

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092123\
 Data File : VY015671.D
 Acq On : 21 Sep 2023 12:52
 Operator : SY/MD
 Sample : 04364-02
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VOC

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_Y\methods\82Y091923S.M

Title : SW846 8260

Signal : TIC: VY015671.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.710	463	474	487	rBV2	18317	56495	3.75%	0.936%
2	5.747	632	644	656	rBV2	9129	29649	1.97%	0.491%
3	6.978	835	846	861	rBV2	12954	42524	2.83%	0.704%
4	7.716	956	967	973	rBV	105804	250633	16.66%	4.152%
5	7.789	973	979	991	rVB	172747	394254	26.20%	6.531%
6	8.142	1025	1037	1047	rBV	115581	265601	17.65%	4.400%
7	8.691	1119	1127	1136	rBV	277922	541228	35.97%	8.966%
8	10.179	1365	1371	1380	rBV	439199	746695	49.63%	12.370%
9	10.581	1433	1437	1445	rVB2	28117	49631	3.30%	0.822%
10	10.947	1492	1497	1503	rBV	31569	55072	3.66%	0.912%
11	11.489	1580	1586	1596	rVB	411650	670755	44.58%	11.112%
12	12.154	1686	1695	1698	rBV5	59475	192801	12.81%	3.194%
13	12.483	1743	1749	1755	rBV	348443	582891	38.74%	9.656%
14	13.196	1861	1866	1868	rBV5	60182	112187	7.46%	1.858%
15	13.422	1895	1903	1922	rVB2	600704	1504632	100.00%	24.926%
16	13.782	1956	1962	1972	rVB3	85438	267243	17.76%	4.427%
17	15.501	2239	2244	2269	rVB5	65491	274159	18.22%	4.542%

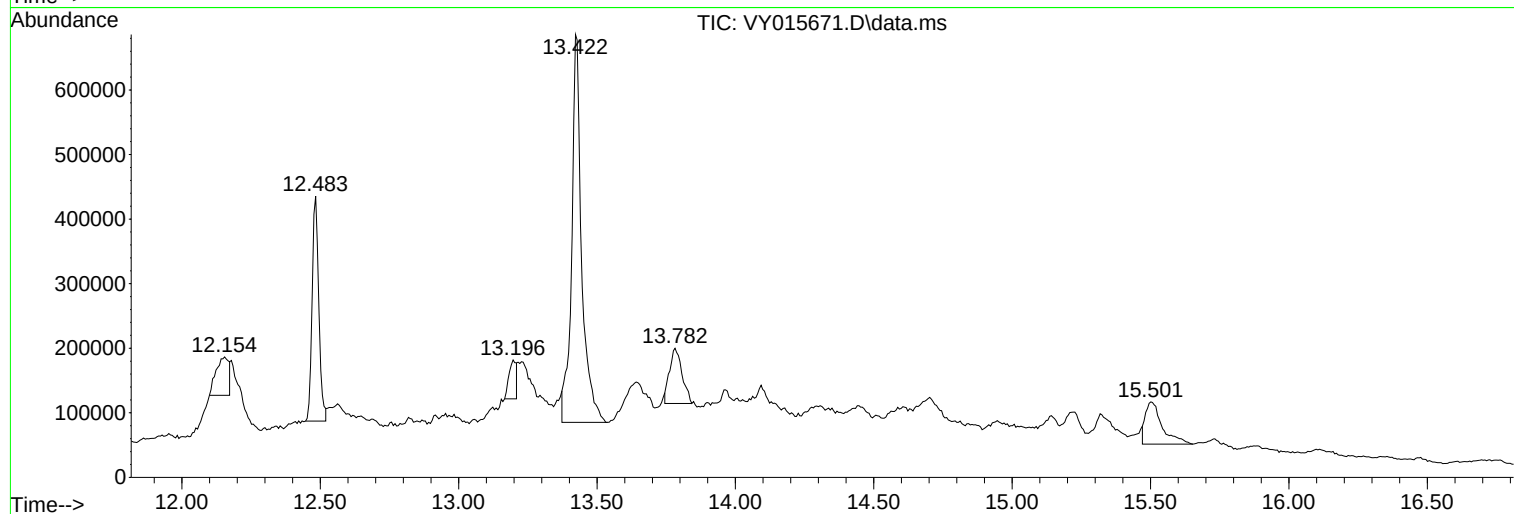
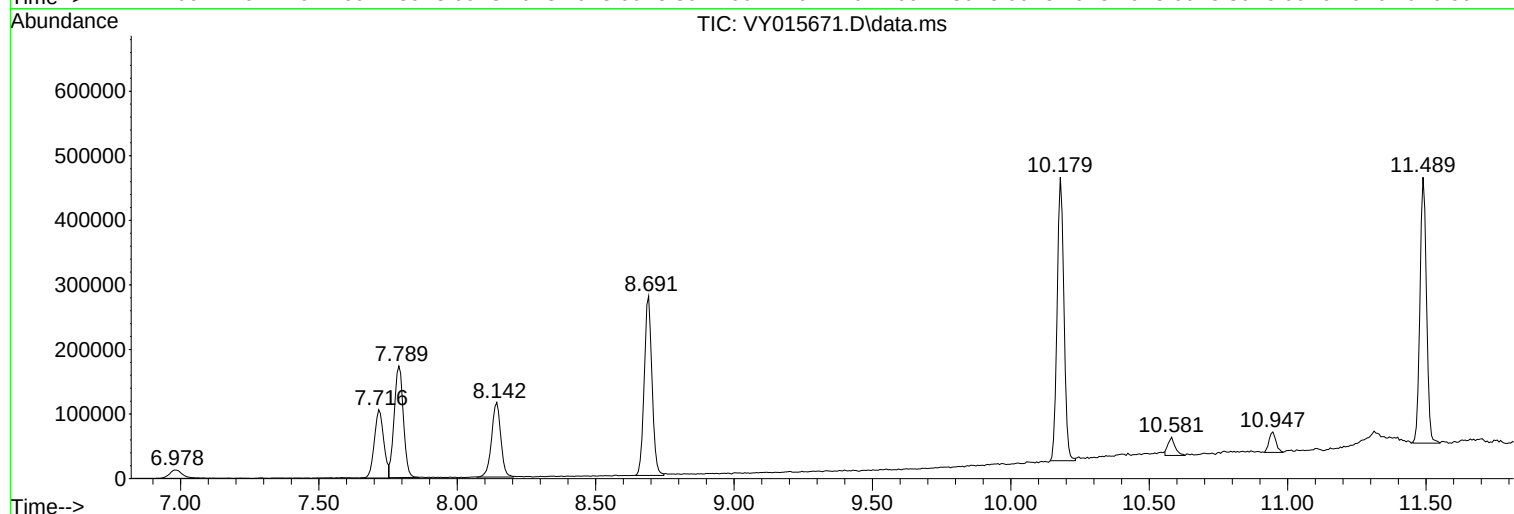
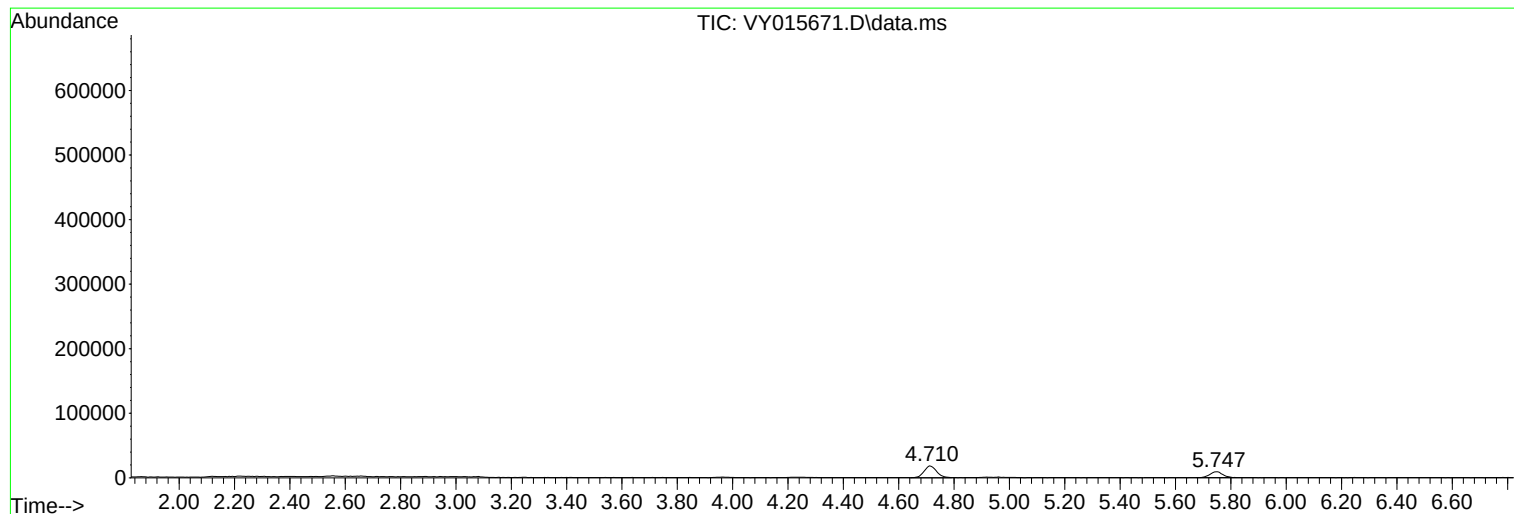
Sum of corrected areas: 6036450

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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



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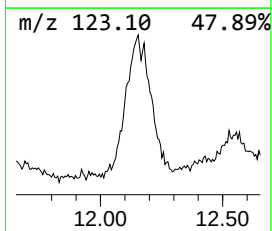
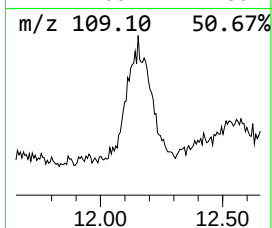
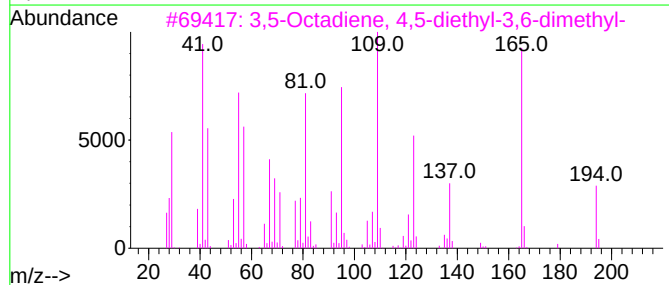
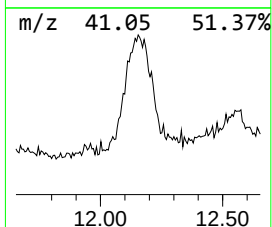
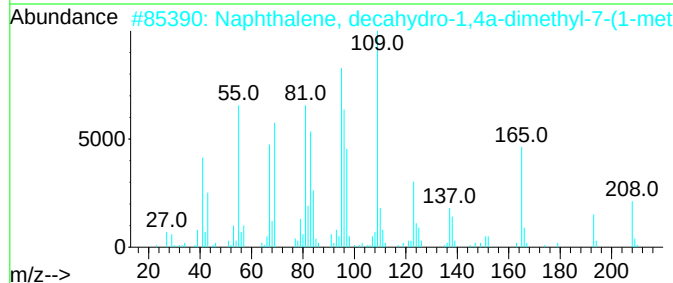
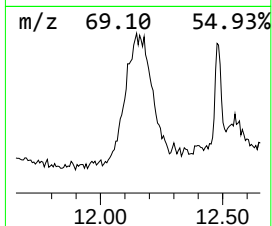
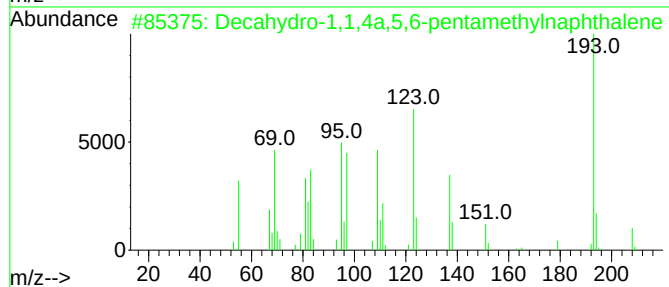
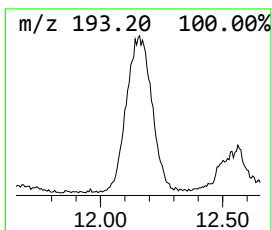
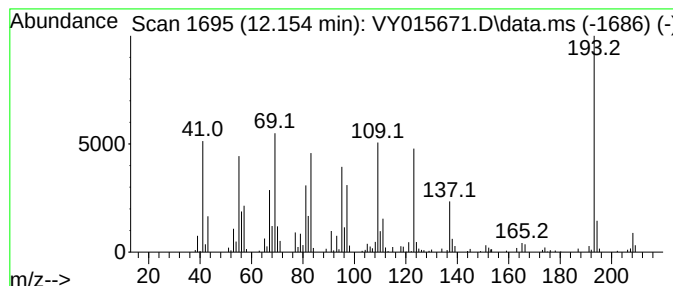
Instrument :
MSVOA_Y
ClientSampleId :
VOC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.154	14.37 ug/l	192801	Chlorobenzene-d5			11.489
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	58
2	Naphthalene, decahydro-1,4a-dime...		208	C15H28	030824-81-8	41
3	3,5-Octadiene, 4,5-diethyl-3,6-d...		194	C14H26	061233-79-2	22
4	Iminostilbene		193	C14H11N	000256-96-2	22
5	Cyclododecanone, 2-methylene-		194	C13H22O	003045-76-9	22



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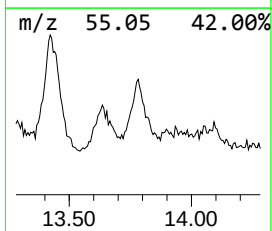
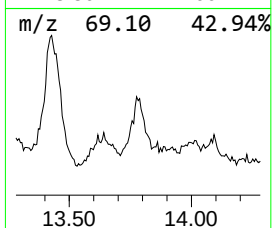
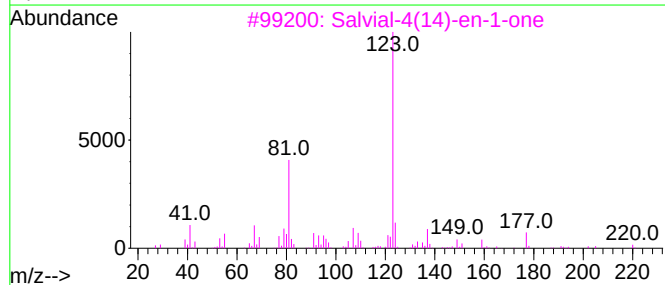
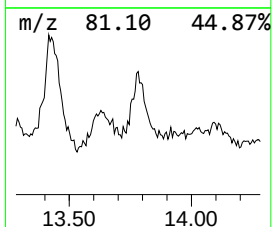
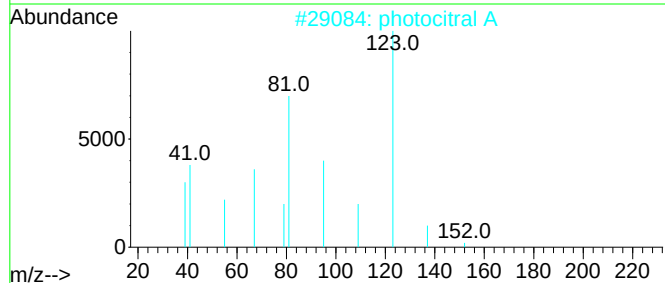
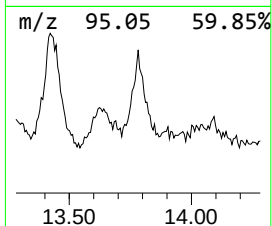
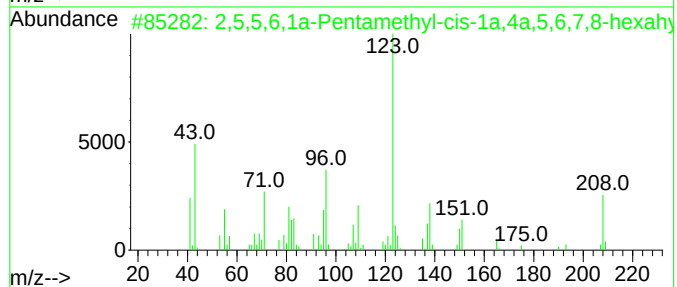
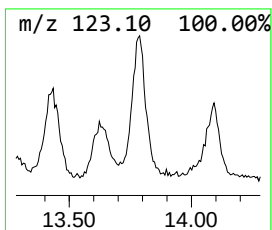
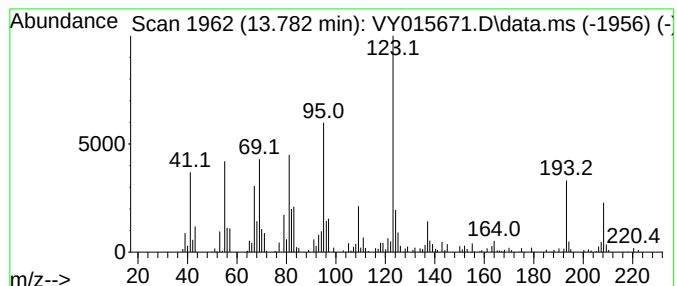
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Peak Number 4 2,5,5,6,1a-Pentamethyl-cis-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.782	8.88 ug/l	267243	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	50		
2	photocitral A	152	C10H16O	055253-28-6	46		
3	Salvial-4(14)-en-1-one	220	C15H24O	073809-82-2	38		
4	p-Hydroxyphenyl methyl carbinol	138	C8H10O2	002380-91-8	38		
5	Propanamide, N-(4-methoxyphenyl)...	193	C11H15NO2	1000307-32-2	35		



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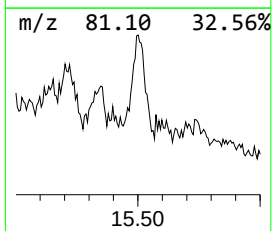
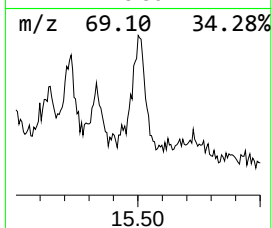
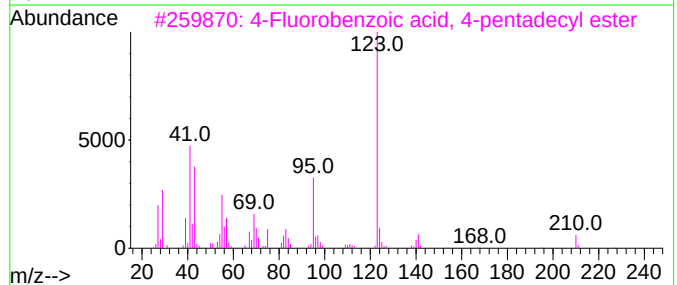
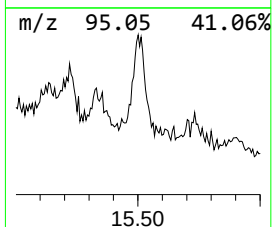
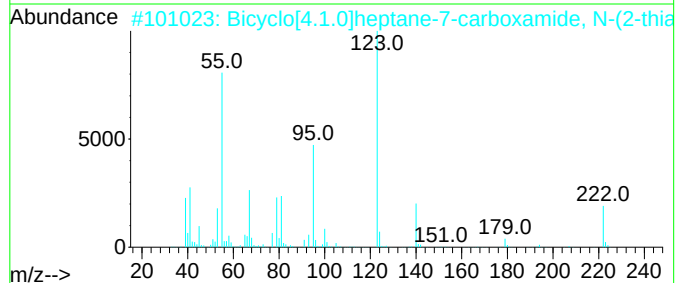
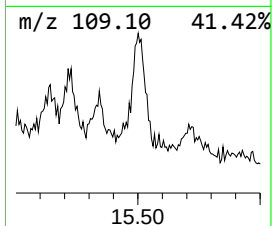
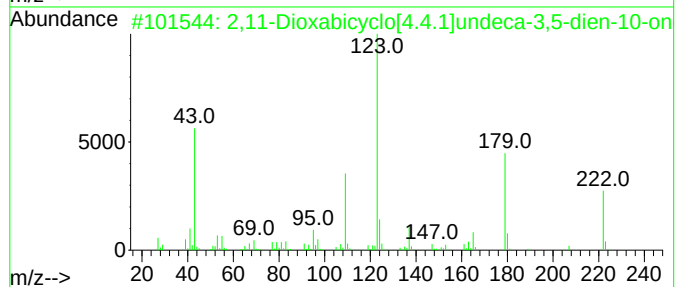
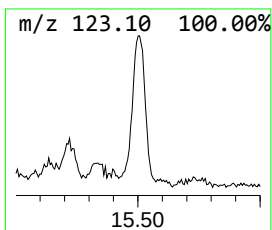
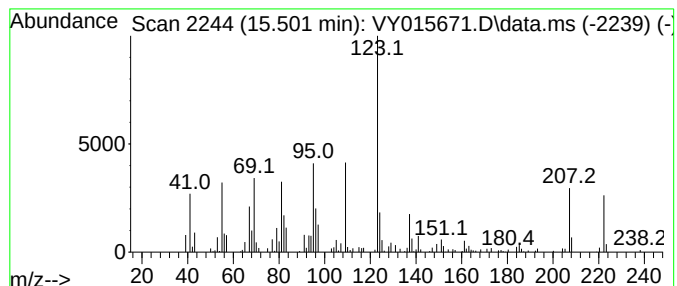
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TIC Integration Parameters: LSCINT.P

Peak Number 5 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	9.11 ug/l	274159	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	52
2			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	43
3			4-Fluorobenzoic acid, 4-pentadec...	350	C22H35FO2	1000280-68-5	43
4			N-[1-(4-Chlorobenzyl)-2-oxoazepa...	374	C20H20ClFN2O2	1000481-70-9	37
5			Phorone	138	C9H14O	000504-20-1	35



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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decahydro-1,1,4...	12.154	14.4	ug/l	192801	3	11.489	670755	50.0
2,5,5,6,1a-Pent...	13.782	8.9	ug/l	267243	4	13.428	1504630	50.0
2,11-Dioxabicyc...	15.501	9.1	ug/l	274159	4	13.428	1504630	50.0