

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
 Data File : BF082779.D
 Acq On : 6 Nov 2015 23:51
 Operator : UM/IZ
 Sample : G4258-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-WP11-1(0-2)

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-BF110715.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	2.144	4	5	18	rVB	98244	248710	4.97%	0.505%
2	2.316	18	20	32	rVB3	28194	74644	1.49%	0.152%
3	4.396	199	202	205	rBV	151187	203449	4.07%	0.413%
4	5.036	255	258	261	rBV	1892054	2320905	46.39%	4.716%
5	5.459	292	295	297	rBV	4798889	5002598	100.00%	10.164%
6	6.476	381	384	386	rBV	4708454	4570493	91.36%	9.286%
7	6.613	393	396	398	rBV	5048660	4592214	91.80%	9.330%
8	6.842	414	416	418	rBV	1321184	1396341	27.91%	2.837%
9	7.002	428	430	433	rBV	3657701	3255026	65.07%	6.614%
10	7.402	462	465	468	rBV	2427190	2933084	58.63%	5.959%
11	7.516	472	475	482	rVB	25400	50210	1.00%	0.102%
12	8.133	526	529	531	rBV	1771330	1760122	35.18%	3.576%
13	9.208	620	623	626	rBV	4103982	4626713	92.49%	9.401%
14	9.608	655	658	660	rBV	1042314	1169449	23.38%	2.376%
15	9.882	679	682	685	rBV	1804974	2200312	43.98%	4.471%
16	10.305	716	719	720	rBV	52519	52031	1.04%	0.106%
17	10.328	720	721	723	rVB	61019	56910	1.14%	0.116%
18	10.671	748	751	754	rBV	3479747	3435164	68.67%	6.980%
19	10.808	760	763	767	rVB	93946	153124	3.06%	0.311%
20	11.254	800	802	803	rBV	110677	99261	1.98%	0.202%
21	11.368	809	812	814	rBV	2695456	2359788	47.17%	4.795%
22	11.676	837	839	842	rVB	78197	67920	1.36%	0.138%
23	11.905	857	859	868	rBV2	135563	259974	5.20%	0.528%
24	12.694	924	928	932	rBV2	39852	58182	1.16%	0.118%
25	12.957	948	951	953	rBV	5148032	4702856	94.01%	9.555%
26	13.997	1040	1042	1045	rBV	1609717	1876167	37.50%	3.812%
27	14.865	1116	1118	1121	rVB	82824	86907	1.74%	0.177%
28	15.425	1164	1167	1170	rBV	1387390	1605078	32.08%	3.261%

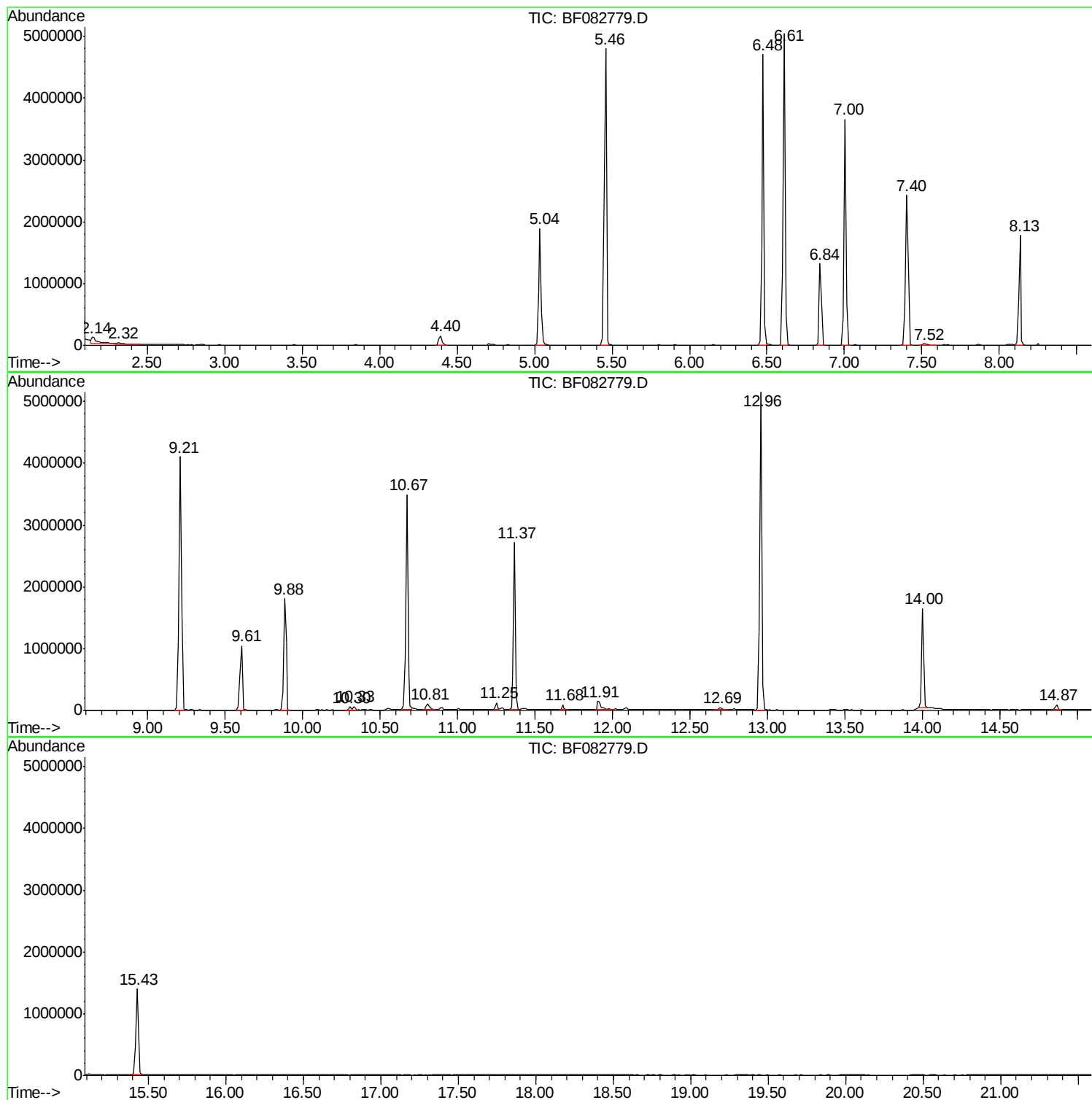
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ClientSampleId :
COFF-WP11-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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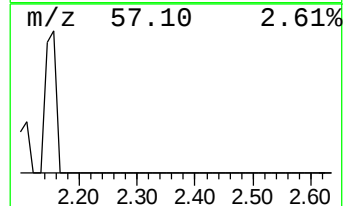
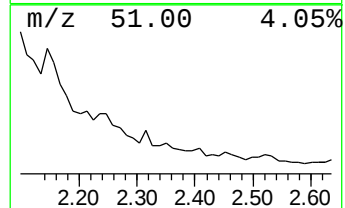
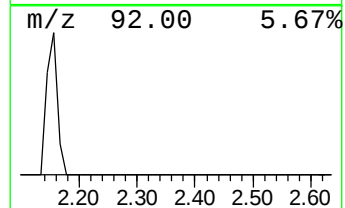
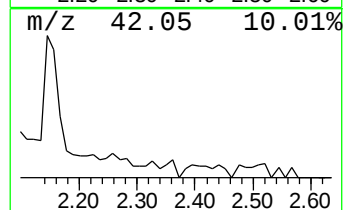
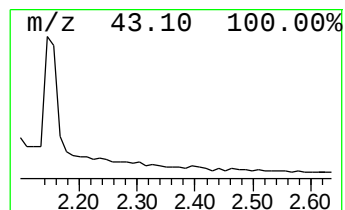
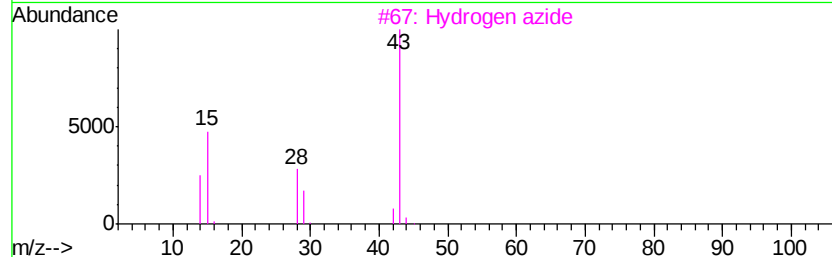
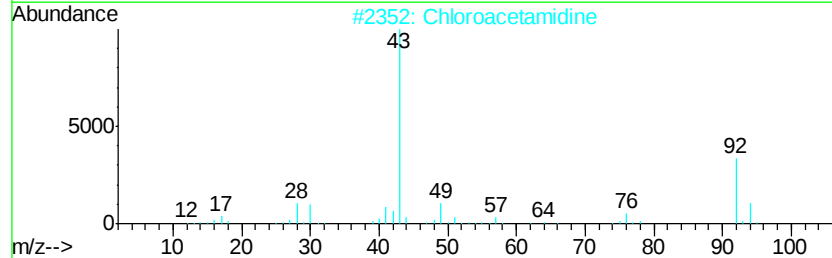
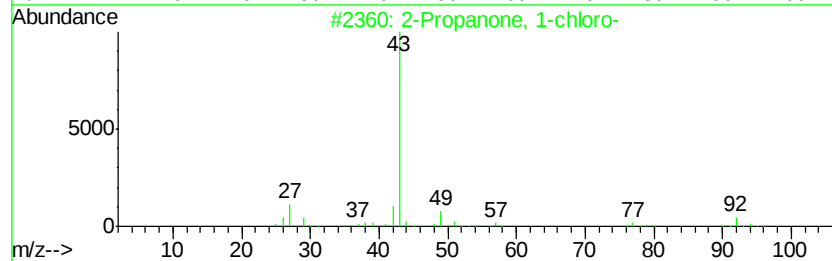
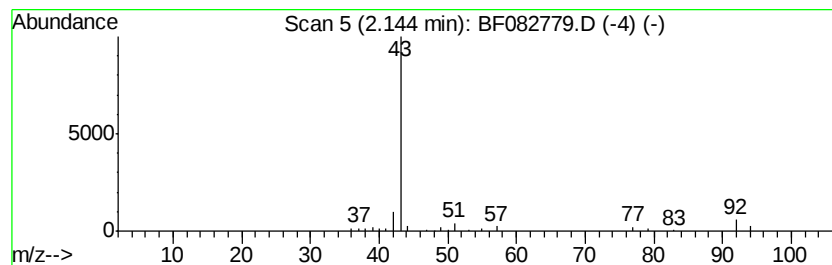
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Propanone, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	3.56 ng	248710	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	86
2			Chloroacetamidine	92	C2H5ClN2	020846-52-0	4
3			Hvdrogen azide	43	HN3	007782-79-8	4
4			2-Acetyl-2-methyl-succinonitrile	136	C7H8N2O	082471-44-1	2
5			Isobutyl nitrite	103	C4H9NO2	000542-56-3	2



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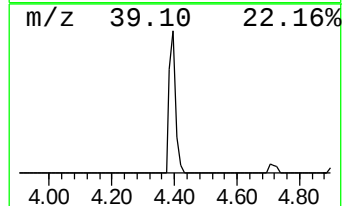
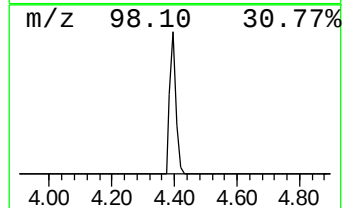
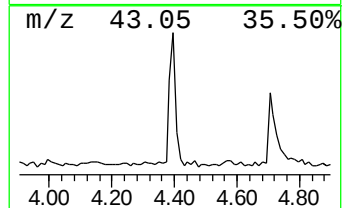
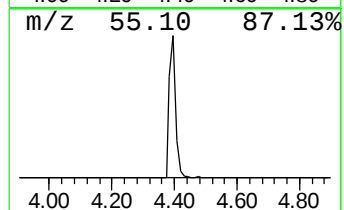
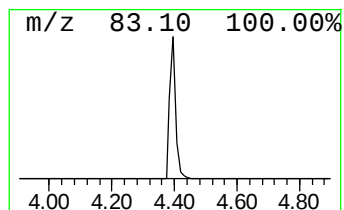
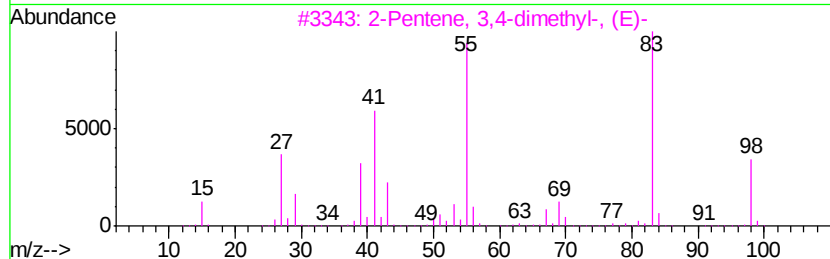
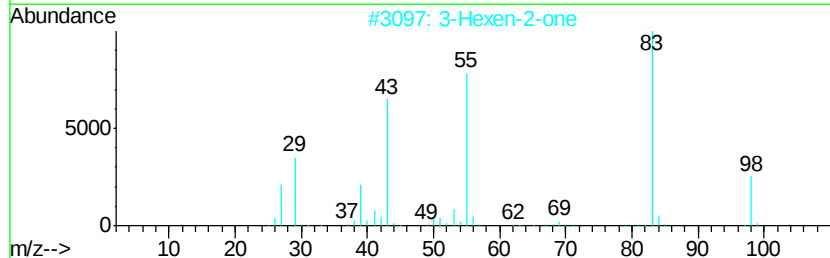
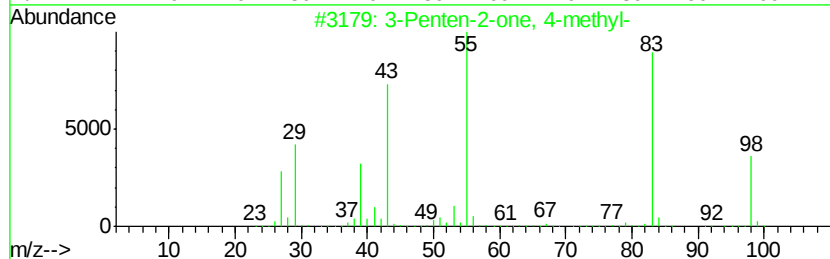
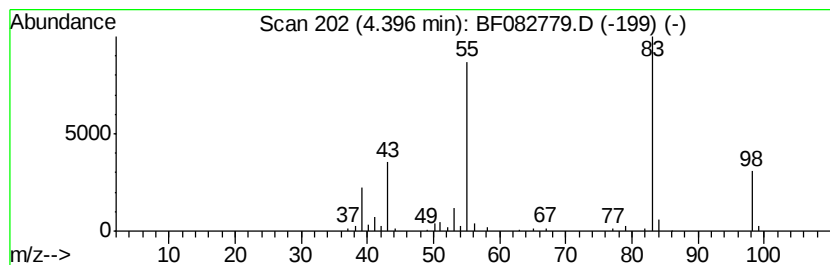
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.91 ng	203449	1,4-Dichlorobenzene-d4	6.84

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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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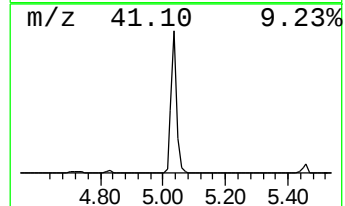
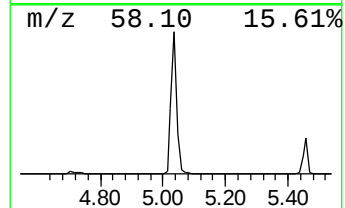
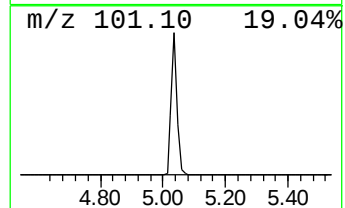
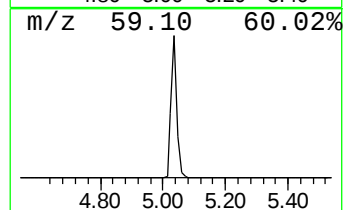
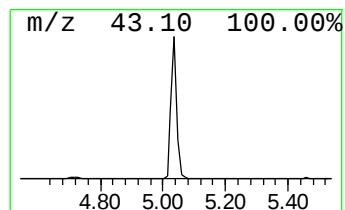
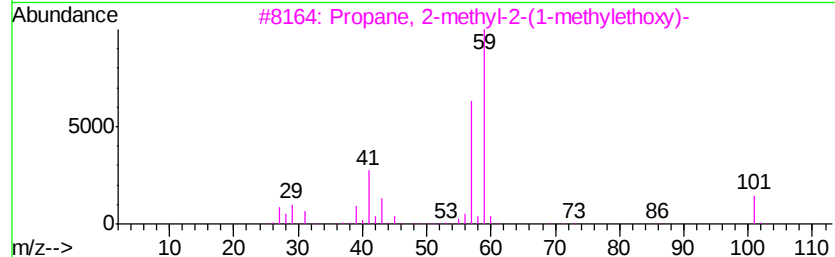
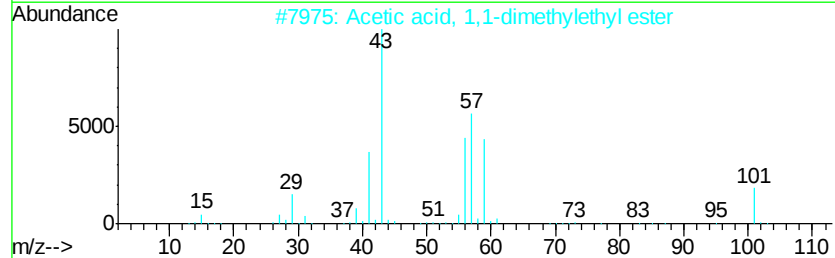
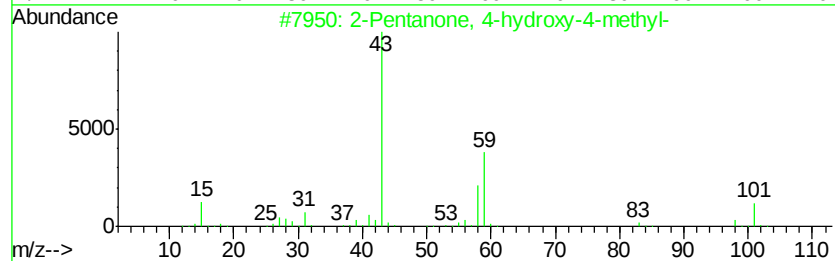
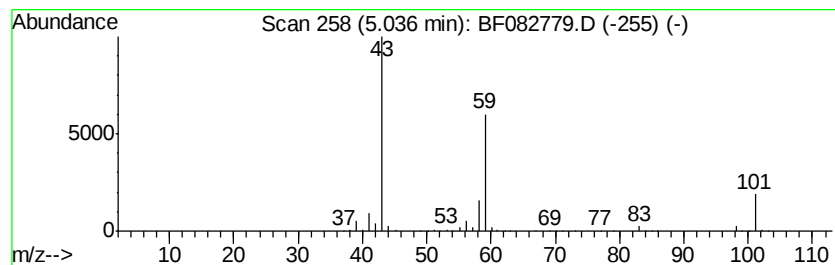
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	33.24 ng	2320910	1,4-Dichlorobenzene-d4	6.84

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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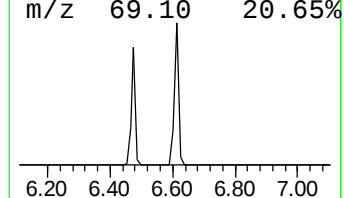
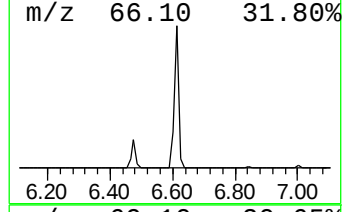
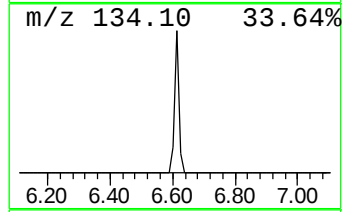
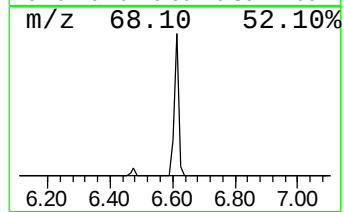
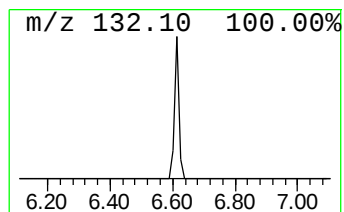
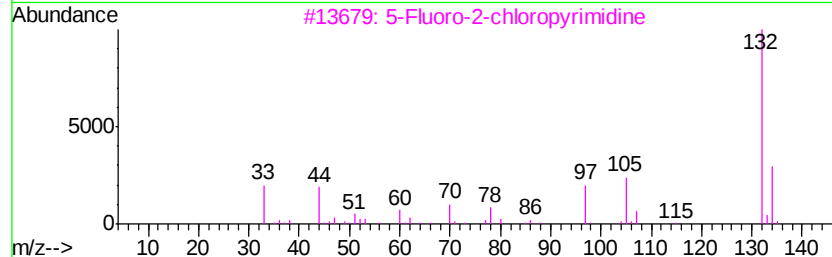
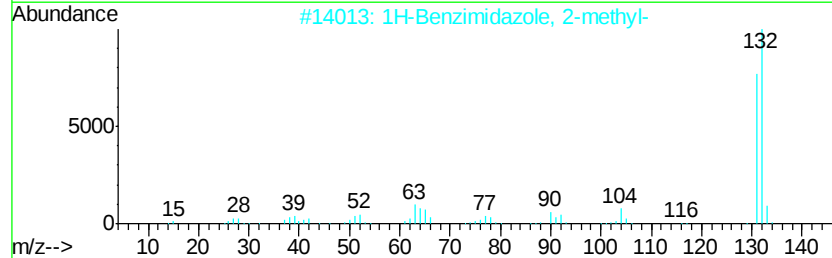
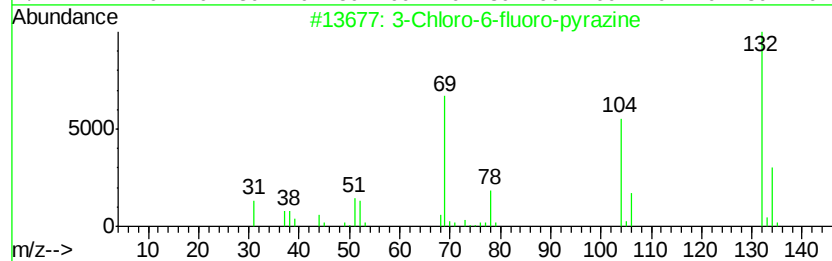
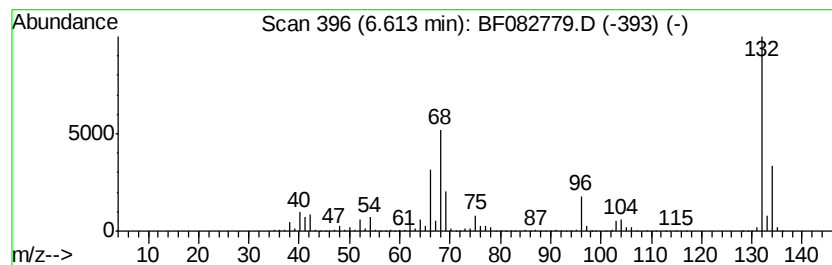
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	65.78 ng	4592210	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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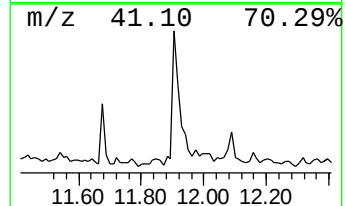
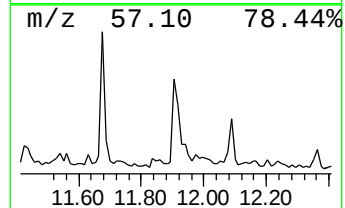
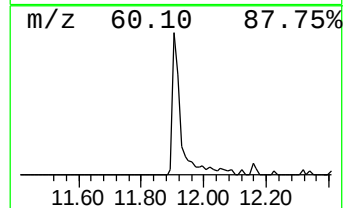
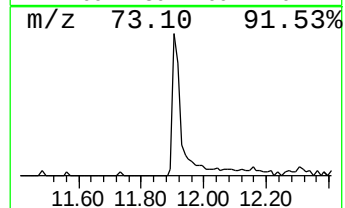
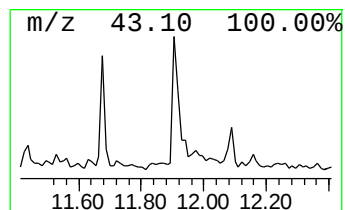
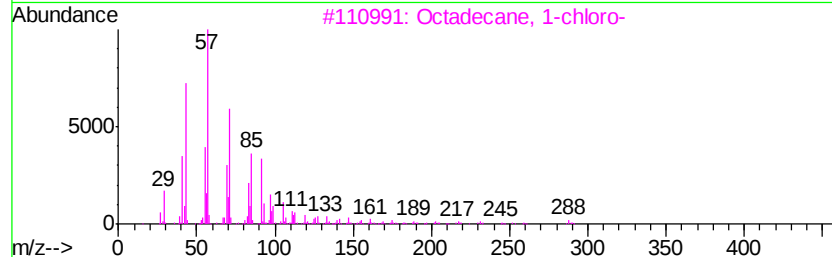
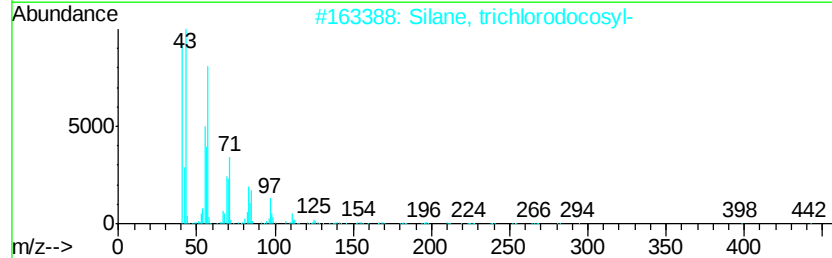
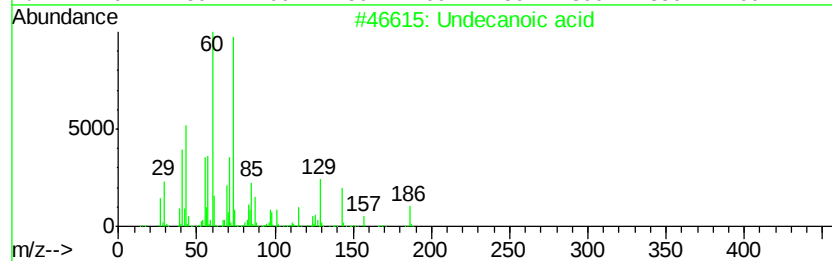
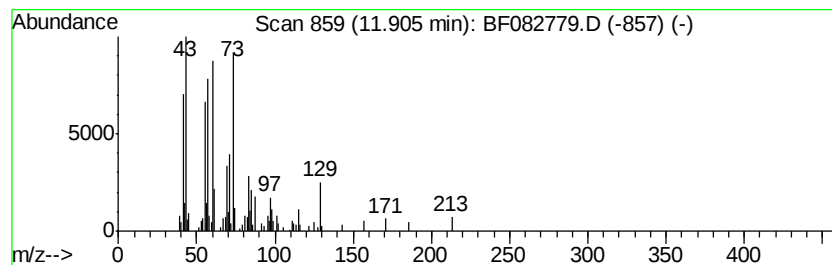
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.20 ng	259974	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	86
2	Silane, trichlorodocosyl-		442	C22H45Cl3Si	007325-84-0	25
3	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	22
4	Undecane		156	C11H24	001120-21-4	18
5	Dodecane		170	C12H26	000112-40-3	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanone, 1-ch...	2.14	3.6	ng	248710	1	6.84	1396340	20.0
3-Penten-2-one, 4...	4.40	2.9	ng	203449	1	6.84	1396340	20.0
2-Pentanone, 4-hy...	5.04	33.2	ng	2320910	1	6.84	1396340	20.0
unknown6.61	6.61	65.8	ng	4592210	1	6.84	1396340	20.0
Undecanoic acid	11.91	2.2	ng	259974	4	11.37	2359790	20.0