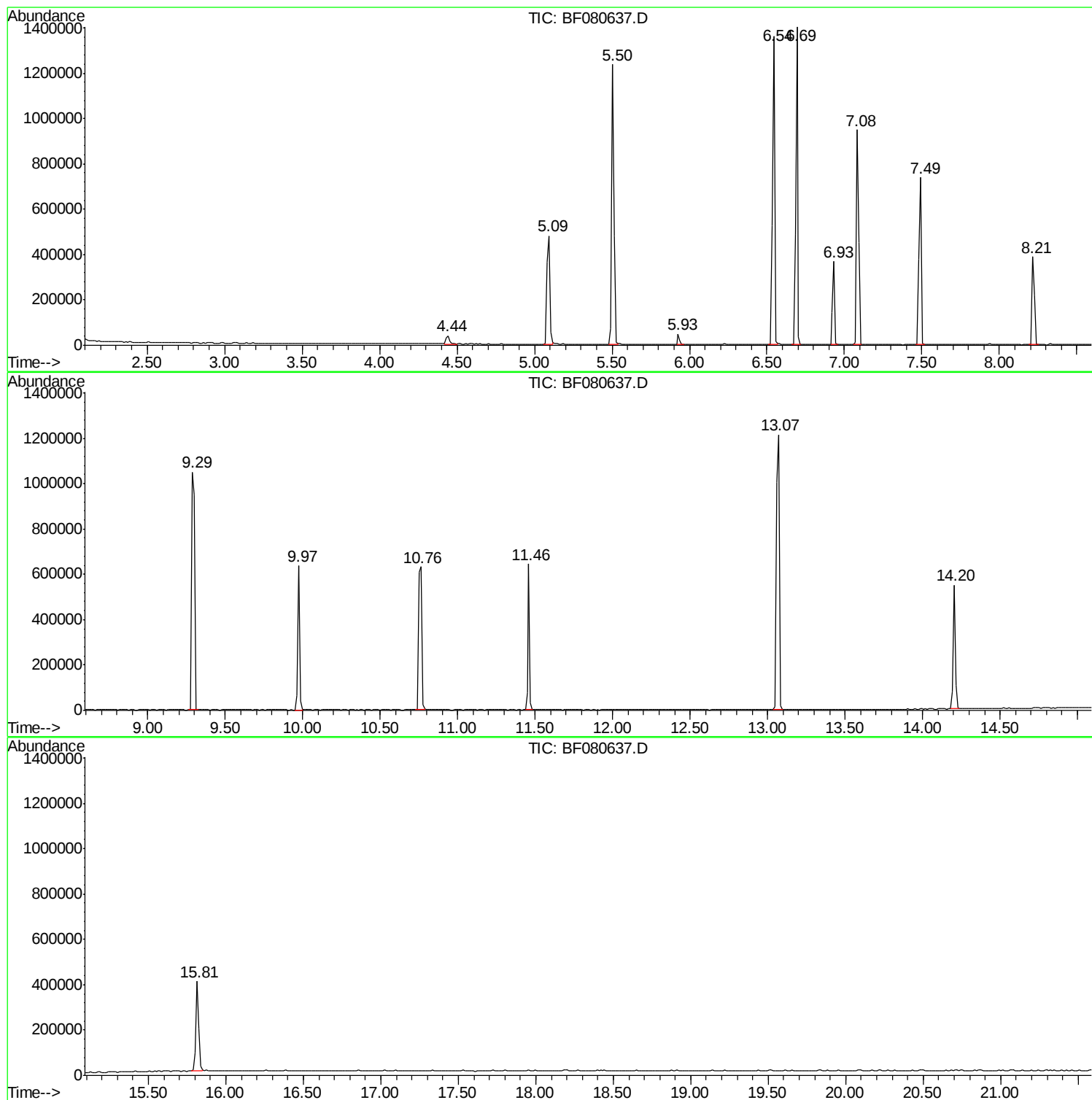
Sum of corrected areas: 12843487

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



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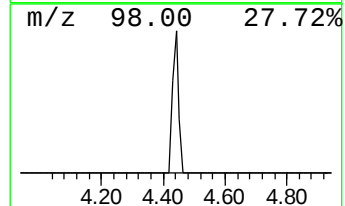
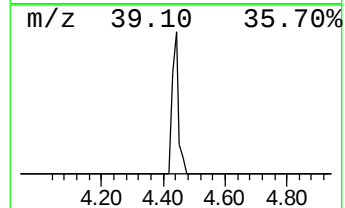
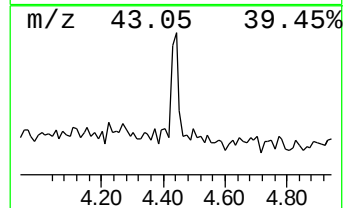
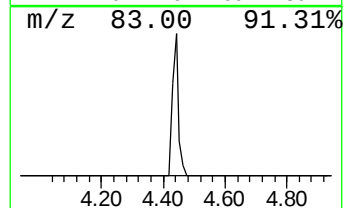
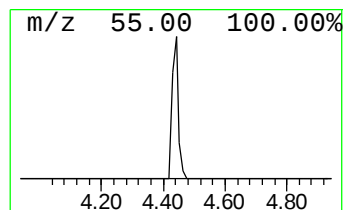
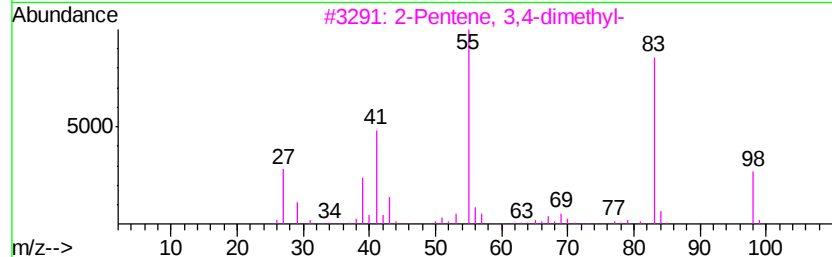
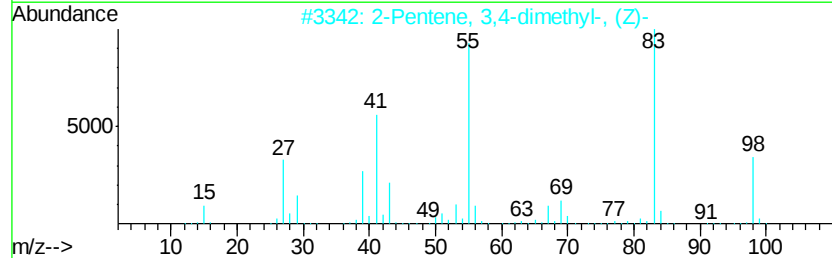
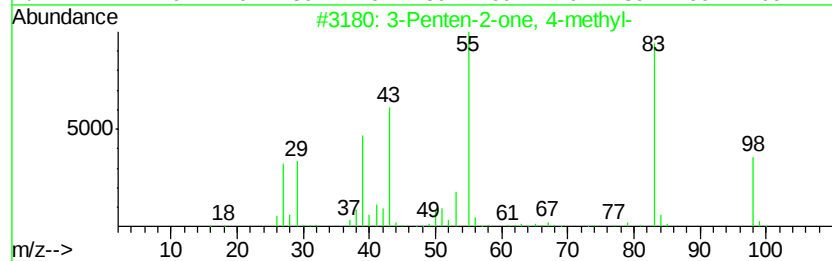
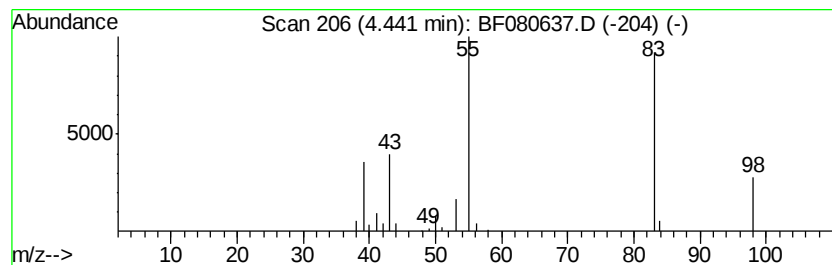
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	3.19 ng	55861	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
3			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64
4			3-Hexen-2-one	98	C6H10O	000763-93-9	64
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	64



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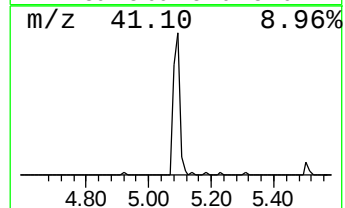
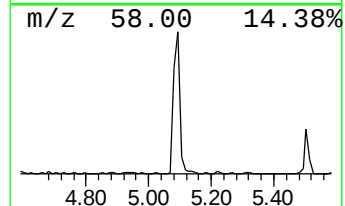
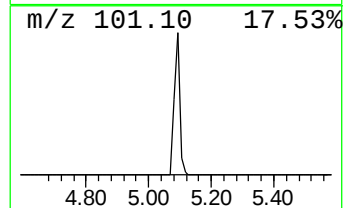
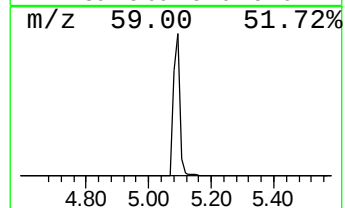
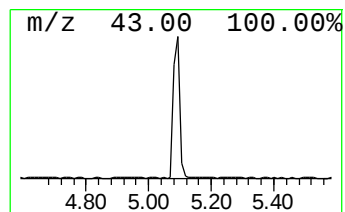
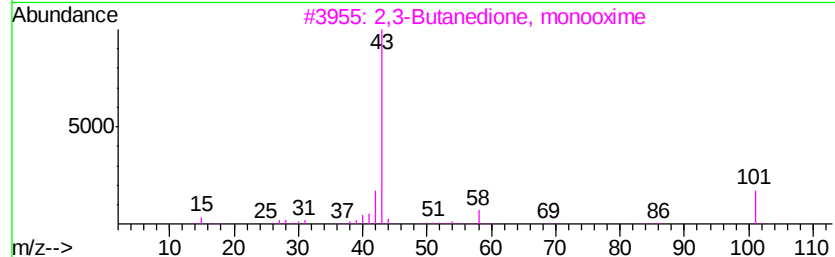
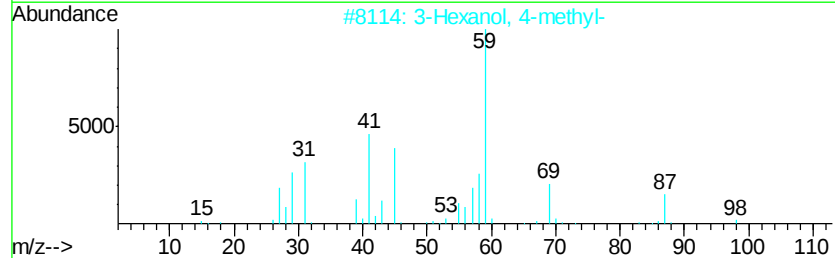
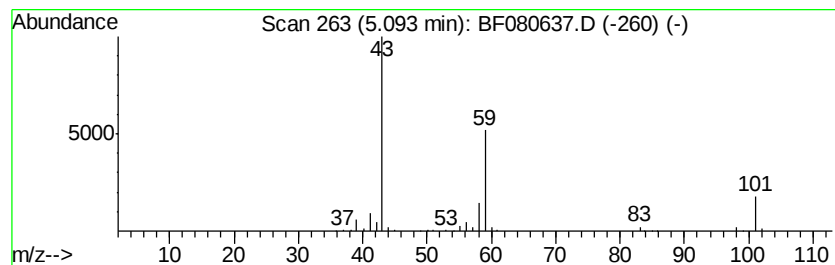
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	35.43 ng	620110	1,4-Dichlorobenzene-d4	6.93

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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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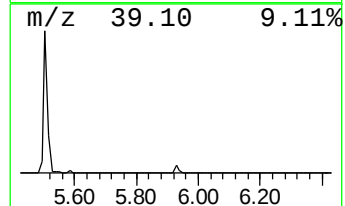
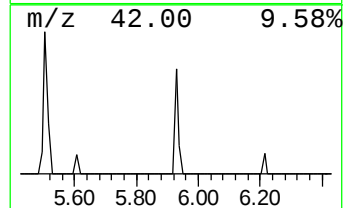
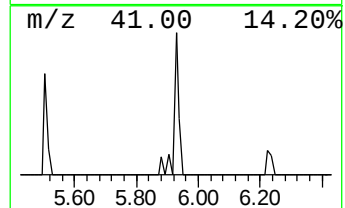
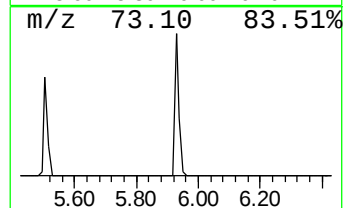
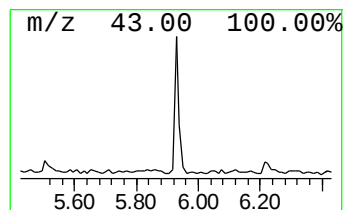
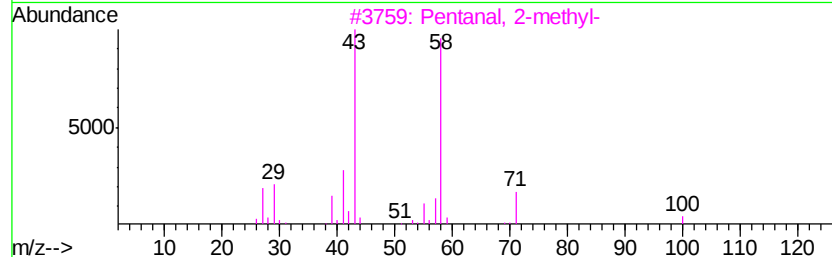
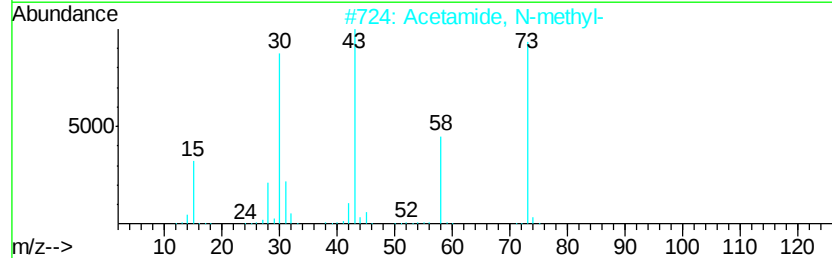
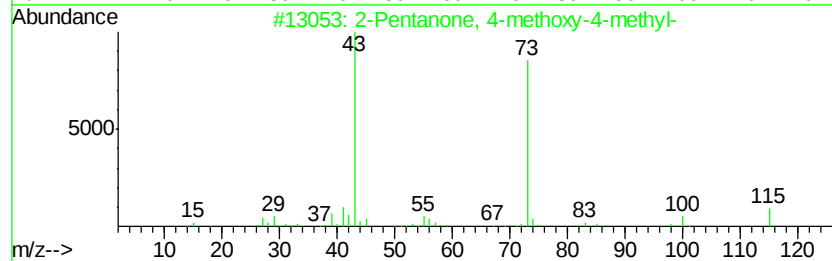
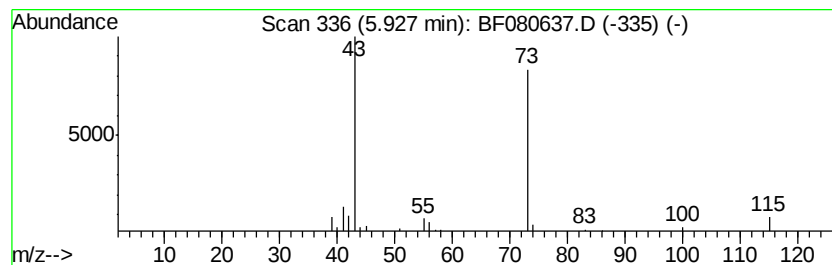
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	2.56 ng	44783	1,4-Dichlorobenzene-d4	6.93

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	50
3		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	9
4		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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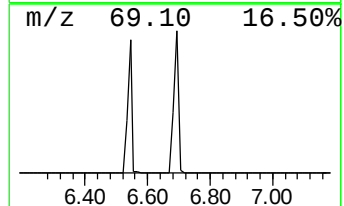
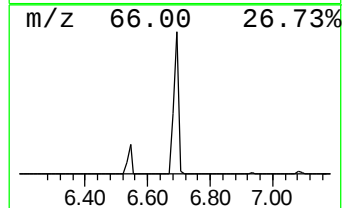
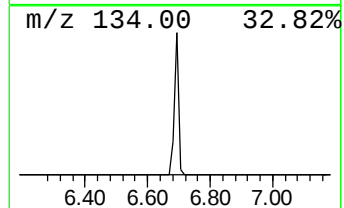
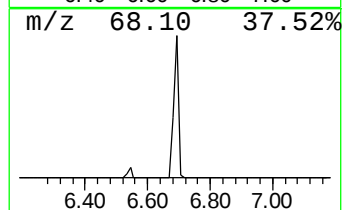
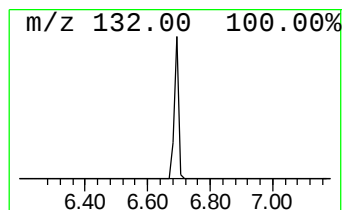
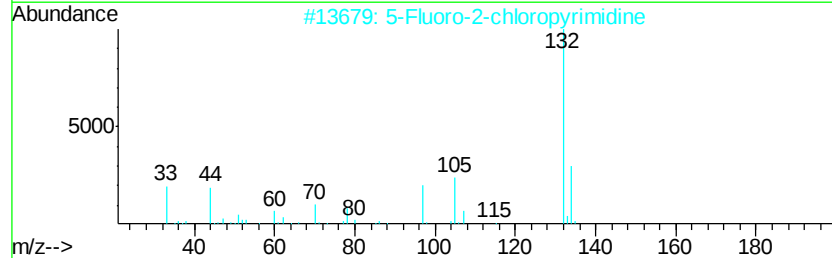
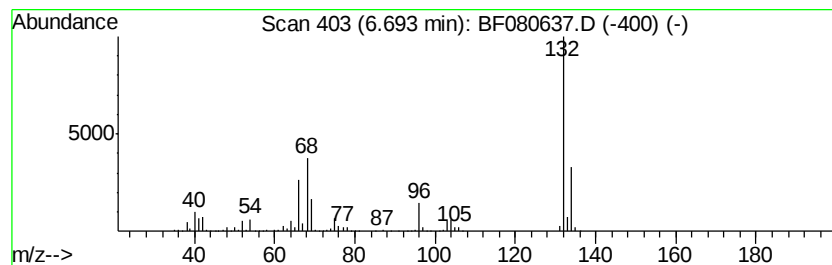
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Peak Number 4 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	75.29 ng	1317760	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.44	3.2	ng	55861	1	6.93	350045	20.0
2-Pentanone, 4-hy...	5.09	35.4	ng	620110	1	6.93	350045	20.0
2-Pentanone, 4-me...	5.93	2.6	ng	44783	1	6.93	350045	20.0
unknown6.69	6.69	75.3	ng	1317760	1	6.93	350045	20.0