

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
 Data File : BF081057.D
 Acq On : 18 Aug 2015 23:01
 Operator : UM/IZ
 Sample : PB85016BL
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB85016BL

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-BF081715.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	3.999	174	176	182	rBV	51048	82458	3.30%	0.386%
2	4.741	236	241	250	rBV	1025817	1744819	69.72%	8.165%
3	5.187	277	280	282	rBV	1896728	2092603	83.62%	9.792%
4	5.599	314	316	319	rBV	82122	69157	2.76%	0.324%
5	6.250	370	373	376	rBV	1643009	1848540	73.87%	8.650%
6	6.376	381	384	386	rBV	1729154	2103209	84.04%	9.842%
7	6.605	402	404	406	rBV	582260	482258	19.27%	2.257%
8	6.765	415	418	420	rBV	1526530	1569160	62.70%	7.343%
9	7.176	451	454	456	rBV	1381723	1387195	55.43%	6.491%
10	7.885	514	516	519	rBV	470355	594851	23.77%	2.784%
11	8.970	608	611	613	rBV	2428612	2231525	89.17%	10.442%
12	9.633	666	669	672	rBB	824819	716513	28.63%	3.353%
13	10.422	735	738	740	rBV	1358575	1482557	59.24%	6.938%
14	11.108	795	798	800	rBV	907641	815333	32.58%	3.815%
15	12.537	920	923	924	rBV	65830	65977	2.64%	0.309%
16	12.697	934	937	939	rBV	2364426	2502510	100.00%	11.710%
17	13.234	982	984	986	rBB	72134	57656	2.30%	0.270%
18	13.279	986	988	989	rBV	38147	31335	1.25%	0.147%
19	13.611	1015	1017	1019	rBV	29955	29299	1.17%	0.137%
20	13.725	1024	1027	1029	rBV	794240	782211	31.26%	3.660%
21	13.920	1042	1044	1047	rVB	41010	35491	1.42%	0.166%
22	14.514	1094	1096	1099	rVB	25365	25054	1.00%	0.117%
23	15.074	1141	1145	1147	rBV	416813	620189	24.78%	2.902%

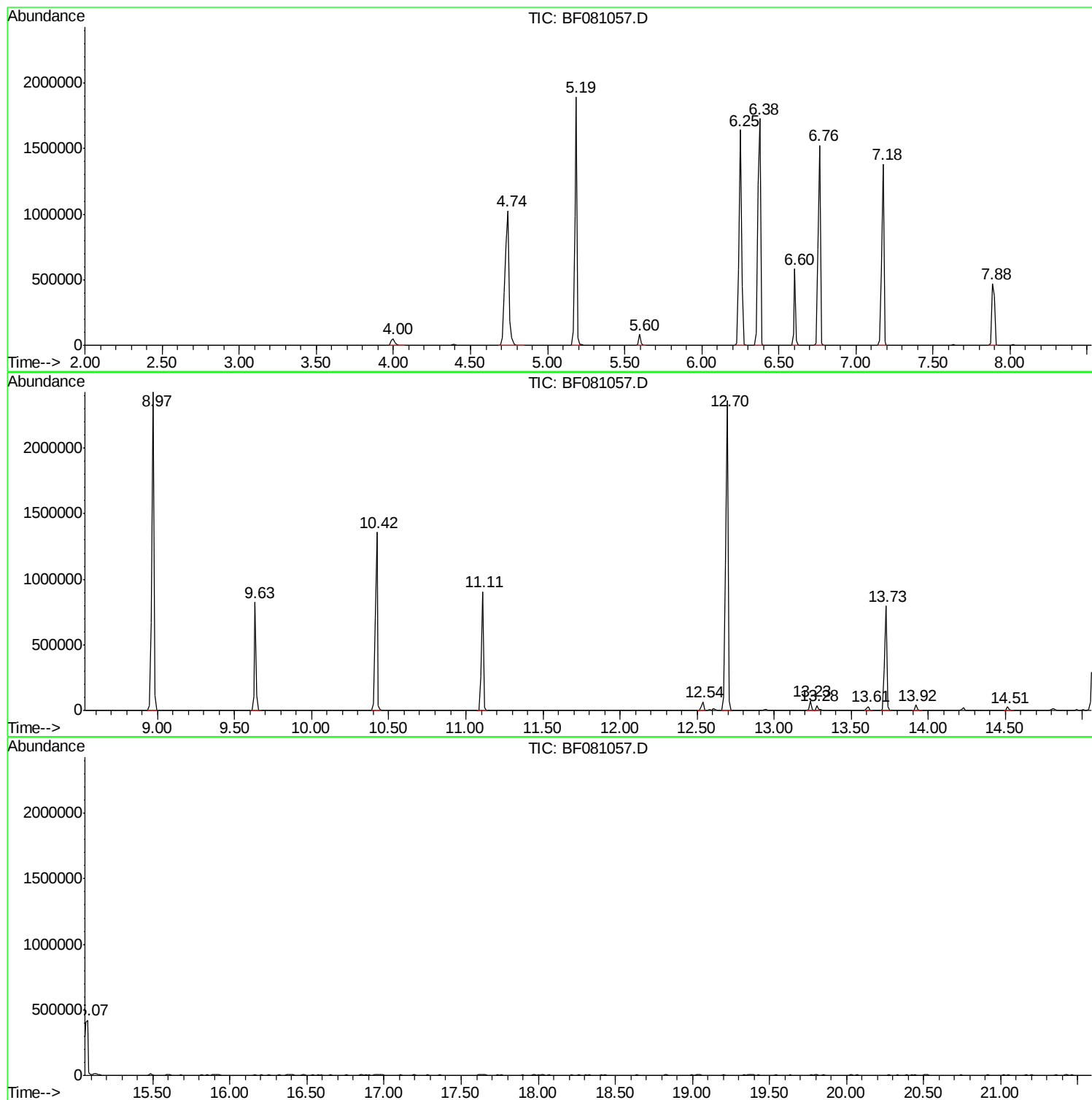
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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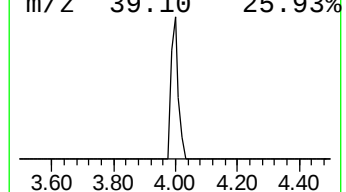
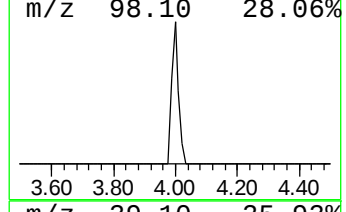
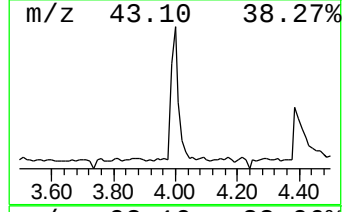
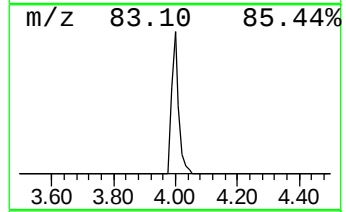
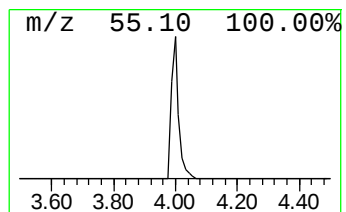
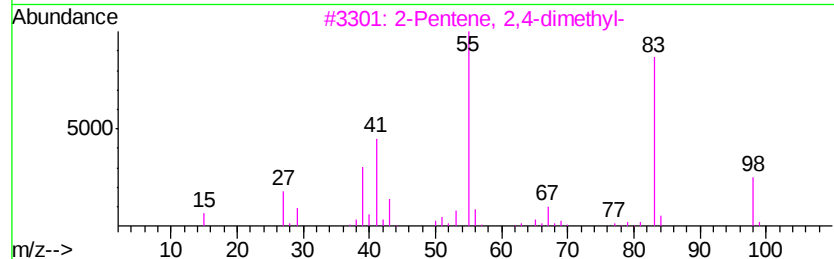
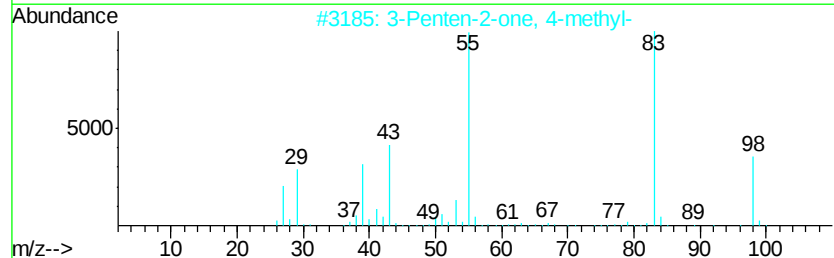
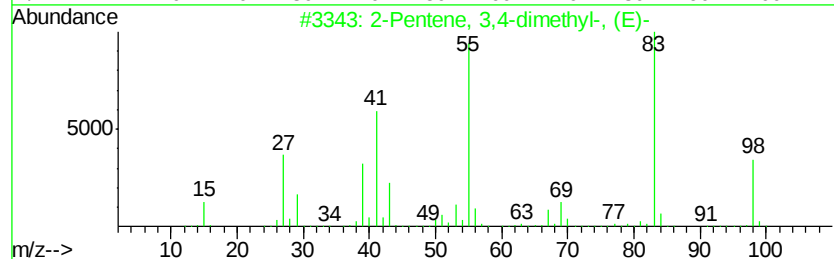
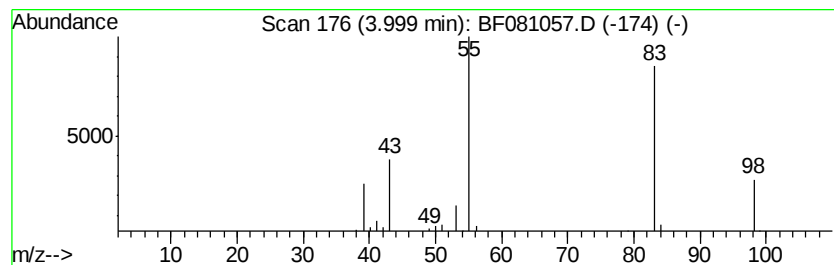
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	3.42 ng	82458	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	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	86
4			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5			3-Hexen-2-one	98	C6H10O	000763-93-9	86



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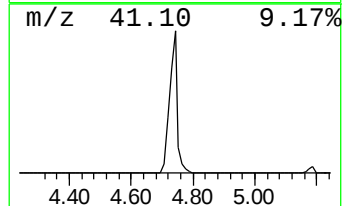
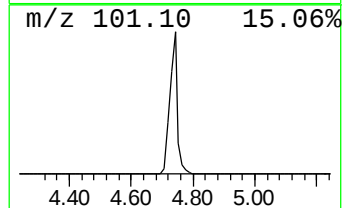
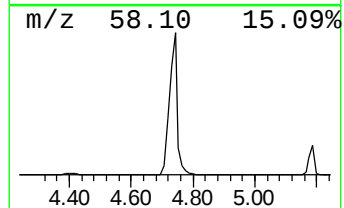
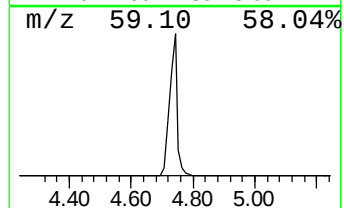
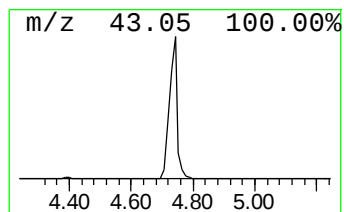
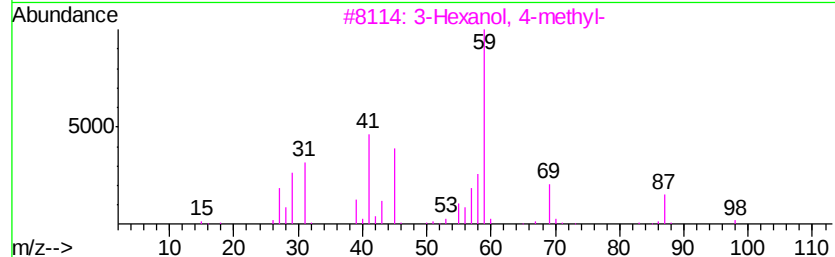
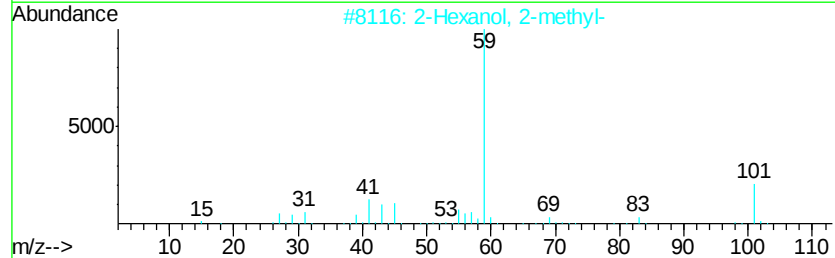
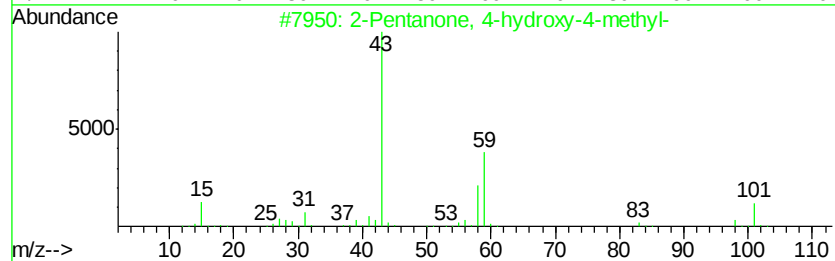
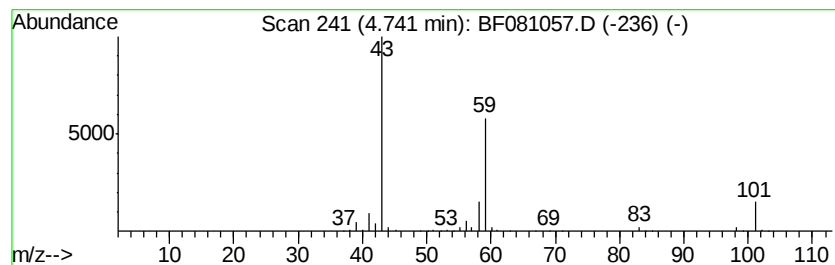
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	72.36 ng	1744820	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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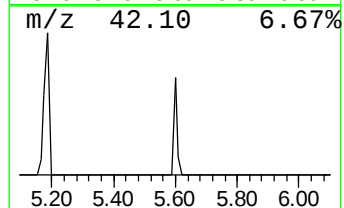
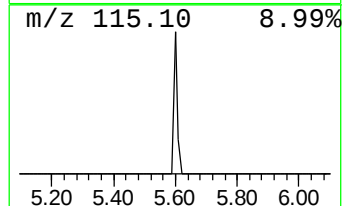
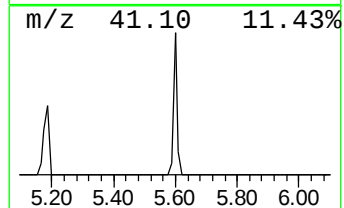
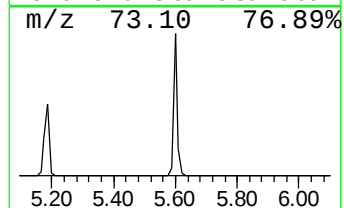
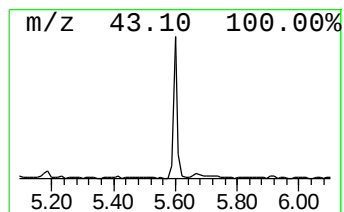
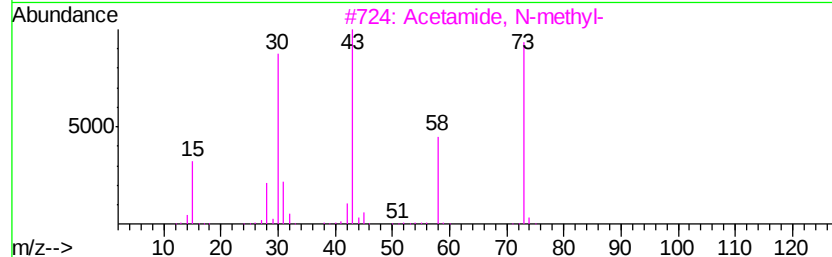
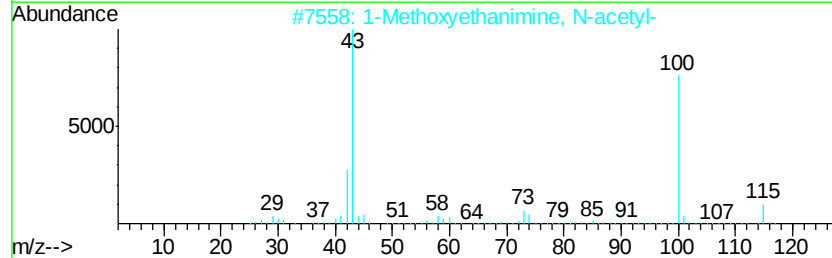
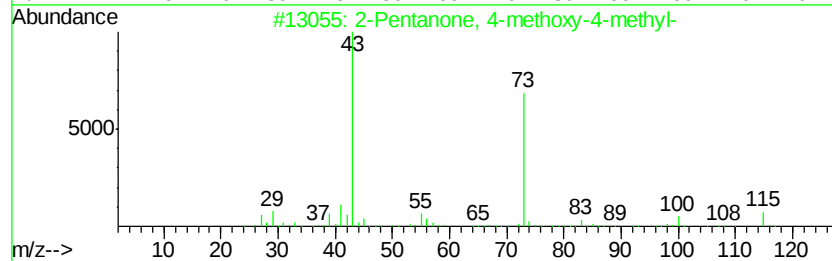
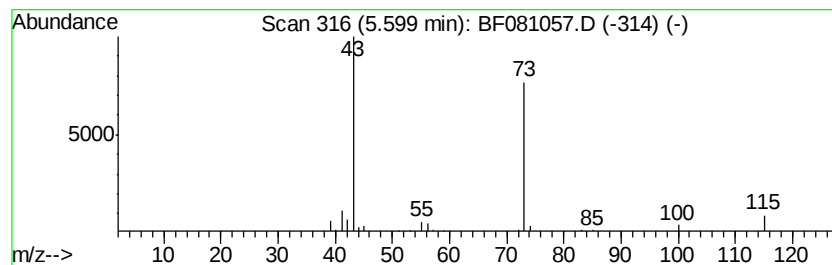
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	2.87 ng	69157	1,4-Dichlorobenzene-d4	6.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	43
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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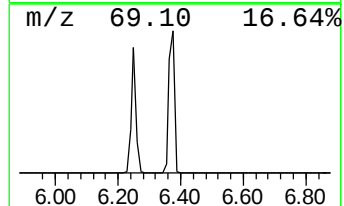
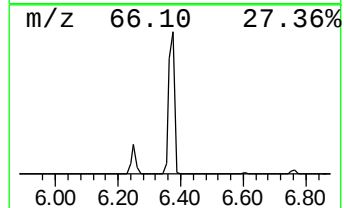
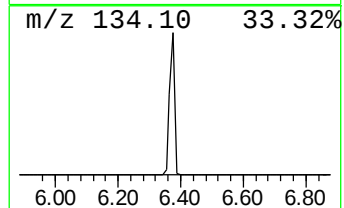
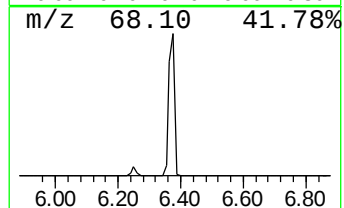
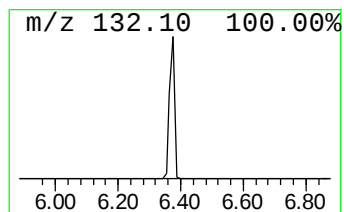
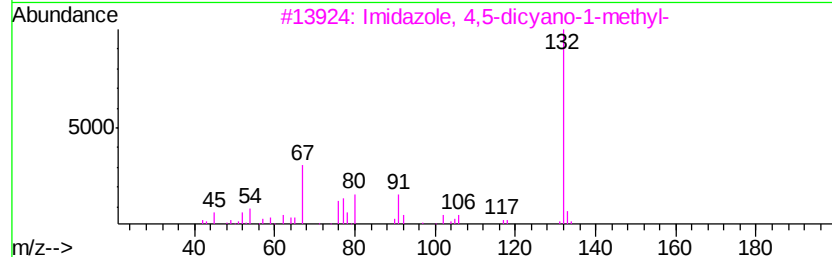
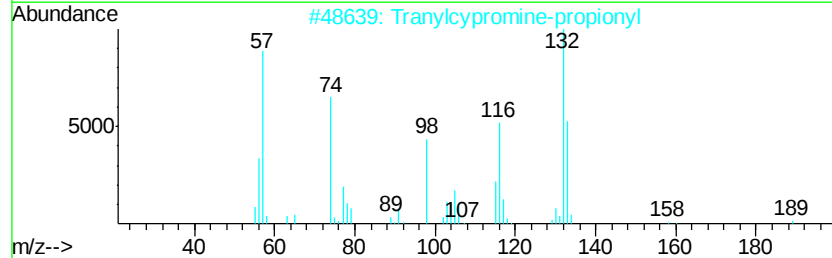
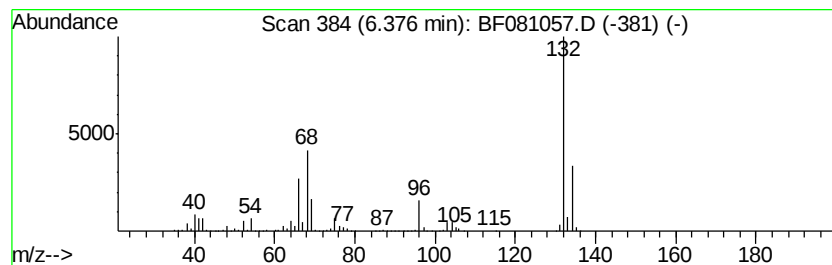
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Peak Number 4 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	87.22 ng	2103210	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentene, 3,4-di...	4.00	3.4	ng	82458	1	6.60	482258	20.0
2-Pentanone, 4-hy...	4.74	72.4	ng	1744820	1	6.60	482258	20.0
2-Pentanone, 4-me...	5.60	2.9	ng	69157	1	6.60	482258	20.0
unknown6.38	6.38	87.2	ng	2103210	1	6.60	482258	20.0