

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
 Data File : VU055880.D
 Acq On : 25 Oct 2023 15:33
 Operator : MD/SY
 Sample : 04952-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOAR0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	15	21	37	rBV2	161144	178260	7.06%	0.851%
2	1.489	56	62	75	rBV2	86979	111327	4.41%	0.532%
3	1.599	89	96	116	rBV2	384775	503155	19.93%	2.402%
4	1.891	180	187	206	rVB	214193	327744	12.98%	1.565%
5	2.560	380	395	414	rBV	533589	885554	35.08%	4.228%
6	3.354	630	642	656	rVB5	7941	17702	0.70%	0.085%
7	3.483	679	682	691	rVB4	749	1063	0.04%	0.005%
8	3.550	697	703	707	rBV3	733	911	0.04%	0.004%
9	3.686	739	745	746	rBV3	2648	2018	0.08%	0.010%
10	3.962	814	831	844	rVB8	5656	17574	0.70%	0.084%
11	4.431	964	977	980	rBV4	2983	5524	0.22%	0.026%
12	4.528	991	1007	1011	rBV2	8312	18763	0.74%	0.090%
13	4.615	1025	1034	1064	rVB	178860	447831	17.74%	2.138%
14	4.853	1104	1108	1113	rVB6	832	698	0.03%	0.003%
15	5.058	1155	1172	1200	rBV	443298	1000691	39.64%	4.778%
16	5.284	1236	1242	1244	rBV5	843	890	0.04%	0.004%
17	5.329	1244	1256	1261	rBV3	5191	9854	0.39%	0.047%
18	5.454	1285	1295	1311	rVB6	7327	16562	0.66%	0.079%
19	5.583	1327	1335	1346	rBV7	2683	6133	0.24%	0.029%
20	5.628	1346	1349	1353	rVB2	1120	828	0.03%	0.004%
21	5.721	1356	1378	1409	rBV2	920262	2524561	100.00%	12.053%
22	5.978	1449	1458	1469	rVB8	4161	8927	0.35%	0.043%
23	6.116	1495	1501	1503	rBV4	1436	1353	0.05%	0.006%
24	6.245	1527	1541	1566	rBV	663953	1293666	51.24%	6.177%
25	6.502	1609	1621	1629	rBV2	8406	19244	0.76%	0.092%
26	6.685	1664	1678	1695	rBV	555339	1103187	43.70%	5.267%
27	6.859	1729	1732	1739	rVB6	1662	1612	0.06%	0.008%
28	6.975	1762	1768	1770	rBV4	1911	1737	0.07%	0.008%
29	7.065	1790	1796	1797	rBV4	1027	781	0.03%	0.004%
30	7.184	1816	1833	1844	rBV4	8748	26604	1.05%	0.127%
31	7.377	1881	1893	1904	rBV6	10637	21598	0.86%	0.103%
32	7.428	1904	1909	1910	rBV3	1693	1371	0.05%	0.007%
33	7.560	1937	1950	1970	rBV	312051	554661	21.97%	2.648%
34	7.692	1989	1991	1998	rVB6	1710	1613	0.06%	0.008%
35	7.756	2003	2011	2020	rVB5	5563	9920	0.39%	0.047%
36	7.894	2033	2054	2076	rBV	1151594	2024927	80.21%	9.668%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	8.174	2130	2141	2156	rBV	215265	373856	14.81%	1.785%
38	8.357	2190	2198	2203	rBV8	2532	3865	0.15%	0.018%
39	8.406	2206	2213	2224	rVB4	7639	13795	0.55%	0.066%
40	8.486	2224	2238	2247	rBV2	31603	60821	2.41%	0.290%
41	8.550	2247	2258	2272	rVB	161014	270943	10.73%	1.294%
42	8.631	2272	2283	2314	rBV	679526	1317408	52.18%	6.290%
43	8.856	2347	2353	2359	rBV8	2305	3556	0.14%	0.017%
44	8.920	2364	2373	2376	rBV9	1751	2825	0.11%	0.013%
45	9.058	2409	2416	2417	rBV3	2836	2591	0.10%	0.012%
46	9.068	2417	2419	2430	rVB8	4323	5712	0.23%	0.027%
47	9.168	2446	2450	2451	rBV4	1289	807	0.03%	0.004%
48	9.338	2490	2503	2512	rVV4	10626	20359	0.81%	0.097%
49	9.412	2514	2526	2569	rVV	974548	1864256	73.84%	8.901%
50	9.563	2570	2573	2578	rBV6	1626	1452	0.06%	0.007%
51	9.692	2600	2613	2625	rVB3	25230	47730	1.89%	0.228%
52	9.865	2662	2667	2669	rBV3	1652	1483	0.06%	0.007%
53	10.013	2706	2713	2716	rBV6	3923	3991	0.16%	0.019%
54	10.100	2735	2740	2752	rVB4	7578	11978	0.47%	0.057%
55	10.232	2778	2781	2783	rVV3	1358	907	0.04%	0.004%
56	10.364	2811	2822	2825	rBV8	4423	7924	0.31%	0.038%
57	10.483	2850	2859	2867	rBV4	7644	12901	0.51%	0.062%
58	10.521	2867	2871	2872	rBV2	1027	746	0.03%	0.004%
59	10.692	2921	2924	2930	rVB8	3296	3309	0.13%	0.016%
60	10.753	2930	2943	2973	rVB	850273	1402763	55.56%	6.697%
61	10.901	2976	2989	3009	rBV5	11600	28012	1.11%	0.134%
62	10.997	3009	3019	3035	rBV4	19446	42771	1.69%	0.204%
63	11.090	3041	3048	3066	rVB4	10957	20818	0.82%	0.099%
64	11.229	3087	3091	3094	rBV4	803	719	0.03%	0.003%
65	11.290	3101	3110	3118	rBV3	12935	21883	0.87%	0.104%
66	11.373	3134	3136	3140	rVV4	1144	821	0.03%	0.004%
67	11.412	3140	3148	3156	rVV4	6067	9084	0.36%	0.043%
68	11.467	3156	3165	3176	rVB	29412	46824	1.85%	0.224%
69	11.608	3200	3209	3214	rBV3	8783	13504	0.53%	0.064%
70	11.743	3245	3251	3259	rVB9	5996	7950	0.31%	0.038%
71	11.807	3259	3271	3290	rBV	1101771	1787918	70.82%	8.536%
72	11.994	3326	3329	3335	rVB6	1689	1643	0.07%	0.008%
73	12.090	3352	3359	3369	rBV2	15876	26589	1.05%	0.127%
74	12.190	3377	3390	3414	rBV	1220026	2042164	80.89%	9.750%
75	12.370	3442	3446	3448	rBV4	2851	2608	0.10%	0.012%
76	12.460	3468	3474	3480	rBV5	5479	7808	0.31%	0.037%

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 Title : VOC Analysis

77	12.569	3502	3508	3516	rVB4	9730	12862	0.51%	0.061%
78	12.679	3536	3542	3547	rBV5	8212	11997	0.48%	0.057%
79	12.820	3577	3586	3589	rBV7	3840	5309	0.21%	0.025%
80	12.939	3615	3623	3628	rBV10	5293	8433	0.33%	0.040%
81	13.029	3644	3651	3661	rVB4	7142	12157	0.48%	0.058%
82	13.113	3667	3677	3682	rBV9	4346	8271	0.33%	0.039%
83	13.251	3712	3720	3727	rBV3	10775	14342	0.57%	0.068%
84	13.296	3728	3734	3742	rVB6	5679	8095	0.32%	0.039%
85	13.383	3758	3761	3762	rBV3	1181	738	0.03%	0.004%
86	13.454	3774	3783	3794	rBV3	20390	34637	1.37%	0.165%
87	13.560	3813	3816	3820	rBV4	1863	1460	0.06%	0.007%
88	13.621	3830	3835	3845	rVB9	6321	9112	0.36%	0.044%
89	13.733	3863	3870	3877	rVV9	2597	4249	0.17%	0.020%
90	13.785	3878	3886	3894	rVB8	4849	8121	0.32%	0.039%
91	13.836	3894	3902	3912	rBV8	7179	16141	0.64%	0.077%
92	14.184	4003	4010	4023	rVB7	16698	28329	1.12%	0.135%
93	14.280	4028	4040	4052	rBV7	26074	46381	1.84%	0.221%
94	14.486	4096	4104	4112	rBV10	3801	5708	0.23%	0.027%
95	14.679	4153	4164	4178	rVB10	8760	20816	0.82%	0.099%
96	14.772	4191	4193	4196	rBV3	1430	860	0.03%	0.004%
97	14.807	4197	4204	4207	rBV7	3578	4607	0.18%	0.022%
98	14.875	4219	4225	4237	rVB8	7832	12548	0.50%	0.060%
99	15.013	4264	4268	4281	rVB8	5864	10379	0.41%	0.050%
100	15.418	4389	4394	4404	rVB9	8131	13177	0.52%	0.063%

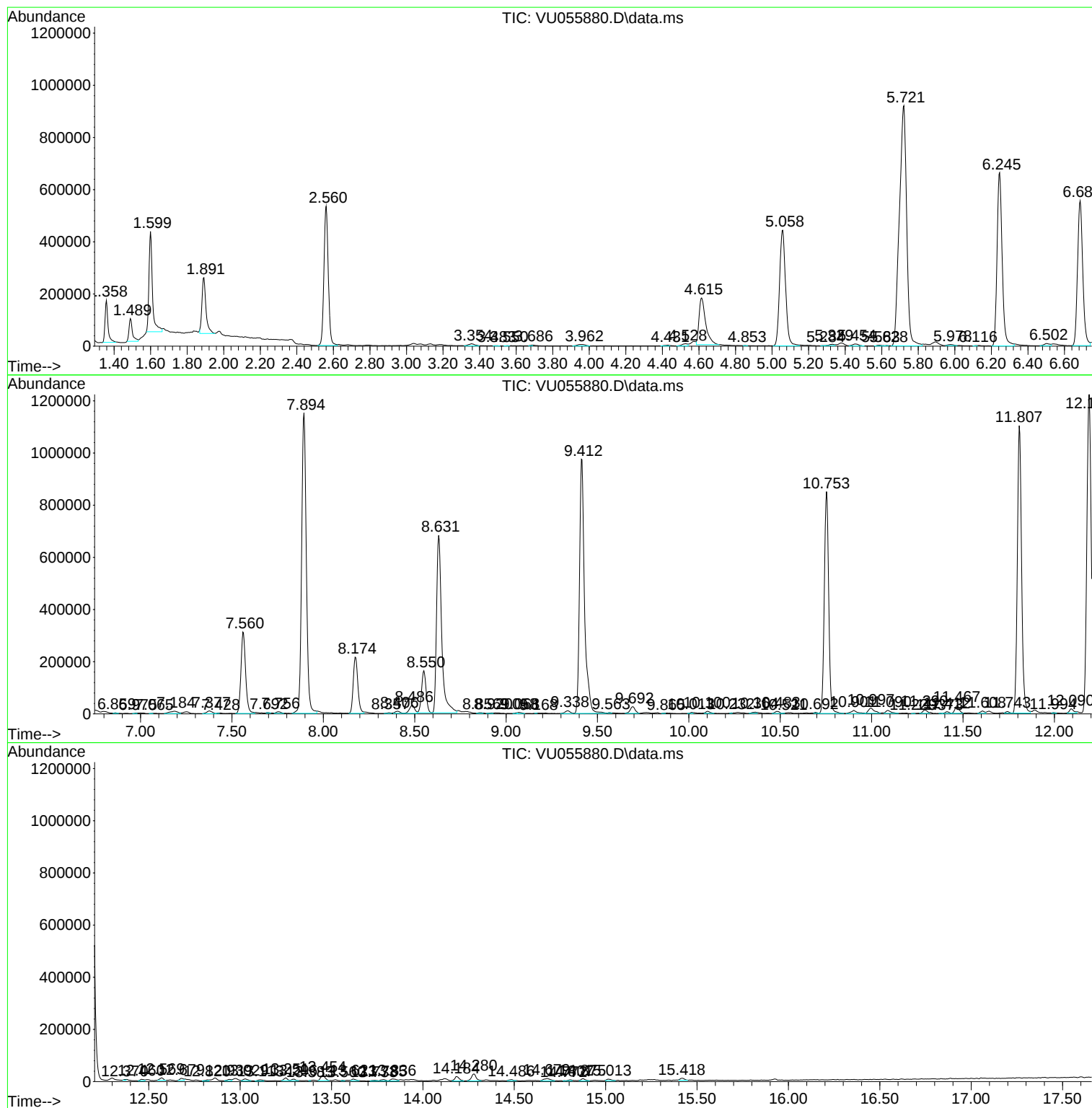
Sum of corrected areas: 20944667

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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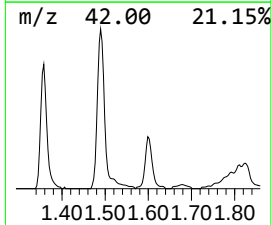
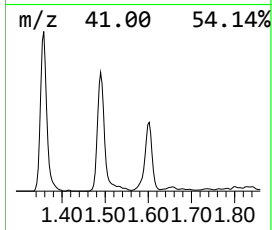
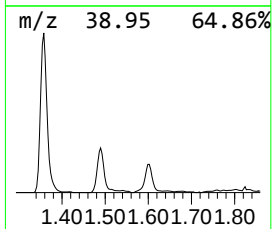
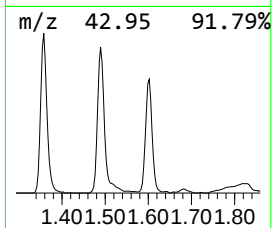
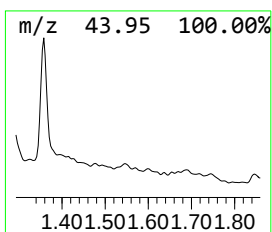
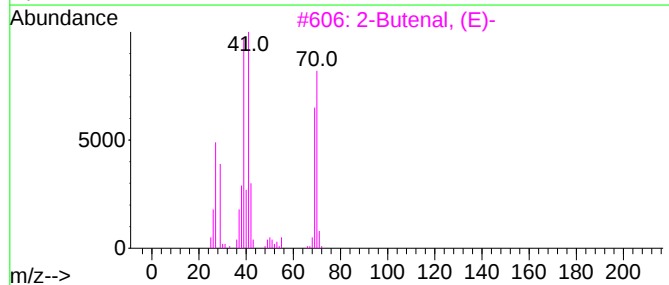
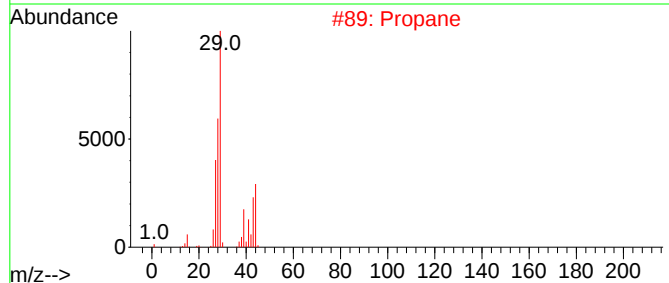
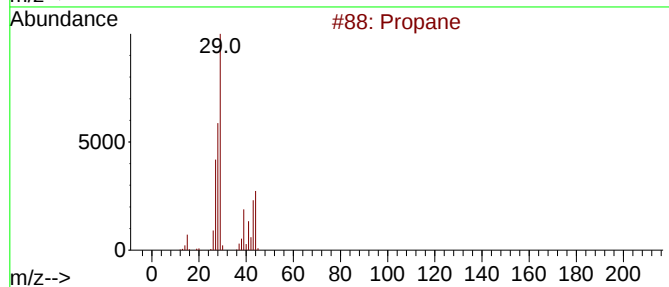
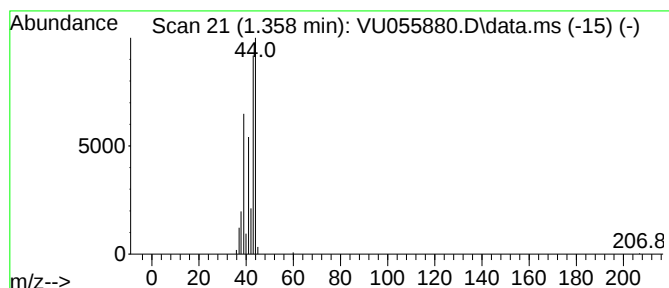
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	6.89 ug/L	178260	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propane	44	C3H8	000074-98-6	83
3			2-Butenal, (E)-	70	C4H6O	000123-73-9	40
4			2-Hexynoic acid	112	C6H8O2	000764-33-0	39
5			Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	38



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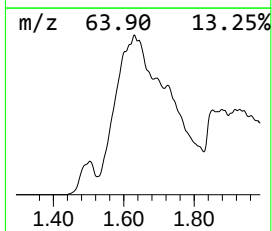
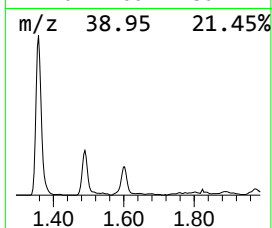
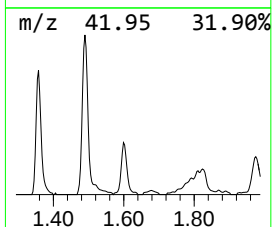
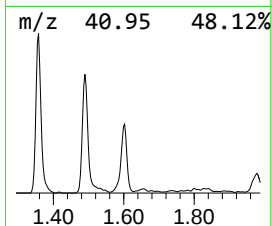
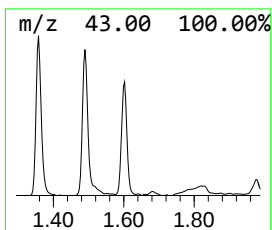
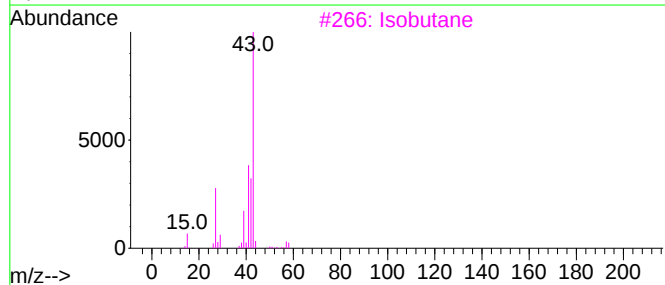
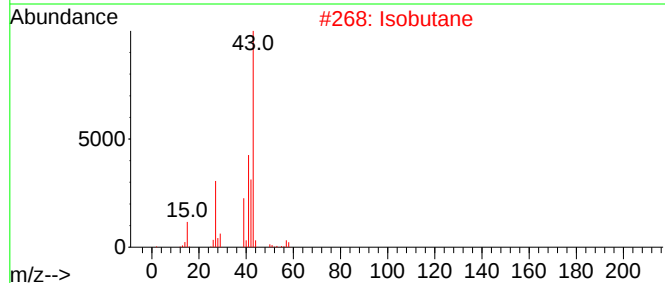
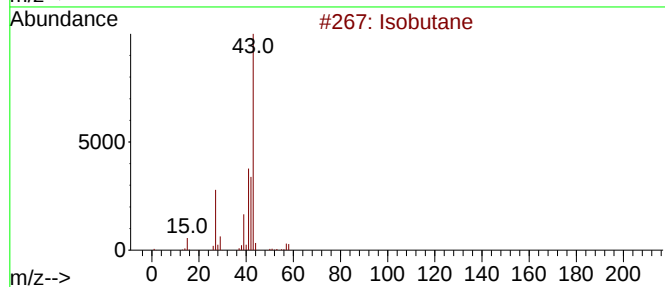
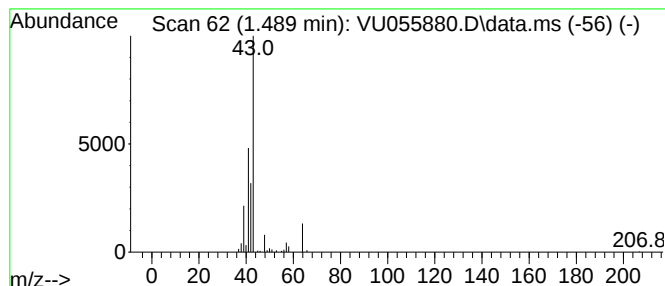
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.489	4.30 ug/L	111327	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	53
2		Isobutane	58	C4H10	000075-28-5	50
3		Isobutane	58	C4H10	000075-28-5	50
4		Isobutane	58	C4H10	000075-28-5	38
5		Isobutane	58	C4H10	000075-28-5	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.358	6.9	ug/L	178260	1	6.245	1293670	50.0
(DEL) Alkane: S...	1.489	4.3	ug/L	111327	1	6.245	1293670	50.0