

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042021\
 Data File : VY004530.D
 Acq On : 20 Apr 2021 15:44
 Operator : SY/MD
 Sample : M2090-15
 Misc : 5.79G/5ML/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SEDGWICK-VOC-9

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\82Y041221S.M

Title : SW846 8260

Signal : TIC: VY004530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.235	45	68	70	rBV5	9811	50425	8.13%	1.903%
2	2.564	113	122	123	rBV4	12247	29609	4.77%	1.117%
3	3.954	342	350	364	rVB	11695	32088	5.17%	1.211%
4	4.729	469	477	487	rBV3	4812	14857	2.40%	0.561%
5	7.728	960	969	974	rBV	33180	78220	12.61%	2.951%
6	7.801	974	981	990	rVB	94503	214838	34.63%	8.106%
7	8.149	1030	1038	1052	rVB	56206	122893	19.81%	4.637%
8	8.697	1119	1128	1138	rVB	144390	288166	46.45%	10.873%
9	10.185	1364	1372	1379	rBV	238426	404095	65.14%	15.247%
10	11.496	1579	1587	1593	rBV	201580	339151	54.67%	12.797%
11	11.703	1615	1621	1626	rBV4	4040	7602	1.23%	0.287%
12	12.337	1719	1725	1731	rBV	21707	35459	5.72%	1.338%
13	12.489	1740	1750	1758	rBV3	354705	620333	100.00%	23.406%
14	12.739	1783	1791	1793	rBV	4731	7108	1.15%	0.268%
15	12.806	1798	1802	1809	rVB3	7149	12049	1.94%	0.455%
16	13.123	1849	1854	1859	rBV	11396	16825	2.71%	0.635%
17	13.428	1898	1904	1913	rVB	184292	296670	47.82%	11.194%
18	13.751	1952	1957	1961	rBV6	4186	7727	1.25%	0.292%
19	13.965	1987	1992	1999	rVB2	13944	23290	3.75%	0.879%
20	14.081	2007	2011	2017	rVB5	4122	6810	1.10%	0.257%
21	14.684	2103	2110	2116	rBV7	5585	13341	2.15%	0.503%
22	15.239	2195	2201	2206	rVB	12875	20782	3.35%	0.784%
23	16.294	2369	2374	2380	rVB5	4610	7929	1.28%	0.299%

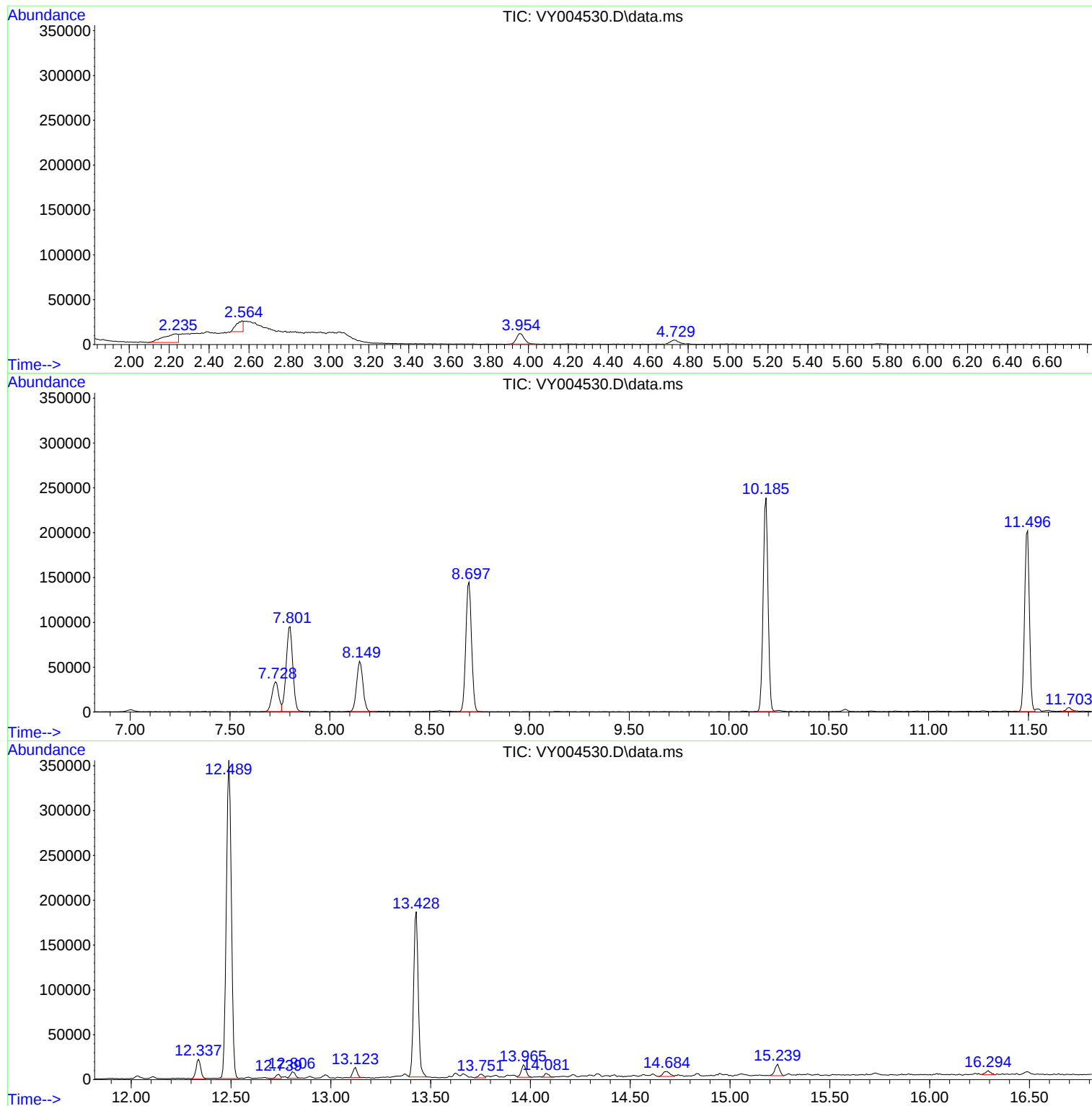
Sum of corrected areas: 2650267

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
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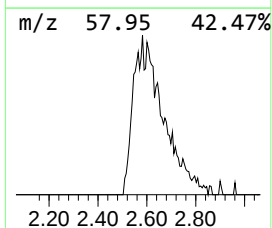
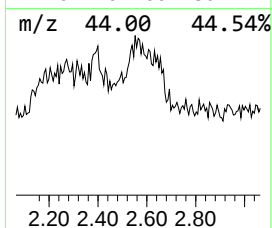
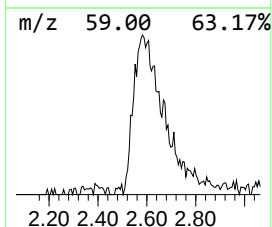
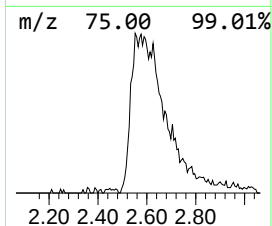
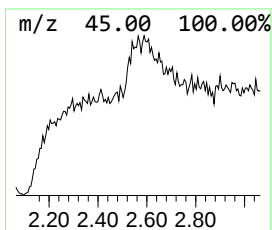
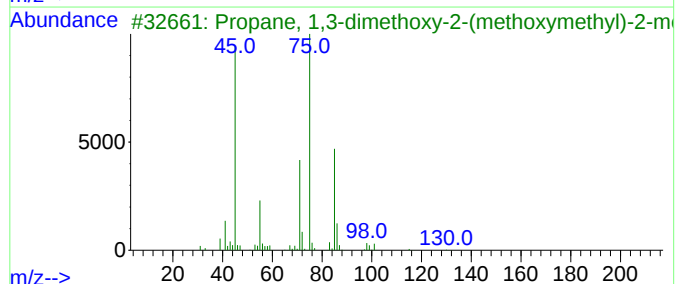
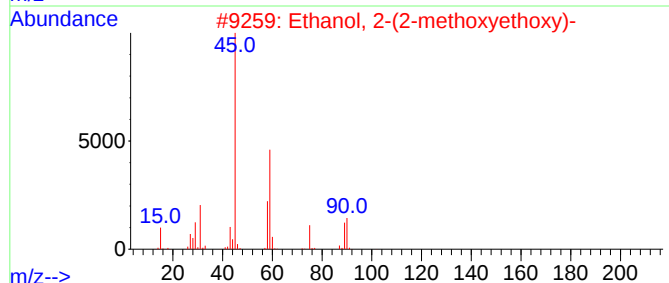
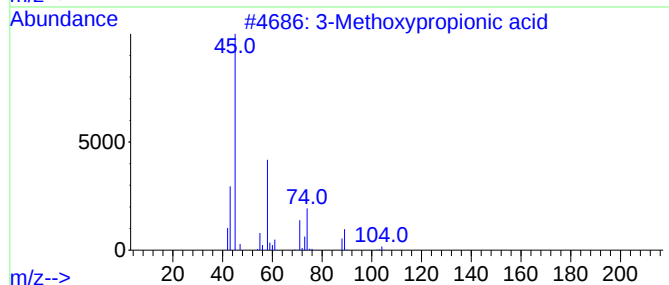
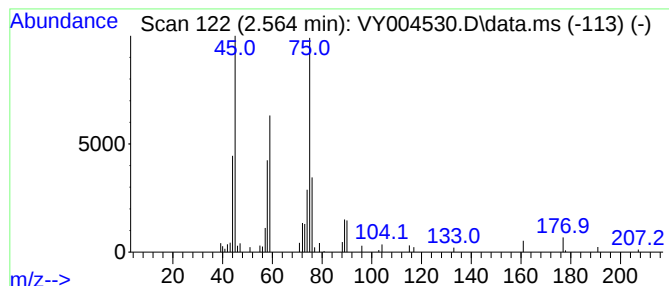
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.564 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.564	6.89 ug/l	29609	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methoxypropionic acid	104	C4H8O3	002544-06-1	35
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	32
3			Propane, 1,3-dimethoxy-2-(methox...	162	C8H18O3	015476-20-7	25
4			1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	25
5			Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	16



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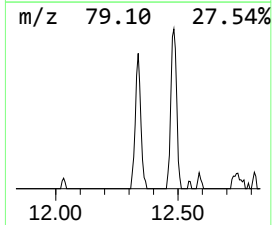
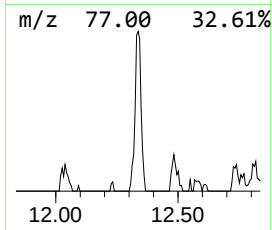
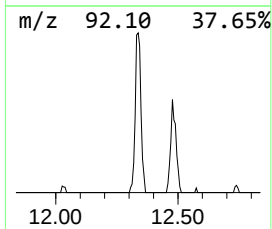
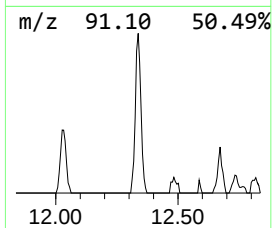
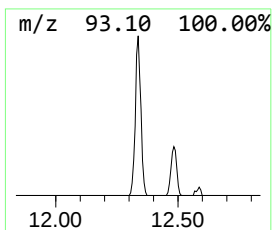
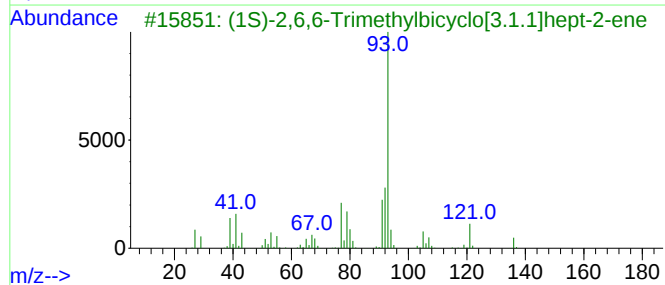
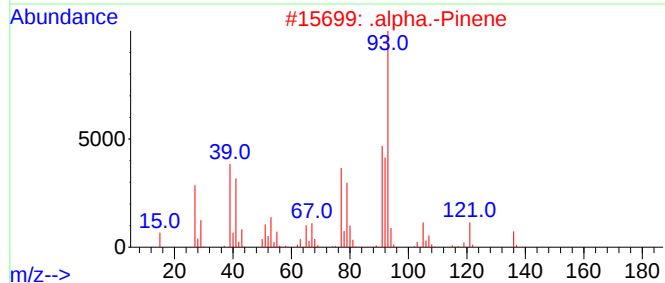
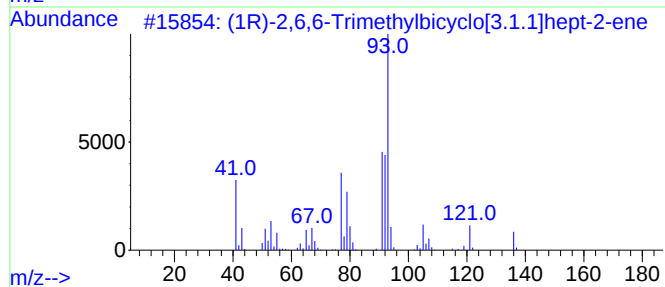
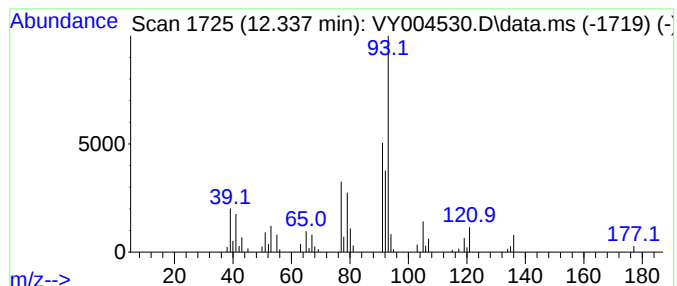
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Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	5.23 ug/l	35459	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	96
2			.alpha.-Pinene	136	C10H16	000080-56-8	95
3			(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91
4			Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
5			Cyclohexene, 4-methylene-1-(1-methyl-2-propenyl)-	136	C10H16	000099-84-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.564	2.564	6.9	ug/l	29609	1	7.801	214838	50.0
(1R)-2,6,6-Trim...	12.337	5.2	ug/l	35459	3	11.496	339151	50.0