

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077914.D
Acq On : 24 Mar 2015 16:29
Operator : TP/IZ
Sample : PB82241BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB82241BL

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-BF031115.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	1.276	32	34	37	rVB	684643	872304	65.06%	8.010%
2	1.653	65	67	74	rVV	128612	257149	19.18%	2.361%
3	1.767	74	77	102	rVB	309510	609204	45.43%	5.594%
4	4.030	273	275	283	rVB	40982	65626	4.89%	0.603%
5	4.876	345	349	351	rBV	663997	957183	71.39%	8.789%
6	5.402	392	395	398	rBV	576741	599242	44.69%	5.502%
7	5.905	437	439	442	rBV	36334	33624	2.51%	0.309%
8	6.693	505	508	510	rBV	502529	593973	44.30%	5.454%
9	6.830	517	520	522	rBV	568833	644729	48.08%	5.920%
10	7.116	542	545	547	rBV	267272	244838	18.26%	2.248%
11	7.299	559	561	564	rBV	756104	686983	51.24%	6.308%
12	7.813	603	606	608	rBV	448052	489019	36.47%	4.490%
13	8.693	680	683	685	rBV	355382	328028	24.46%	3.012%
14	10.042	798	801	803	rBV	1126138	1107420	82.59%	10.169%
15	10.865	870	873	875	rBV	304714	377234	28.13%	3.464%
16	11.837	956	958	961	rBV	411446	397873	29.67%	3.653%
17	12.694	1031	1033	1036	rBV	423618	403020	30.06%	3.701%
18	14.694	1205	1208	1210	rBV	1199303	1340835	100.00%	12.312%
19	15.974	1318	1320	1323	rBV	311483	450717	33.61%	4.139%
20	17.757	1473	1476	1479	rBV	369473	431461	32.18%	3.962%

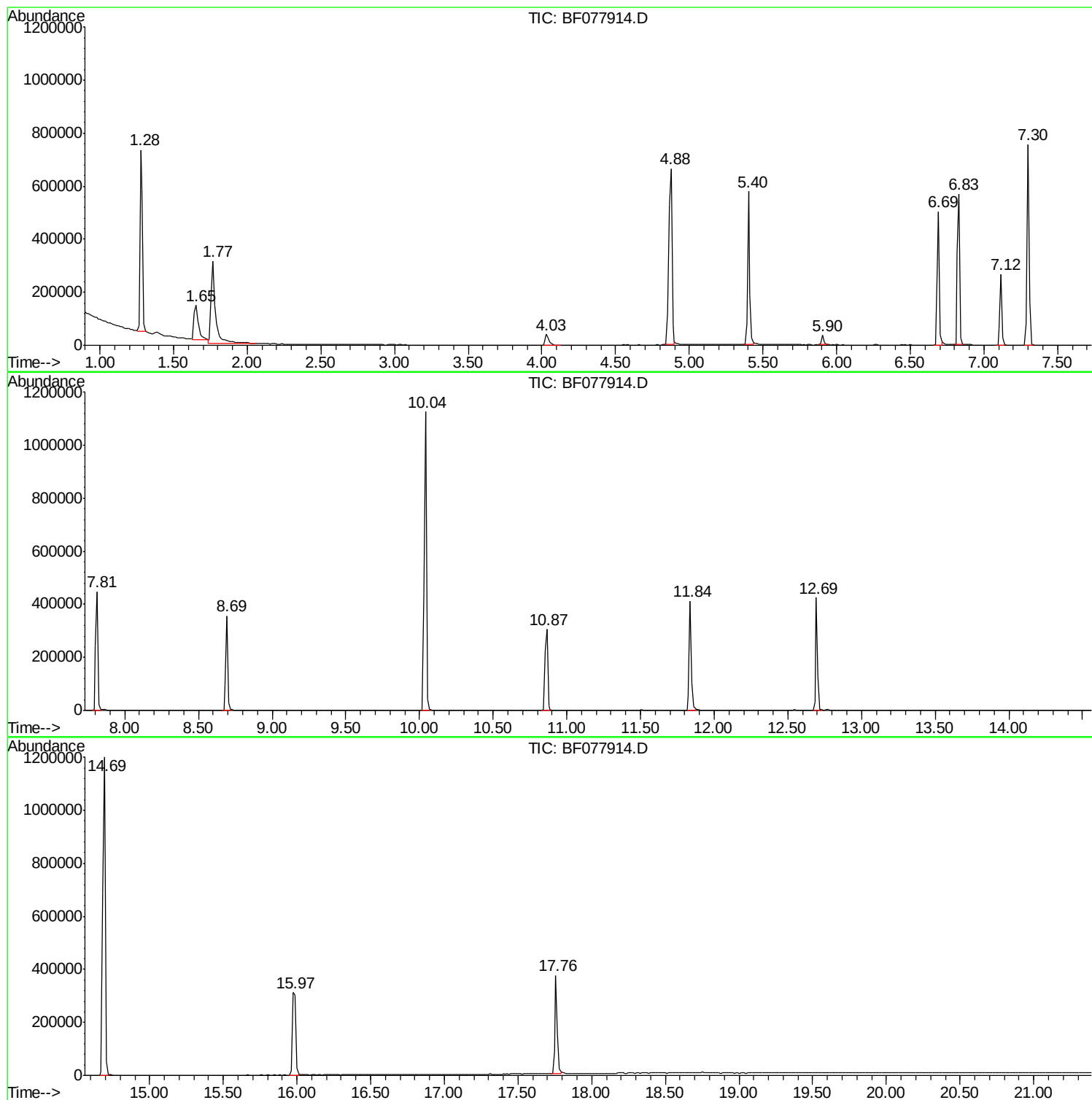
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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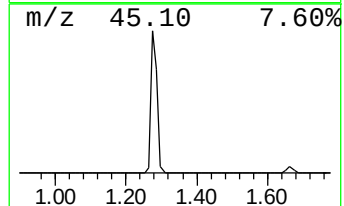
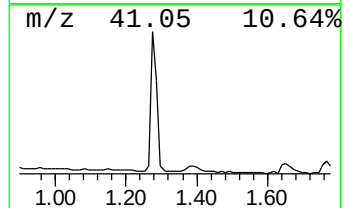
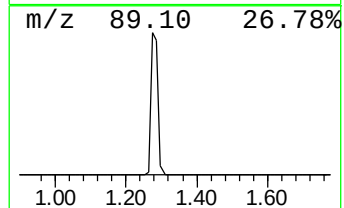
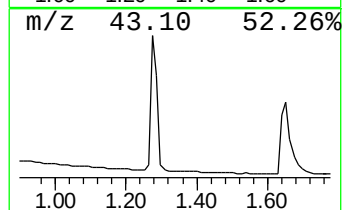
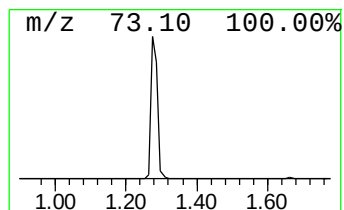
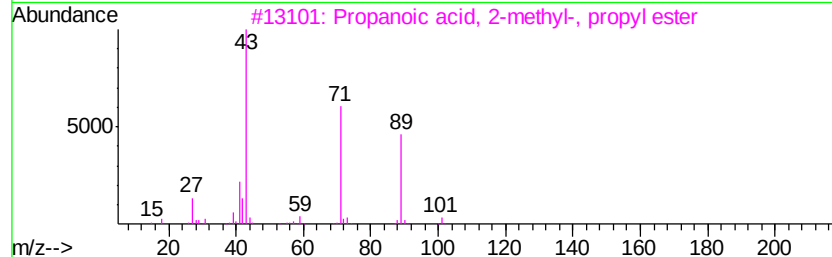
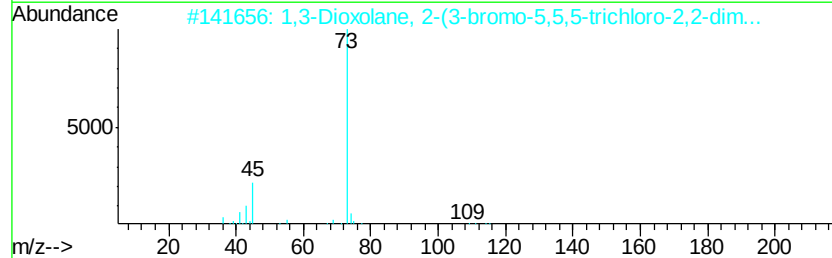
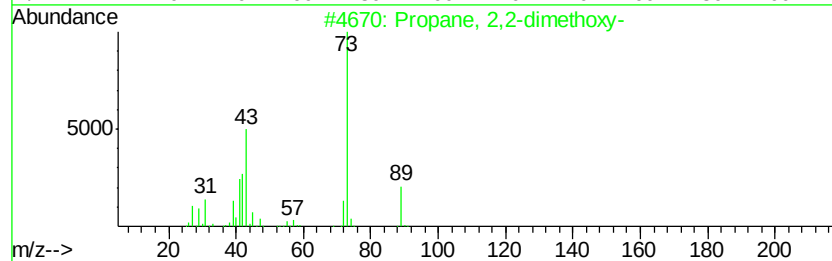
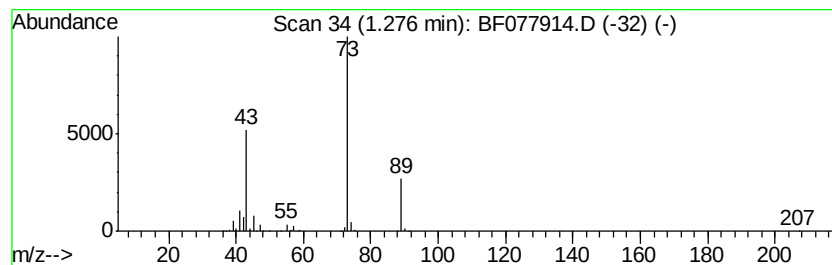
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.28	71.26 ng	872304	1,4-Dichlorobenzene-d4	7.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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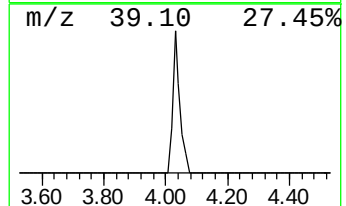
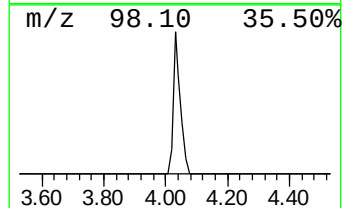
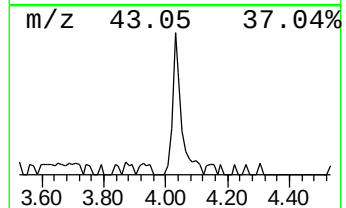
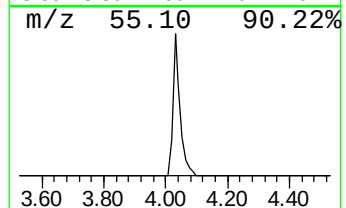
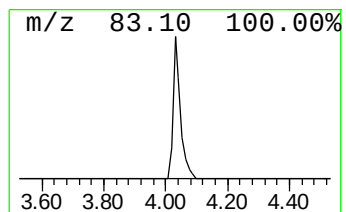
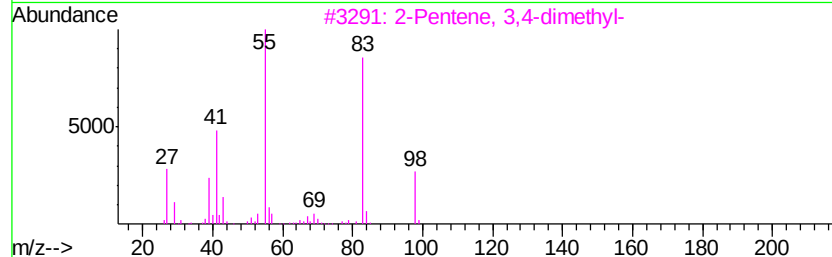
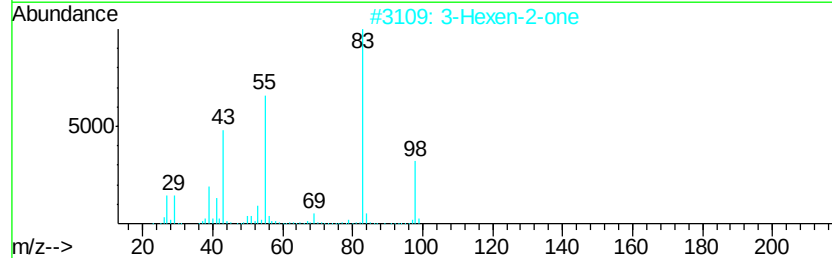
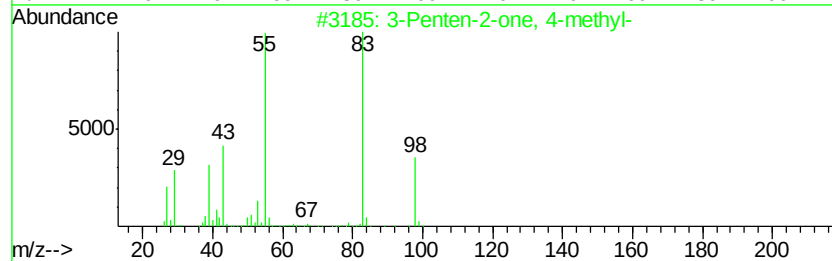
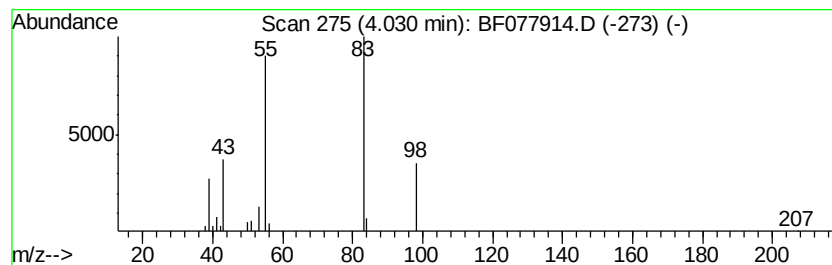
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TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	5.36 ng	65626	1,4-Dichlorobenzene-d4	7.12

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	86
3		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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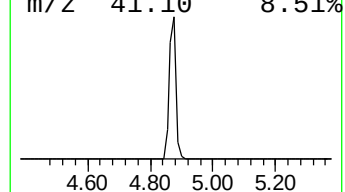
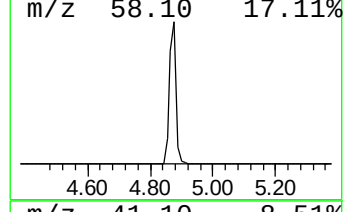
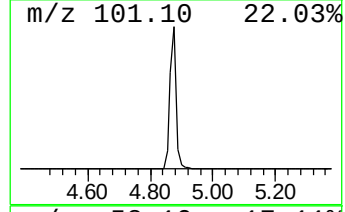
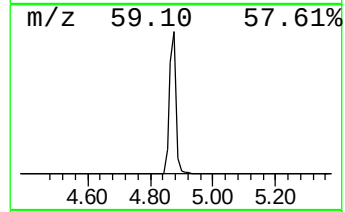
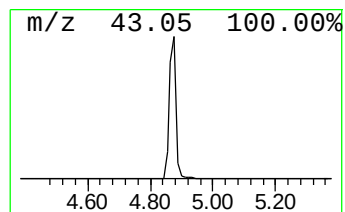
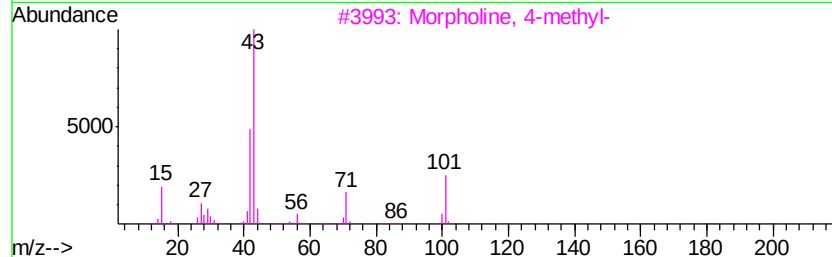
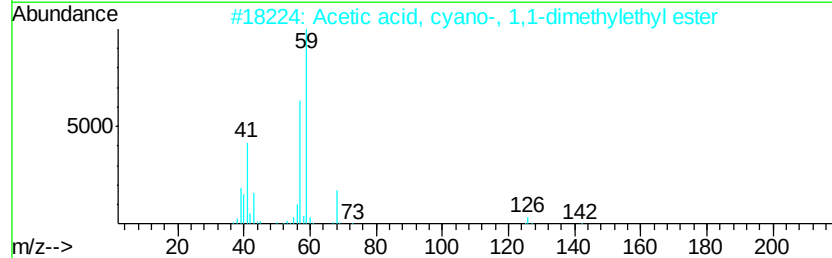
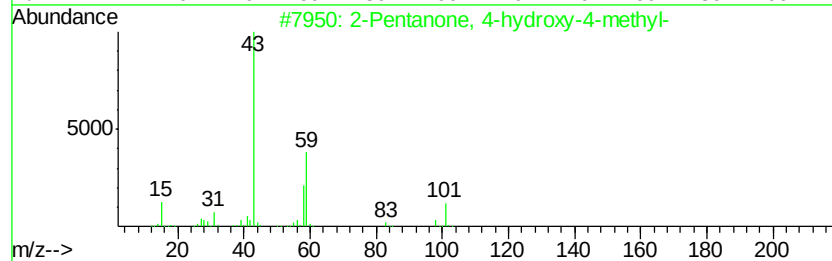
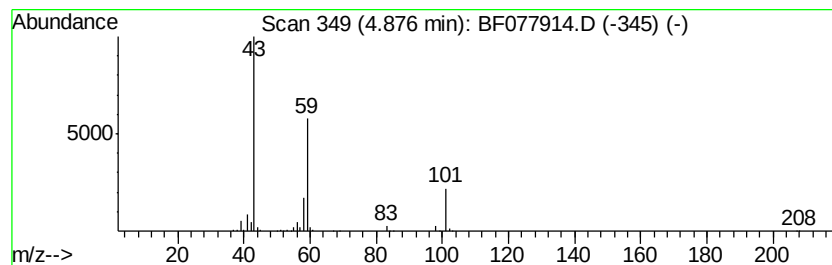
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	78.19 ng	957183	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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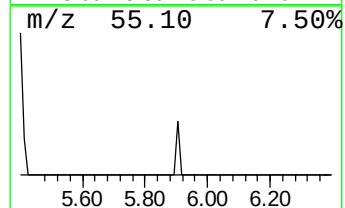
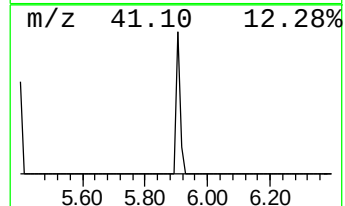
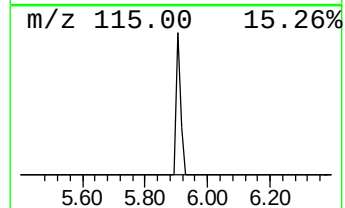
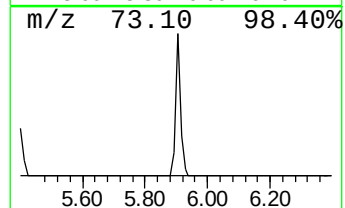
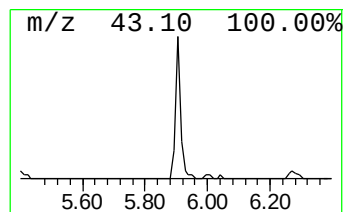
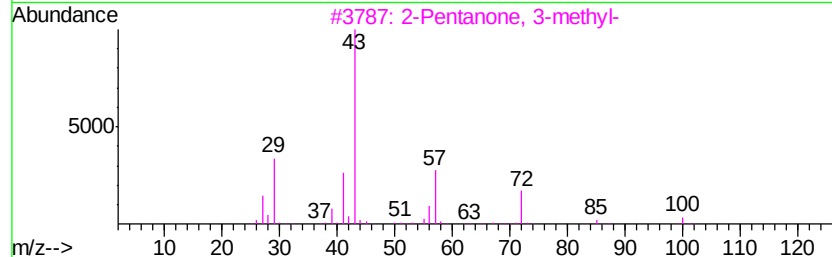
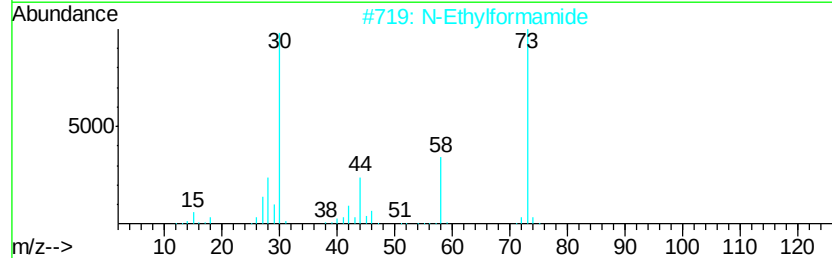
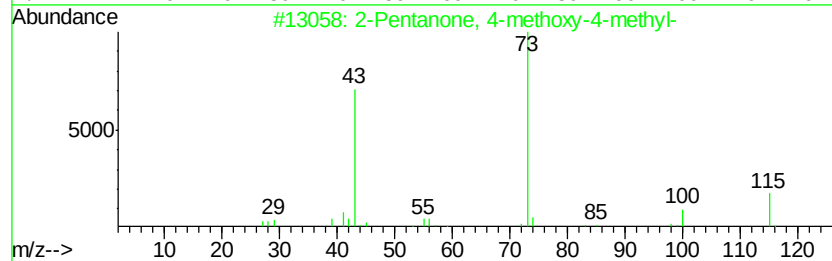
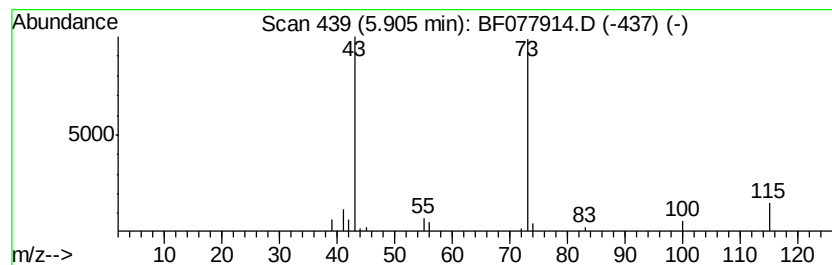
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Peak Number 6 unknown5.90 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.75 ng	33624	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-Ethylformamide	73	C3H7NO	000627-45-2	16
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
4		1H-Tetrazole-1-acetic acid	128	C3H4N4O2	021732-17-2	9
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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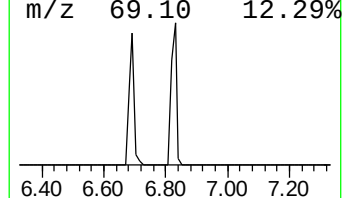
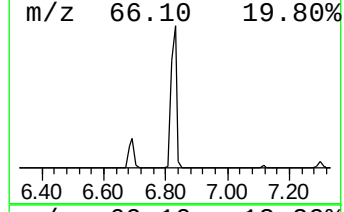
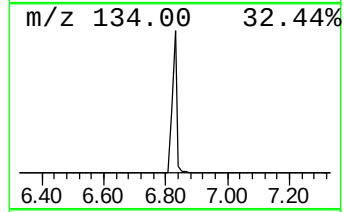
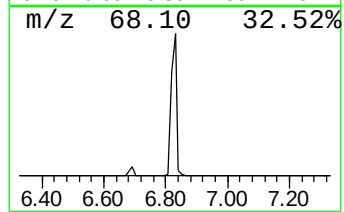
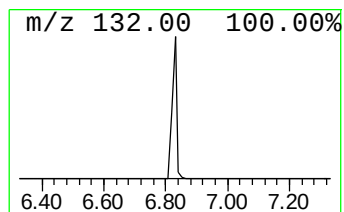
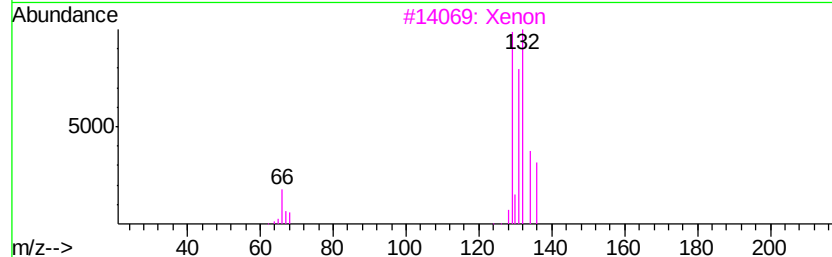
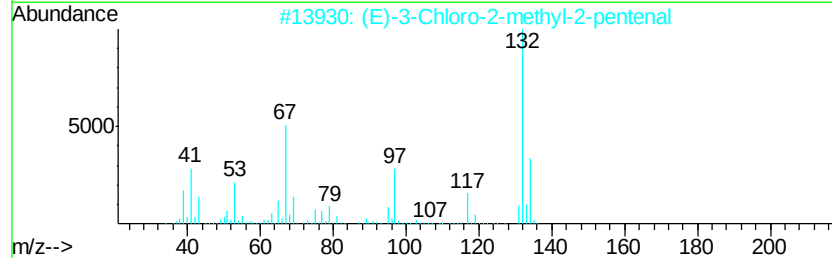
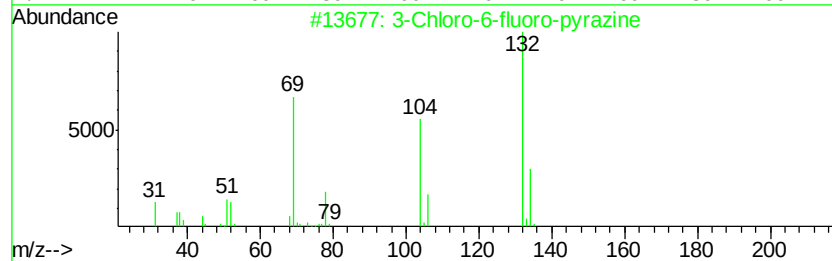
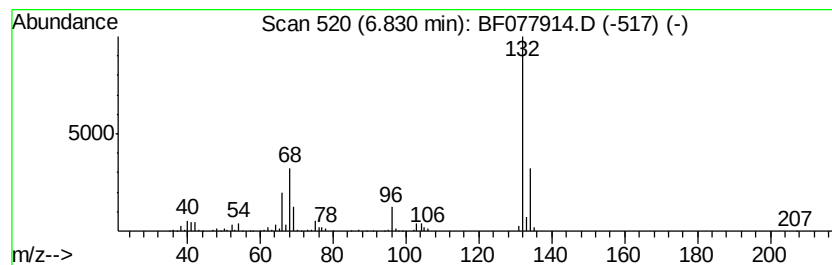
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Peak Number 7 unknown6.83 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	52.67 ng	644729	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Xenon	132	Xe	007440-63-3	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
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
Propane, 2,2-dime...	1.28	71.3	ng	872304	1	7.12	244838	20.0
3-Penten-2-one, 4...	4.03	5.4	ng	65626	1	7.12	244838	20.0
2-Pentanone, 4-hy...	4.88	78.2	ng	957183	1	7.12	244838	20.0
unknown5.90	5.90	2.8	ng	33624	1	7.12	244838	20.0
unknown6.83	6.83	52.7	ng	644729	1	7.12	244838	20.0