

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY080122\
 Data File : VY009802.D
 Acq On : 01 Aug 2022 17:25
 Operator : KP/MD
 Sample : N3976-03
 Misc : 4.27g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP2-0729

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\82Y072622S.M
 Title : SW846 8260

Signal : TIC: VY009802.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.698	461	472	487	rBV2	28522	90882	11.92%	2.041%
2	5.734	633	642	654	rBV2	7347	22653	2.97%	0.509%
3	7.710	954	966	972	rBV	92753	223670	29.32%	5.024%
4	7.783	972	978	990	rVB	187889	415048	54.42%	9.322%
5	8.136	1027	1036	1046	rBV	88681	191324	25.08%	4.297%
6	8.685	1118	1126	1138	rVB	293041	575271	75.42%	12.921%
7	10.179	1363	1371	1379	rBV	391233	653323	85.65%	14.674%
8	10.947	1491	1497	1508	rBV	11645	20452	2.68%	0.459%
9	11.489	1578	1586	1597	rBV	482623	762742	100.00%	17.132%
10	12.483	1740	1749	1756	rBV2	247483	427090	55.99%	9.593%
11	12.569	1756	1763	1768	rVV5	3048	7730	1.01%	0.174%
12	12.623	1768	1772	1782	rVB	8555	19825	2.60%	0.445%
13	12.831	1797	1806	1812	rBV4	9133	23032	3.02%	0.517%
14	13.068	1823	1845	1857	rBV	29372	61723	8.09%	1.386%
15	13.178	1857	1863	1869	rBV	15620	24148	3.17%	0.542%
16	13.282	1869	1880	1885	rBV	51167	88272	11.57%	1.983%
17	13.422	1895	1903	1908	rVV	451047	700196	91.80%	15.727%
18	13.477	1908	1912	1922	rVB	46013	102678	13.46%	2.306%
19	13.642	1932	1939	1948	rBV3	14635	26681	3.50%	0.599%
20	13.965	1985	1992	2004	rVB3	5992	15384	2.02%	0.346%

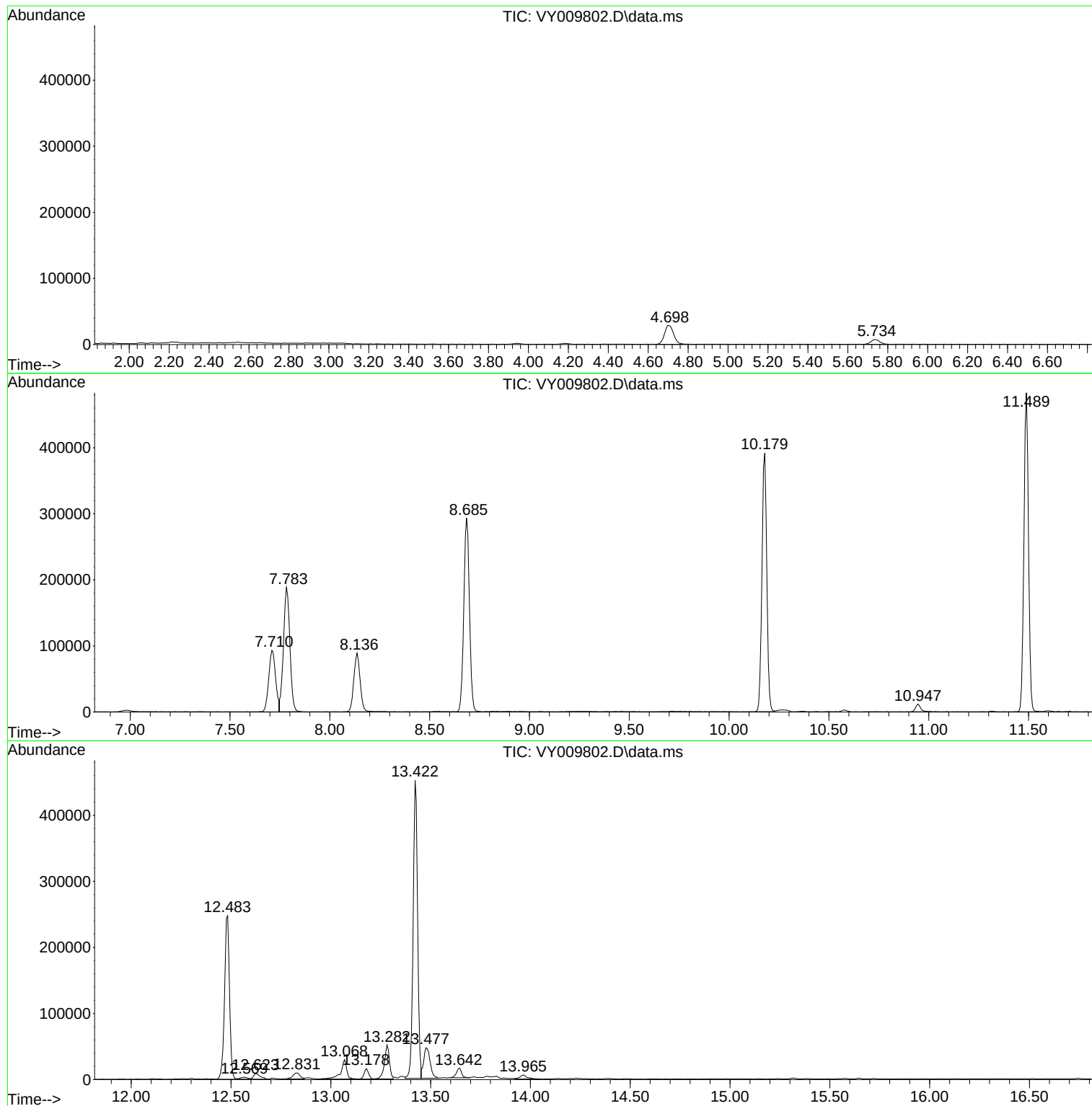
Sum of corrected areas: 4452124

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072622S.M
Quant Title : SW846 8260

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



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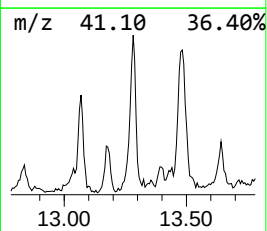
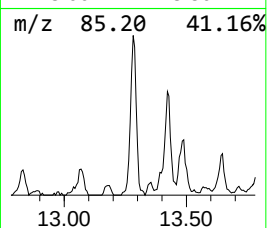
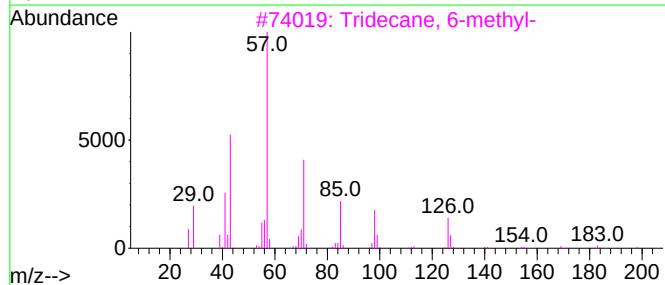
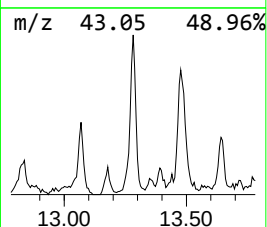
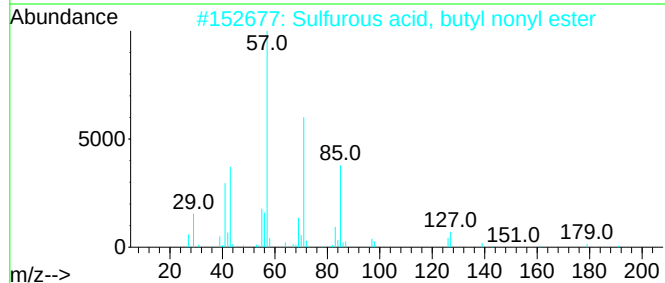
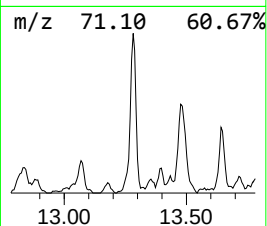
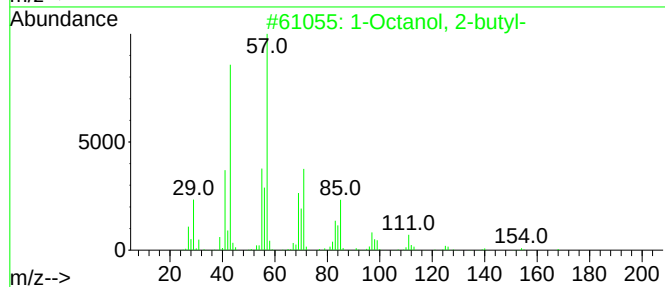
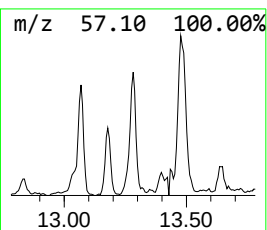
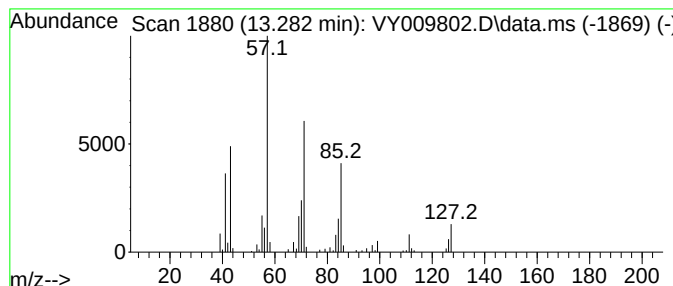
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072622S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Octanol, 2-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	6.30 ug/l	88272	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	59
2		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	50
3		Tridecane, 6-methyl-	198	C14H30	013287-21-3	47
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	47
5		Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	47



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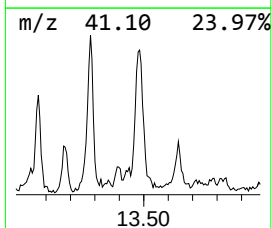
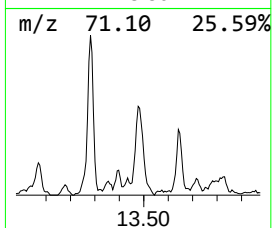
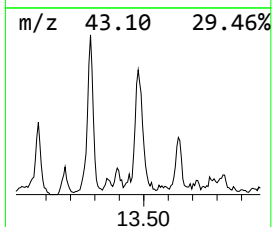
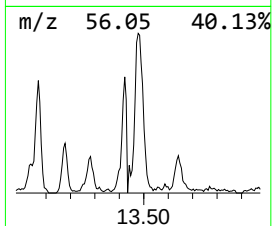
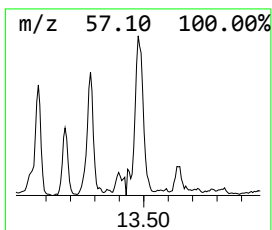
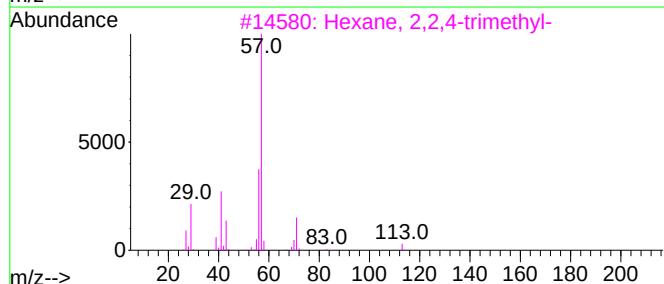
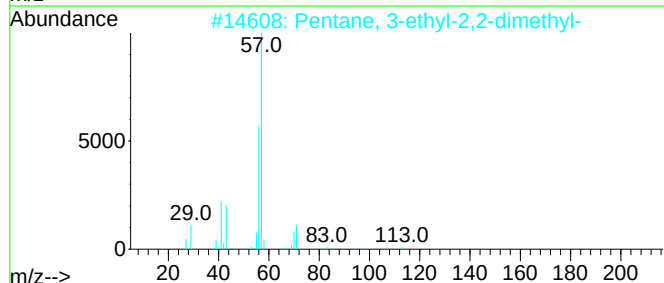
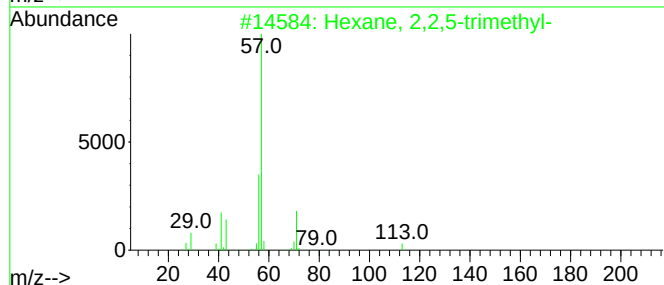
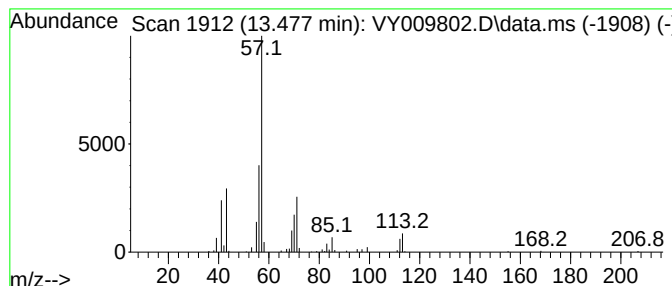
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexane, 2,2,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	7.33 ug/l	102678	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	59
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
4			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
5			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Octanol, 2-bu...	13.282	6.3	ug/l	88272	4	13.422	700196	50.0
Hexane, 2,2,5-t...	13.477	7.3	ug/l	102678	4	13.422	700196	50.0