

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072823\
 Data File : VY014913.D
 Acq On : 28 Jul 2023 16:56
 Operator : SY/MD
 Sample : 03813-01
 Misc : 4.89g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 PLAUDERVILLE-1

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\82Y071323S.M
 Title : SW846 8260

Signal : TIC: VY014913.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	59	64	66	rBV2	6469	10050	1.32%	0.162%
2	3.942	340	348	357	rBV	5051	14380	1.90%	0.231%
3	4.198	381	390	401	rBV	6316	20185	2.66%	0.325%
4	4.704	460	473	487	rBV	20357	66492	8.76%	1.070%
5	5.728	632	641	652	rVB3	6591	21127	2.78%	0.340%
6	6.972	832	845	871	rBV	99615	338804	44.65%	5.453%
7	7.710	957	966	972	rBV	108743	257348	33.91%	4.142%
8	7.783	972	978	990	rVB	176515	401376	52.90%	6.460%
9	8.130	1022	1035	1047	rBV2	127435	332821	43.86%	5.357%
10	8.685	1117	1126	1134	rBV	275677	550306	72.52%	8.857%
11	10.173	1363	1370	1378	rBV	441546	758811	100.00%	12.213%
12	10.258	1378	1384	1387	rBV4	6426	12571	1.66%	0.202%
13	10.575	1427	1436	1443	rBV	102500	185132	24.40%	2.980%
14	10.941	1490	1496	1508	rBV	55296	102430	13.50%	1.649%
15	11.038	1508	1512	1518	rVB4	6701	11094	1.46%	0.179%
16	11.313	1552	1557	1564	rVB2	35981	60324	7.95%	0.971%
17	11.483	1577	1585	1594	rBV	433707	707510	93.24%	11.387%
18	12.105	1681	1687	1696	rVB2	5816	10553	1.39%	0.170%
19	12.331	1715	1724	1728	rBV4	7966	13883	1.83%	0.223%
20	12.477	1738	1748	1755	rBV3	413153	744892	98.17%	11.989%
21	12.544	1755	1759	1762	rBV5	7362	12407	1.64%	0.200%
22	12.623	1767	1772	1781	rVB	17531	40017	5.27%	0.644%
23	12.825	1795	1805	1811	rBV5	18563	53028	6.99%	0.853%
24	12.983	1827	1831	1837	rBV6	2940	7881	1.04%	0.127%
25	13.062	1840	1844	1851	rVB	27597	43532	5.74%	0.701%
26	13.178	1856	1863	1869	rVB2	19930	32392	4.27%	0.521%
27	13.276	1869	1879	1884	rBV	36592	68436	9.02%	1.101%
28	13.337	1884	1889	1892	rBV3	9956	18081	2.38%	0.291%
29	13.422	1897	1903	1908	rVV	429428	699426	92.17%	11.257%
30	13.477	1908	1912	1924	rVB3	29785	64916	8.55%	1.045%
31	13.635	1932	1938	1942	rBV2	12246	21171	2.79%	0.341%
32	13.776	1955	1961	1966	rBV4	5757	11137	1.47%	0.179%
33	13.959	1986	1991	1999	rBV2	12636	21082	2.78%	0.339%
34	14.306	2043	2048	2055	rVB2	26985	44918	5.92%	0.723%
35	14.465	2067	2074	2085	rBV	224027	352561	46.46%	5.674%
36	14.562	2085	2090	2096	rBV	31934	50509	6.66%	0.813%

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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\82Y071323S.M
Title : SW846 8260

37	15.312	2205	2213	2219	rBV	30879	51496	6.79%	0.829%
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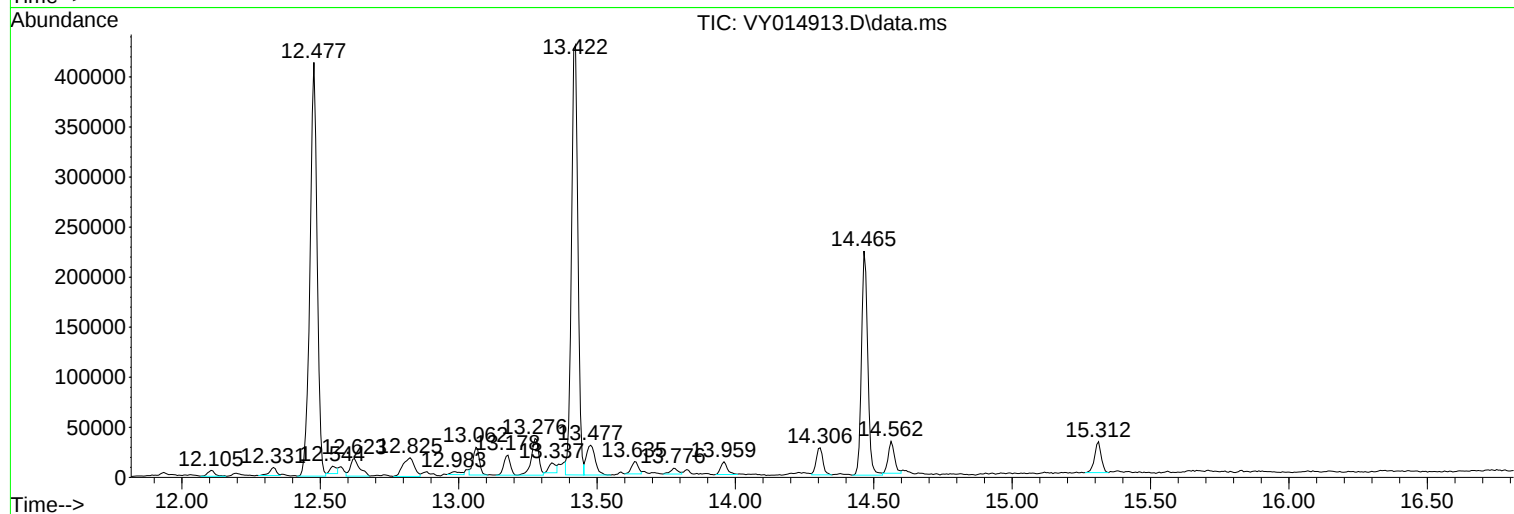
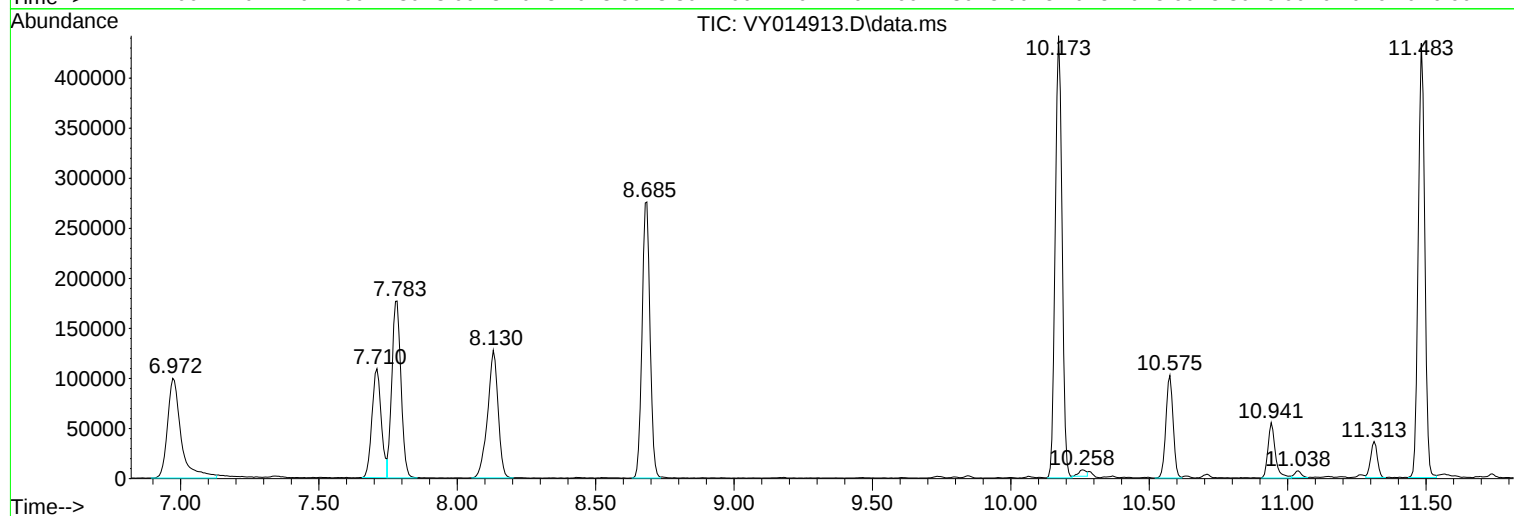
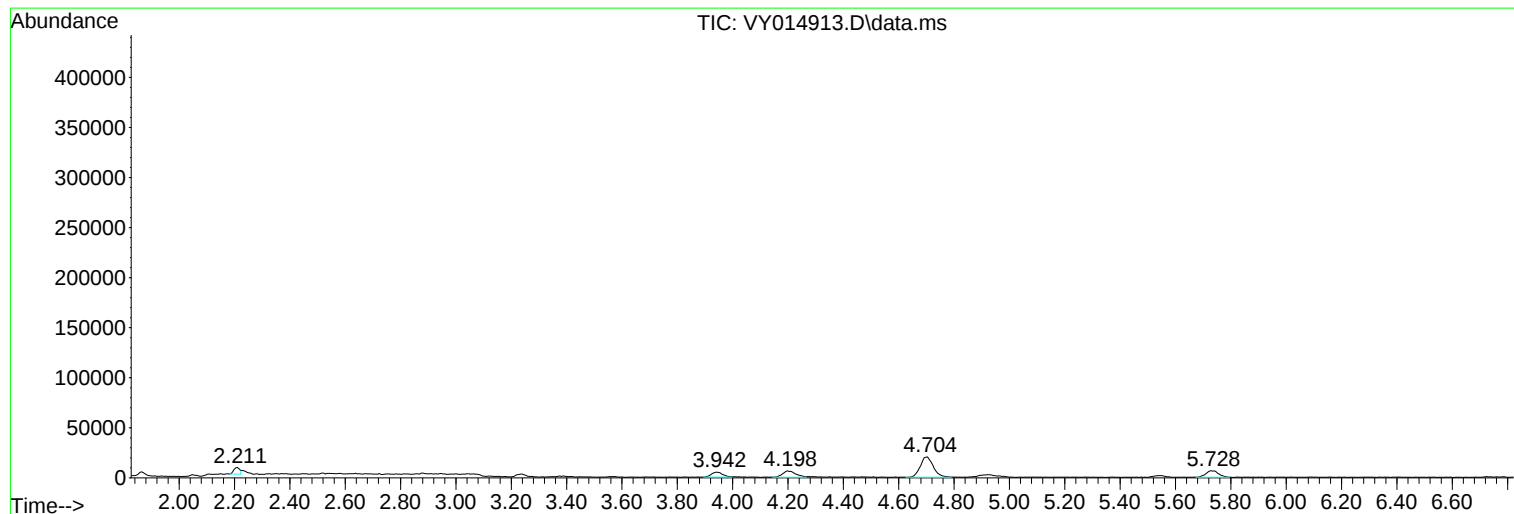
Sum of corrected areas: 6213079

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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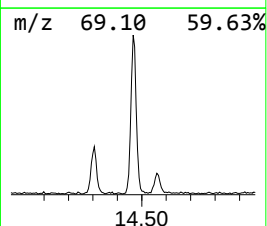
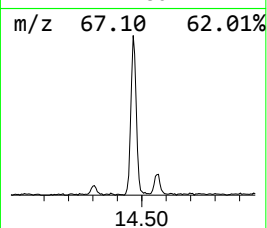
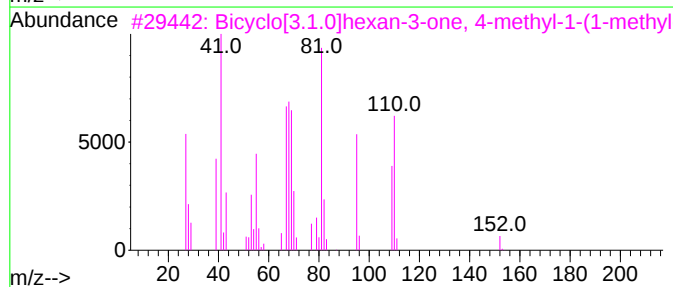
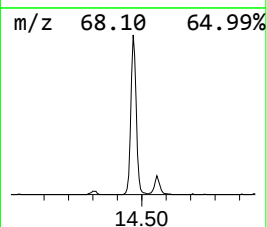
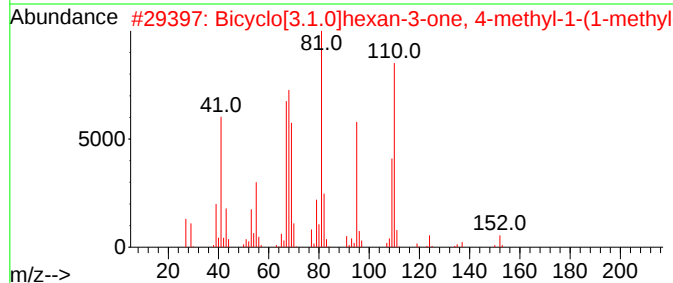
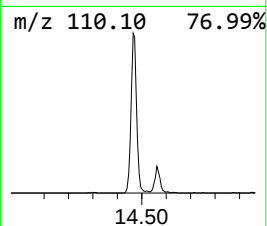
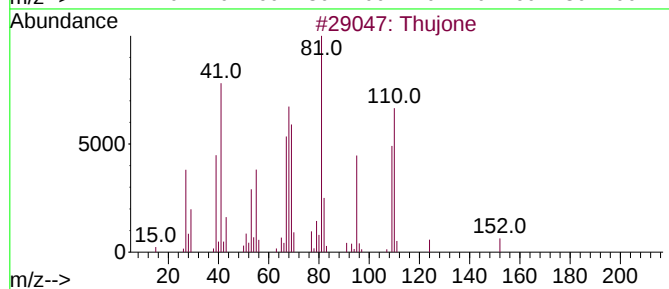
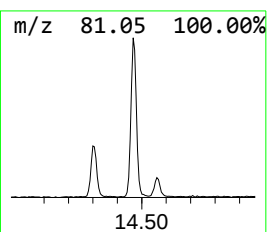
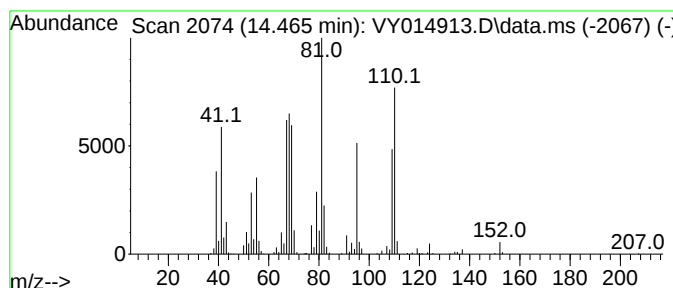
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Thujone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.464	25.20 ug/l	352561	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thujone	152	C10H16O	000546-80-5	98
2			Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	94
3			Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	000471-15-8	93
4			3,5-Octadiene, (Z,Z)-	110	C8H14	007348-80-3	74
5			5-Hexenal, 4-methylene-	110	C7H10O	017844-21-2	60



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Thujone	14.464	25.2	ug/l	352561	4	13.422	699426	50.0