

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091815\
 Data File : BF081702.D
 Acq On : 18 Sep 2015 18:04
 Operator : UM/IZ
 Sample : G3704-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-7-9-15-15

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-BF090115.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	1.236	9	13	15	rBV	2789922	3668946	66.51%	17.049%
2	1.304	15	19	26	rVB3	20977	59579	1.08%	0.277%
3	1.441	29	31	37	rBV	145755	395991	7.18%	1.840%
4	1.533	37	39	92	rVB	1418359	5516444	100.00%	25.634%
5	4.424	290	292	309	rBV	77344	207315	3.76%	0.963%
6	5.316	367	370	392	rBV	298337	653699	11.85%	3.038%
7	7.579	566	568	573	rBV	178384	364249	6.60%	1.693%
8	7.682	573	577	587	rVB	794781	1367360	24.79%	6.354%
9	8.162	616	619	623	rBV	167767	271272	4.92%	1.261%
10	8.493	644	648	651	rBV	752030	1229873	22.29%	5.715%
11	9.465	729	733	736	rBV	518849	1096952	19.89%	5.097%
12	11.065	869	873	883	rBV	202087	343780	6.23%	1.597%
13	12.814	1023	1026	1028	rBV	44998	85082	1.54%	0.395%
14	12.860	1028	1030	1036	rVB	39689	70152	1.27%	0.326%
15	13.705	1099	1104	1107	rBV	956888	1920209	34.81%	8.923%
16	15.191	1230	1234	1242	rBB	210703	366230	6.64%	1.702%
17	17.100	1396	1401	1413	rBB	643364	1167490	21.16%	5.425%
18	18.689	1537	1540	1550	rBB	204972	392927	7.12%	1.826%
19	22.072	1832	1836	1839	rBV	1412790	1790384	32.46%	8.320%
20	23.341	1945	1947	1950	rBV	287688	333022	6.04%	1.548%
21	24.781	2071	2073	2078	rBV	204123	219004	3.97%	1.018%

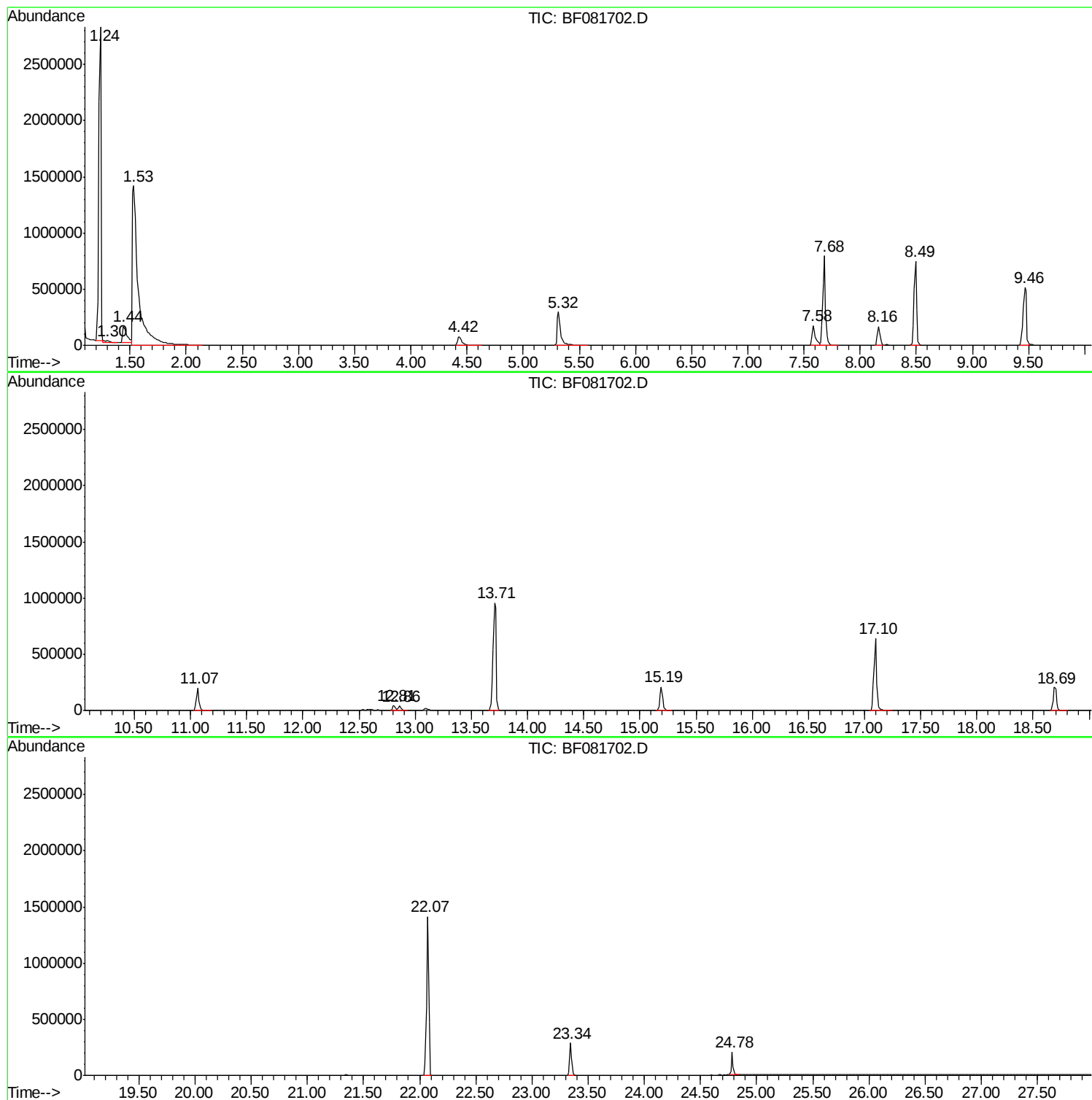
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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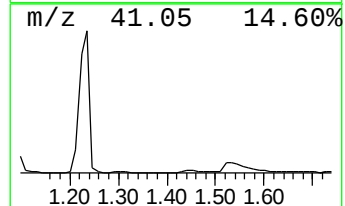
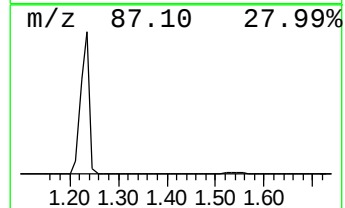
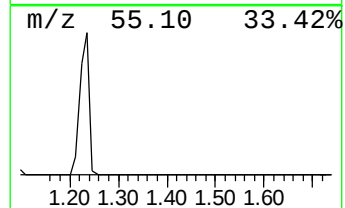
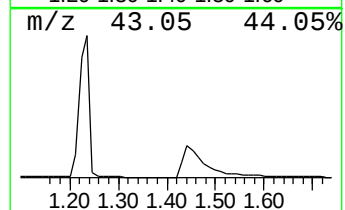
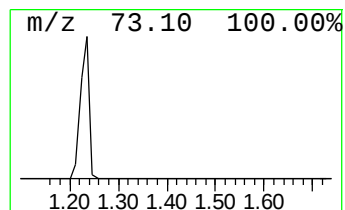
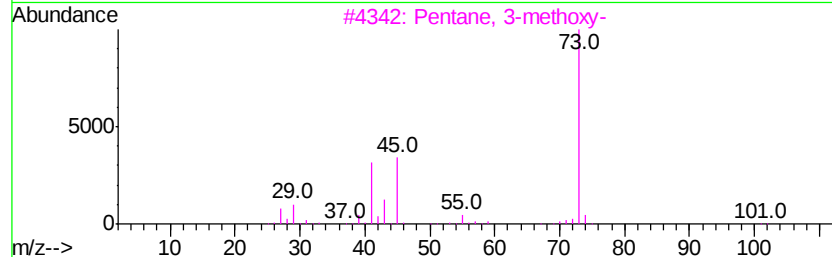
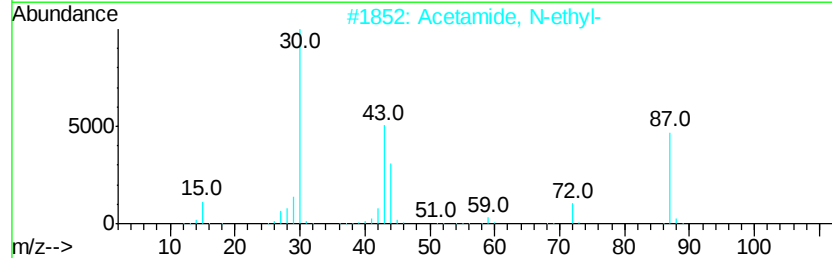
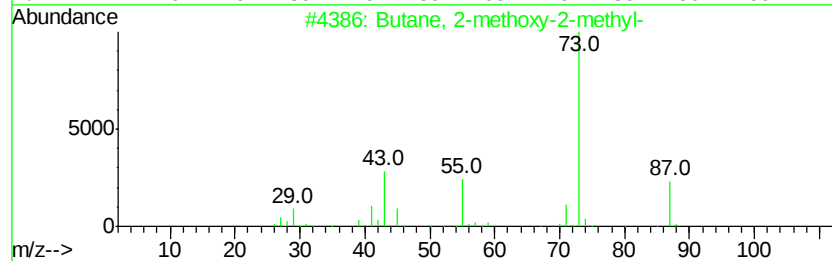
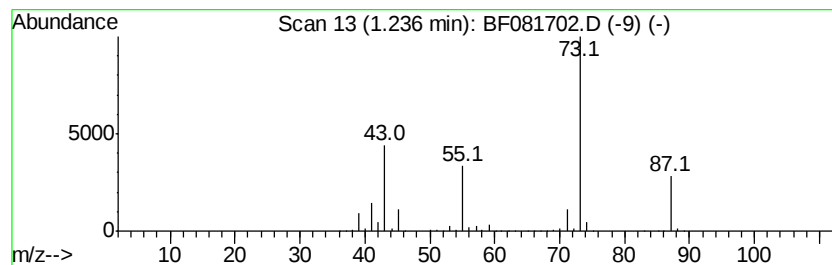
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.24	270.50 ng	3668950	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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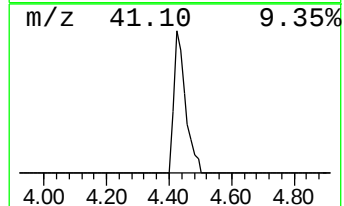
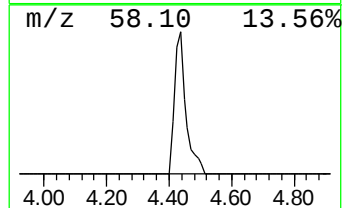
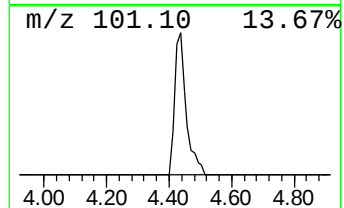
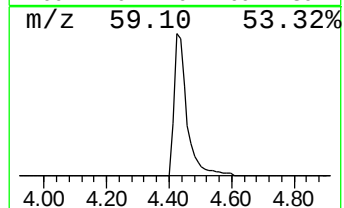
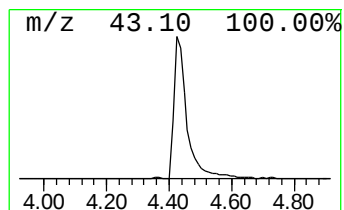
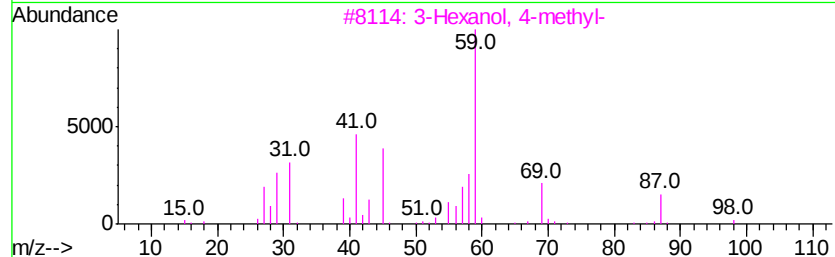
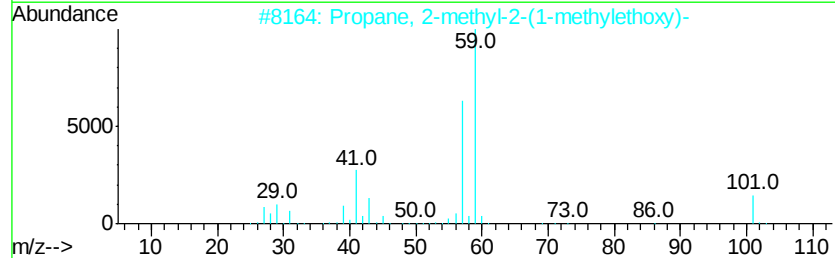
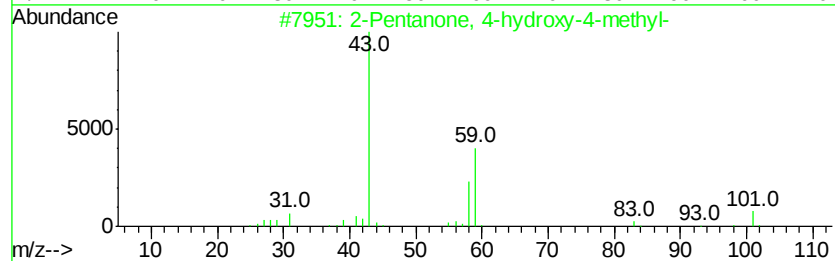
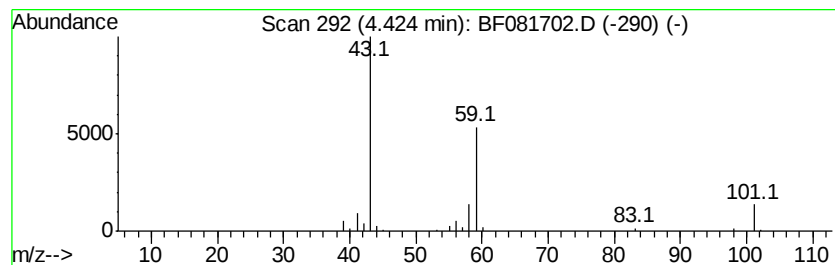
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	15.28 ng	207315	1,4-Dichlorobenzene-d4	8.16

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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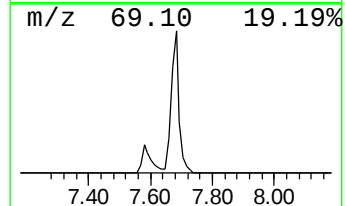
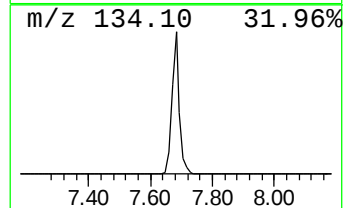
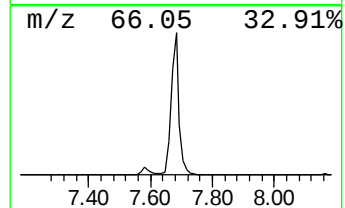
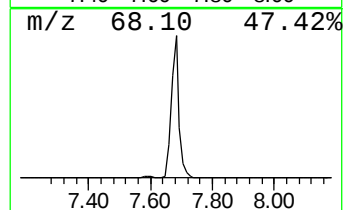
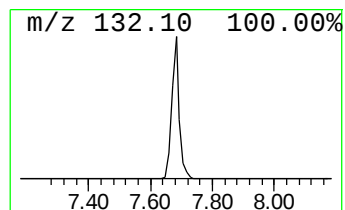
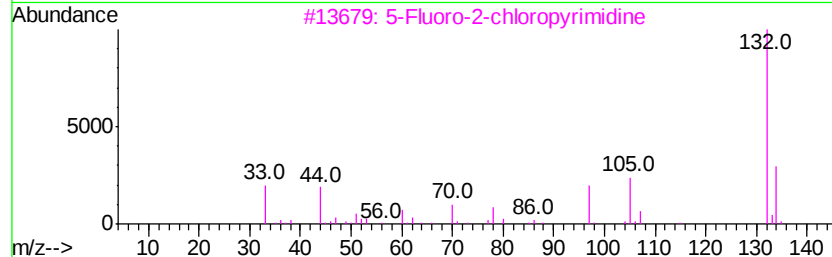
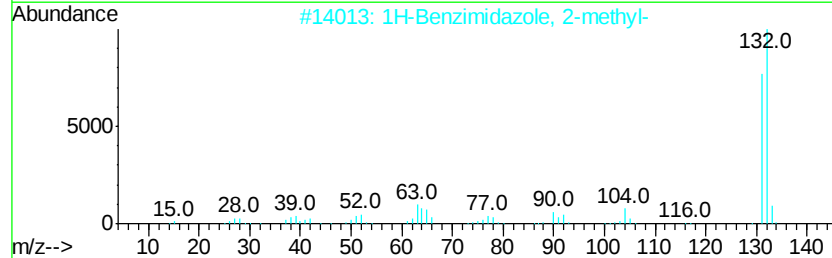
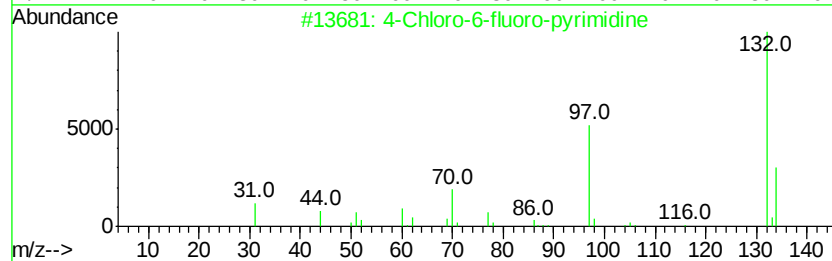
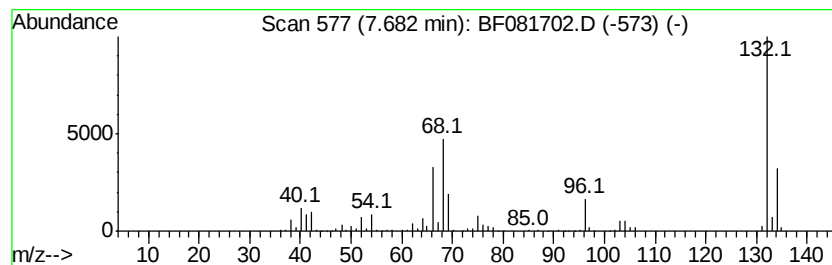
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	100.81 ng	1367360	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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ClientSampleId :
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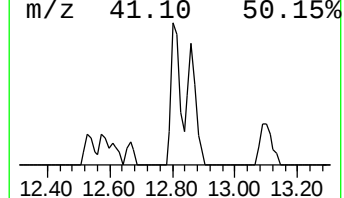
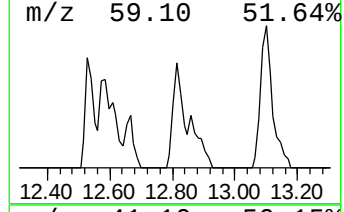
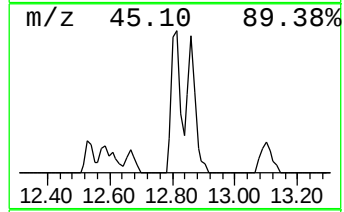
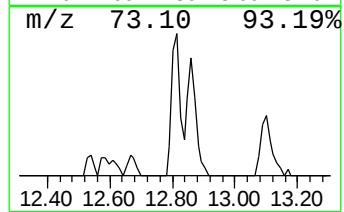
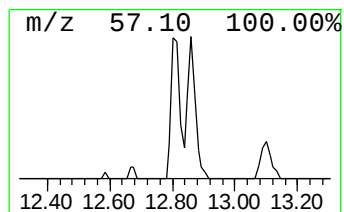
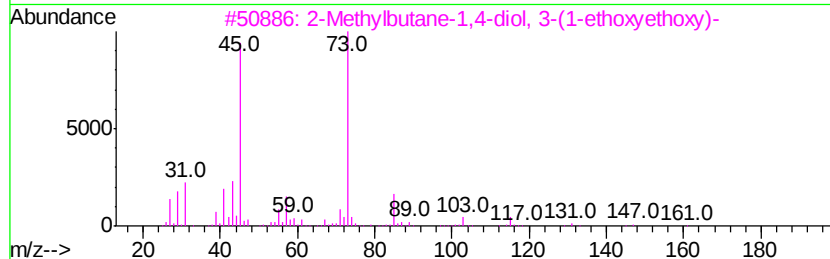
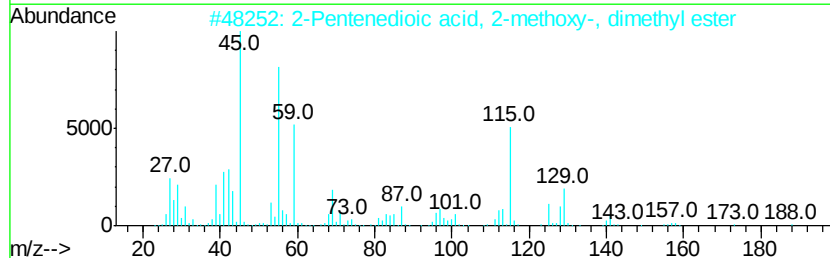
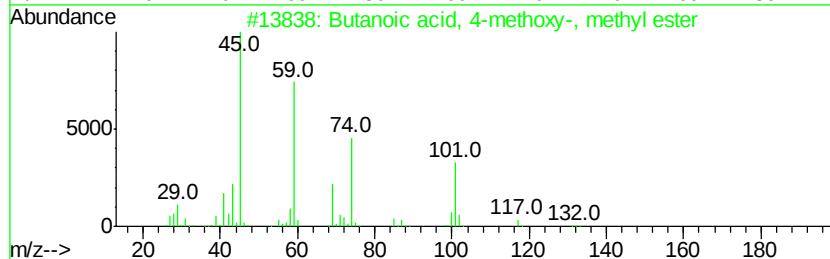
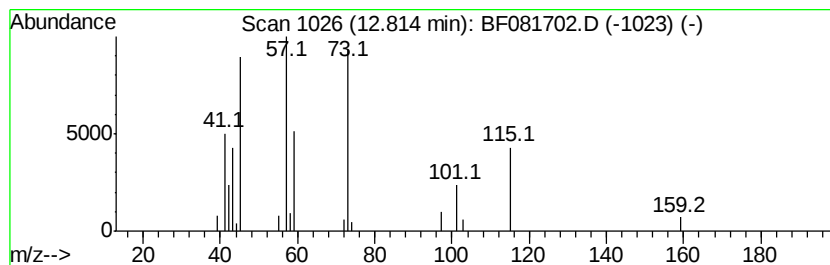
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 unknown12.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	4.95 ng	85082	Naphthalene-d8	11.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	37
2		2-Pentenedioic acid, 2-methoxy-, ...	188	C8H12O5	056009-33-7	36
3		2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	17
4		1,3-Dioxan-5-ol	104	C4H8O3	004740-78-7	17
5		Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	9



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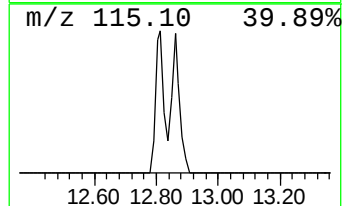
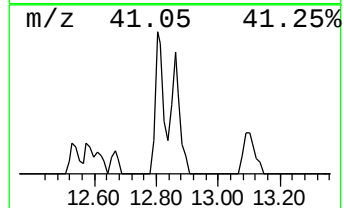
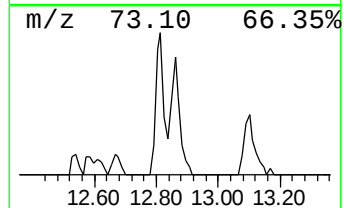
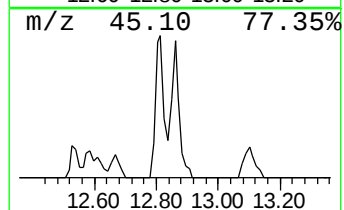
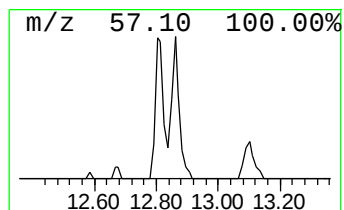
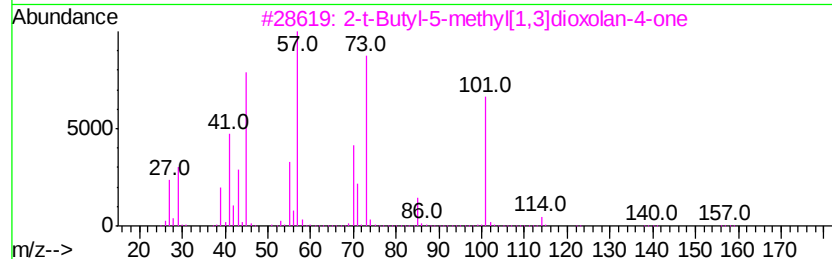
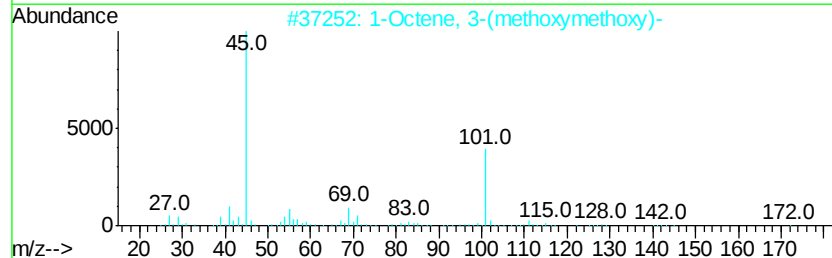
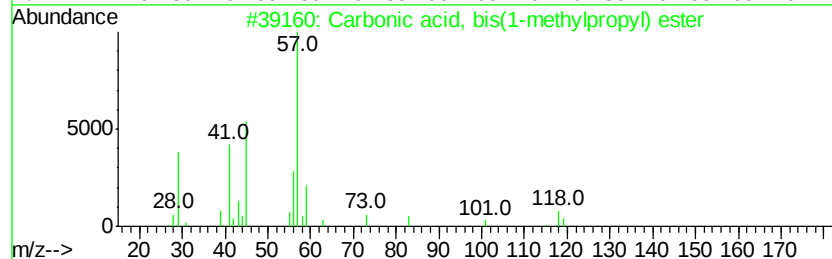
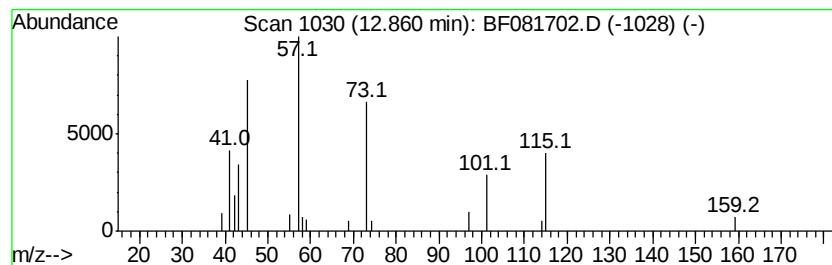
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Peak Number 9 unknown12.86 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	4.08 ng	70152	Naphthalene-d8	11.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	25
2		1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	9
3		2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	9
4		2-t-Butyl-4-methyl-5-oxo-[1,3]di...	202	C9H14O5	1000191-45-5	9
5		Phloroglucitol	132	C6H12O3	002041-15-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.24	270.5	ng	3668950	1	8.16	271272	20.0
2-Pentanone, 4-hy...	4.42	15.3	ng	207315	1	8.16	271272	20.0
unknown7.68	7.68	100.8	ng	1367360	1	8.16	271272	20.0
unknown12.81	12.81	5.0	ng	85082	2	11.07	343780	20.0
unknown12.86	12.86	4.1	ng	70152	2	11.07	343780	20.0