

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
 Data File : VU044852.D
 Acq On : 25 Sep 2021 21:15
 Operator : SY/MD
 Sample : M3895-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 210922099-02-VOA

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_U\Method\82U092421W.M
 Title : SW846 8260

Signal : TIC: VU044852.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	39	44	53	rVB	48071	45496	1.00%	0.292%
2	2.633	389	402	426	rBV2	39229	81987	1.81%	0.527%
3	3.186	551	574	618	rBV	1183077	2875346	63.31%	18.469%
4	4.636	1001	1025	1068	rBV	1746401	4541539	100.00%	29.171%
5	4.809	1071	1079	1099	rVB3	26285	69338	1.53%	0.445%
6	5.054	1139	1155	1191	rVB	479264	1066130	23.48%	6.848%
7	5.292	1215	1229	1243	rBV	151263	318325	7.01%	2.045%
8	5.378	1243	1256	1280	rVB	269418	555663	12.24%	3.569%
9	5.706	1342	1358	1371	rBV	191410	392560	8.64%	2.521%
10	5.780	1371	1381	1388	rVV	33720	72743	1.60%	0.467%
11	5.832	1389	1397	1423	rVB3	39821	92920	2.05%	0.597%
12	6.253	1511	1528	1546	rBV	404856	757391	16.68%	4.865%
13	7.902	2025	2041	2056	rVV	621555	1075129	23.67%	6.906%
14	8.034	2072	2082	2095	rVB	35178	62836	1.38%	0.404%
15	8.796	2306	2319	2335	rBV6	26380	59053	1.30%	0.379%
16	9.420	2499	2513	2534	rBV	561623	933954	20.56%	5.999%
17	9.693	2580	2598	2610	rVV	75866	133147	2.93%	0.855%
18	10.102	2715	2725	2744	rBV	51449	87523	1.93%	0.562%
19	10.635	2875	2891	2905	rBV	428111	686795	15.12%	4.411%
20	11.471	3115	3151	3160	rBV2	35442	76768	1.69%	0.493%
21	11.815	3242	3258	3276	rBV	574139	990314	21.81%	6.361%
22	12.098	3338	3346	3358	rVB	34841	56704	1.25%	0.364%
23	12.954	3601	3612	3622	rBV	146820	242214	5.33%	1.556%
24	13.031	3623	3636	3665	rVB	23861	85689	1.89%	0.550%
25	13.693	3831	3842	3851	rBV2	56711	97580	2.15%	0.627%
26	13.847	3874	3890	3902	rBV8	24273	51464	1.13%	0.331%
27	14.285	4015	4026	4046	rBV6	24984	60072	1.32%	0.386%

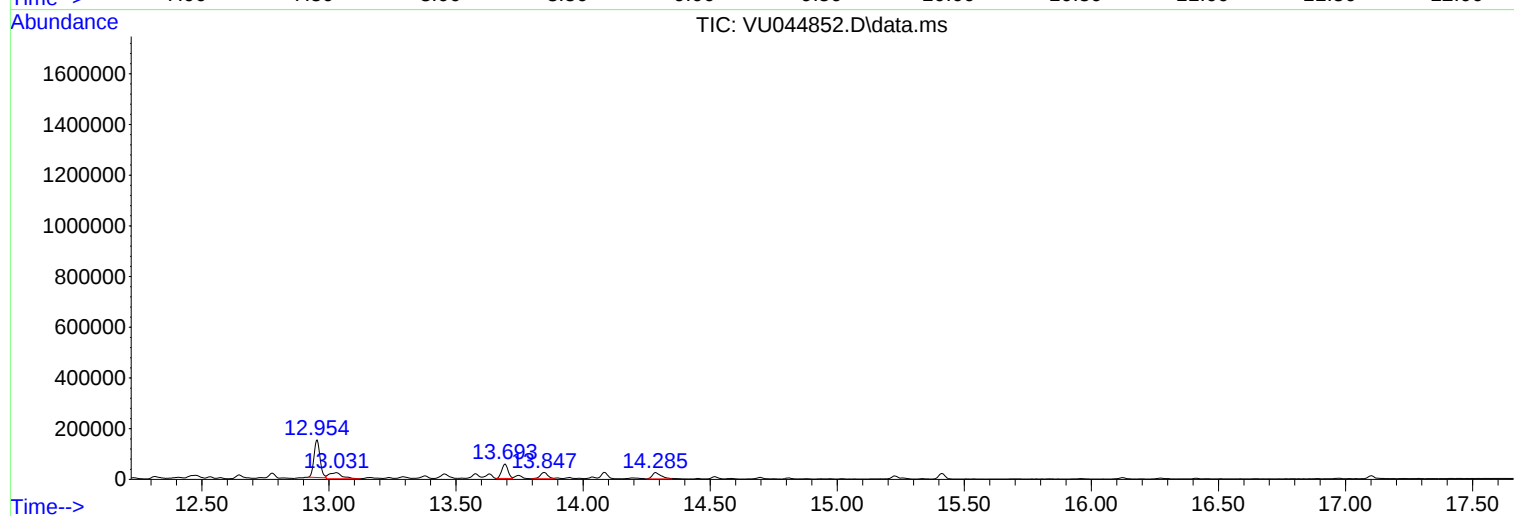
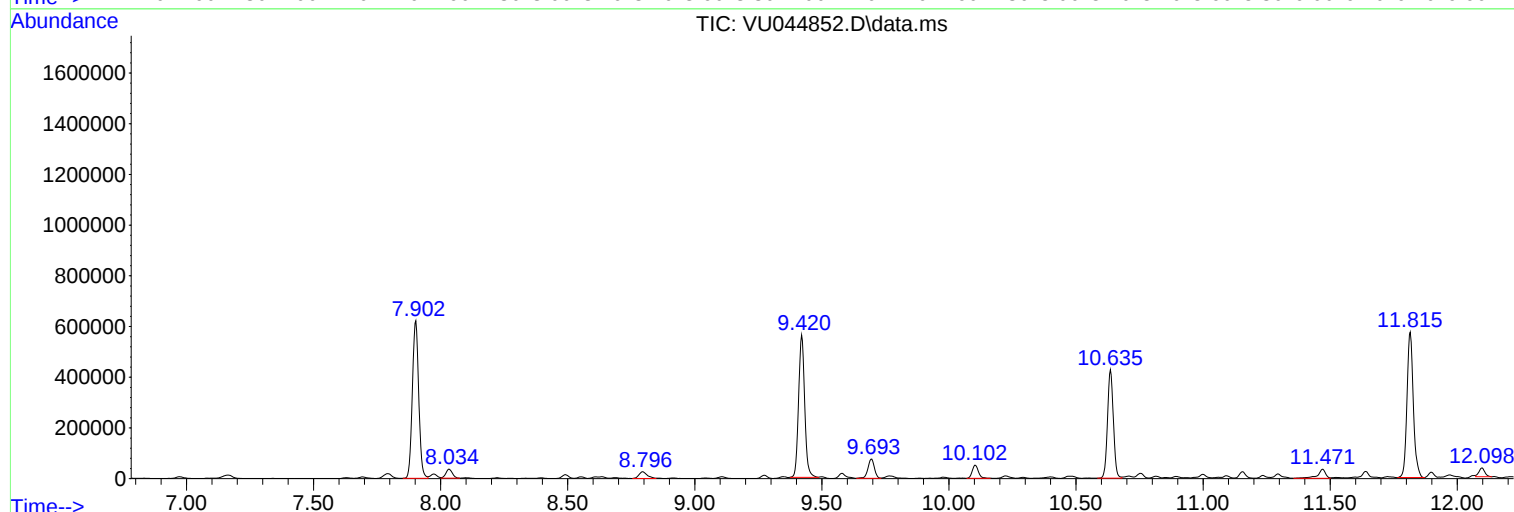
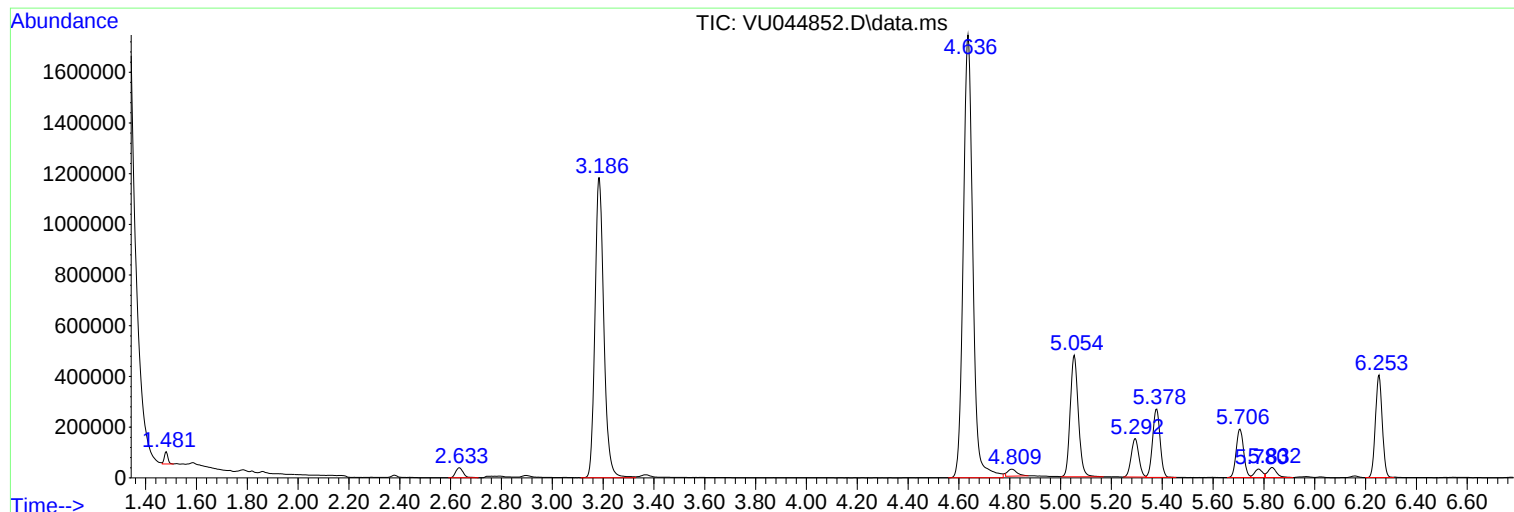
Sum of corrected areas: 15568680

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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



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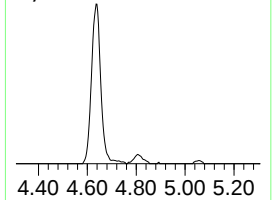
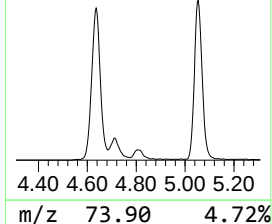
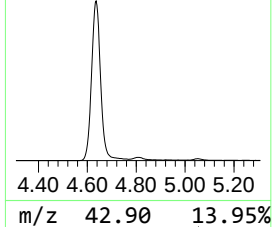
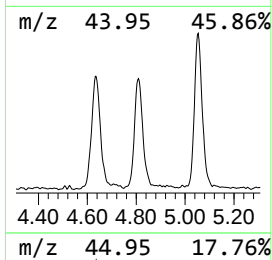
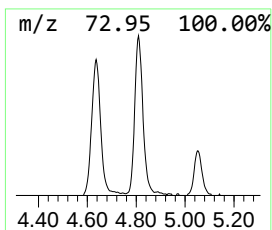
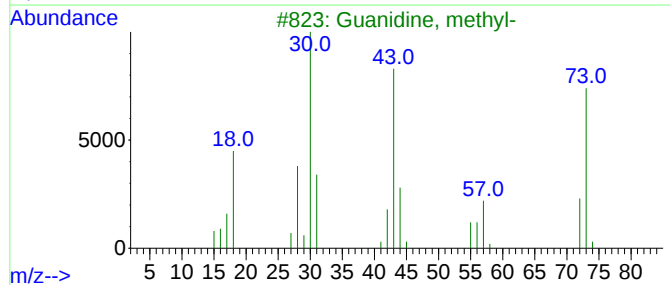
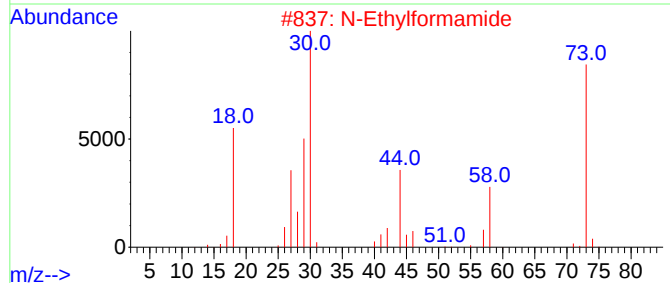
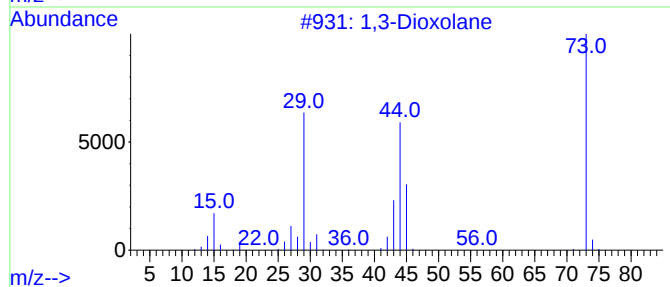
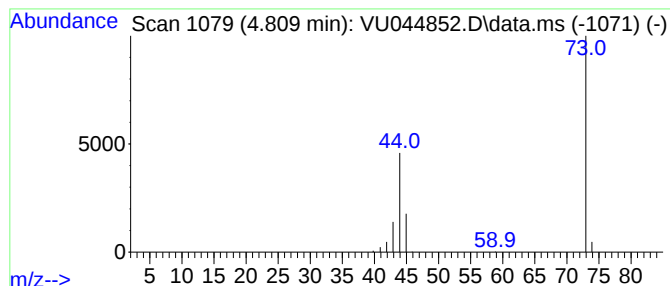
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 2 1,3-Dioxolane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.809	6.24 ug/l	69338	Pentafluorobenzene	5.378

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane	74	C3H6O2	000646-06-0	90
2			N-Ethylformamide	73	C3H7NO	000627-45-2	5
3			Guanidine, methyl-	73	C2H7N3	000471-29-4	5
4			Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	4
5			Ethylene oxide	44	C2H4O	000075-21-8	4



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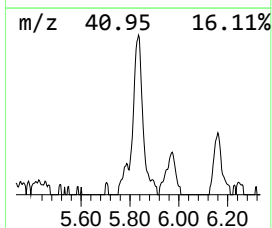
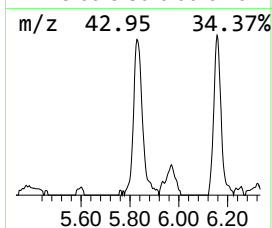
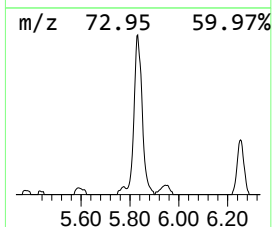
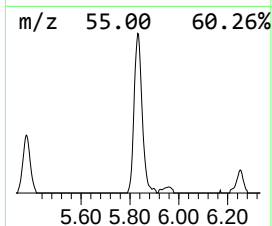
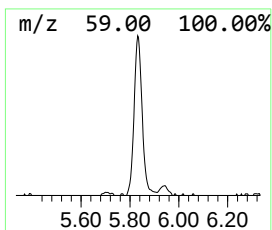
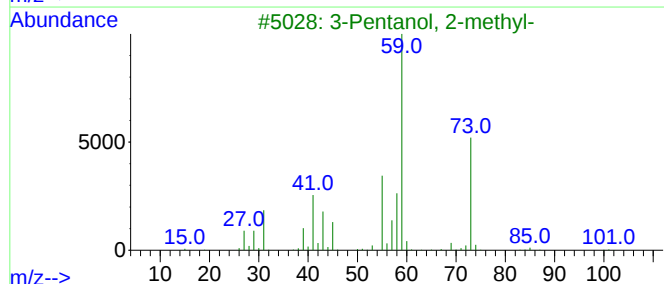
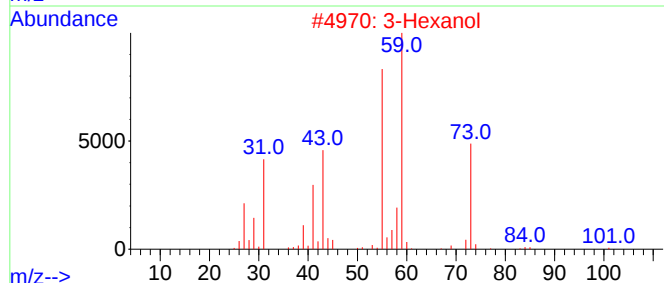
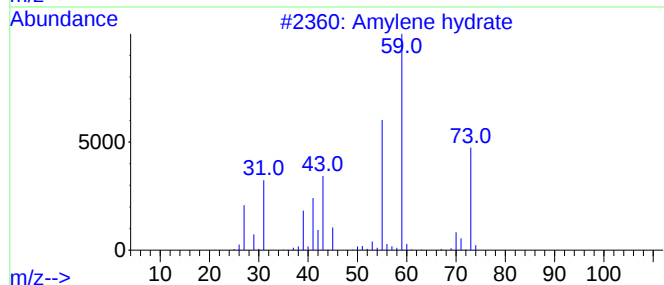
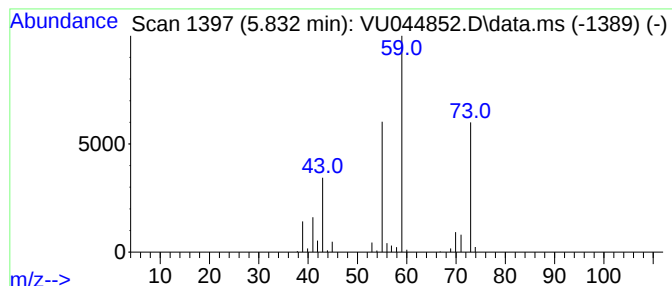
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 3 Amylene hydrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.832	6.13 ug/l	92920	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Hexanol	102	C6H14O	000623-37-0	43
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
4			1-Hepten-4-ol	114	C7H14O	003521-91-3	9
5			1-Butanol, 3-methyl-, formate	116	C6H12O2	000110-45-2	9



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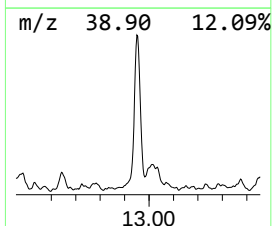
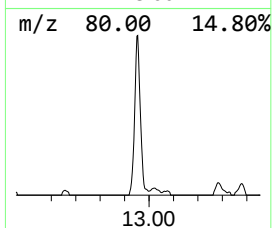
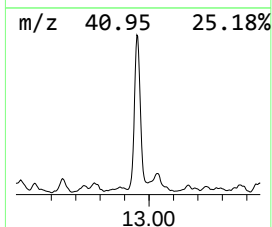
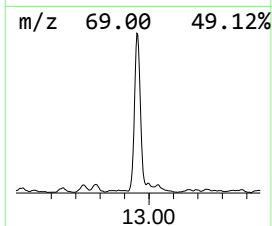
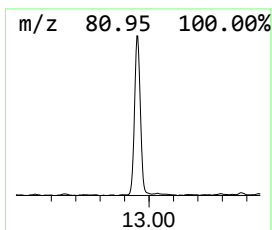
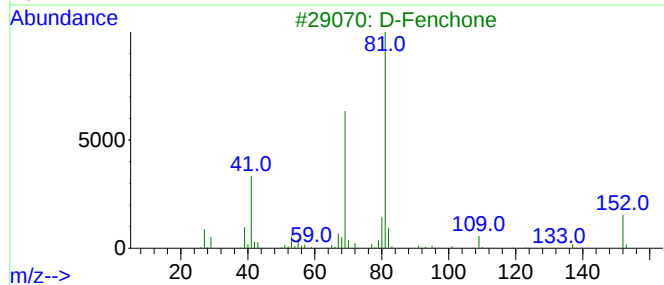
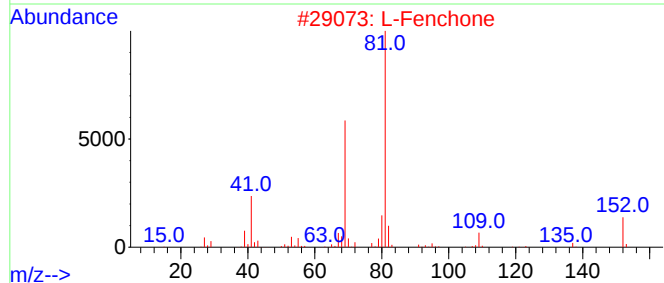
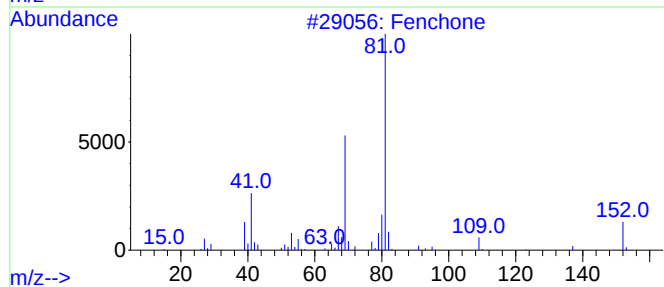
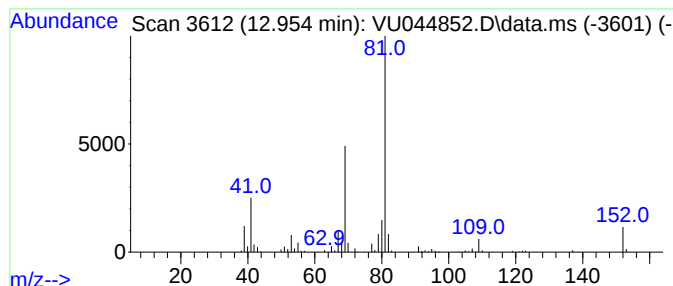
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.954	12.23 ug/l	242214	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	94
2			L-Fenchone	152	C10H16O	007787-20-4	91
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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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
1,3-Dioxolane	4.809	6.2	ug/l	69338	1	5.378	555663	50.0
Amylene hydrate	5.832	6.1	ug/l	92920	2	6.253	757391	50.0
Fenchone	12.954	12.2	ug/l	242214	4	11.815	990314	50.0