

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060922\
 Data File : VN072731.D
 Acq On : 09 Jun 2022 15:27
 Operator : JC\MD
 Sample : N3181-03 20X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TRE-1279

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\82N060822W.M

Title : SW846 8260

Signal : TIC: VN072731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	50	rBV4	10665	29797	1.63%	0.315%
2	2.581	96	101	107	rBV	14566	25703	1.41%	0.272%
3	4.287	376	391	414	rBV	164828	495228	27.14%	5.237%
4	4.575	431	440	452	rBV	22044	67671	3.71%	0.716%
5	7.334	894	909	930	rBV2	95025	332607	18.23%	3.517%
6	7.657	956	964	977	rVB	11183	29617	1.62%	0.313%
7	8.016	1015	1025	1031	rBV	266986	649342	35.59%	6.867%
8	8.081	1031	1036	1049	rVB	261227	591458	32.41%	6.255%
9	8.257	1057	1066	1073	rBV3	14880	36492	2.00%	0.386%
10	8.433	1085	1096	1109	rBV2	323333	739243	40.51%	7.818%
11	8.963	1177	1186	1197	rBV	404129	838634	45.96%	8.869%
12	9.410	1254	1262	1271	rBV2	26542	51863	2.84%	0.548%
13	10.333	1410	1419	1426	rBV2	28329	57443	3.15%	0.607%
14	10.439	1429	1437	1444	rVV	1007660	1824702	100.00%	19.297%
15	10.504	1444	1448	1457	rVB2	41692	81499	4.47%	0.862%
16	11.104	1537	1550	1551	rBV4	19459	36147	1.98%	0.382%
17	11.145	1551	1557	1581	rVB	204531	408308	22.38%	4.318%
18	11.745	1651	1659	1671	rBV	576663	1035166	56.73%	10.947%
19	12.269	1742	1748	1756	rVB4	17851	33264	1.82%	0.352%
20	12.351	1756	1762	1773	rBV2	16202	34781	1.91%	0.368%
21	12.727	1819	1826	1838	rBV	702574	1188020	65.11%	12.564%
22	13.674	1979	1987	1995	rBV	474649	830367	45.51%	8.782%
23	13.768	1998	2003	2010	rVB2	20446	38508	2.11%	0.407%

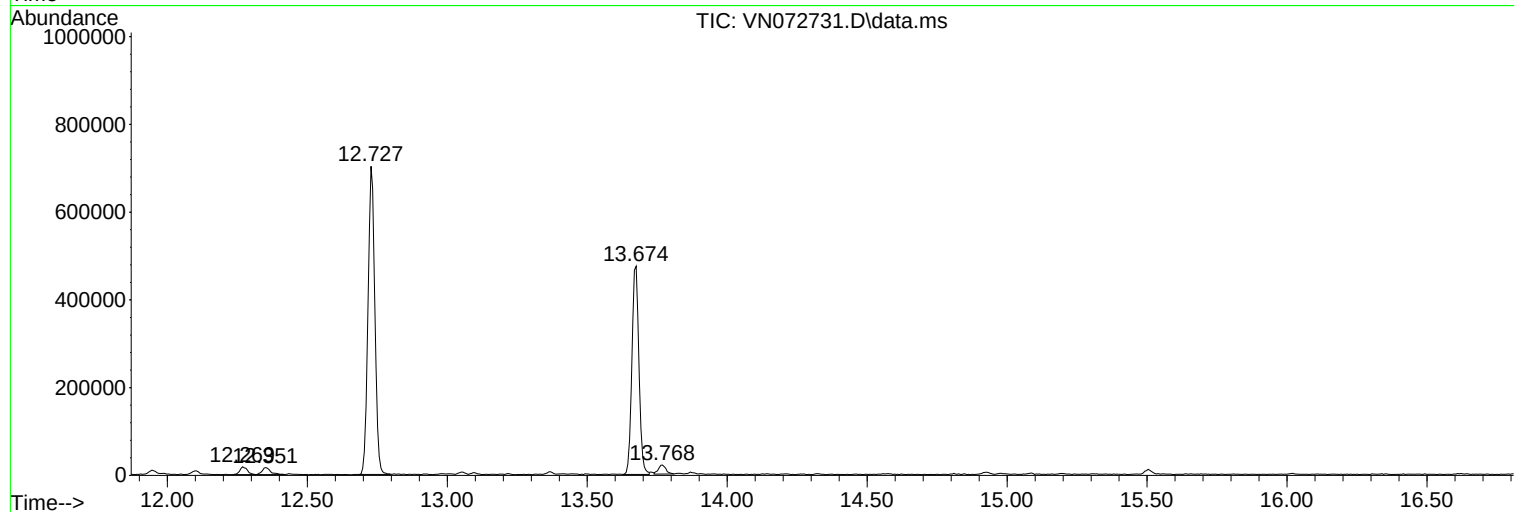
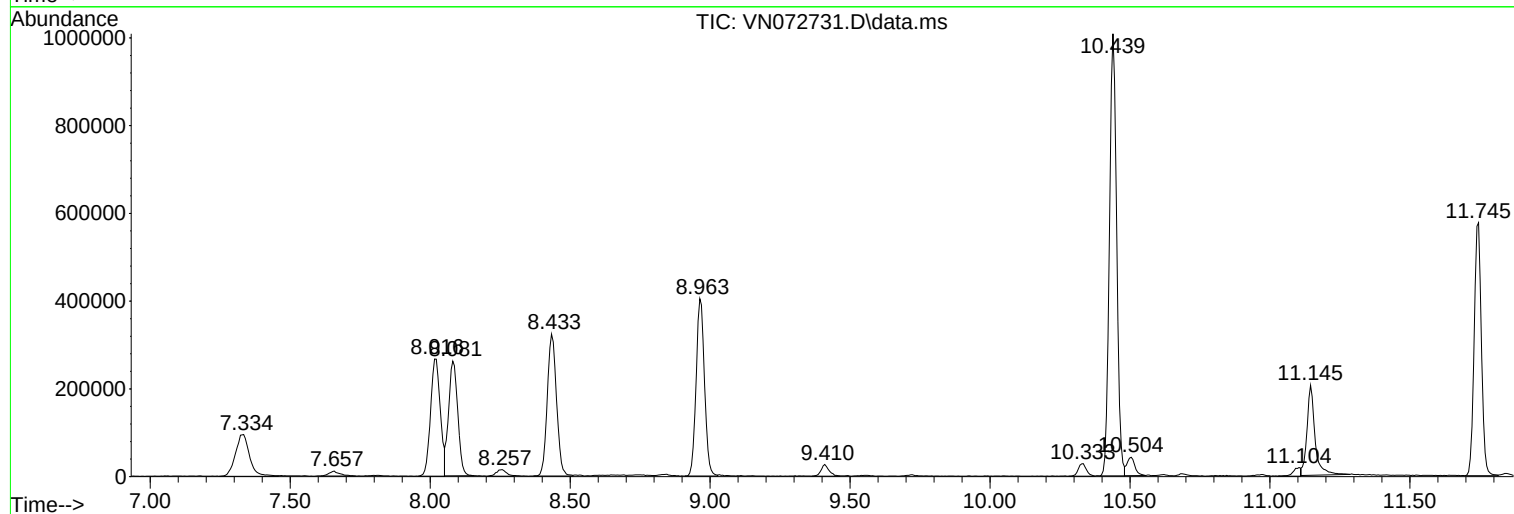
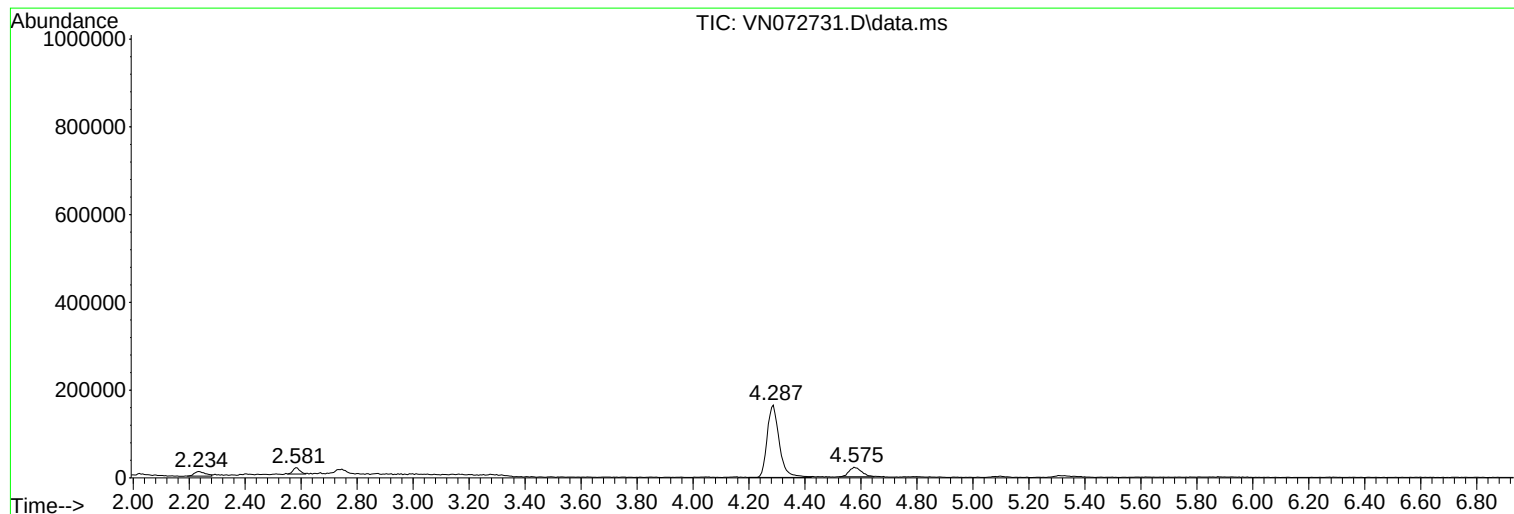
Sum of corrected areas: 9455860

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Instrument :
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ClientSampleId :
TRE-1279

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

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



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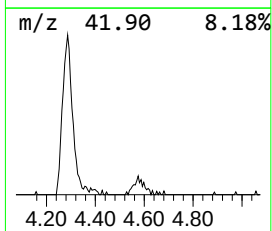
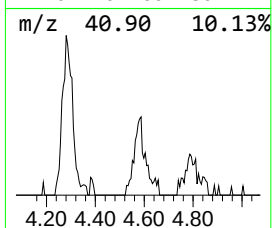
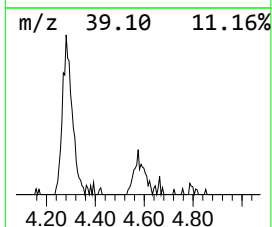
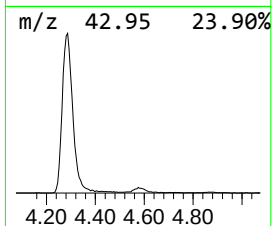
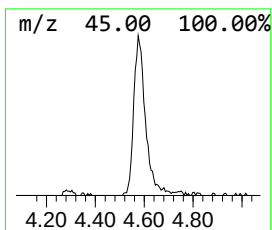
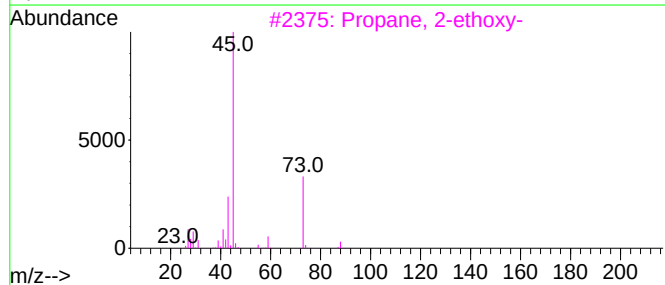
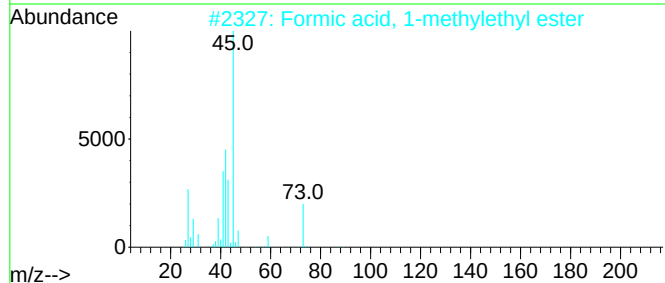
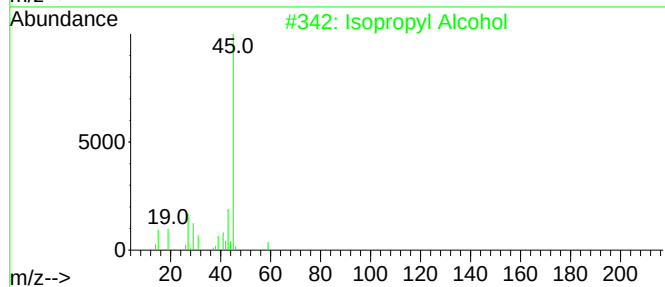
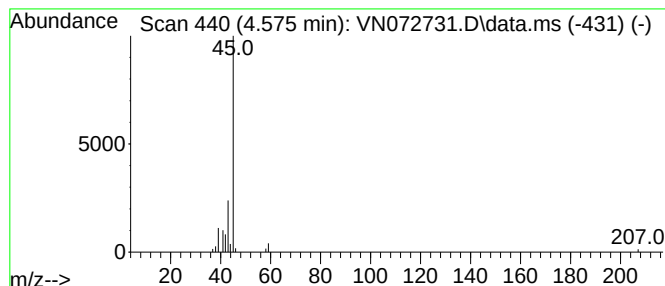
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	5.72 ug/l	67671	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4			2-Methyl-4-methoxy-1-butanol	118	C6H14O2	071052-94-3	9
5			Ethylamine	45	C2H7N	000075-04-7	5



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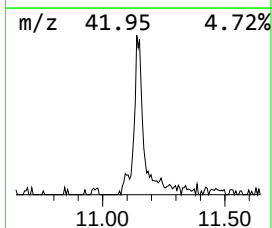
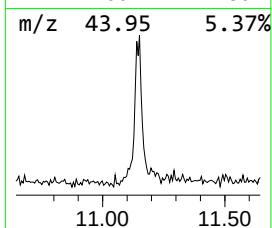
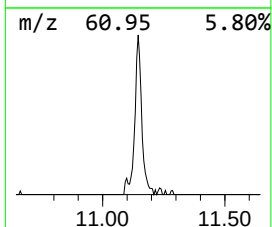
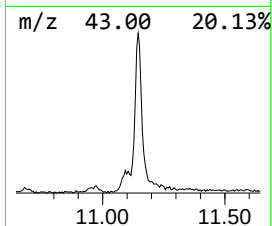
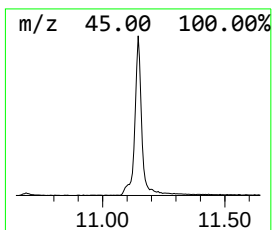
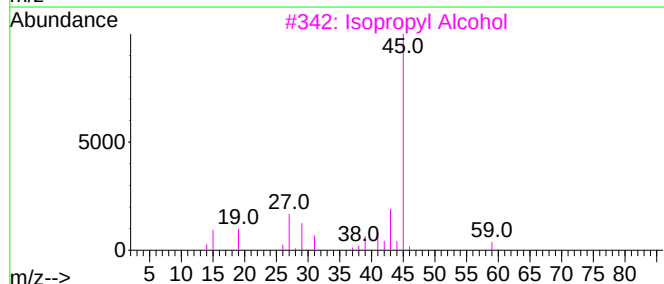
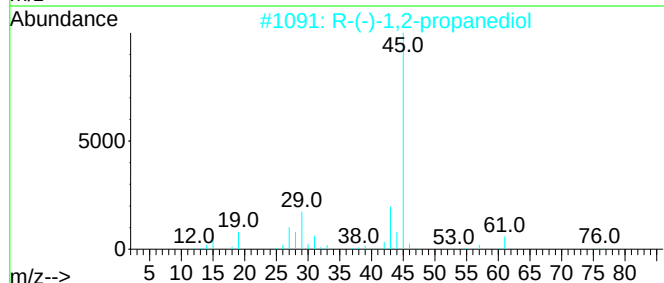
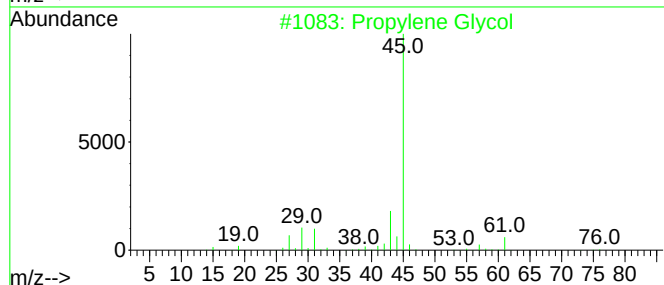
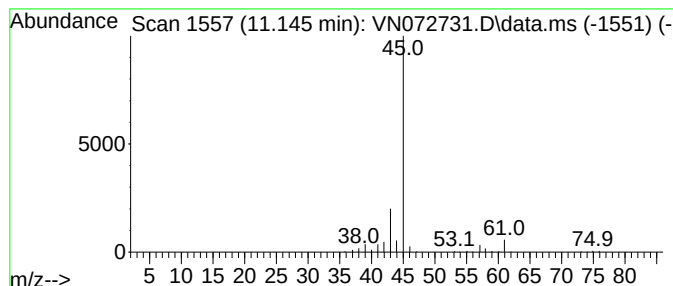
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	19.72 ug/l	408308	Chlorobenzene-d5	11.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	4.575	5.7	ug/l	67671	1	8.081	591458	50.0
Propylene Glycol	11.145	19.7	ug/l	408308	3	11.745	1035170	50.0