

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100517\
 Data File : BF099110.D
 Acq On : 5 Oct 2017 18:25
 Operator : SJ/JU
 Sample : PB102898BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB102898BL

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-BF092317.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	3.657	262	267	276	rBV	64658	96949	2.83%	0.348%
2	4.493	406	409	418	rBV	112939	126576	3.69%	0.455%
3	5.104	509	513	529	rBV	494450	655403	19.12%	2.356%
4	5.492	574	579	582	rBV	2792261	2973362	86.75%	10.688%
5	6.492	743	749	752	rBV	2568769	2913169	84.99%	10.472%
6	6.634	768	773	776	rBV	2948586	3011312	87.85%	10.824%
7	6.863	808	812	815	rBV	891614	720669	21.03%	2.590%
8	7.022	834	839	842	rBV	2431712	2377210	69.35%	8.545%
9	7.428	902	908	911	rBV	1778022	1882871	54.93%	6.768%
10	8.145	1025	1030	1033	rBV	1064997	989492	28.87%	3.557%
11	9.222	1207	1213	1216	rBV	3314199	3427634	100.00%	12.321%
12	9.898	1323	1328	1332	rBV2	1209453	1082543	31.58%	3.891%
13	10.692	1457	1463	1466	rBV	1771882	1854426	54.10%	6.666%
14	11.386	1575	1581	1584	rBV	1328368	1091523	31.84%	3.924%
15	12.974	1844	1851	1854	rBV	3023479	3102456	90.51%	11.152%
16	14.027	2025	2030	2033	rBV	957307	917359	26.76%	3.297%
17	15.498	2274	2280	2288	rBV	468842	596884	17.41%	2.146%

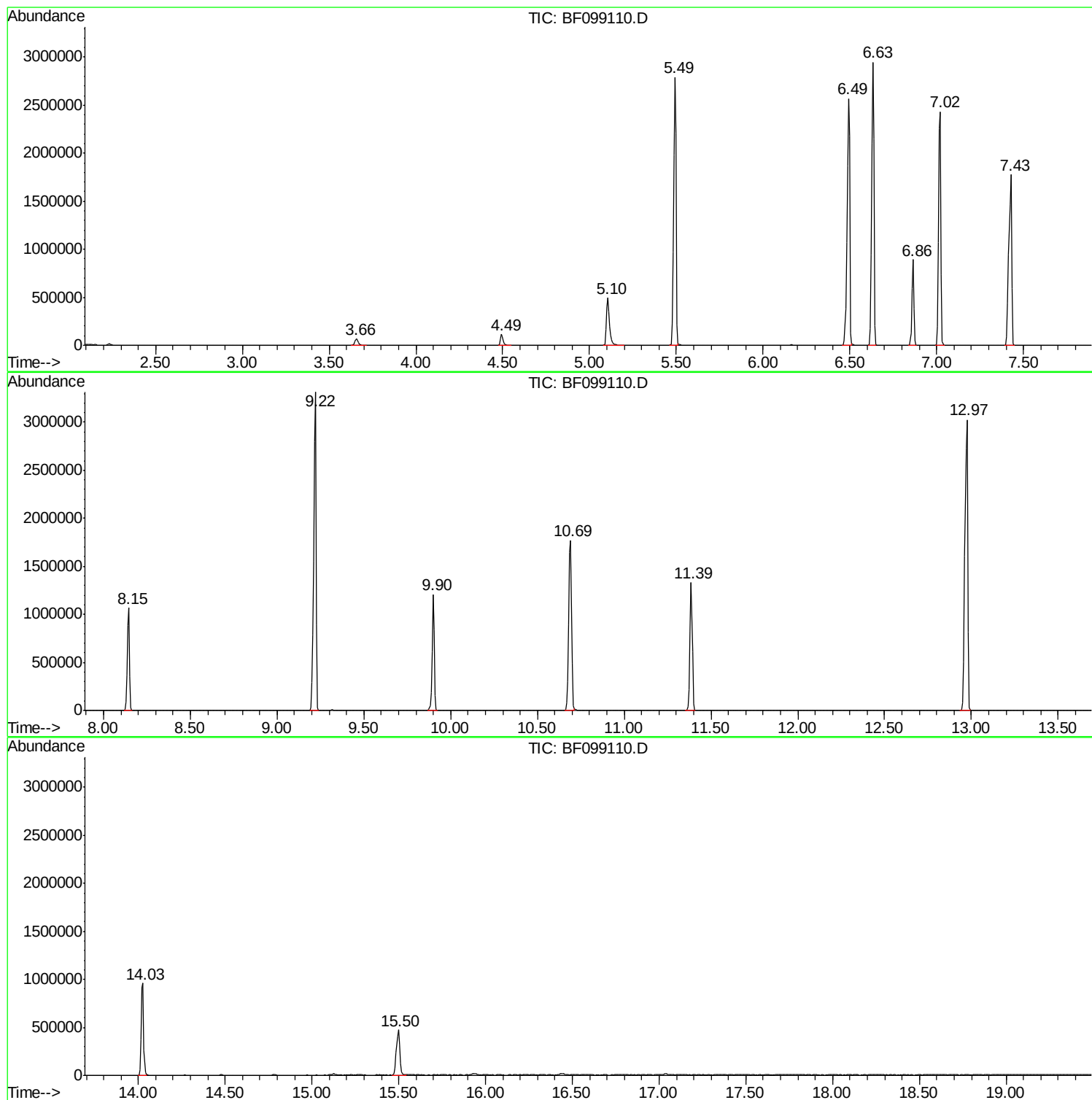
Sum of corrected areas: 27819838

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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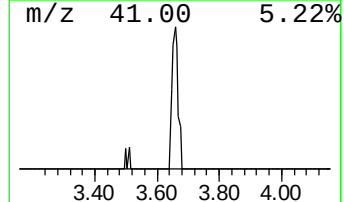
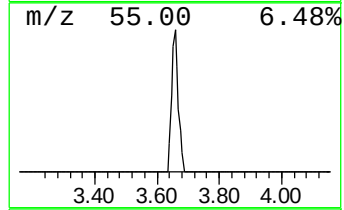
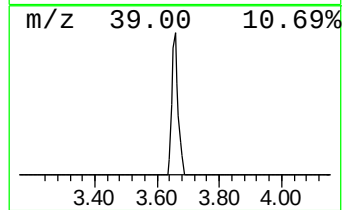
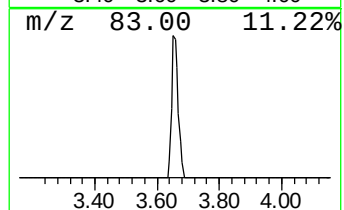
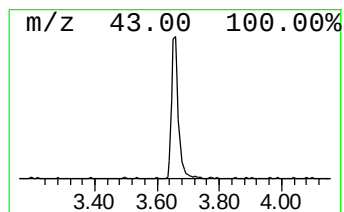
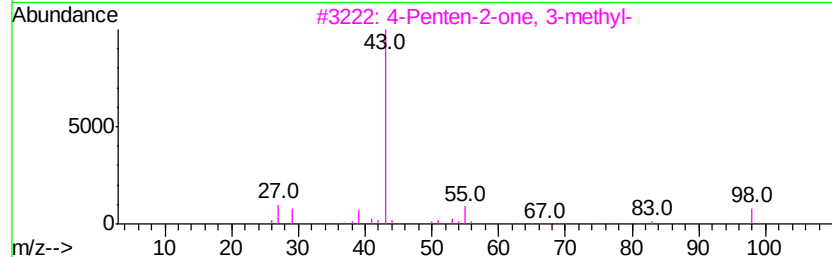
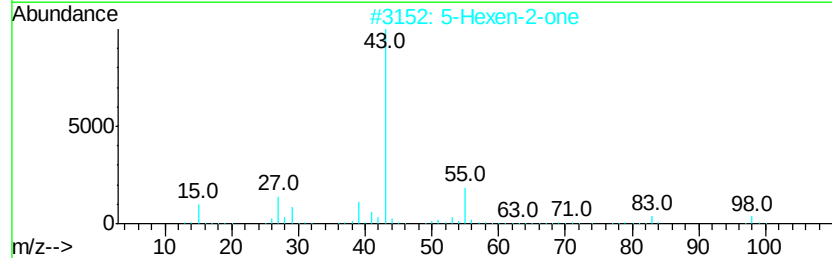
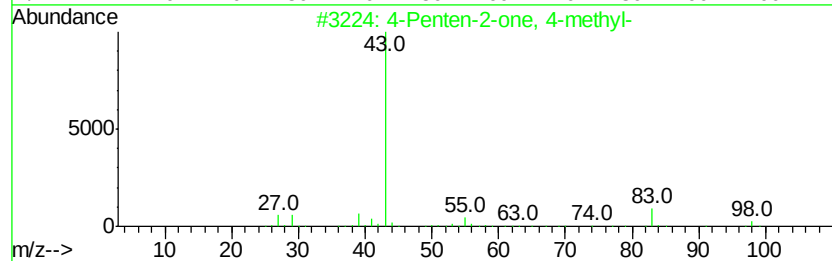
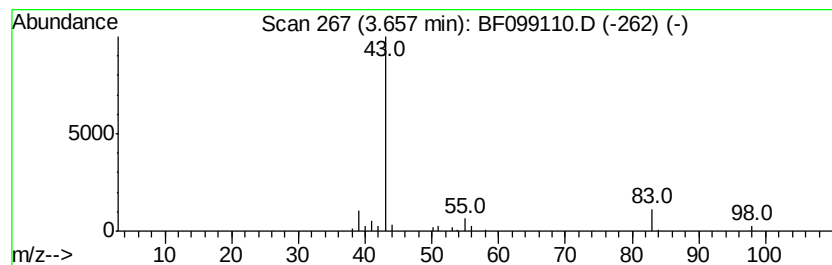
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.66	2.69 ng	96949	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	53
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4		4-Hexen-2-one	98	C6H10O	025659-22-7	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	5



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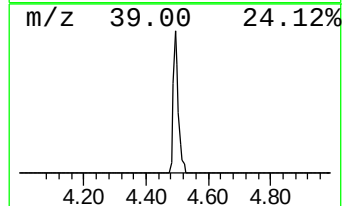
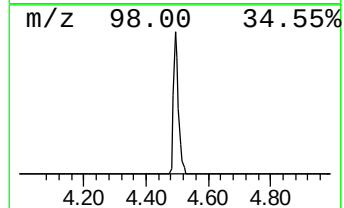
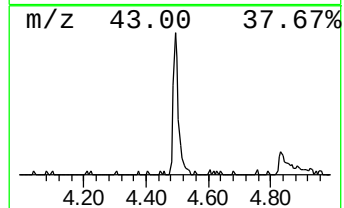
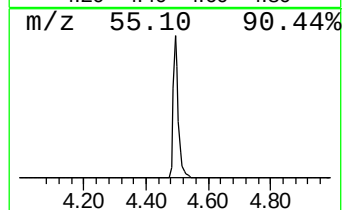
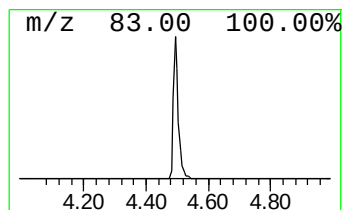
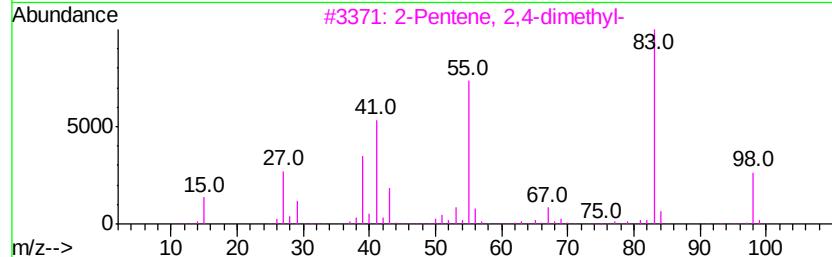
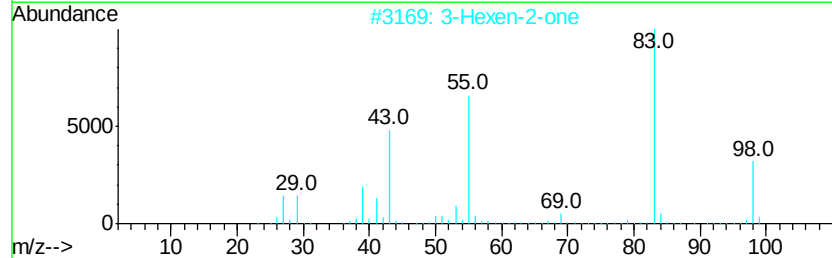
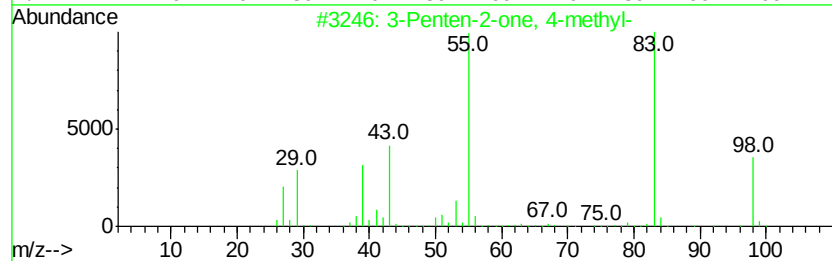
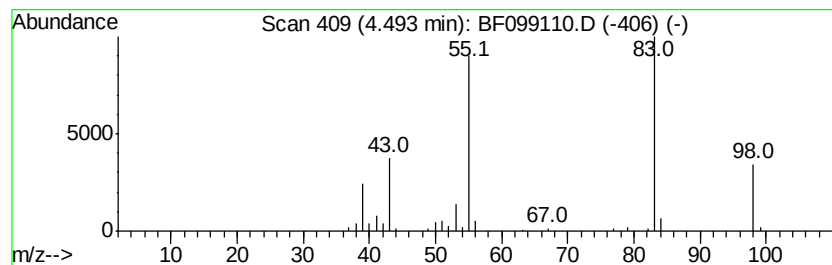
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	3.51 ng	126576	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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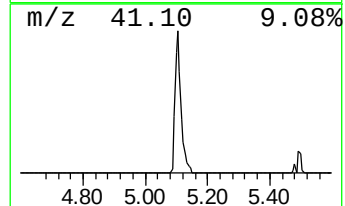
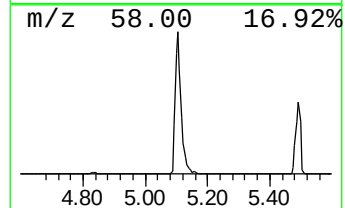
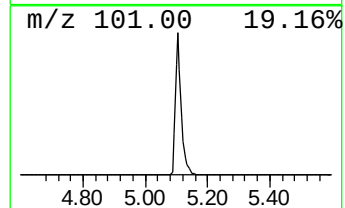
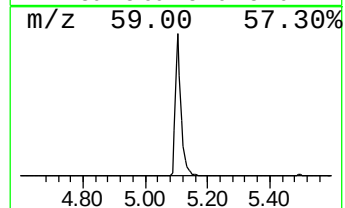
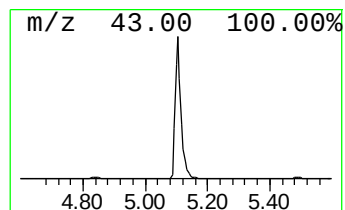
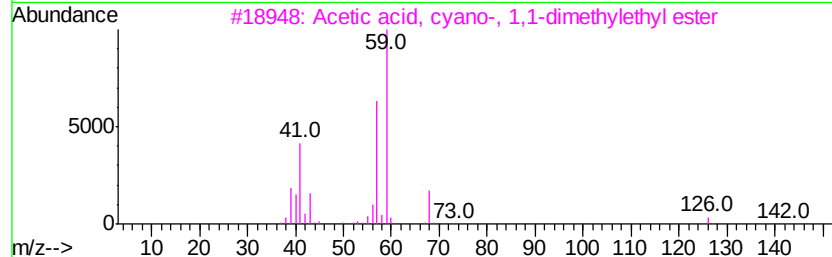
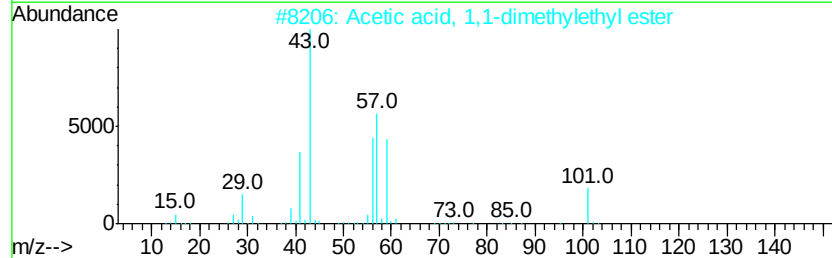
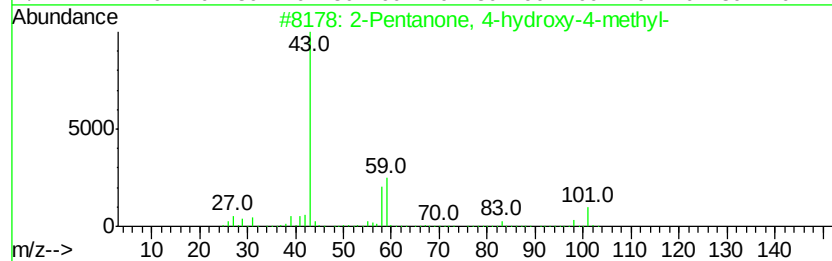
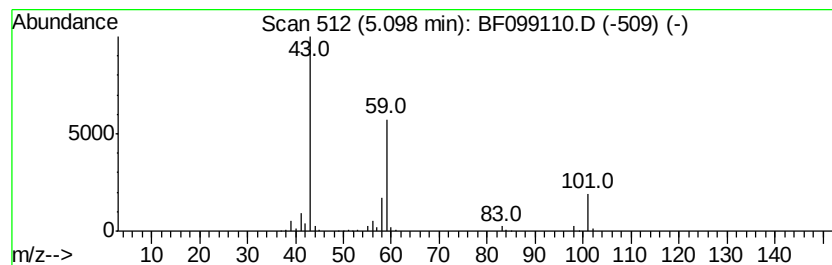
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	18.19 ng	655403	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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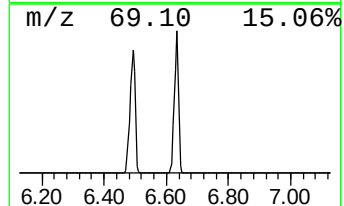
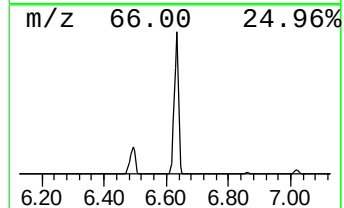
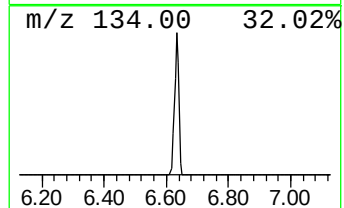
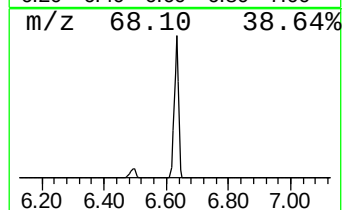
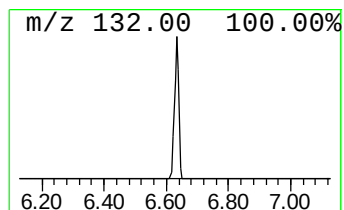
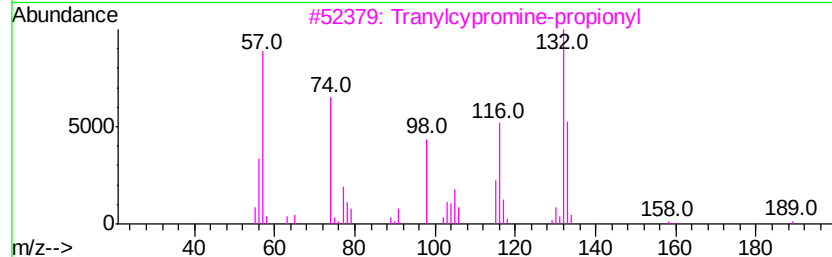
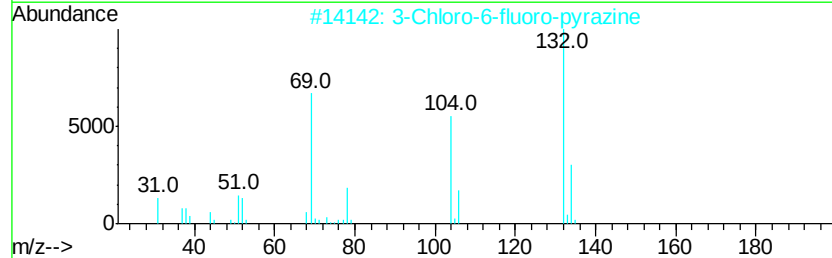
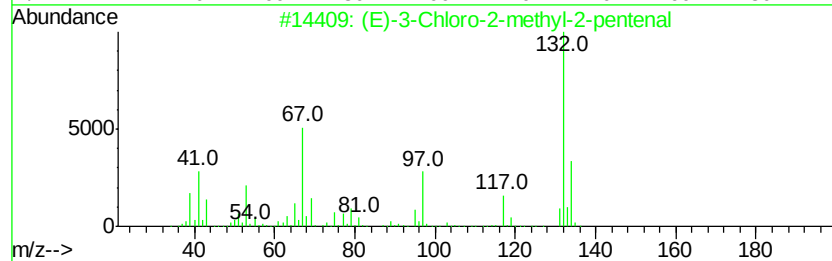
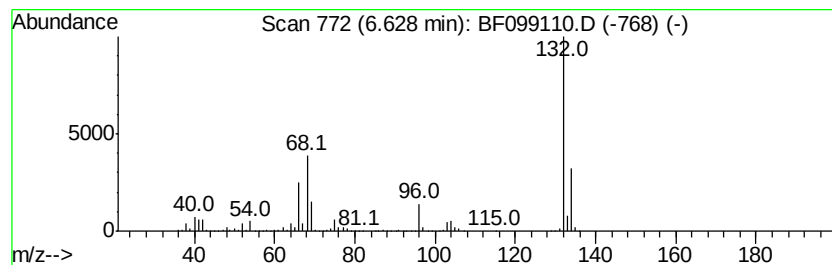
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Peak Number 4 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	83.57 ng	3011310	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.66	2.7	ng	96949	1	6.86	720669	20.0
3-Penten-2-one, 4...	4.49	3.5	ng	126576	1	6.86	720669	20.0
2-Pentanone, 4-hy...	5.10	18.2	ng	655403	1	6.86	720669	20.0
unknown6.63	6.63	83.6	ng	3011310	1	6.86	720669	20.0