

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
 Data File : VN070626.D
 Acq On : 14 Jan 2022 16:29
 Operator : JC/MD
 Sample : N1141-07
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31272

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.310	841	865	907	rBV	161493	593720	12.32%	1.955%
2	4.854	1042	1068	1095	rBV2	23547	84885	1.76%	0.279%
3	7.356	1979	2001	2047	rVB2	83209	287195	5.96%	0.946%
4	8.019	2224	2248	2257	rBV2	635603	1604010	33.29%	5.281%
5	8.075	2259	2269	2289	rVV	1099012	2617245	54.33%	8.617%
6	8.158	2290	2300	2320	rVB5	62137	152047	3.16%	0.501%
7	8.284	2327	2347	2366	rBV3	216097	502002	10.42%	1.653%
8	8.432	2382	2402	2428	rBV	806457	1858505	38.58%	6.119%
9	8.654	2473	2485	2521	rVB6	65107	221089	4.59%	0.728%
10	8.818	2528	2546	2581	rBV4	103384	296025	6.14%	0.975%
11	8.963	2581	2600	2644	rVB	1572592	3319586	68.90%	10.930%
12	9.191	2669	2685	2696	rBV5	29819	65684	1.36%	0.216%
13	9.252	2699	2708	2728	rVB4	28148	61741	1.28%	0.203%
14	9.446	2758	2780	2798	rBV7	28477	87139	1.81%	0.287%
15	10.341	3099	3114	3132	rBV2	45823	92617	1.92%	0.305%
16	10.441	3132	3151	3163	rBV	2571951	4817739	100.00%	15.862%
17	10.502	3163	3174	3200	rVB	1569830	2961189	61.46%	9.750%
18	11.183	3415	3428	3444	rBV	91442	166187	3.45%	0.547%
19	11.747	3621	3638	3665	rBV	1872836	3470767	72.04%	11.427%
20	11.953	3704	3715	3724	rBV4	96834	179626	3.73%	0.591%
21	12.355	3856	3865	3884	rVB	66025	127385	2.64%	0.419%
22	12.734	3991	4006	4026	rVB	1941041	3382699	70.21%	11.137%
23	13.047	4116	4123	4137	rVB5	78144	133527	2.77%	0.440%
24	13.675	4343	4357	4379	rBV	1876941	3290067	68.29%	10.832%

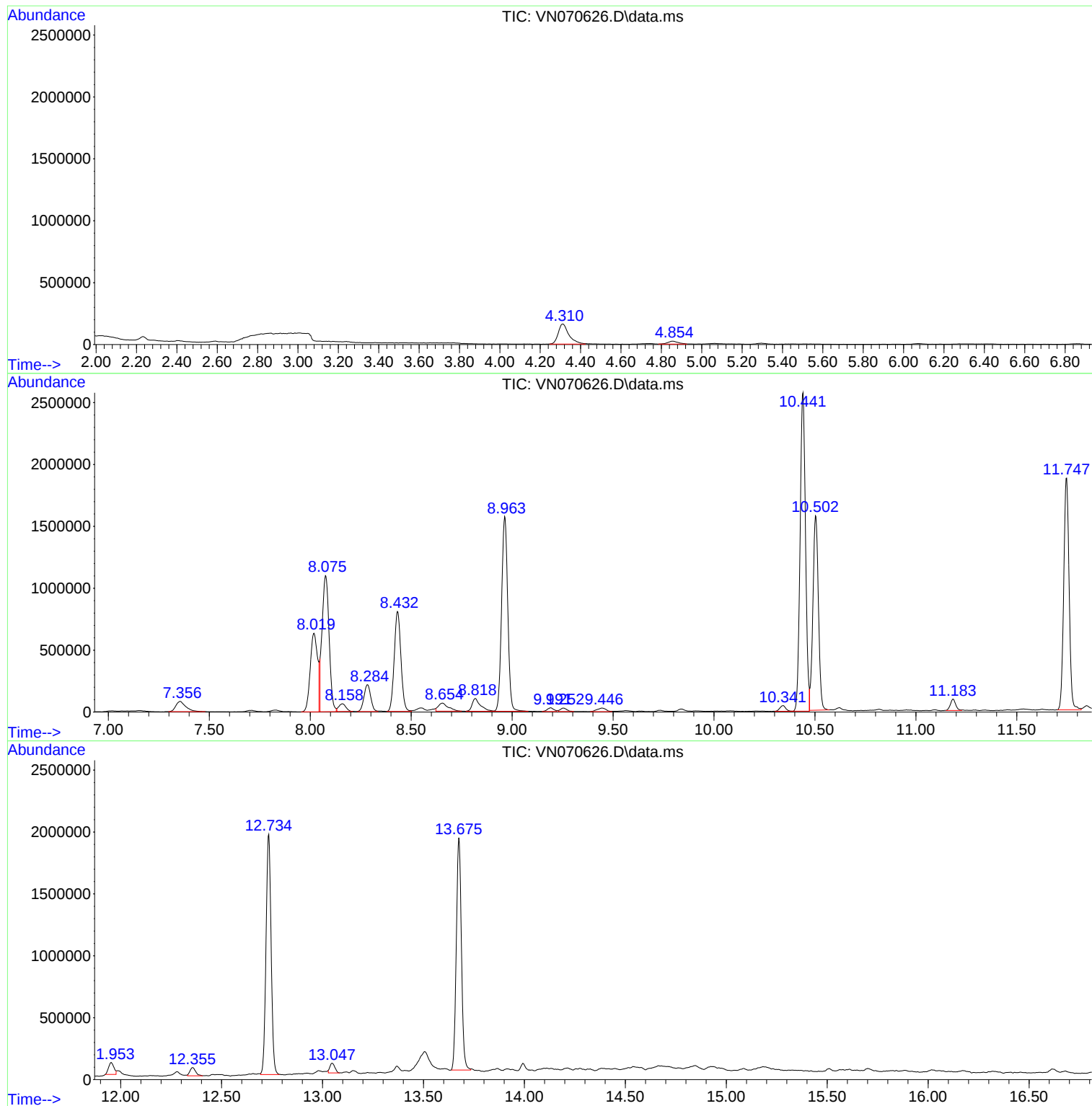
Sum of corrected areas: 30372676

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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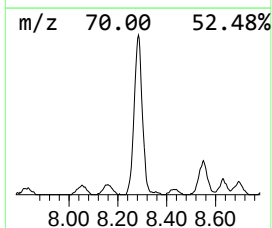
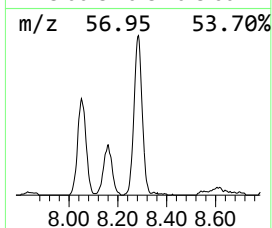
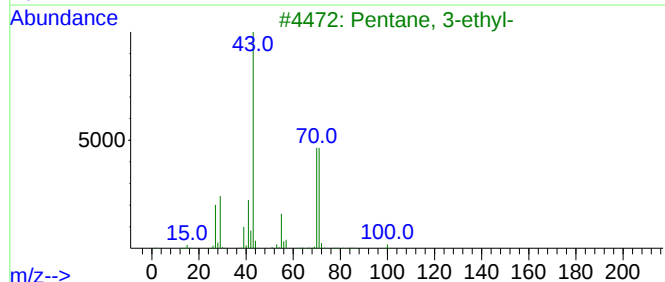
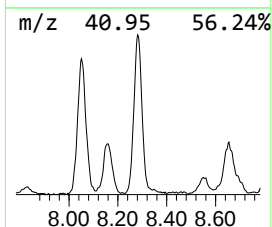
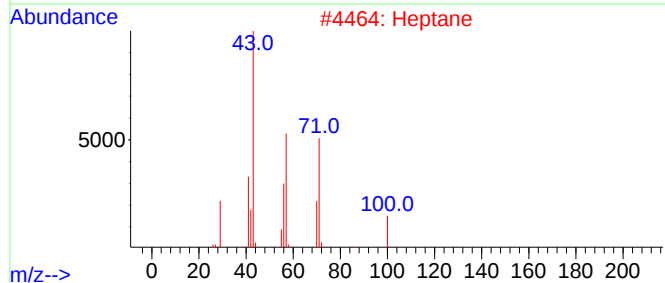
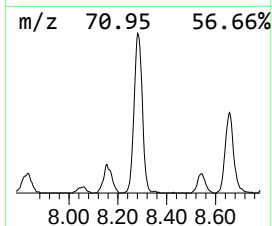
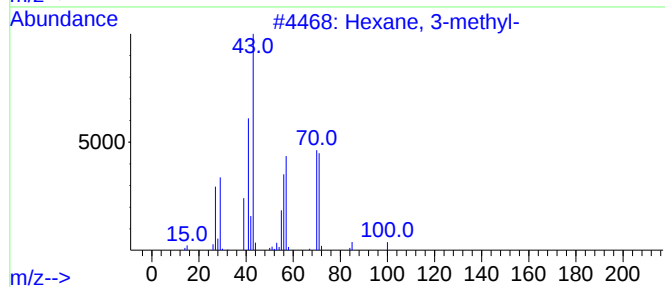
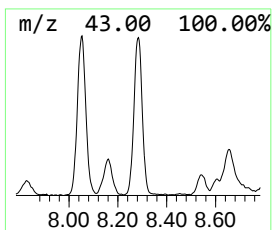
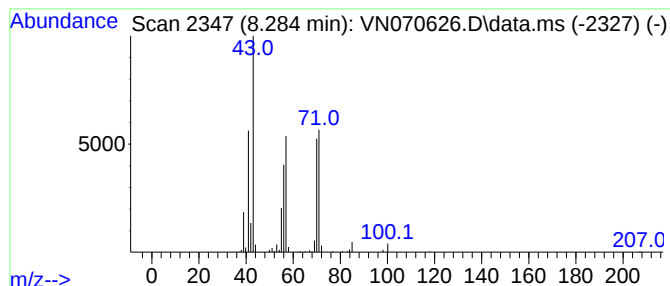
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	9.59 ug/l	502002	Pentafluorobenzene	8.078

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2		Heptane	100	C7H16	000142-82-5	64
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	58
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5		Heptane, 4-methyl-	114	C8H18	000589-53-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	8.284	9.6	ug/l	502002	1	8.078	2617250	50.0