

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012921\
 Data File : VN065673.D
 Acq On : 29 Jan 2021 13:12
 Operator : JC/MD
 Sample : M1253-07
 Misc : 5.86g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VNJ-229

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\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.685	896	916	917	rBV	9401	17199	1.66%	0.262%
2	7.547	1787	1806	1816	rBV	113480	283586	27.31%	4.316%
3	7.621	1816	1829	1853	rVB2	232370	551998	53.15%	8.402%
4	7.984	1917	1942	1968	rBV2	141085	343438	33.07%	5.227%
5	8.544	2100	2116	2134	rBV	354772	740424	71.30%	11.270%
6	9.135	2283	2300	2302	rBV3	11578	17088	1.65%	0.260%
7	10.055	2569	2586	2599	rBV	568191	1038486	100.00%	15.807%
8	10.122	2599	2607	2627	rVB	22475	42847	4.13%	0.652%
9	10.833	2812	2828	2852	rBV	203866	393954	37.94%	5.996%
10	11.376	2983	2997	3022	rBV	466886	835280	80.43%	12.714%
11	12.106	3214	3224	3234	rBV4	11999	22291	2.15%	0.339%
12	12.161	3234	3241	3251	rVV2	8461	14698	1.42%	0.224%
13	12.373	3292	3307	3326	rBV	333702	562762	54.19%	8.566%
14	12.701	3392	3409	3428	rVB	12373	29095	2.80%	0.443%
15	13.013	3500	3506	3514	rVB3	7461	12249	1.18%	0.186%
16	13.174	3546	3556	3561	rBV4	6449	11702	1.13%	0.178%
17	13.228	3562	3573	3587	rVV	422464	668849	64.41%	10.180%
18	13.315	3588	3600	3617	rVB	398820	671448	64.66%	10.220%
19	13.428	3627	3635	3647	rVB5	11358	22494	2.17%	0.342%
20	13.637	3689	3700	3711	rBV6	16477	34472	3.32%	0.525%
21	13.965	3793	3802	3809	rBV9	8041	13707	1.32%	0.209%
22	14.013	3809	3817	3829	rVV9	7816	16981	1.64%	0.258%
23	14.097	3832	3843	3849	rBV9	15388	29575	2.85%	0.450%
24	14.164	3852	3864	3876	rVB5	18434	53902	5.19%	0.820%
25	14.270	3890	3897	3902	rBV3	13338	21266	2.05%	0.324%
26	14.550	3976	3984	3996	rBV3	24444	54599	5.26%	0.831%
27	14.611	3997	4003	4013	rVB8	14816	25584	2.46%	0.389%
28	14.817	4061	4067	4075	rVB5	28102	39985	3.85%	0.609%

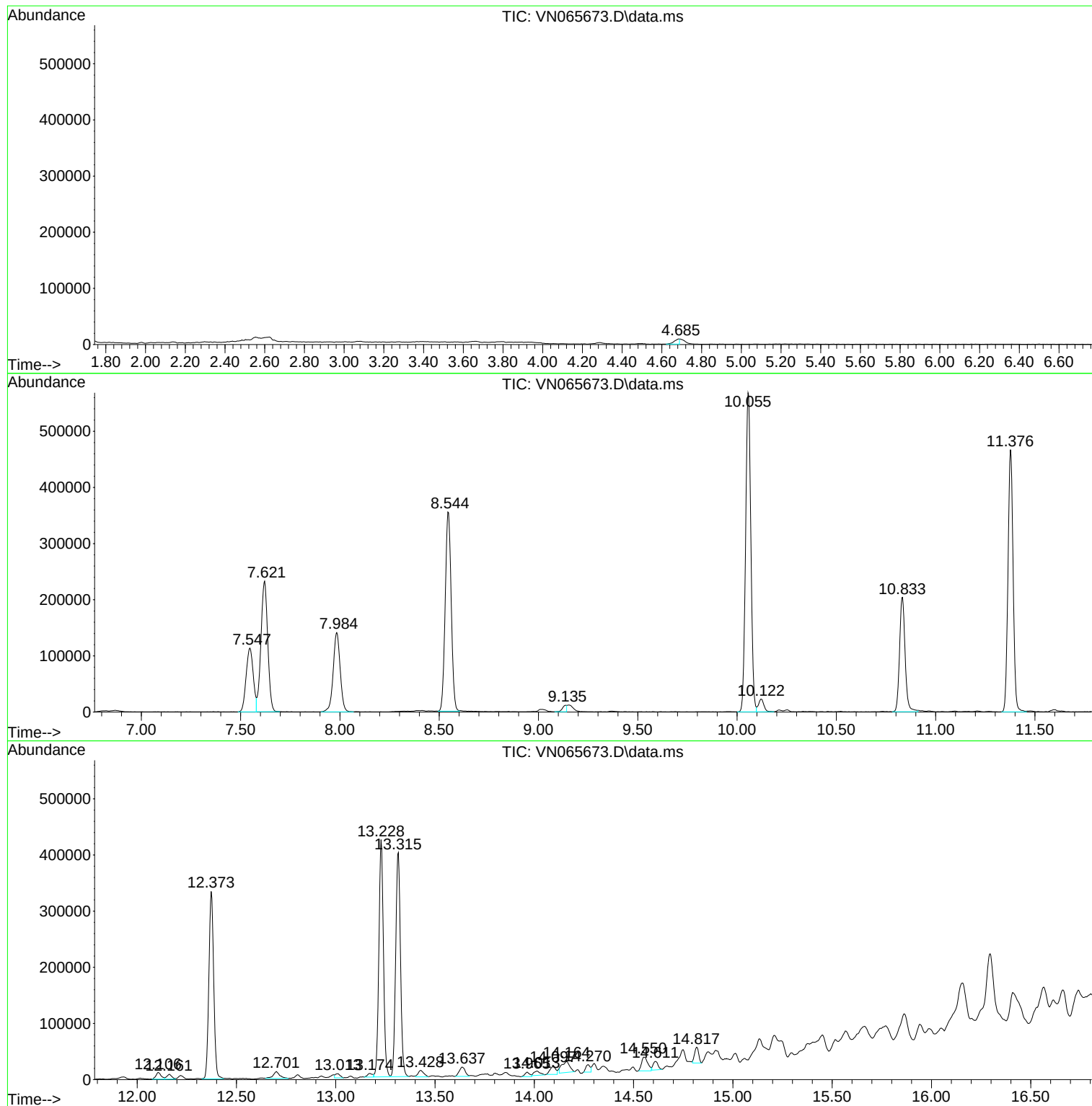
Sum of corrected areas: 6569959

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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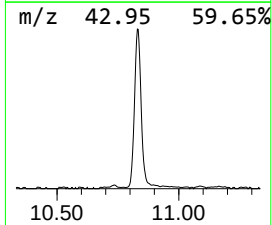
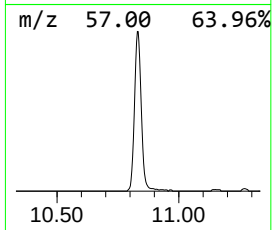
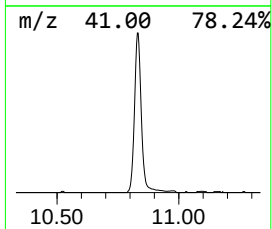
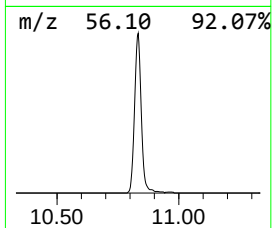
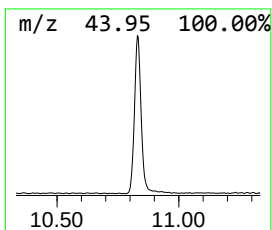
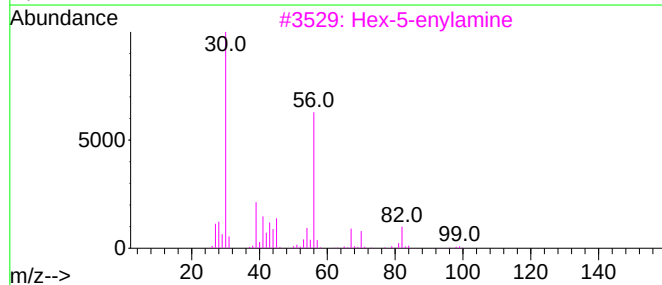
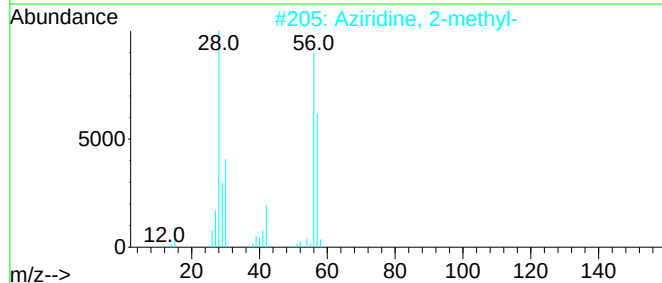
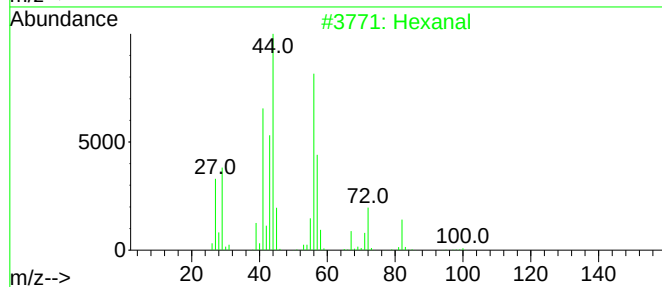
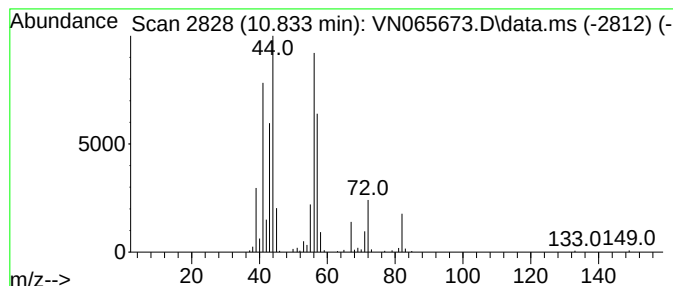
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	23.58 ug/l	393954	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	90
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27
3			Hex-5-enylamine	99	C6H13N	034825-70-2	25
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	25
5			Oxazolidine, 2-methyl-	87	C4H9NO	016250-70-7	25



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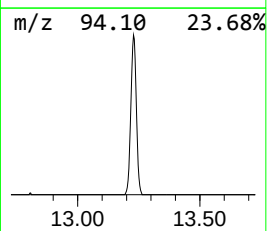
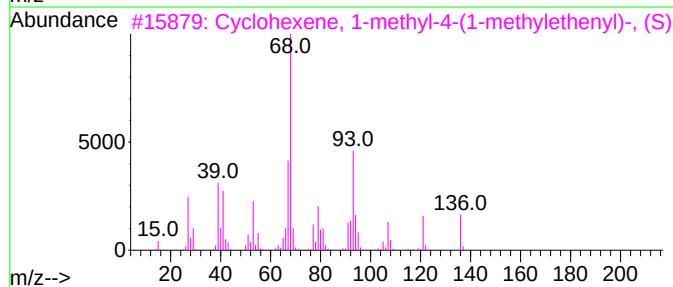
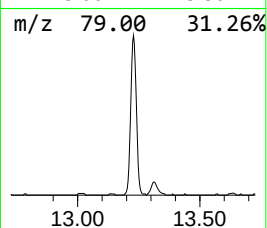
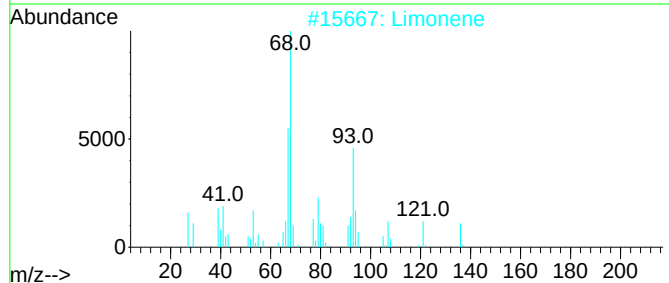
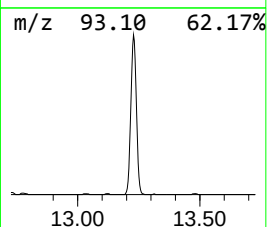
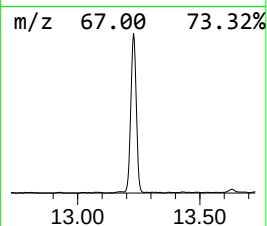
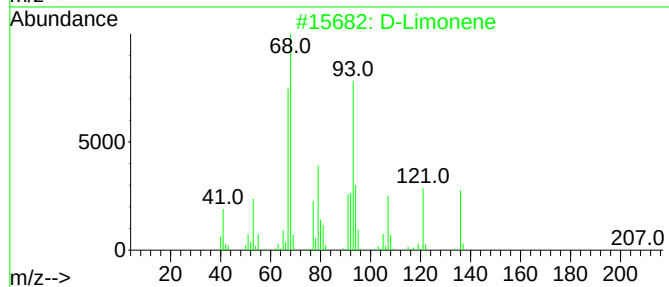
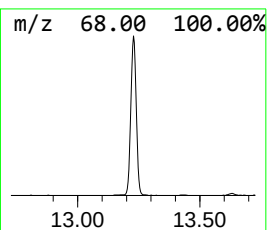
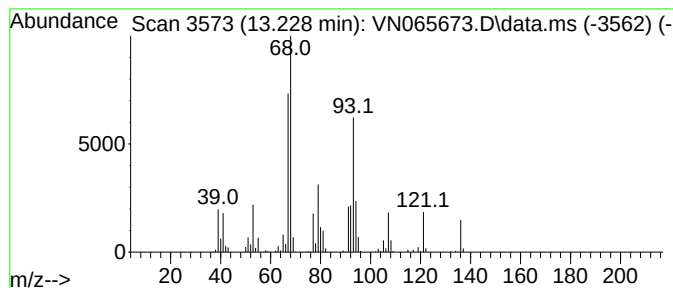
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Peak Number 2 D-Limonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.228	49.81 ug/l	668849	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	97
2			Limonene	136	C10H16	000138-86-3	91
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	81
4			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	72
5			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	10.833	23.6	ug/l	393954	3	11.376	835280	50.0
D-Limonene	13.228	49.8	ug/l	668849	4	13.315	671448	50.0