

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102522\
 Data File : VX032367.D
 Acq On : 25 Oct 2022 16:23
 Operator : JC/MD
 Sample : N5249-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-MW-30-20221019

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_X\Method\82X101922W.M
 Title : SW846 8260

Signal : TIC: VX032367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	22	rVB	168815	175063	27.76%	4.327%
2	1.264	26	29	32	rBV	18870	16762	2.66%	0.414%
3	1.368	40	46	53	rBV2	107000	154622	24.52%	3.822%
4	1.428	53	56	58	rVB	9212	8814	1.40%	0.218%
5	1.496	63	67	73	rVB	18384	19247	3.05%	0.476%
6	1.581	73	81	89	rBV3	2794	6871	1.09%	0.170%
7	1.660	89	94	103	rVB	10791	15001	2.38%	0.371%
8	1.745	103	108	119	rBV	26703	38013	6.03%	0.940%
9	1.910	130	135	138	rBV	26740	35854	5.69%	0.886%
10	1.953	138	142	154	rVB2	41346	70544	11.19%	1.744%
11	2.069	157	161	166	rBV	6923	9921	1.57%	0.245%
12	2.160	171	176	181	rVV	9643	15379	2.44%	0.380%
13	2.721	258	268	278	rBV5	6434	24056	3.82%	0.595%
14	2.825	280	285	290	rBV2	4606	8021	1.27%	0.198%
15	3.105	321	331	340	rVB2	5348	12115	1.92%	0.299%
16	3.331	359	368	376	rBV3	6901	16950	2.69%	0.419%
17	5.385	692	705	722	rBV	76632	224934	35.67%	5.560%
18	5.556	722	733	752	rVB	135528	386907	61.36%	9.563%
19	5.958	788	799	812	rBV	82598	216848	34.39%	5.360%
20	6.763	921	931	945	rBV	198524	475958	75.48%	11.765%
21	7.129	982	991	1000	rVB	9134	21583	3.42%	0.533%
22	8.653	1234	1241	1250	rBV	397137	630560	100.00%	15.586%
23	10.055	1465	1471	1480	rBV	409471	540074	85.65%	13.349%
24	11.079	1634	1639	1650	rBV	331296	419648	66.55%	10.373%
25	12.024	1788	1794	1805	rBV	407087	501950	79.60%	12.407%

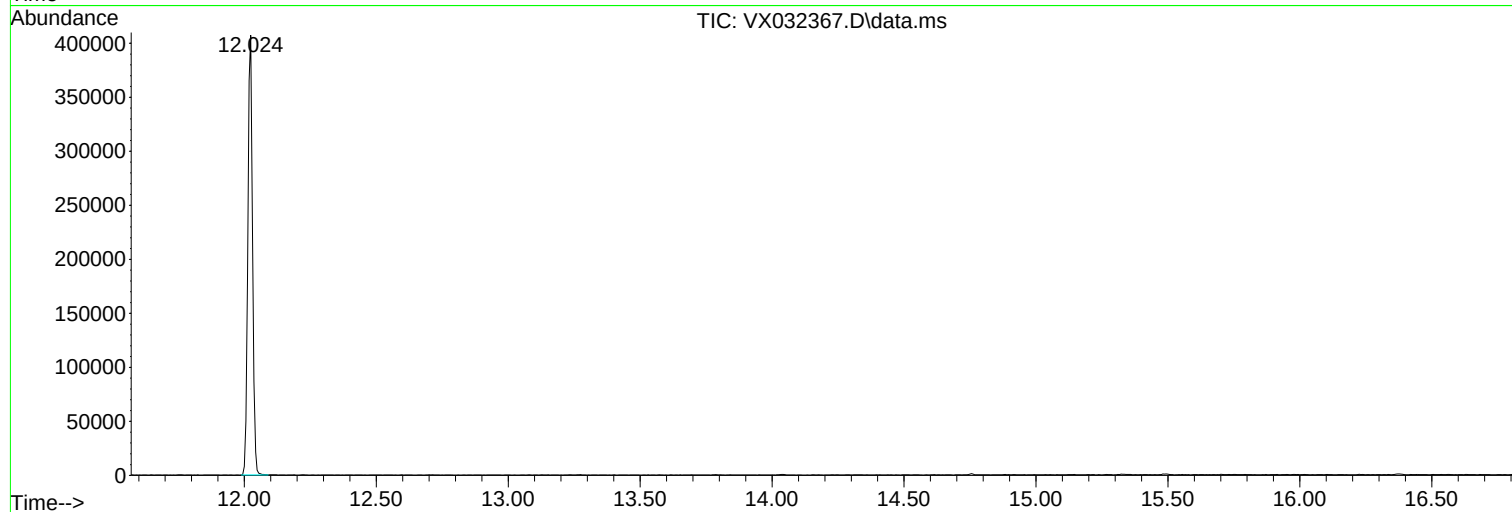
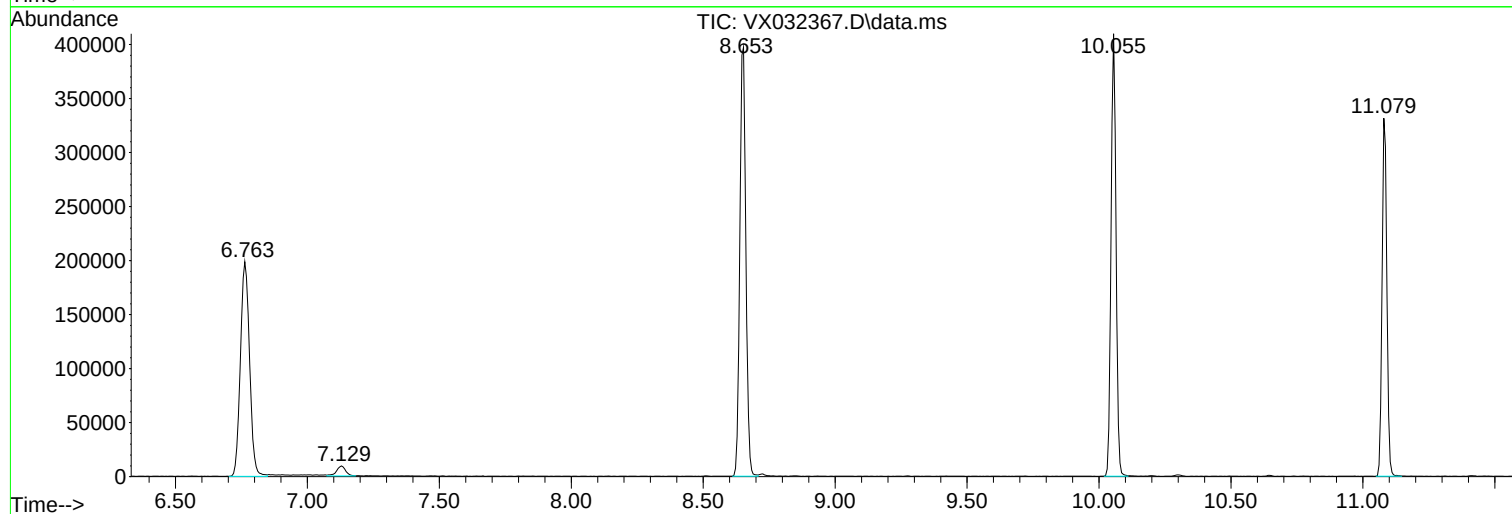
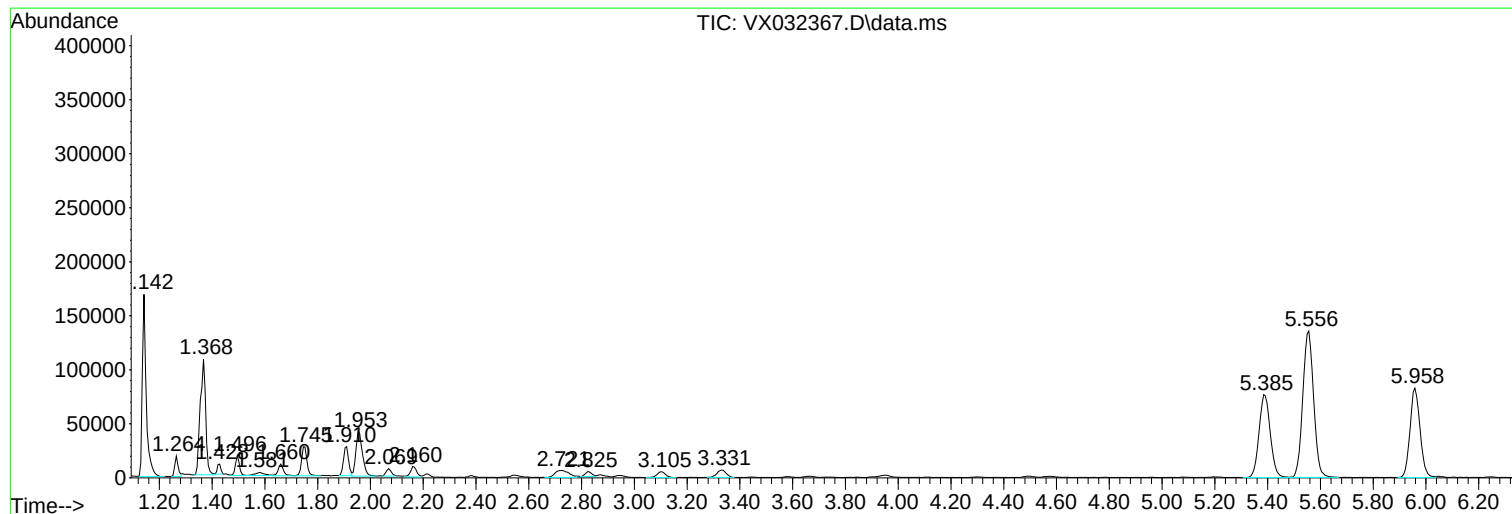
Sum of corrected areas: 4045695

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



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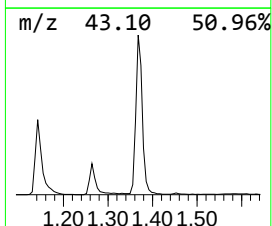
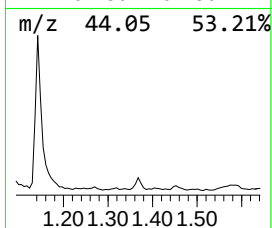
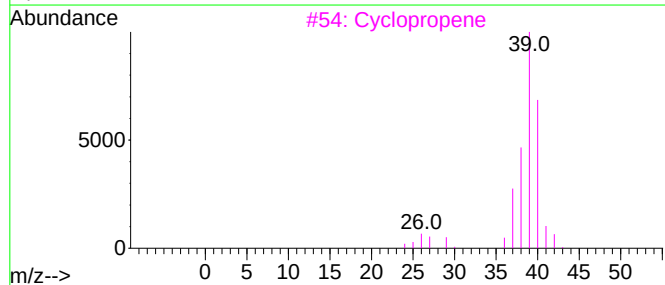
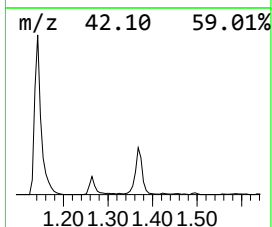
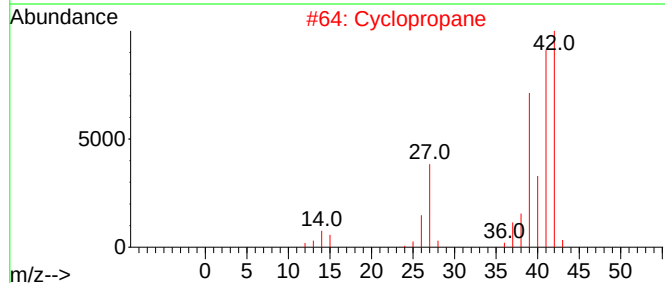
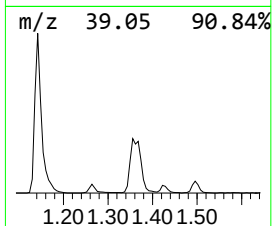
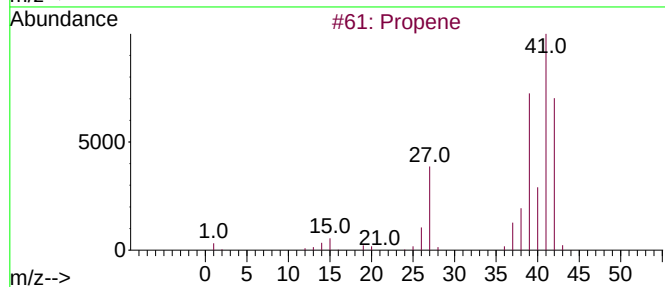
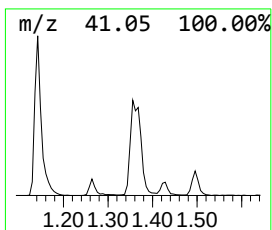
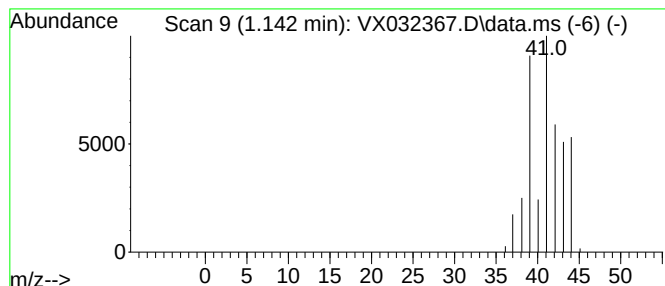
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	22.62 ug/l	175063	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	64
2			Cyclopropane	42	C3H6	000075-19-4	7
3			Cyclopropene	40	C3H4	002781-85-3	4
4			Cyclobutylamine	71	C4H9N	002516-34-9	4
5			Pyrimidine-2,4(1H,3H)-dione, 5-a...	156	C4H4N4O3	1000270-67-7	2



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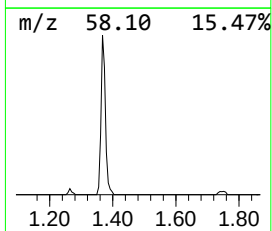
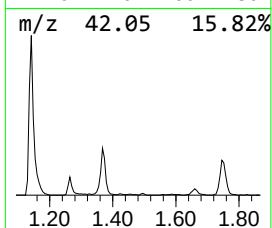
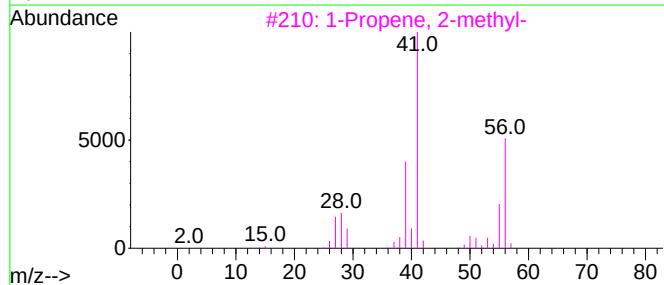
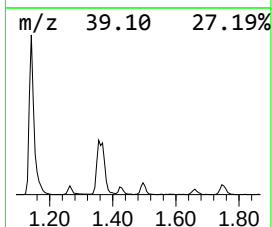
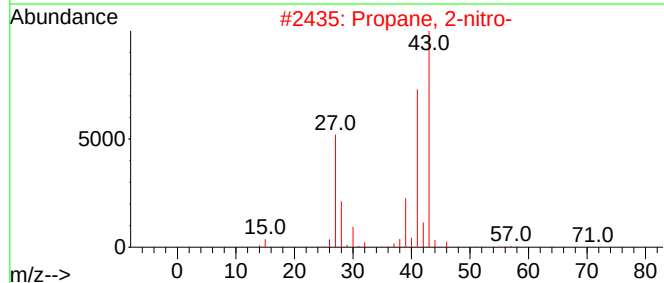
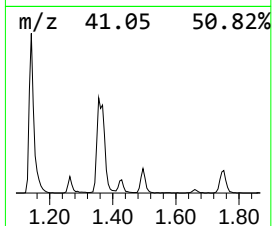
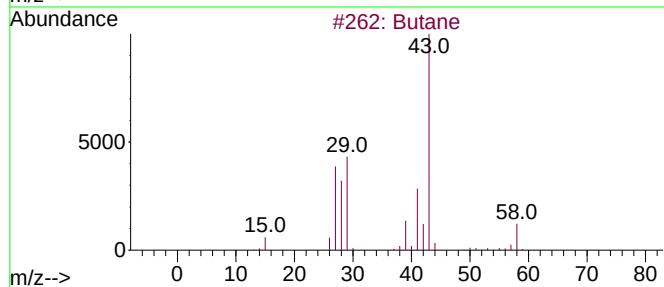
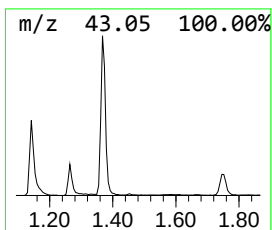
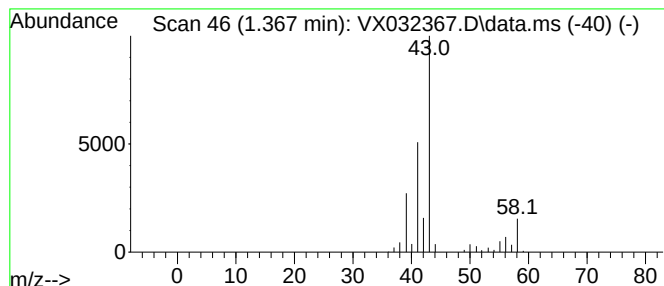
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	19.98 ug/l	154622	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	50
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	33
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Acetone	58	C3H6O	000067-64-1	4



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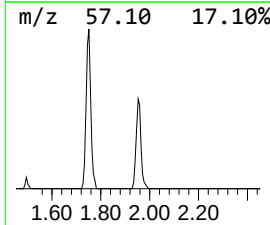
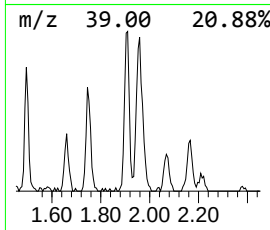
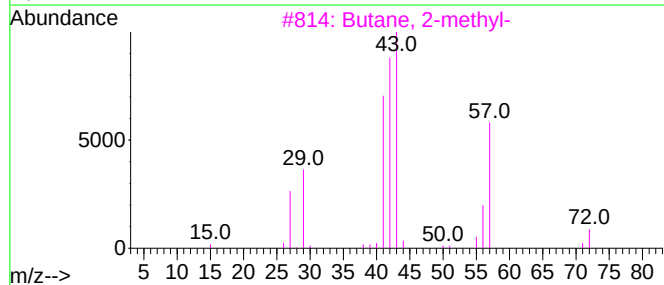
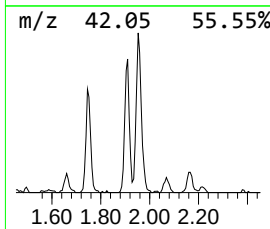
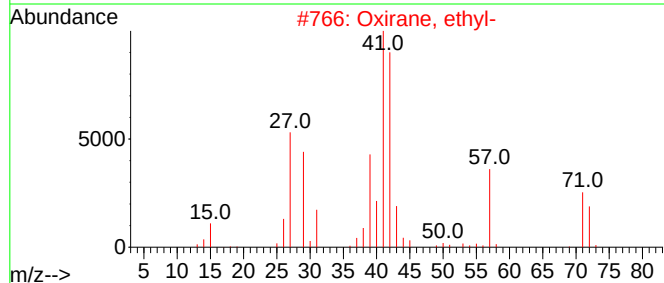
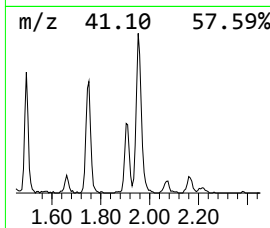
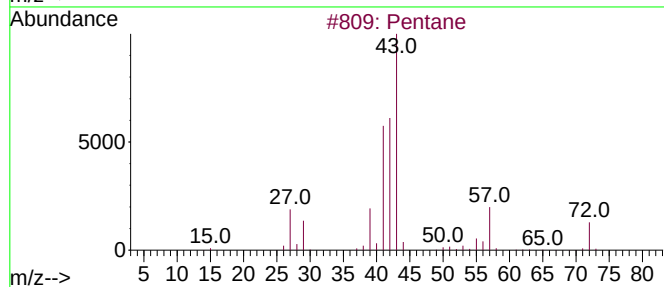
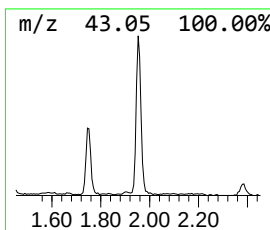
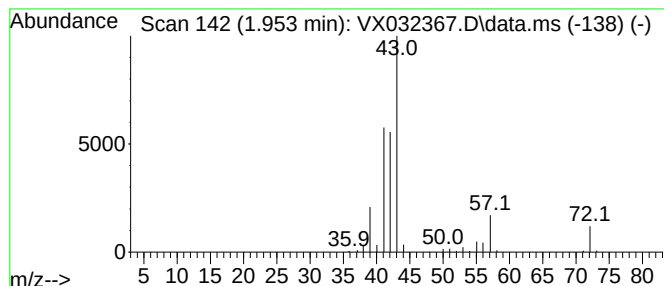
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	9.12 ug/l	70544	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Butane, 2-methyl-	72	C5H12	000078-78-4	36
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	32
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	1.142	22.6	ug/l	175063	1	5.556	386907	50.0
Butane	1.367	20.0	ug/l	154622	1	5.556	386907	50.0
Pentane	1.953	9.1	ug/l	70544	1	5.556	386907	50.0