

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
 Data File : VN068899.D
 Acq On : 13 Oct 2021 15:57
 Operator : JC/MD
 Sample : M4175-03
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31123

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\82N101221W.M

Title : SW846 8260

Signal : TIC: VN068899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	76	89	107	rBV2	18930	44099	2.18%	0.371%
2	7.831	2158	2178	2198	rBV4	9224	24426	1.21%	0.206%
3	8.018	2225	2248	2257	rBV2	256838	628319	31.04%	5.292%
4	8.080	2259	2271	2291	rVV	519936	1278317	63.16%	10.767%
5	8.163	2292	2302	2325	rVB3	26177	63896	3.16%	0.538%
6	8.287	2327	2348	2369	rBV	81006	184855	9.13%	1.557%
7	8.434	2383	2403	2430	rBV	272329	630344	31.14%	5.309%
8	8.566	2432	2452	2464	rBV8	16386	47618	2.35%	0.401%
9	8.820	2534	2547	2572	rVB3	23958	51066	2.52%	0.430%
10	8.965	2580	2601	2630	rBV	698860	1465926	72.42%	12.347%
11	10.443	3132	3152	3166	rBV	1036723	2024068	100.00%	17.048%
12	10.505	3166	3175	3196	rVB	180277	335165	16.56%	2.823%
13	11.746	3620	3638	3668	rBV	954879	1714713	84.72%	14.442%
14	11.958	3704	3717	3739	rVB6	9577	20246	1.00%	0.171%
15	12.733	3990	4006	4032	rVB	755250	1298551	64.16%	10.937%
16	13.055	4115	4126	4136	rVB9	11494	21118	1.04%	0.178%
17	13.425	4253	4264	4284	rVB3	15634	33090	1.63%	0.279%
18	13.677	4342	4358	4378	rVV	908537	1561225	77.13%	13.150%
19	13.771	4382	4393	4405	rVB3	24132	37958	1.88%	0.320%
20	13.994	4466	4476	4487	rVB8	16409	25627	1.27%	0.216%
21	14.343	4589	4606	4626	rBV5	10641	30806	1.52%	0.259%
22	14.664	4719	4726	4741	rVB5	29217	48032	2.37%	0.405%
23	14.820	4773	4784	4792	rBV5	49900	80132	3.96%	0.675%
24	14.917	4811	4820	4835	rBV3	14545	31795	1.57%	0.268%
25	15.265	4941	4950	4960	rBV7	12235	23057	1.14%	0.194%
26	15.477	5019	5029	5031	rBV7	16448	20849	1.03%	0.176%
27	15.512	5035	5042	5071	rVB2	53192	113235	5.59%	0.954%
28	15.705	5105	5114	5127	rVB6	19081	34190	1.69%	0.288%

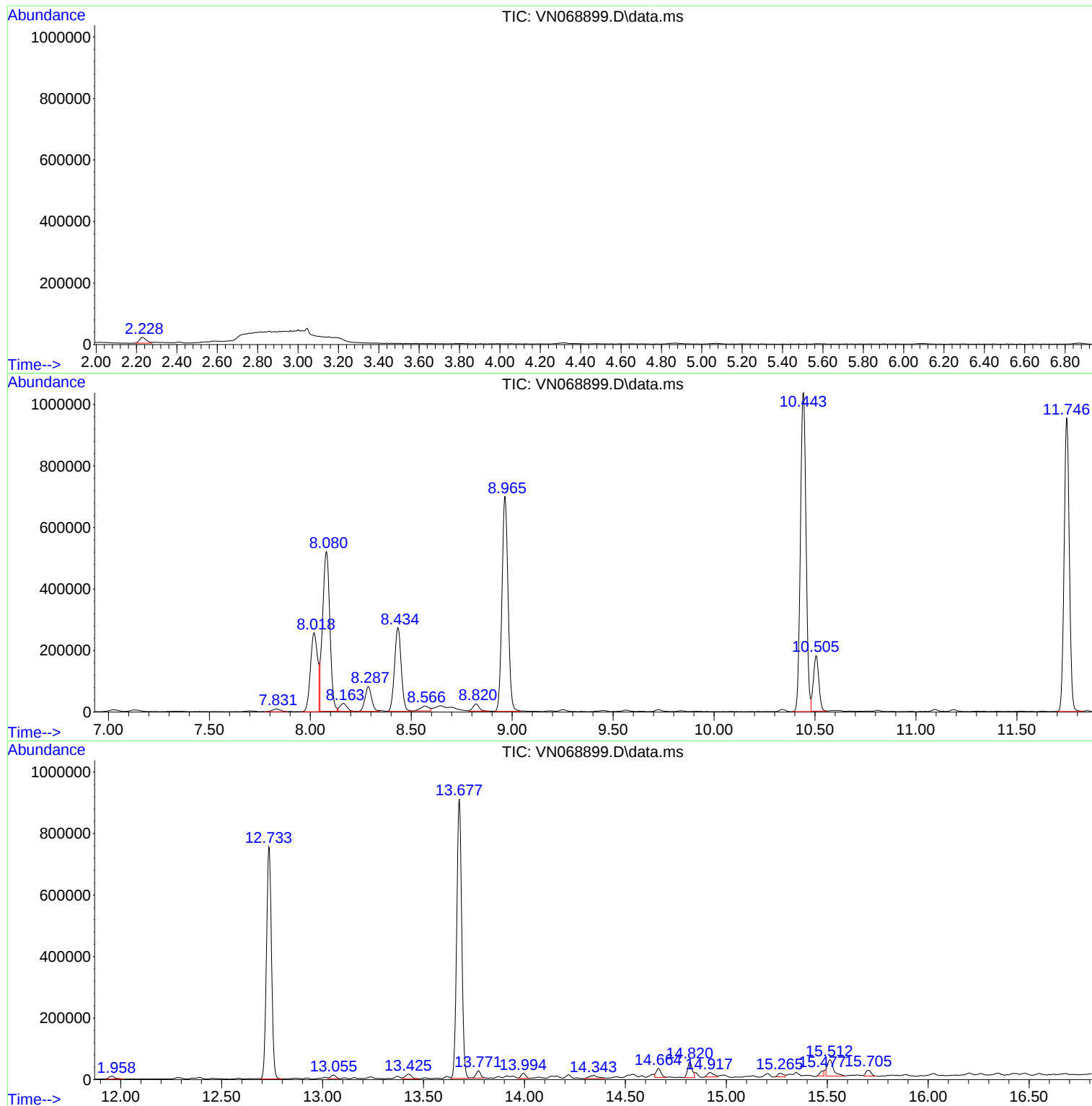
Sum of corrected areas: 11872723

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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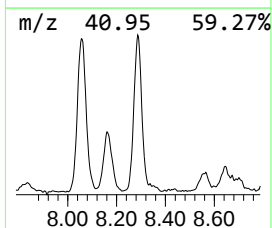
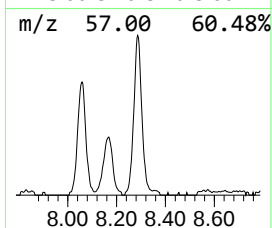
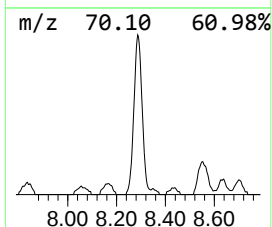
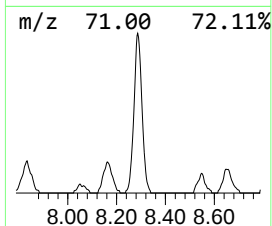
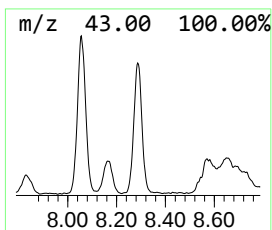
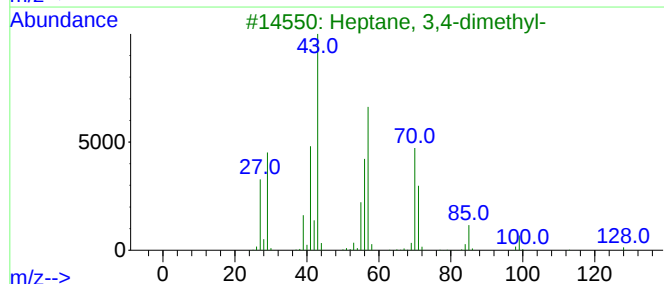
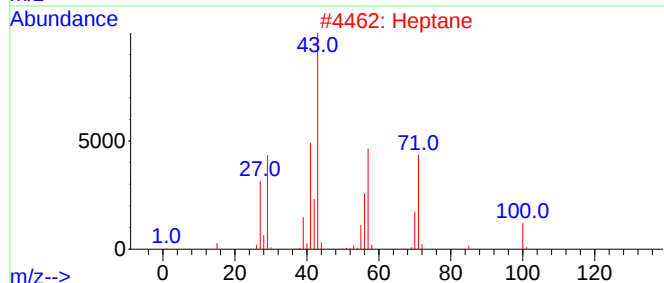
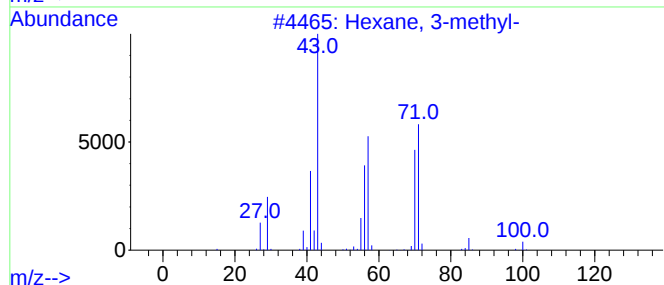
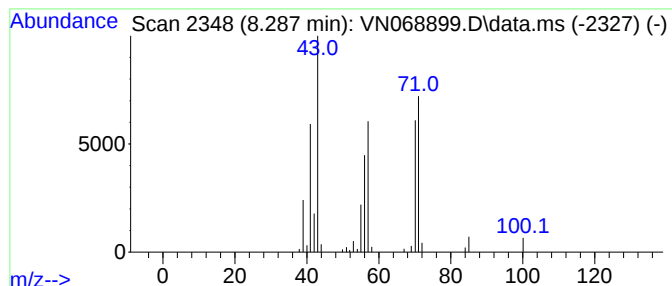
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	7.23 ug/l	184855	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	72
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	8.287	7.2	ug/l	184855	1	8.080	1278320	50.0