

Data Path : V:\HPCHEM1\BNA_F\DATA\BF121515\
 Data File : BF083804.D
 Acq On : 15 Dec 2015 8:14
 Operator : UM/IZ
 Sample : PB87256BL
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87256BL

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-BF121315.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	4.453	204	207	210	rBV	476460	536225	14.72%	2.074%
2	5.104	260	264	266	rBV	1307795	2019385	55.44%	7.811%
3	5.504	297	299	302	rBV	1426139	1846722	50.70%	7.144%
4	5.904	332	334	336	rBB	93737	81657	2.24%	0.316%
5	6.522	385	388	391	rBV	1492794	1760446	48.34%	6.810%
6	6.670	398	401	403	rBV	1517811	2006417	55.09%	7.761%
7	6.899	419	421	423	rBB	729239	621547	17.07%	2.404%
8	7.059	432	435	437	rBB	2321561	2345700	64.40%	9.074%
9	7.459	467	470	472	rBV	1737356	1786268	49.04%	6.910%
10	8.179	531	533	536	rBB	868921	799115	21.94%	3.091%
11	9.265	624	628	630	rBV	3036578	3642154	100.00%	14.089%
12	9.939	684	687	689	rBV	929683	954745	26.21%	3.693%
13	10.716	753	755	758	rBV2	1224260	1470719	40.38%	5.689%
14	11.414	814	816	819	rBV	998234	946267	25.98%	3.660%
15	12.831	938	940	942	rBB	79931	61376	1.69%	0.237%
16	13.002	952	955	958	rBV	3167507	3383659	92.90%	13.089%
17	13.539	999	1002	1003	rBB	34476	42676	1.17%	0.165%
18	14.042	1044	1046	1049	rBV	808655	877195	24.08%	3.393%
19	15.482	1169	1172	1175	rBV	551307	669317	18.38%	2.589%

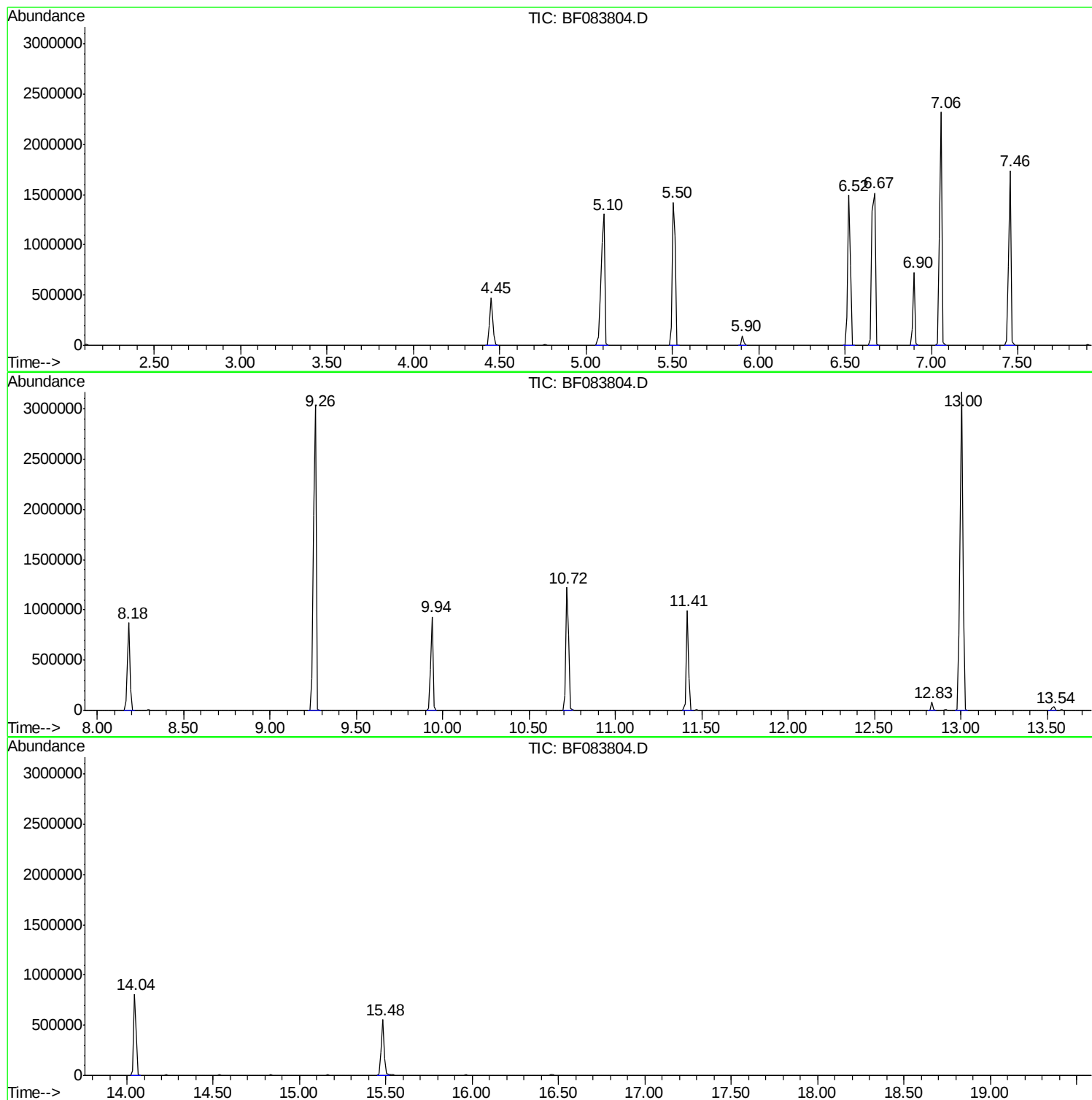
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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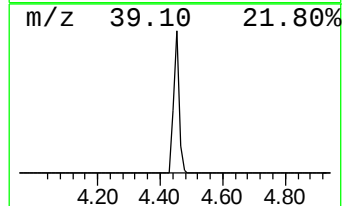
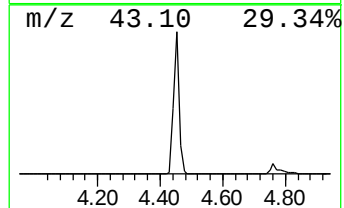
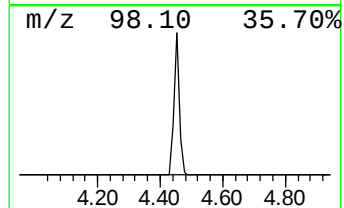
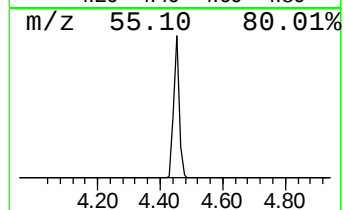
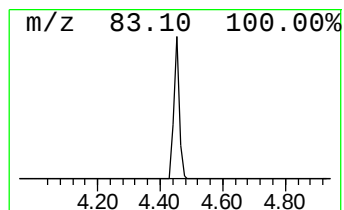
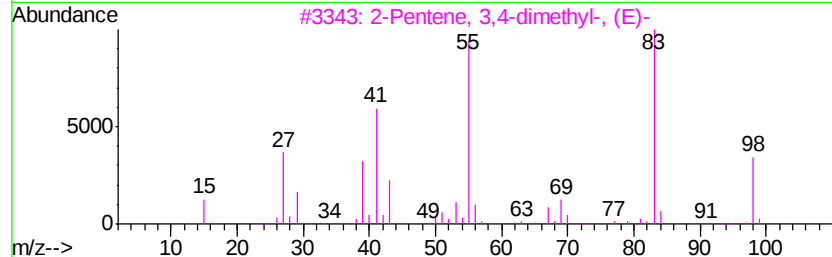
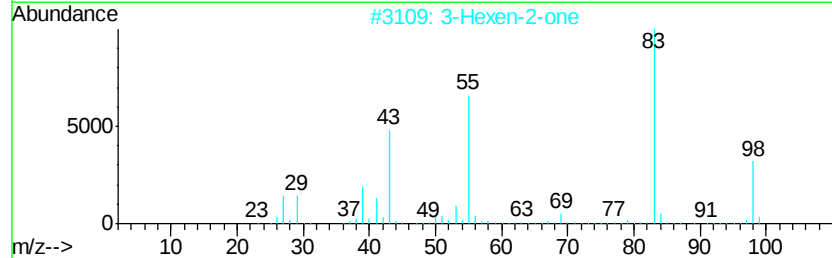
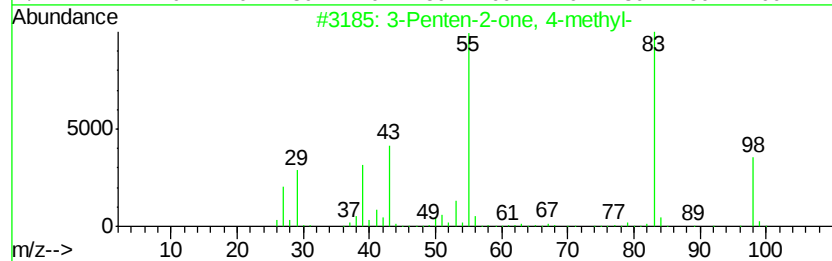
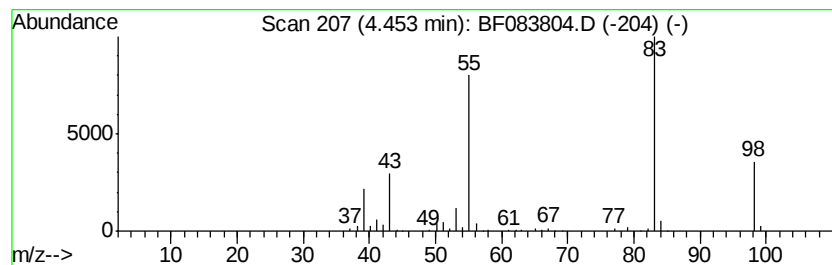
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.45	17.25 ng	536225	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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	78
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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ClientSampled :
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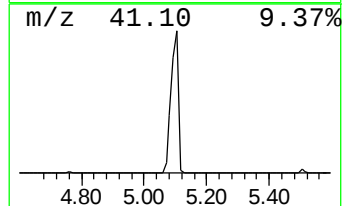
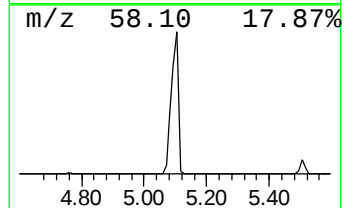
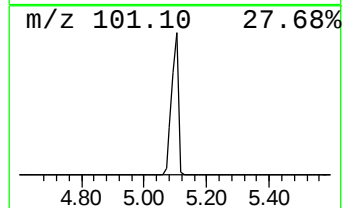
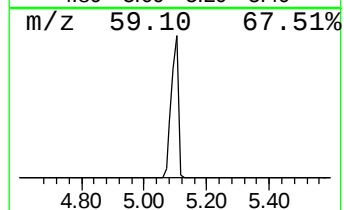
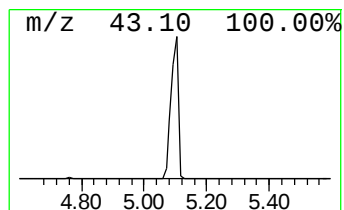
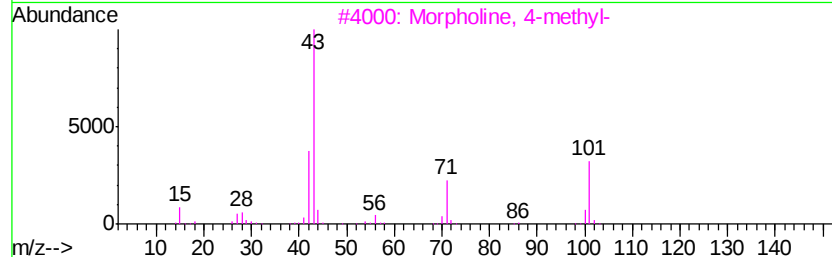
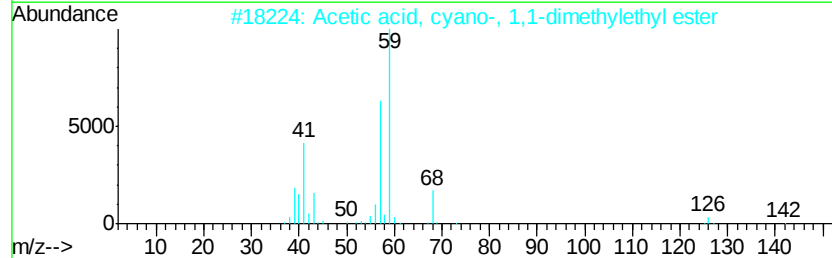
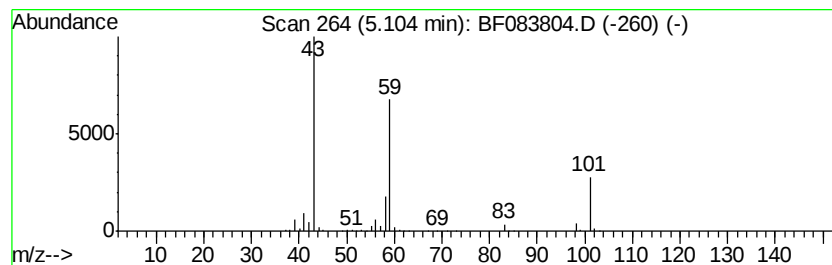
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	64.98 ng	2019390	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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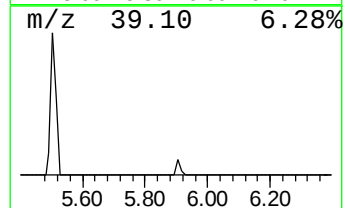
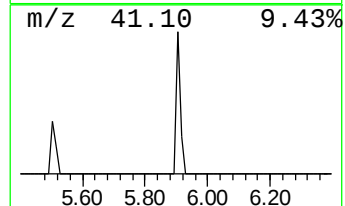
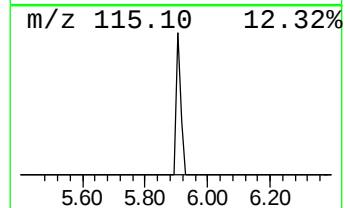
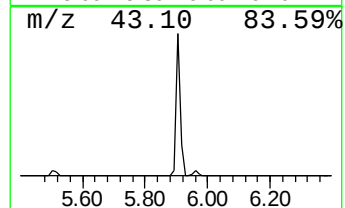
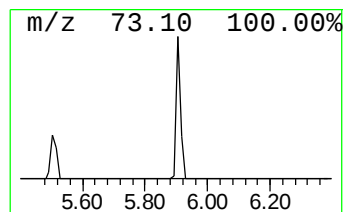
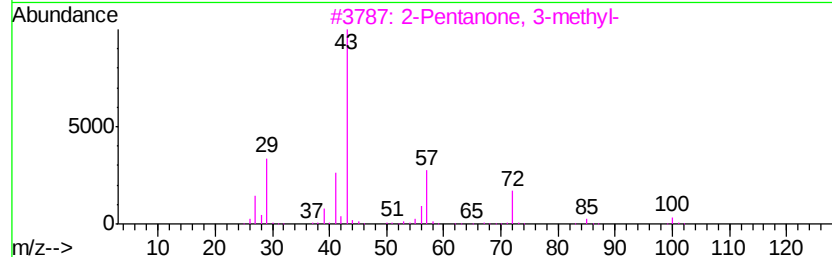
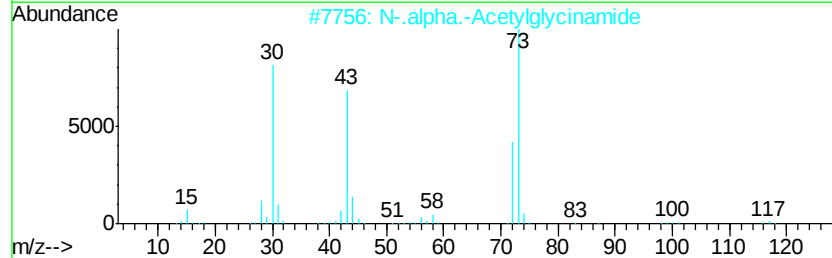
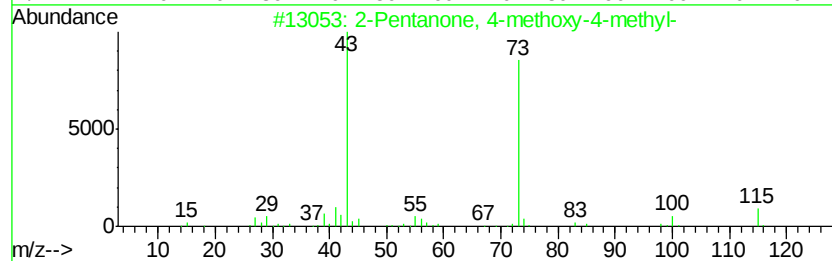
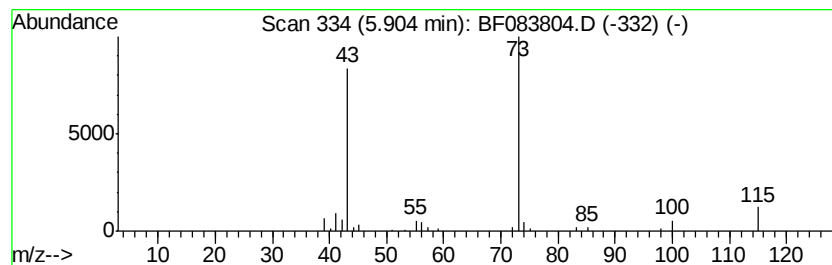
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.63 ng	81657	1,4-Dichlorobenzene-d4	6.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	N-.alpha.-Acetylglucineamide	116	C4H8N2O2	002620-63-5	33	
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10	
4	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9	
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9	



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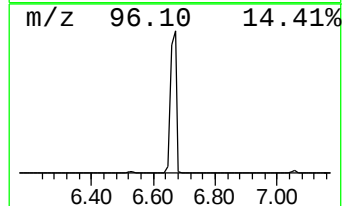
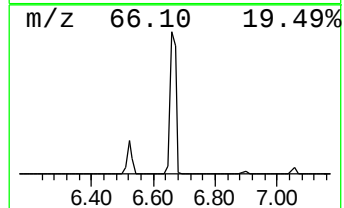
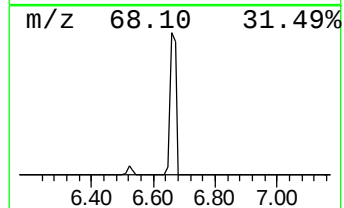
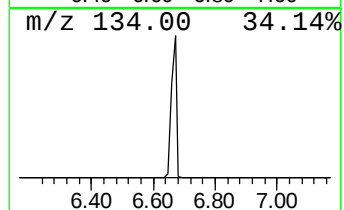
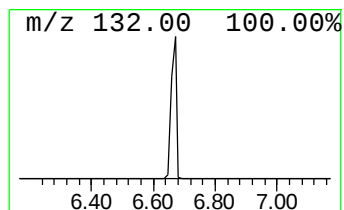
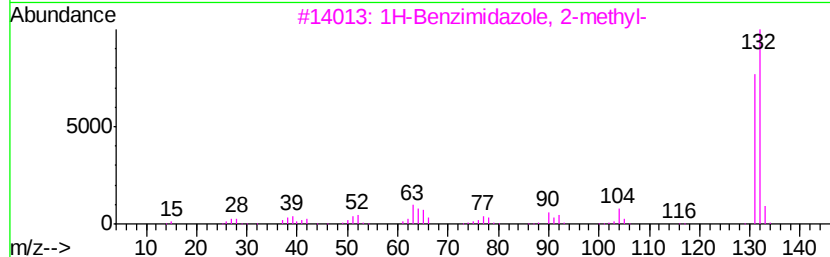
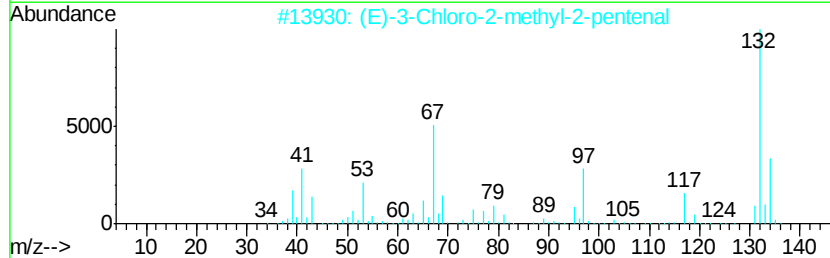
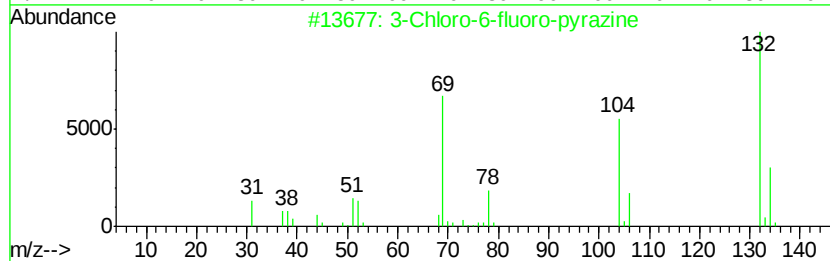
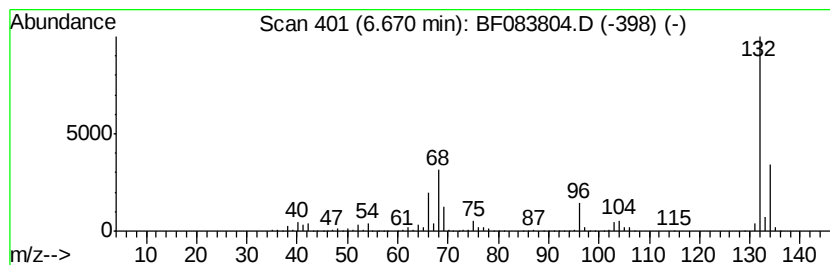
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Peak Number 4 unknown6.67 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	64.56 ng	2006420	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.45	17.3	ng	536225	1	6.90	621547	20.0
2-Pentanone, 4-hy...	5.10	65.0	ng	2019390	1	6.90	621547	20.0
2-Pentanone, 4-me...	5.90	2.6	ng	81657	1	6.90	621547	20.0
unknown6.67	6.67	64.6	ng	2006420	1	6.90	621547	20.0