

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
 Data File : VN075718.D
 Acq On : 12 Dec 2022 17:17
 Operator : JC\MD
 Sample : N5978-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-02

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_N\methods\82N120922W.M
 Title : SW846 8260

Signal : TIC: VN075718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.142	11	15	24	rVB2	9930	20211	1.77%	0.276%
2	2.301	36	42	46	rBV2	17164	42841	3.74%	0.586%
3	2.524	70	80	86	rBV5	5019	17509	1.53%	0.239%
4	2.818	127	130	139	rVB3	8870	19285	1.68%	0.264%
5	3.259	197	205	217	rVB4	15633	39252	3.43%	0.536%
6	5.295	540	551	552	rBV	8685	19790	1.73%	0.270%
7	5.359	553	562	584	rVB6	25496	106313	9.29%	1.453%
8	5.830	627	642	657	rVB2	49727	169565	14.82%	2.318%
9	7.336	886	898	913	rBV	126195	361117	31.55%	4.936%
10	8.171	1031	1040	1045	rBV2	155912	372761	32.57%	5.095%
11	8.230	1045	1050	1065	rVV3	314060	847116	74.01%	11.578%
12	8.588	1102	1111	1124	rVB	154718	368601	32.21%	5.038%
13	8.736	1127	1136	1138	rBV5	5705	13057	1.14%	0.178%
14	8.788	1143	1145	1152	rVV4	7289	11898	1.04%	0.163%
15	8.859	1152	1157	1164	rVB3	6159	13315	1.16%	0.182%
16	9.106	1189	1199	1211	rBV	415799	831482	72.65%	11.364%
17	9.341	1231	1239	1251	rVB3	24127	57760	5.05%	0.789%
18	9.606	1272	1284	1296	rBB8	22430	75201	6.57%	1.028%
19	10.153	1371	1377	1382	rVB3	9496	17864	1.56%	0.244%
20	10.571	1440	1448	1467	rBV	619465	1144528	100.00%	15.643%
21	10.753	1469	1479	1487	rVV7	12647	34152	2.98%	0.467%
22	10.835	1487	1493	1499	rVB2	8783	14412	1.26%	0.197%
23	10.918	1501	1507	1514	rBV2	15773	28856	2.52%	0.394%
24	11.006	1514	1522	1528	rBV5	9028	19548	1.71%	0.267%
25	11.418	1583	1592	1599	rBV2	11792	26028	2.27%	0.356%
26	11.871	1661	1669	1680	rBV	517680	937523	81.91%	12.814%
27	12.700	1804	1810	1816	rVB	13553	22292	1.95%	0.305%
28	12.853	1828	1836	1847	rVB	406344	683169	59.69%	9.337%
29	13.335	1914	1918	1925	rVB2	8407	13267	1.16%	0.181%
30	13.600	1956	1963	1971	rVB4	10943	24891	2.17%	0.340%
31	13.794	1989	1996	2004	rBV	499840	822701	71.88%	11.244%
32	14.000	2026	2031	2038	rVB2	18345	29389	2.57%	0.402%
33	14.335	2083	2088	2096	rBV2	7858	11483	1.00%	0.157%
34	14.447	2101	2107	2114	rVB2	20017	36188	3.16%	0.495%
35	14.588	2126	2131	2136	rBV	7946	13450	1.18%	0.184%
36	14.653	2136	2142	2152	rVB3	12274	23990	2.10%	0.328%

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ClientSampleId :
TOLL-MW-02

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

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37	15.041	2203	2208	2215	rVB5	11063	25704	2.25%	0.351%
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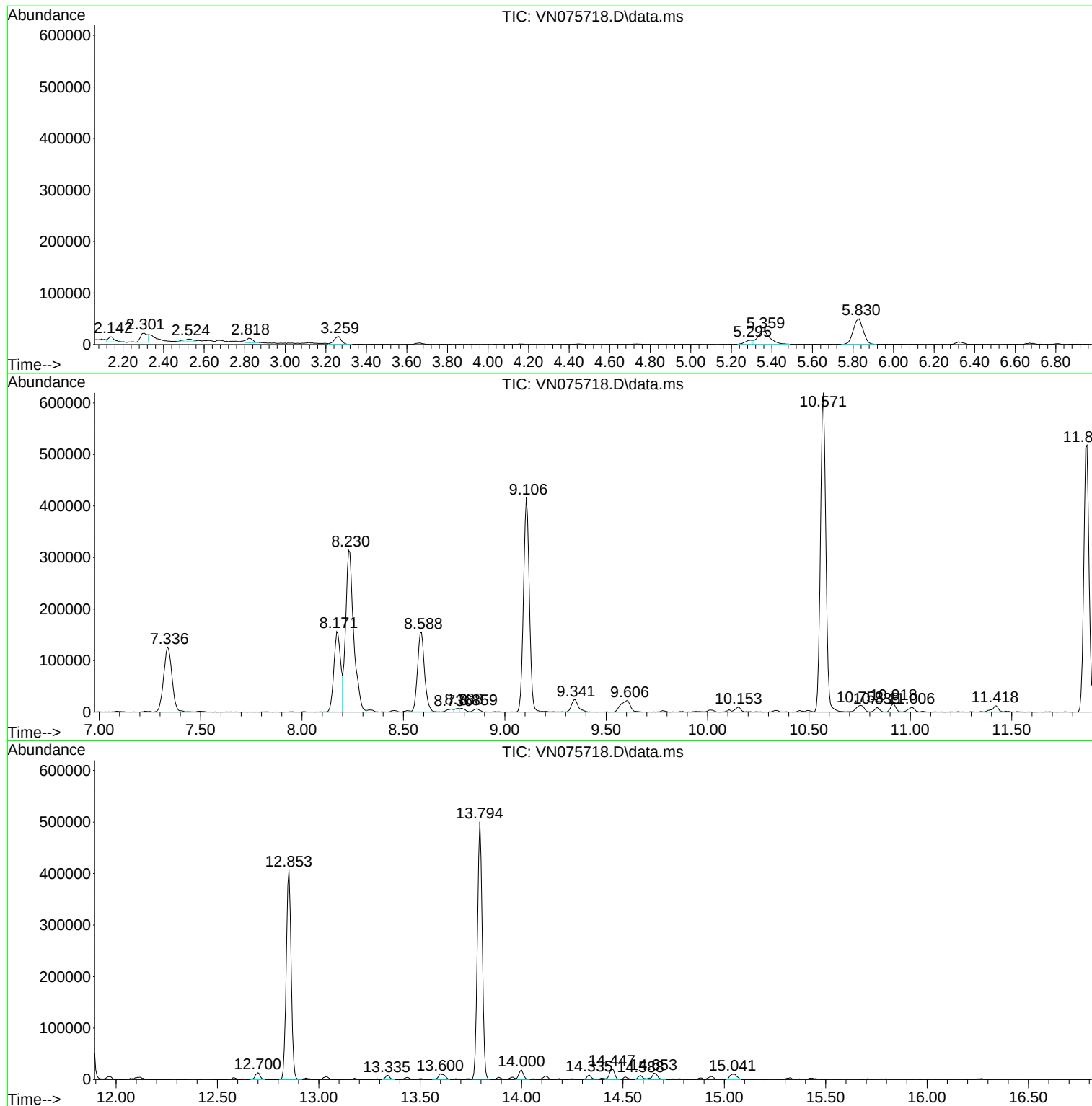
Sum of corrected areas: 7316509

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



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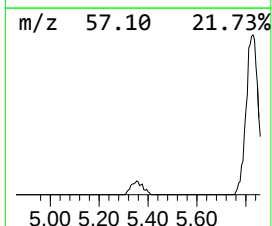
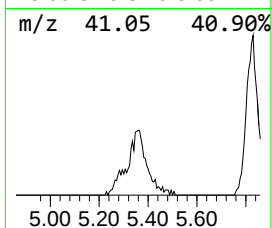
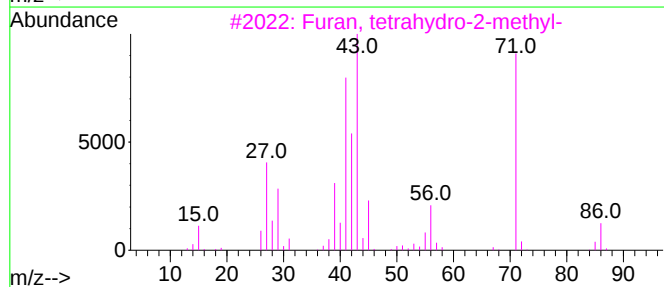
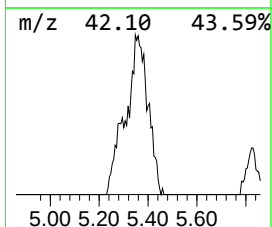
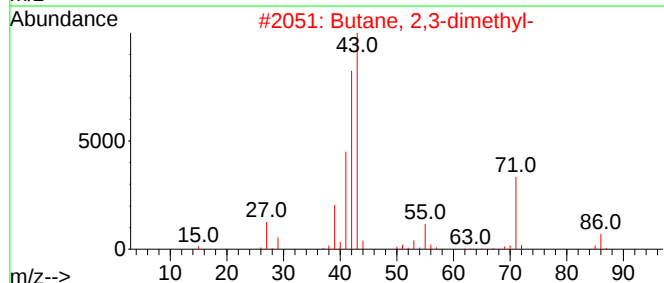
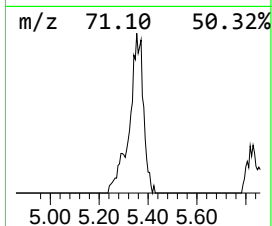
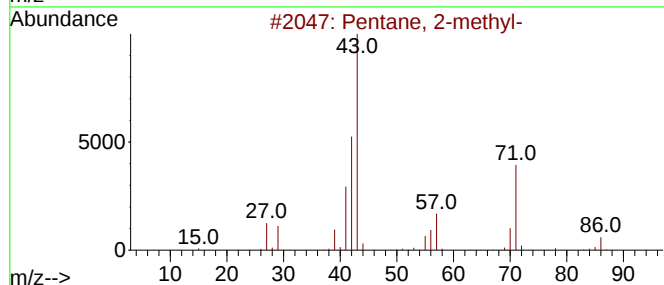
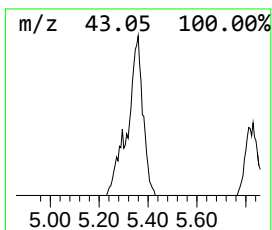
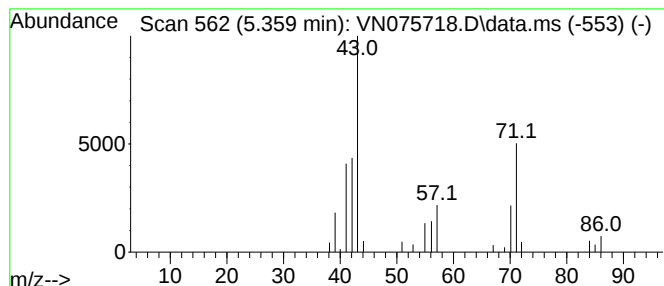
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.359	6.28 ug/l	106313	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	83
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	49
4			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	37



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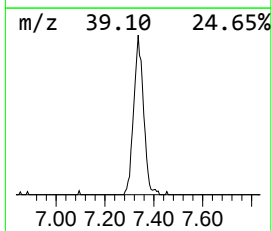
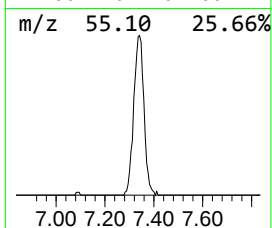
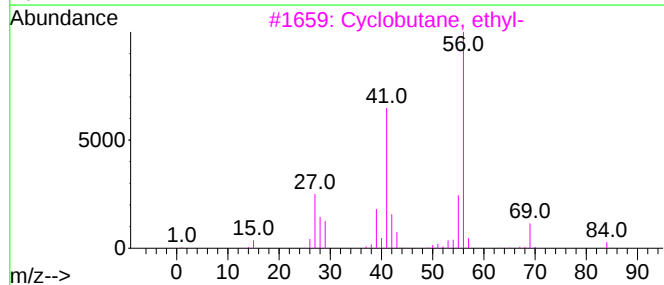
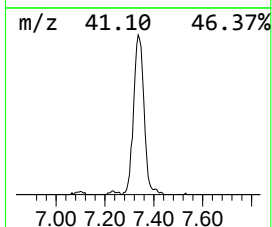
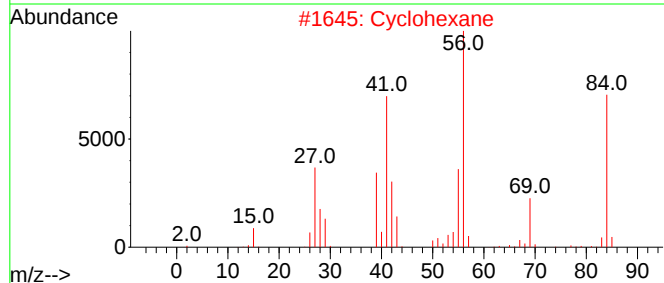
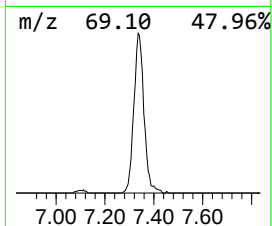
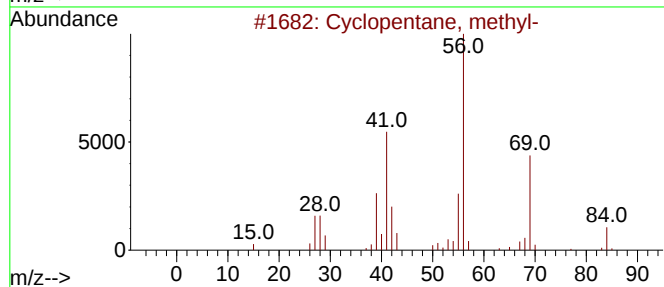
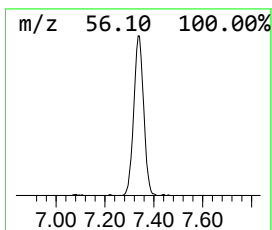
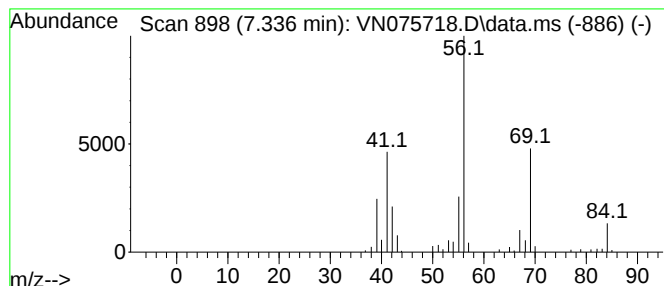
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Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.336	21.31 ug/l	361117	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclohexane	84	C6H12	000110-82-7	87
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5		Cyclobutane, butyl-	112	C8H16	013152-44-8	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2-methyl-	5.359	6.3	ug/l	106313	1	8.230	847116	50.0
Cyclopentane, m...	7.336	21.3	ug/l	361117	1	8.230	847116	50.0