

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060823\
 Data File : VY014082.D
 Acq On : 08 Jun 2023 18:49
 Operator : KP/MD
 Sample : 03072-01
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 30999

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\82Y060123S.M

Title : SW846 8260

Signal : TIC: VY014082.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	20	rVB3	17354	30008	3.23%	0.479%
2	1.997	23	29	35	rBV2	6928	11366	1.23%	0.181%
3	2.223	60	66	75	rBV	21349	37073	4.00%	0.591%
4	2.387	88	93	101	rBV	12805	25512	2.75%	0.407%
5	3.832	321	330	337	rBV	5142	12880	1.39%	0.205%
6	3.960	342	351	374	rVV2	32837	116574	12.57%	1.859%
7	4.204	381	391	400	rBV	7344	21390	2.31%	0.341%
8	4.326	405	411	421	rVB2	3116	9334	1.01%	0.149%
9	4.716	466	475	483	rBV	11907	34324	3.70%	0.547%
10	5.588	607	618	628	rBV6	3199	11448	1.23%	0.183%
11	5.746	635	644	657	rBV5	6964	22133	2.39%	0.353%
12	6.703	793	801	802	rBV2	8967	14480	1.56%	0.231%
13	6.990	831	848	860	rBV3	14073	47698	5.14%	0.761%
14	7.722	958	968	973	rBV	132784	312480	33.68%	4.984%
15	7.789	973	979	991	rVB	199155	456924	49.25%	7.288%
16	8.142	1027	1037	1048	rBV	134549	307169	33.11%	4.900%
17	8.551	1097	1104	1113	rBV4	3893	10666	1.15%	0.170%
18	8.691	1117	1127	1142	rVV	318492	630772	67.99%	10.061%
19	9.142	1195	1201	1209	rBV2	12702	26649	2.87%	0.425%
20	9.264	1216	1221	1232	rBV2	11328	23160	2.50%	0.369%
21	10.069	1347	1353	1363	rBV	25920	49681	5.36%	0.792%
22	10.178	1363	1371	1379	rBV	545171	927704	100.00%	14.797%
23	10.495	1415	1423	1429	rBV6	5978	13250	1.43%	0.211%
24	10.581	1429	1437	1441	rBV2	8044	14390	1.55%	0.230%
25	10.837	1474	1479	1488	rVB	10287	19238	2.07%	0.307%
26	10.934	1488	1495	1502	rBV3	27331	51243	5.52%	0.817%
27	11.489	1578	1586	1596	rBV	529989	855536	92.22%	13.646%
28	11.703	1615	1621	1624	rBV5	4789	9865	1.06%	0.157%
29	11.733	1624	1626	1632	rVB4	7166	11876	1.28%	0.189%
30	12.026	1668	1674	1681	rVB	23907	38295	4.13%	0.611%
31	12.105	1681	1687	1694	rVB	18036	27571	2.97%	0.440%
32	12.209	1698	1704	1714	rBV3	19333	36642	3.95%	0.584%
33	12.337	1718	1725	1729	rBV2	10591	16961	1.83%	0.271%
34	12.483	1742	1749	1760	rVB	427874	681906	73.50%	10.877%
35	12.806	1787	1802	1809	rBV3	41666	93391	10.07%	1.490%
36	12.910	1814	1819	1825	rVV4	11114	26466	2.85%	0.422%

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37	13.160	1852	1860	1867	rVB6	14920	33015	3.56%	0.527%
38	13.269	1871	1878	1882	rBV3	20773	33475	3.61%	0.534%
39	13.428	1897	1904	1915	rBV	525714	839147	90.45%	13.385%
40	13.525	1915	1920	1926	rVB	76790	108146	11.66%	1.725%
41	13.788	1959	1963	1969	rVB7	5698	10884	1.17%	0.174%
42	13.849	1969	1973	1977	rVV3	12412	18859	2.03%	0.301%
43	13.897	1977	1981	1987	rVV5	10196	17608	1.90%	0.281%
44	13.964	1987	1992	1999	rVB	12676	22848	2.46%	0.364%
45	14.105	2008	2015	2022	rBV2	14434	25220	2.72%	0.402%
46	14.208	2022	2032	2037	rVB	27529	49362	5.32%	0.787%
47	14.452	2069	2072	2078	rVB6	6285	9881	1.07%	0.158%
48	14.623	2096	2100	2104	rVV4	8281	12946	1.40%	0.206%
49	14.757	2119	2122	2131	rVB4	11088	18107	1.95%	0.289%
50	14.958	2151	2155	2163	rVB5	11426	23167	2.50%	0.370%
51	15.318	2211	2214	2219	rVB	7757	10644	1.15%	0.170%

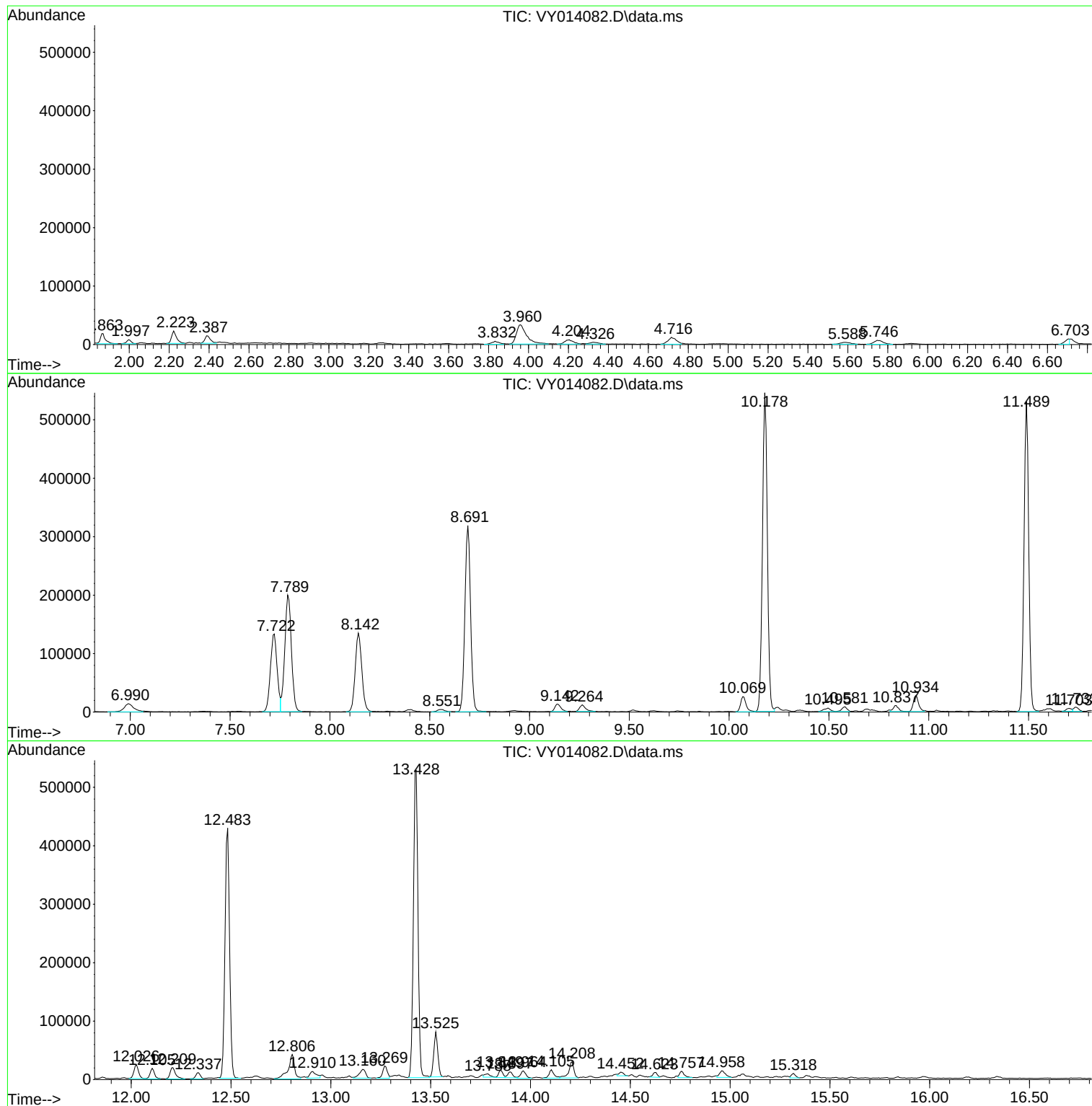
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.M
Quant Title : SW846 8260

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



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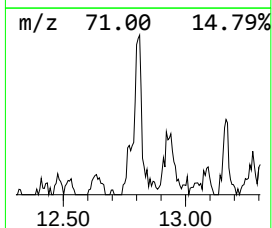
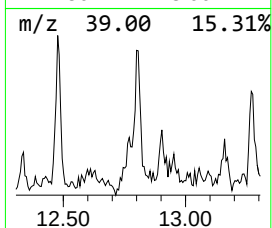
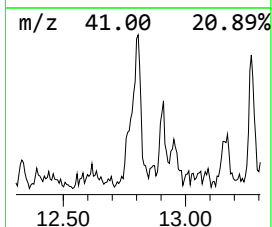
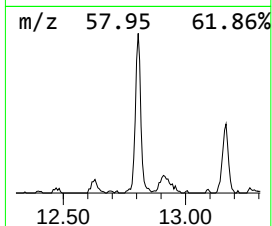
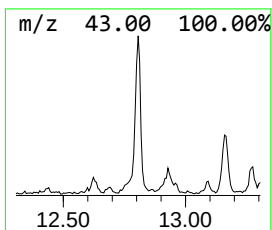
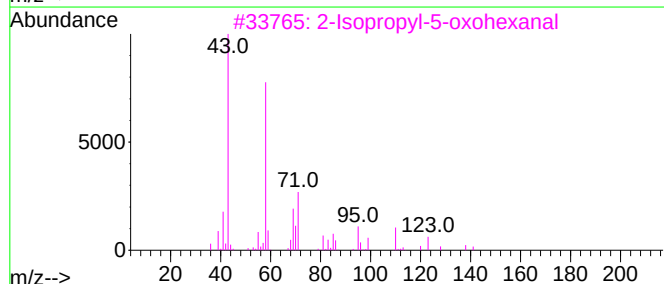
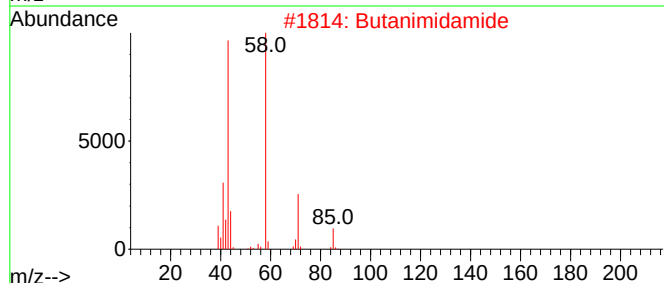
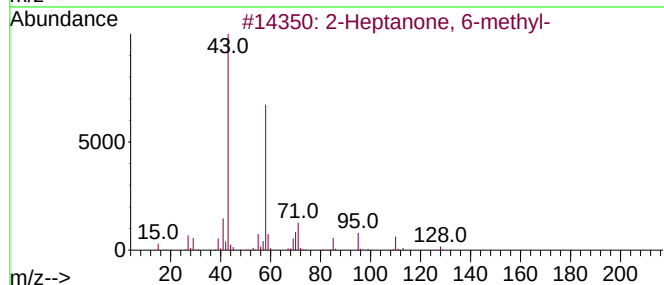
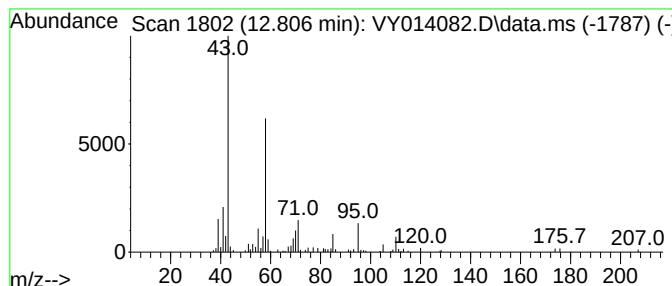
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.M
Quant Title : SW846 8260

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

Peak Number 1 2-Heptanone, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	5.56 ug/l	93391	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2			Butanimidamide	86	C4H10N2	000107-90-4	53
3			2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	50
4			2-Octanone	128	C8H16O	000111-13-7	50
5			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	43



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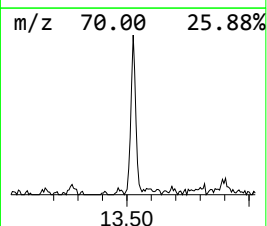
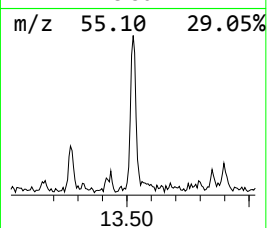
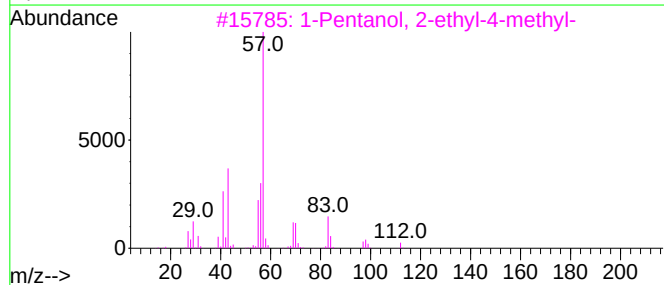
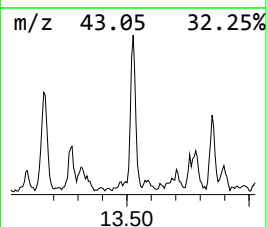
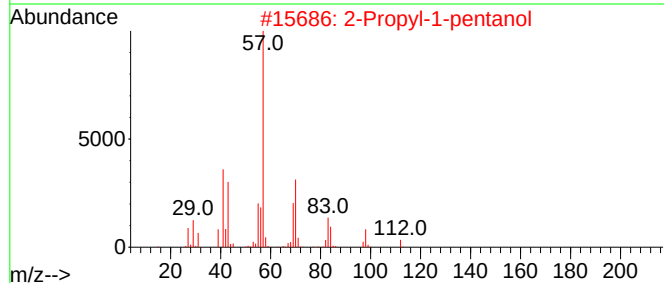
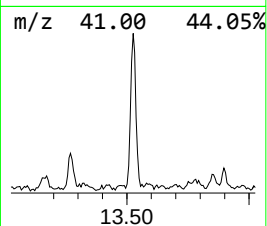
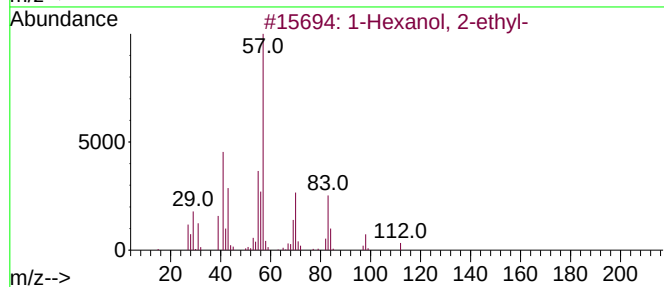
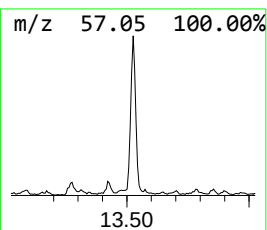
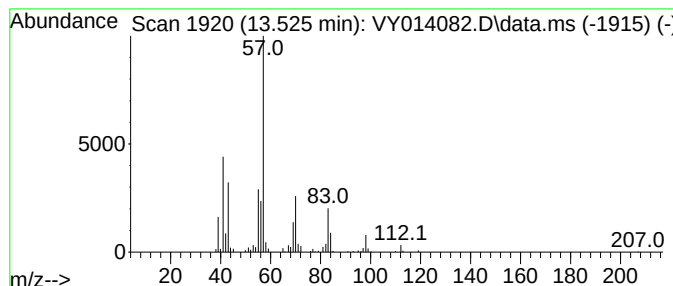
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Quant Title : SW846 8260

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.525	6.44 ug/l	108146	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Heptanone, 6-...	12.806	5.6	ug/l	93391	4	13.428	839147	50.0
1-Hexanol, 2-et...	13.525	6.4	ug/l	108146	4	13.428	839147	50.0