

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
 Data File : BF084398.D
 Acq On : 12 Jan 2016 00:27
 Operator : SJ/UM
 Sample : H1074-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HSR-WC-14-010516

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-BF123115.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	2.704	51	54	59	rVB	289894	391771	3.64%	0.437%
2	4.407	200	203	207	rBV	204017	245848	2.28%	0.274%
3	5.059	257	260	269	rVB	2869464	4167772	38.72%	4.650%
4	5.482	294	297	299	rBV	9142450	10152688	94.32%	11.328%
5	6.499	383	386	389	rBV	6996487	8200807	76.18%	9.150%
6	6.625	394	397	400	rBV	7852030	9918369	92.14%	11.066%
7	6.853	415	417	419	rBV	2878746	2309235	21.45%	2.576%
8	7.013	428	431	433	rBV	8835928	8186229	76.05%	9.134%
9	7.425	463	467	469	rBV	6741129	7788401	72.35%	8.690%
10	8.145	527	530	533	rBV	2094715	3317289	30.82%	3.701%
11	9.219	621	624	626	rBV	10441298	10764606	100.00%	12.010%
12	9.893	680	683	685	rBV	3654016	3238223	30.08%	3.613%
13	10.682	749	752	755	rBV	5434062	6180412	57.41%	6.896%
14	11.379	810	813	815	rBV	2979739	2802323	26.03%	3.127%
15	12.968	949	952	954	rBV	8454683	8422659	78.24%	9.397%
16	14.008	1041	1043	1046	rBV	1685529	1908803	17.73%	2.130%
17	15.437	1165	1168	1171	rBV	1165125	1631948	15.16%	1.821%

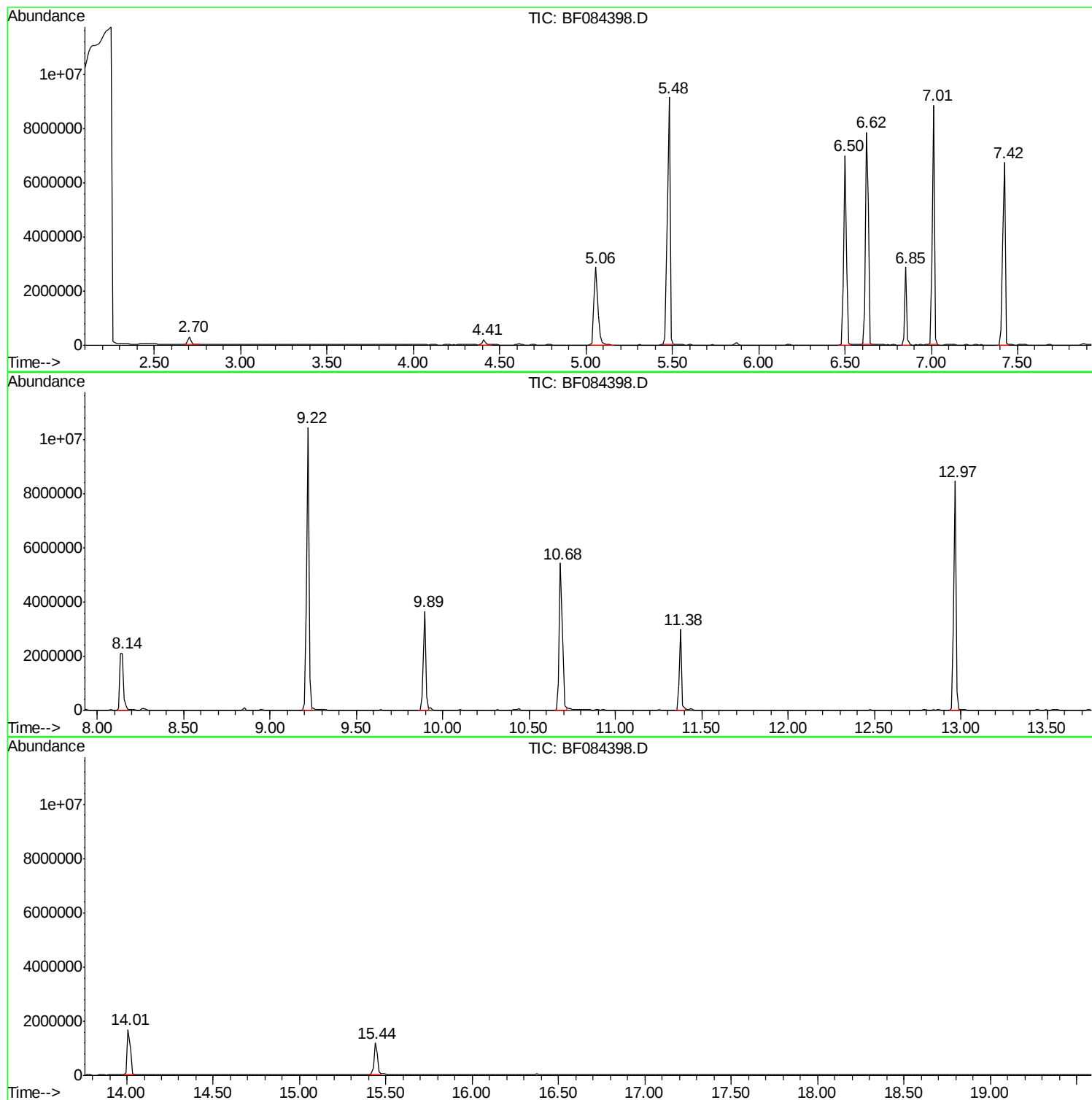
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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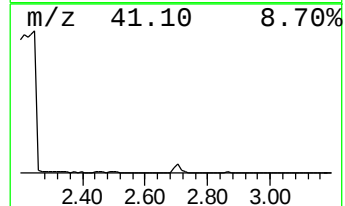
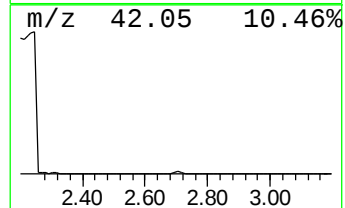
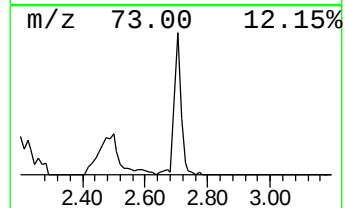
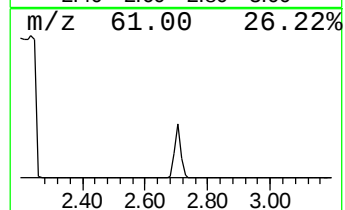
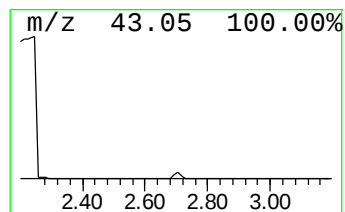
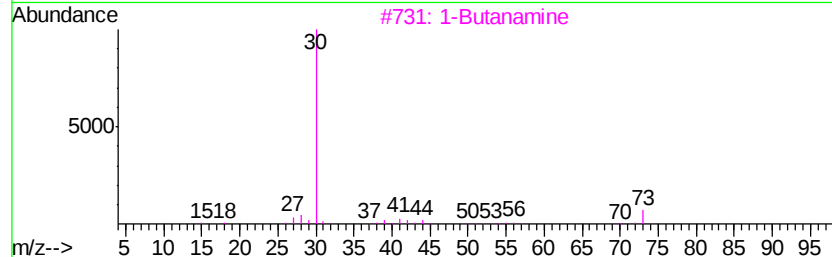
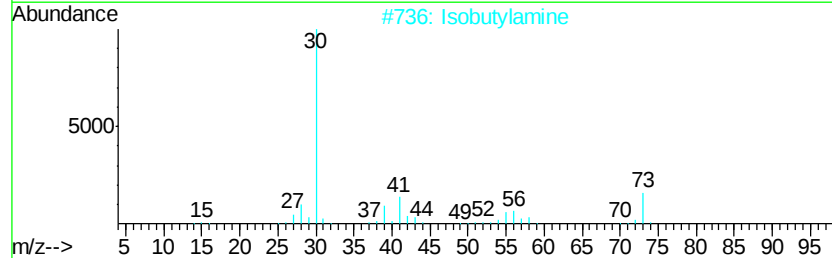
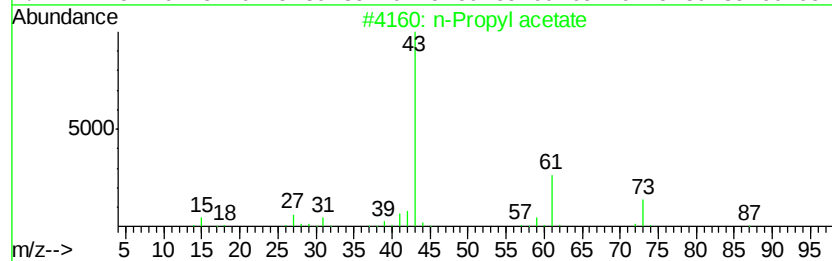
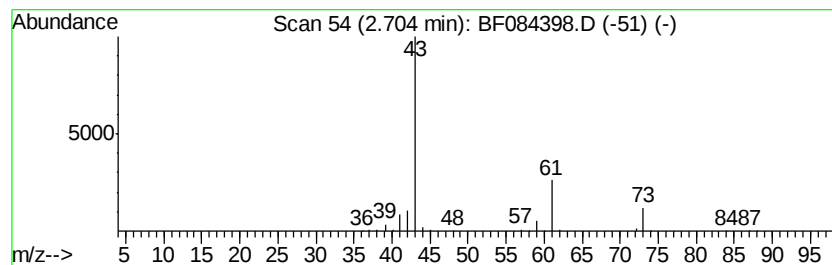
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.70	3.39 ng	391771	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isobutylamine	73	C4H11N	000078-81-9	7
3		1-Butanamine	73	C4H11N	000109-73-9	5
4		Pentane	72	C5H12	000109-66-0	4
5		Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	4



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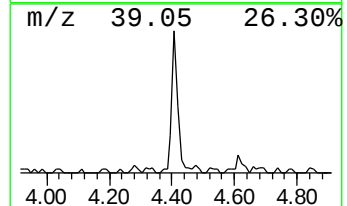
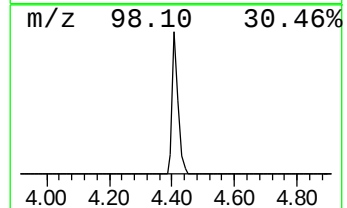
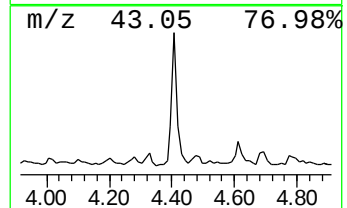
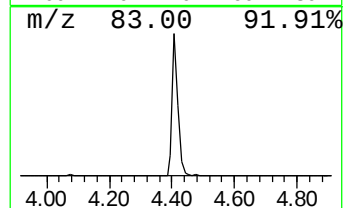
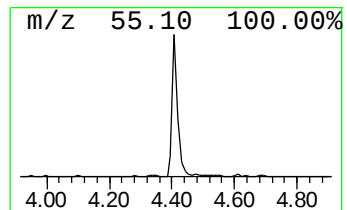
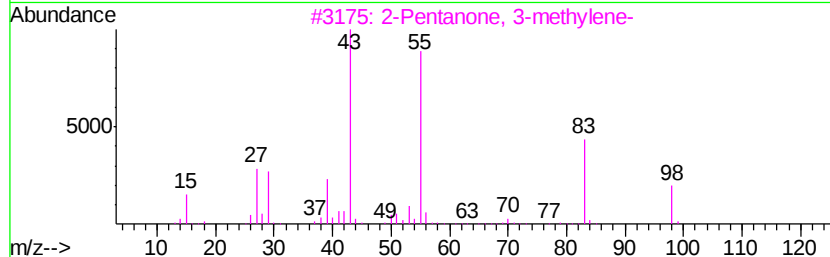
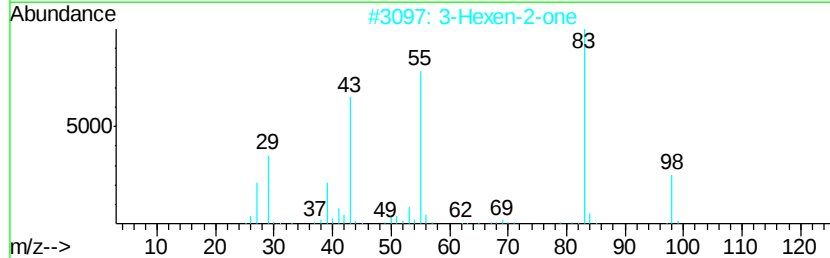
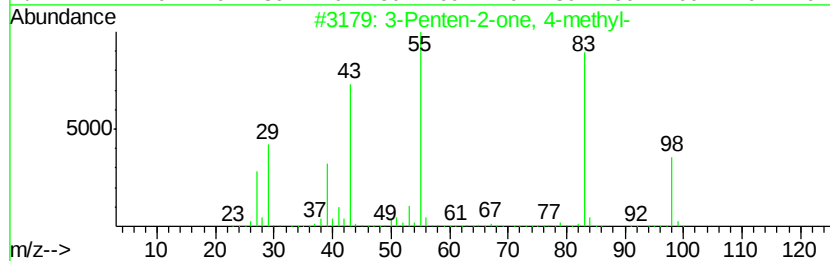
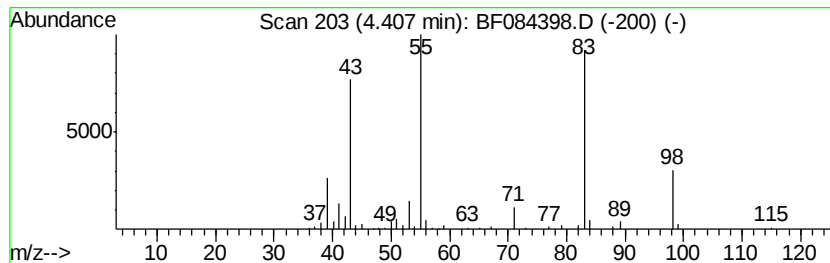
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.13 ng	245848	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	87
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	64
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	64



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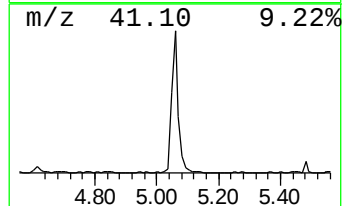
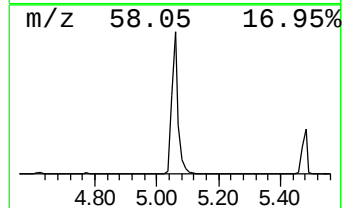
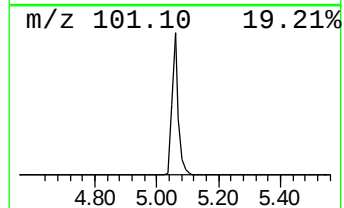
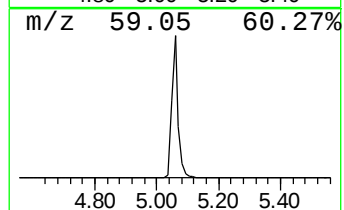
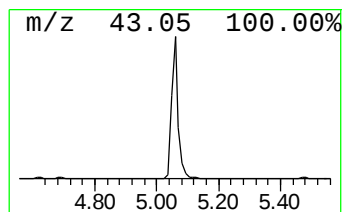
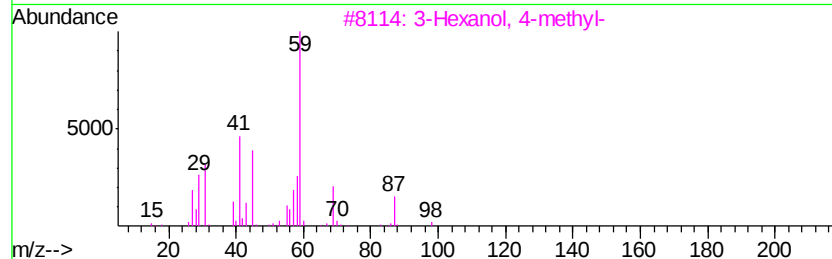
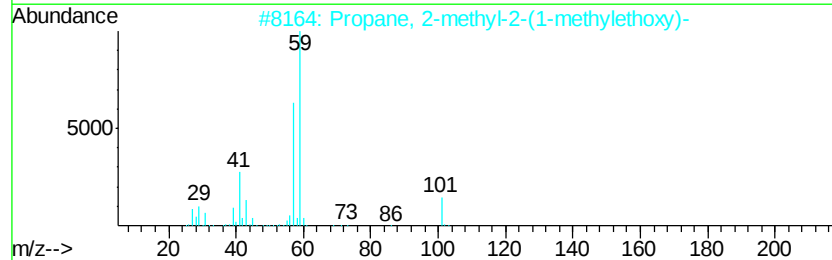
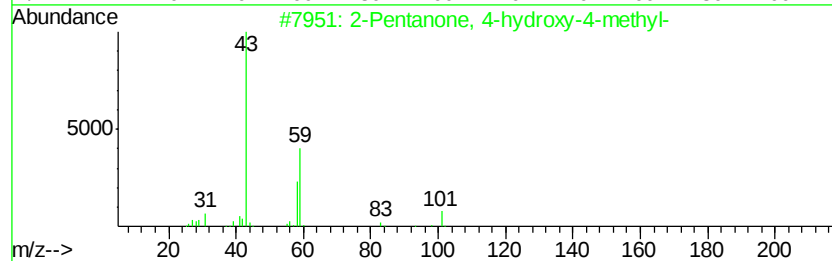
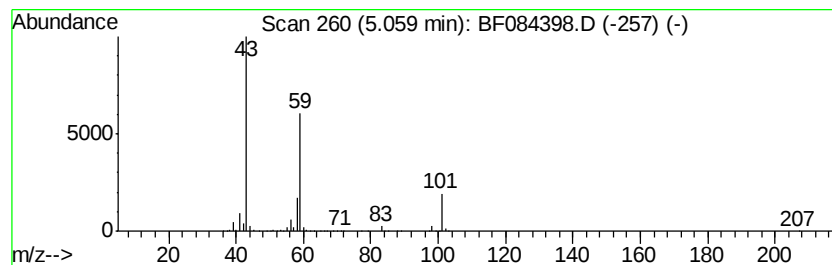
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	36.10 ng	4167770	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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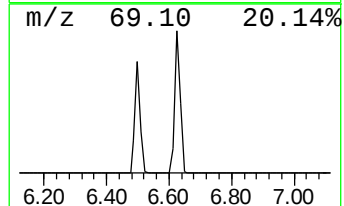
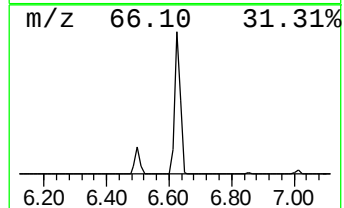
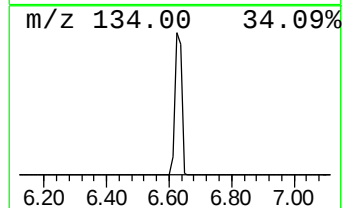
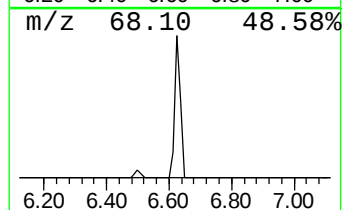
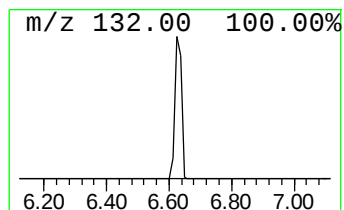
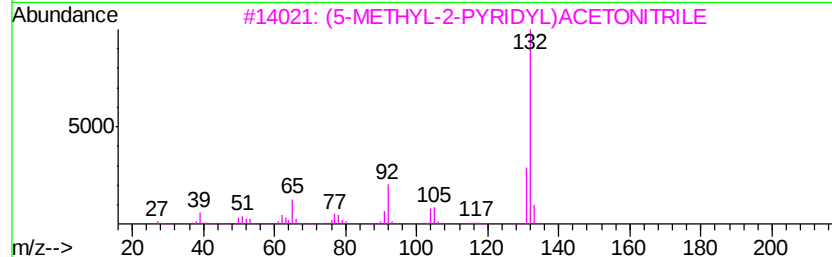
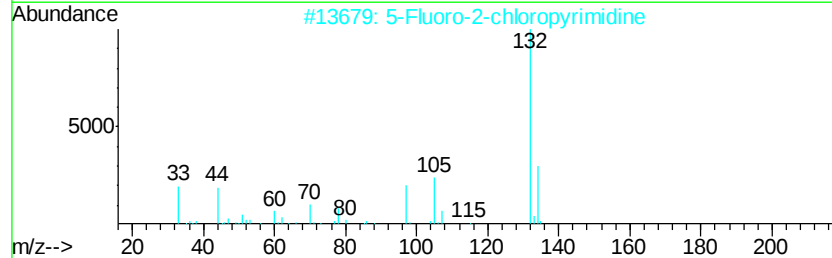
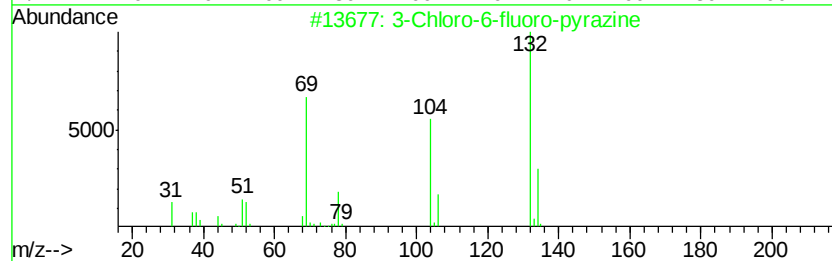
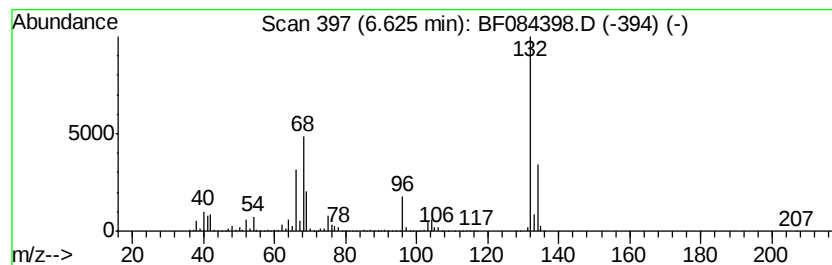
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Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	85.90 ng	9918370	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
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
n-Propyl acetate	2.70	3.4	ng	391771	1	6.85	2309240	20.0
3-Penten-2-one, 4...	4.41	2.1	ng	245848	1	6.85	2309240	20.0
2-Pentanone, 4-hy...	5.06	36.1	ng	4167770	1	6.85	2309240	20.0
unknown6.62	6.62	85.9	ng	9918370	1	6.85	2309240	20.0