

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102524\
Data File : VN084522.D
Acq On : 25 Oct 2024 17:38
Operator : JC\MD
Sample : P4550-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VPB190-HYD-20241023

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:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.M

Title : SW846 8260

Signal : TIC: VN084522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1047	1056	1061	rBV	120672	293264	45.73%	7.455%
2	8.224	1061	1066	1080	rVB	187947	416406	64.93%	10.586%
3	8.577	1117	1126	1137	rBV	135431	297211	46.34%	7.556%
4	9.100	1206	1215	1226	rBV	284466	583949	91.05%	14.845%
5	11.865	1677	1685	1695	rBV	360809	641336	100.00%	16.304%
6	12.847	1845	1852	1863	rVB	260071	439513	68.53%	11.173%
7	13.076	1883	1891	1899	rBV	104056	180619	28.16%	4.592%
8	13.176	1901	1908	1915	rBV	43892	73546	11.47%	1.870%
9	13.788	2004	2012	2022	rBV	336516	562948	87.78%	14.311%
10	14.023	2045	2052	2059	rBV2	99424	164034	25.58%	4.170%
11	14.118	2060	2068	2076	rVB	167767	280773	43.78%	7.138%

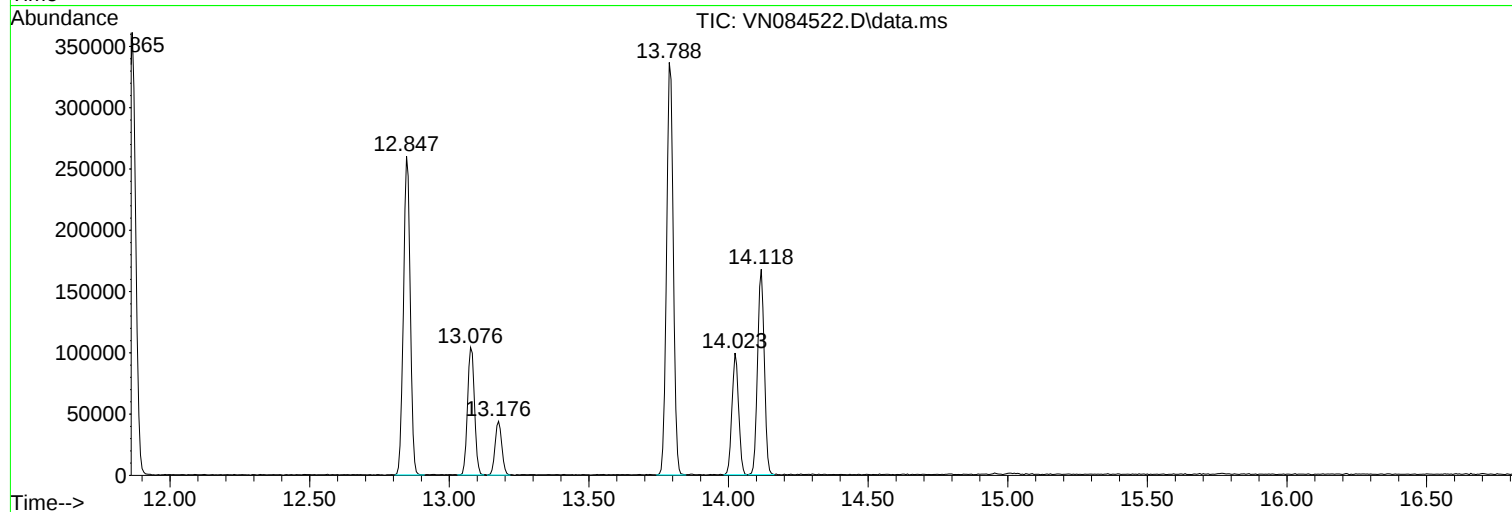
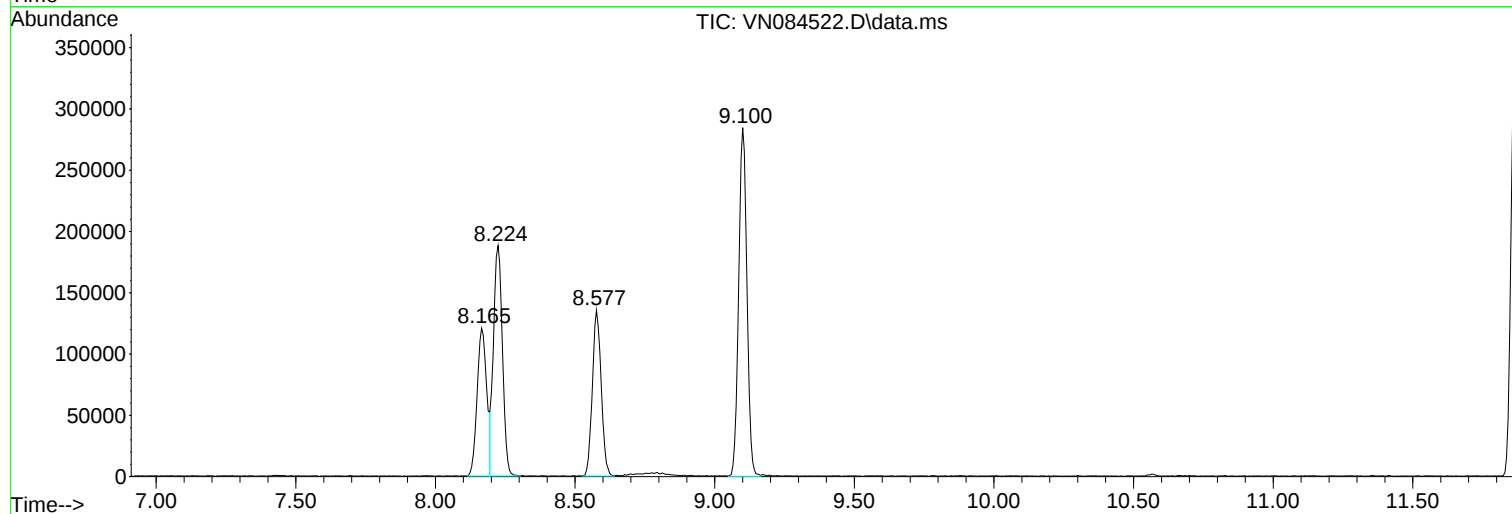
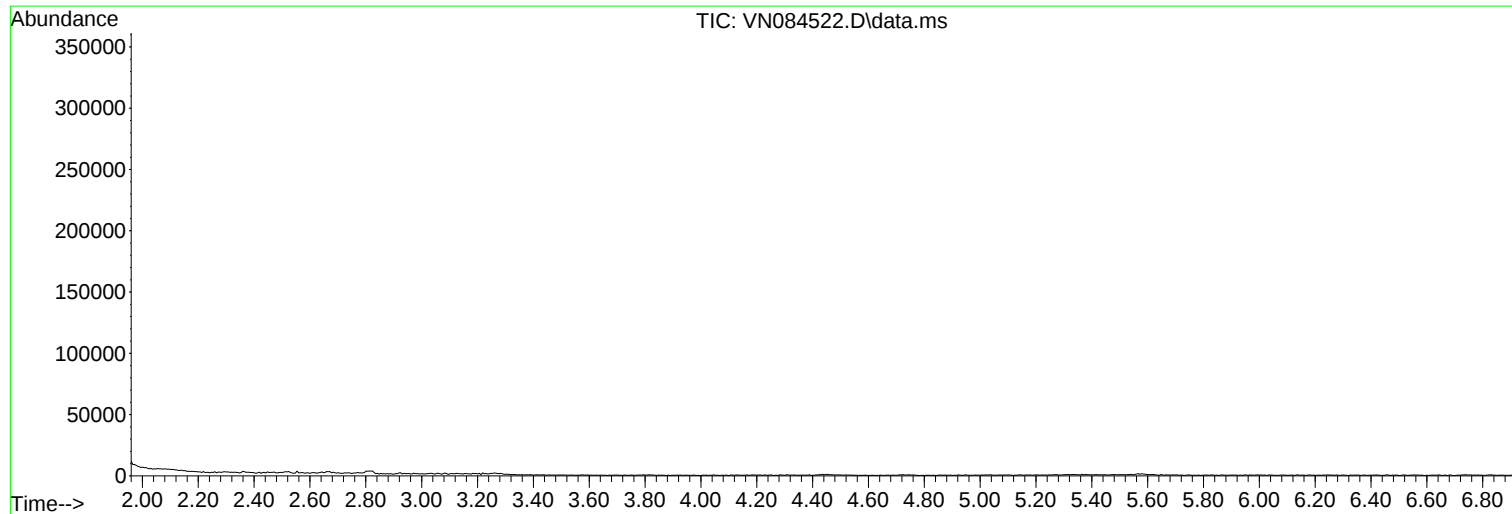
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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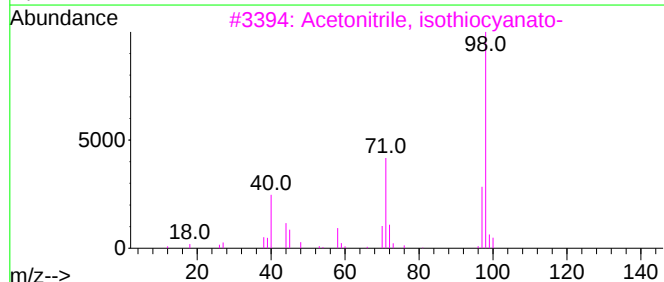
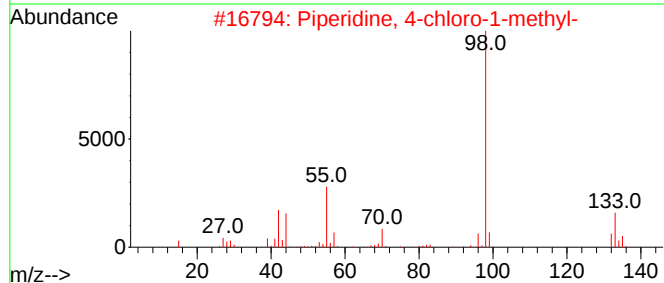
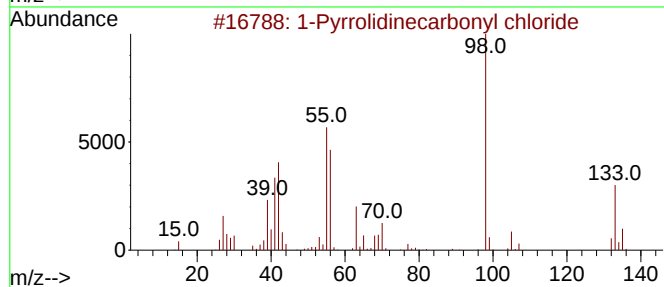
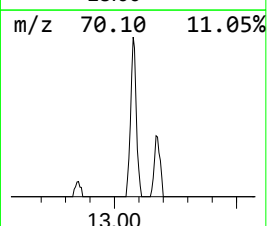
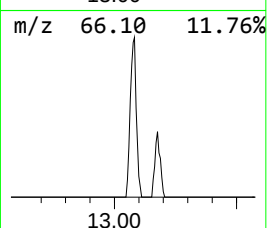
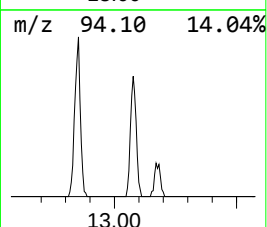
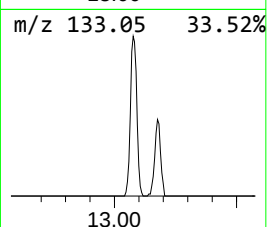
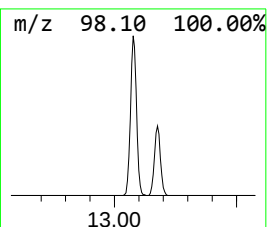
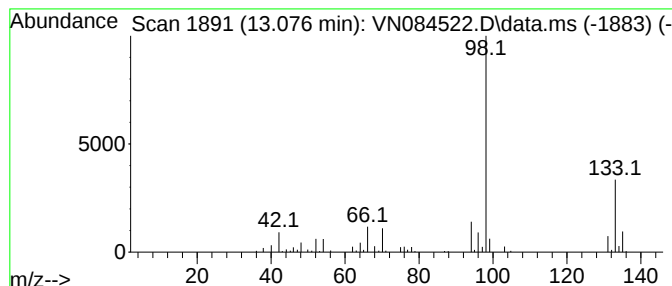
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Pyrrolidinecarbonyl chloride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.076	16.04 ug/l	180619	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrrolidinecarbonyl chloride	133	C5H8ClNO	001192-63-8	59
2			Piperidine, 4-chloro-1-methyl-	133	C6H12ClN	005570-77-4	45
3			Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	38
4			Benzen-d5-amine	98	C6H2D5N	004165-61-1	37
5			Encainide	352	C22H28N2O2	037612-13-8	33



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Instrument :
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ClientSampleId :
VPB190-HYD-20241023

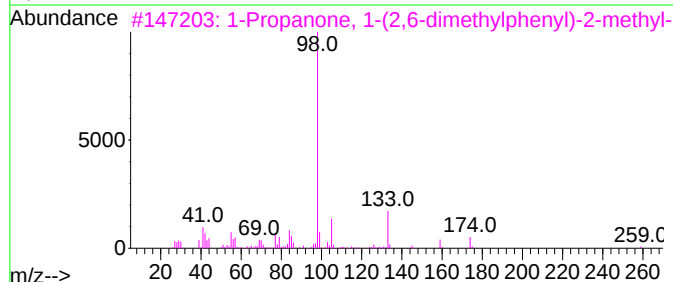
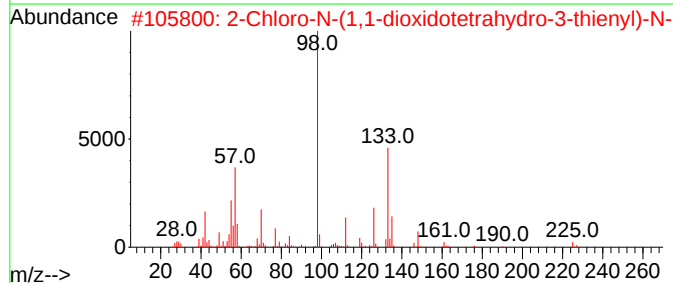
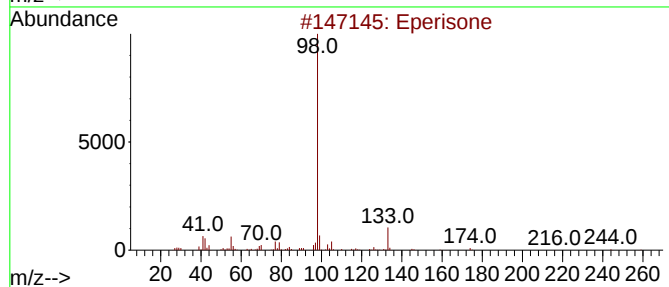
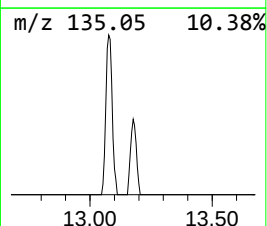
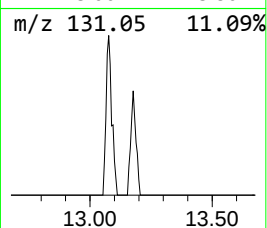
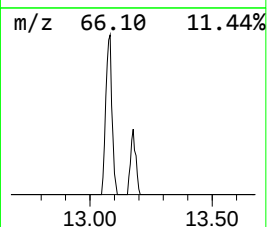
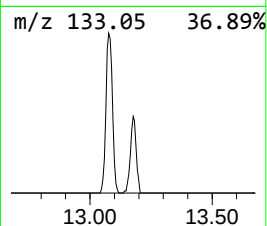
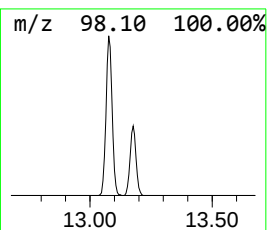
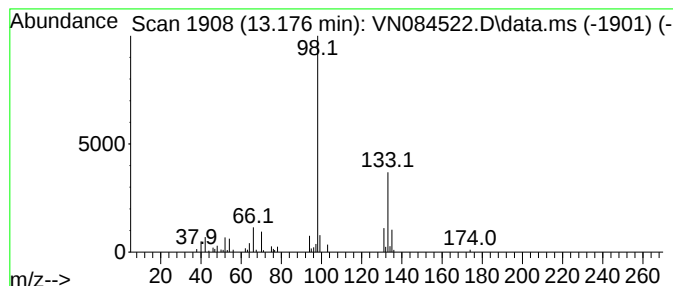
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Quant Title : SW846 8260

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Peak Number 2 Eperisone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.176	6.53 ug/l	73546	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eperisone	259	C17H25NO	064840-90-0	59
2			2-Chloro-N-(1,1-dioxidotetrahydr...	225	C7H12ClNO3S	007365-23-3	59
3			1-Propanone, 1-(2,6-dimethylphen...	259	C17H25NO	158176-61-5	59
4			Encainide	352	C22H28N2O2	037612-13-8	50
5			5-Phenyl-3-piperidin-1-ylmethyl-...	275	C14H17N3OS	023269-66-1	38



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Instrument :
MSVOA_N
ClientSampleId :
VPB190-HYD-20241023

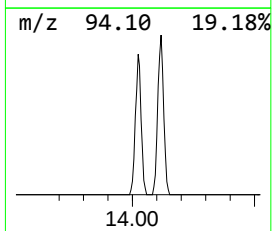
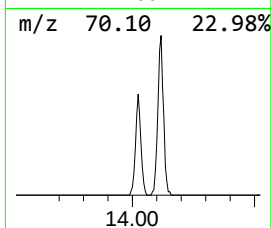
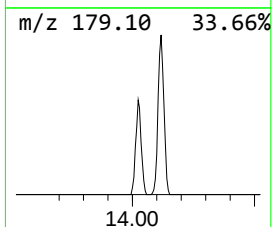
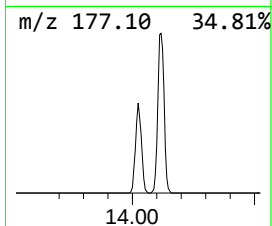
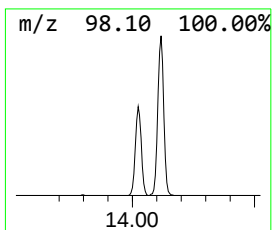
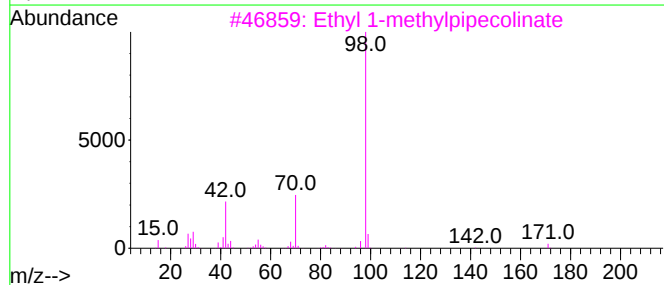
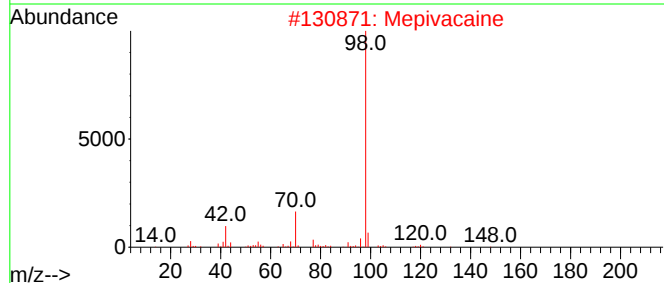
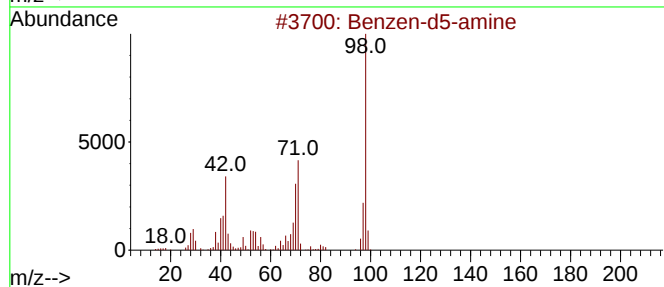
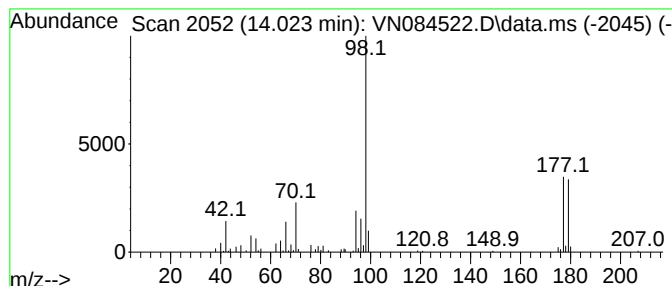
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Quant Title : SW846 8260

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Peak Number 3 unknown14.023 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.023	14.57 ug/l	164034	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzen-d5-amine	98	C6H2D5N	004165-61-1	47
2			Mepivacaine	246	C15H22N2O	000096-88-8	43
3			Ethyl 1-methylpipercolinate	171	C9H17NO2	030727-18-5	37
4			1-Methyl-2-piperidinethanol	129	C7H15NO	020845-34-5	37
5			(R)-1-Ethyl-2-pyrrolidinecarboxa...	142	C7H14N2O	1000237-69-9	32



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Instrument :
MSVOA_N
ClientSampleId :
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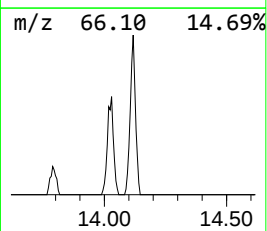
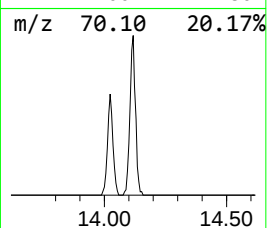
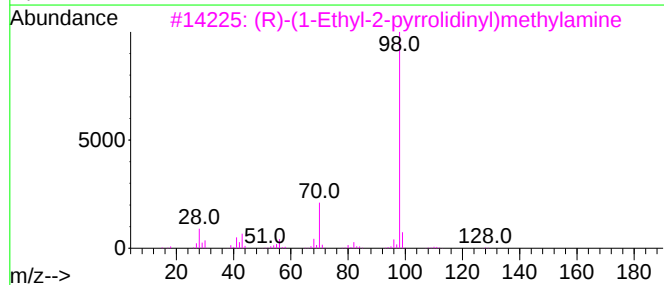
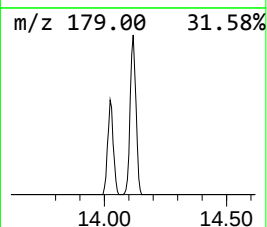
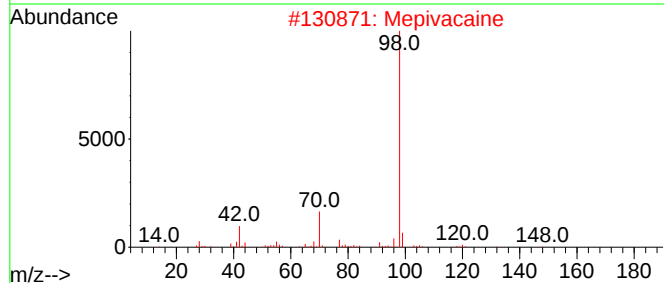
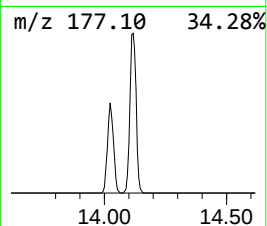
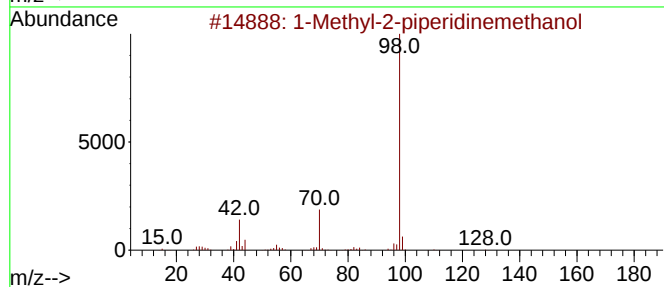
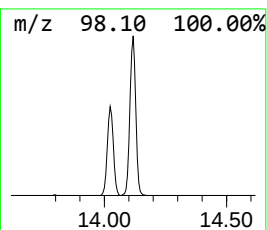
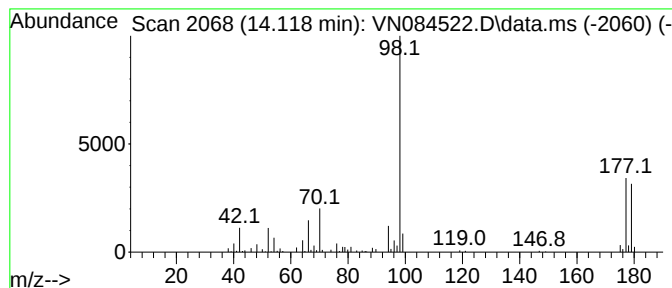
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Peak Number 4 unknown14.118 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.118	24.94 ug/l	280773	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	47
2			Mepivacaine	246	C15H22N2O	000096-88-8	47
3			(R)-(1-Ethyl-2-pyrrolidinyl)meth...	128	C7H16N2	022795-97-7	38
4			2-Piperidinecarboxylic acid, 2-m...	143	C7H13NO2	072518-41-3	38
5			Ethyl 1-methylpipercolinate	171	C9H17NO2	030727-18-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pyrrolidineca...	13.076	16.0	ug/l	180619	4	13.788	562948	50.0
Eperisone	13.176	6.5	ug/l	73546	4	13.788	562948	50.0
unknown14.023	14.023	14.6	ug/l	164034	4	13.788	562948	50.0
unknown14.118	14.118	24.9	ug/l	280773	4	13.788	562948	50.0