LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055902.D
Acq On : 26 Oct 2023 13:31
Operator : MD/SY
Sample : 04961-06ME
Misc : 5.59g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

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: VU055902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.470	48	56	66	rBV	39288	88827	1.93%	0.453%
2	1.595	90	95	124	rVB	105027	194337	4.23%	0.990%
3	2.544	375	390	413	rBV	198616	349417	7.61%	1.780%
4	2.750	451	454	455	rBV2	1186	573	0.01%	0.003%
5	2.763	456	458	459	rBV	1172	529	0.01%	0.003%
6	2.878	491	494	496	rBV	756	468	0.01%	0.002%
7	2.959	514	519	521	rVB3	738	674	0.01%	0.003%
8	2.975	521	524	529	rBV3	482	485	0.01%	0.002%
9	3.033	532	542	555	rBV4	5973	13790	0.30%	0.070%
10	3.174	571	586	610	rBV	23441	57501	1.25%	0.293%
11	3.422	659	663	667	rBV2	416	487	0.01%	0.002%
12	3.679	733	743	752	rBV5	2622	5288	0.12%	0.027%
13	4.177	894	898	905	rBV	438	539	0.01%	0.003%
14	4.502	993	999	1004	rBV3	818	944	0.02%	0.005%
15	4.628	1023	1038	1087	rBV	133139	475270	10.35%	2.422%
16	4.920	1125	1129	1132	rVB4	829	646	0.01%	0.003%
17	5.055	1154	1171	1198	rBV	281878	676029	14.73%	3.444%
18	5.184	1208	1211	1213	rBV3	558	417	0.01%	0.002%
19	5.206	1216	1218	1224	rVV3	1259	1018	0.02%	0.005%
20	5.328	1244	1256	1259	rBV7	6763	11040	0.24%	0.056%
21	5.425	1284	1286	1292	rVB	921	595	0.01%	0.003%
22	5.486	1302	1305	1311	rVB2	500	455	0.01%	0.002%
23	5.534	1316	1320	1323	rBV2	628	504	0.01%	0.003%
24	5.566	1323	1330	1336	rBV5	419	522	0.01%	0.003%
25	5.714	1355	1376	1407	rBV2	556954	1524547	33.21%	7.768%
26	5.984	1449	1460	1468	rVV7	3246	7030	0.15%	0.036%
27	6.126	1498	1504	1512	rVB8	1449	2404	0.05%	0.012%
28	6.245	1527	1541	1568	rBV	630717	1287927	28.05%	6.562%
29	6.537	1615	1632	1644	rBV4	30823	68003	1.48%	0.346%
30	6.685	1664	1678	1707	rVB	360911	747672	16.29%	3.809%
31	6.975	1766	1768	1774	rVB4	743	604	0.01%	0.003%
32	7.007	1774	1778	1782	rBV3	544	493	0.01%	0.003%
33	7.055	1788	1793	1799	rBV5	879	786	0.02%	0.004%
34	7.090	1799	1804	1810	rBV2	1248	1466	0.03%	0.007%
35	7.193	1824	1836	1843	rBV6	6873	14824	0.32%	0.076%
36	7.338	1876	1881	1884	rBV5	665	612	0.01%	0.003%

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Misc : 5.59g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

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

37	7.486	1921	1927	1928	rBV5	1234	1172	0.03%	0.006%
38	7.563	1939	1951	1976	rBV	185470	370601	8.07%	1.888%
39	7.705	1988	1995	1999	rBV8	2549	3594	0.08%	0.018%
40	7.785	2013	2020	2027	rBV6	3755	5475	0.12%	0.028%
41	7.840	2035	2037	2041	rVB3	787	552	0.01%	0.003%
42	7.894	2041	2054	2073	rBV	567985	1044251	22.75%	5.320%
43	8.126	2121	2126	2131	rVV5	2033	2542	0.06%	0.013%
44	8.180	2131	2143	2170	rVB2	115014	256098	5.58%	1.305%
45	8.322	2182	2187	2189	rVV4	636	567	0.01%	0.003%
46	8.354	2189	2197	2203	rVV5	2107	3939	0.09%	0.020%
47	8.380	2203	2205	2208	rVV2	1083	623	0.01%	0.003%
48	8.396	2208	2210	2215	rVB3	801	416	0.01%	0.002%
49	8.467	2224	2232	2233	rBV5	2324	2233	0.05%	0.011%
50	8.547	2240	2257	2275	rBV	2659104	4590905	100.00%	23.391%
51	8.650	2276	2289	2320	rVB	584983	1196107	26.05%	6.094%
52	8.901	2364	2367	2368	rBV4	1020	597	0.01%	0.003%
53	8.917	2369	2372	2373	rBV3	1720	831	0.02%	0.004%
54	8.971	2386	2389	2391	rVB4	1253	730	0.02%	0.004%
55	8.997	2393	2397	2399	rBV4	761	515	0.01%	0.003%
56	9.116	2431	2434	2439	rVB7	969	900	0.02%	0.005%
57	9.158	2442	2447	2449	rBV3	1369	1249	0.03%	0.006%
58	9.209	2456	2463	2473	rVB8	4251	7297	0.16%	0.037%
59	9.335	2493	2502	2514	rVB9	3513	5899	0.13%	0.030%
60	9.418	2514	2528	2558	rBV	890779	1704563	37.13%	8.685%
61	9.569	2571	2575	2576	rBV4	1494	1110	0.02%	0.006%
62	9.656	2600	2602	2606	rBV	895	690	0.02%	0.004%
63	9.698	2606	2615	2623	rBV5	6654	11968	0.26%	0.061%
64	9.868	2666	2668	2670	rVV3	1091	628	0.01%	0.003%
65	10.010	2708	2712	2713	rBV	1077	699	0.02%	0.004%
66	10.116	2735	2745	2748	rBV6	3538	5621	0.12%	0.029%
67	10.200	2763	2771	2776	rVB5	1120	1555	0.03%	0.008%
68	10.248	2776	2786	2794	rBV6	4613	8014	0.17%	0.041%
69	10.341	2812	2815	2821	rBV7	1289	1553	0.03%	0.008%
70	10.393	2824	2831	2840	rVB6	5562	9390	0.20%	0.048%
71	10.438	2840	2845	2846	rBV2	627	421	0.01%	0.002%
72	10.492	2860	2862	2866	rVB2	607	418	0.01%	0.002%
73	10.557	2872	2882	2890	rBV4	2897	4918	0.11%	0.025%
74	10.621	2895	2902	2907	rBV5	4474	5874	0.13%	0.030%
75	10.759	2931	2945	2964	rBV	738878	1224216	26.67%	6.237%
76	11.010	3019	3023	3025	rBV5	1424	1163	0.03%	0.006%

LSC Area Percent Report

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Misc : 5.59g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

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

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Peak separation: 5

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

77	11.055	3033	3037	3046	rVV7	2152	2978	0.06%	0.015%
78	11.113	3046	3055	3070	rVB3	18547	29816	0.65%	0.152%
79	11.203	3079	3083	3088	rVB5	1541	1657	0.04%	0.008%
80	11.229	3088	3091	3094	rBV	724	480	0.01%	0.002%
81	11.248	3094	3097	3103	rBV5	929	1049	0.02%	0.005%
82	11.309	3106	3116	3126	rBV9	4096	6642	0.14%	0.034%
83	11.367	3130	3134	3135	rBV3	2774	1696	0.04%	0.009%
84	11.412	3141	3148	3156	rVB2	14127	18843	0.41%	0.096%
85	11.476	3164	3168	3171	rBV3	2334	1997	0.04%	0.010%
86	11.569	3191	3197	3201	rBV7	1572	1929	0.04%	0.010%
87	11.621	3206	3213	3214	rBV5	1834	2064	0.04%	0.011%
88	11.811	3260	3272	3287	rBV	1082662	1741975	37.94%	8.875%
89	12.000	3326	3331	3336	rVB7	4527	5300	0.12%	0.027%
90	12.084	3355	3357	3360	rBV3	988	781	0.02%	0.004%
91	12.193	3377	3391	3412	rBV	856288	1440506	31.38%	7.339%
92	12.325	3424	3432	3444	rBV2	45112	63576	1.38%	0.324%
93	12.666	3530	3538	3546	rBV8	7845	12544	0.27%	0.064%
94	12.942	3607	3624	3636	rBV8	13157	43175	0.94%	0.220%
95	13.045	3651	3656	3664	rVB4	8693	10919	0.24%	0.056%
96	13.132	3677	3683	3692	rVB7	7441	10753	0.23%	0.055%
97	13.344	3746	3749	3758	rBV6	2444	3672	0.08%	0.019%
98	13.428	3767	3775	3800	rVB2	61133	107865	2.35%	0.550%
99	13.582	3816	3823	3832	rBV3	28979	43319	0.94%	0.221%
100	14.447	4085	4092	4100	rVB2	42226	56917	1.24%	0.290%

Sum of corrected areas: 19627070

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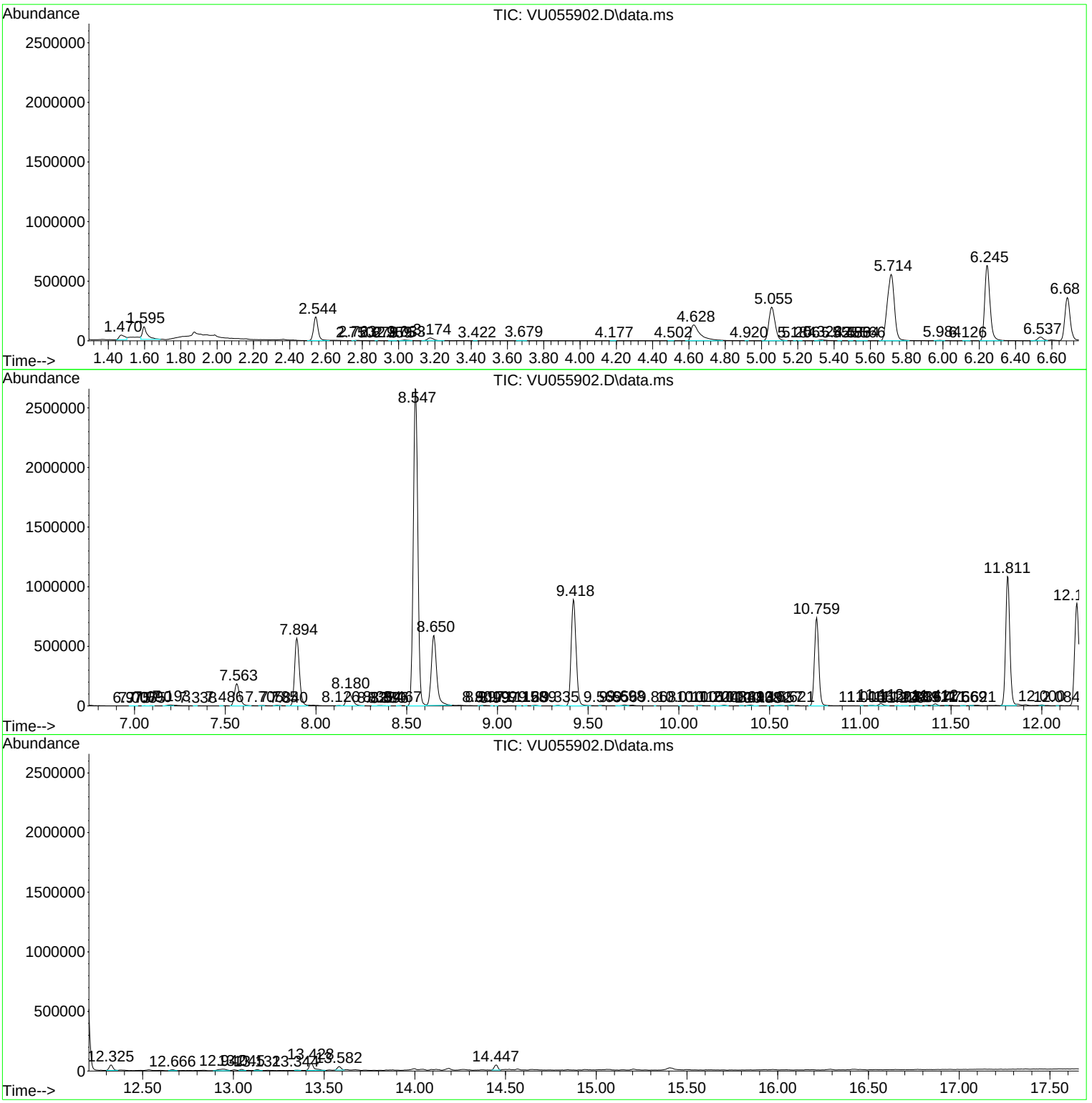
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

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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Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

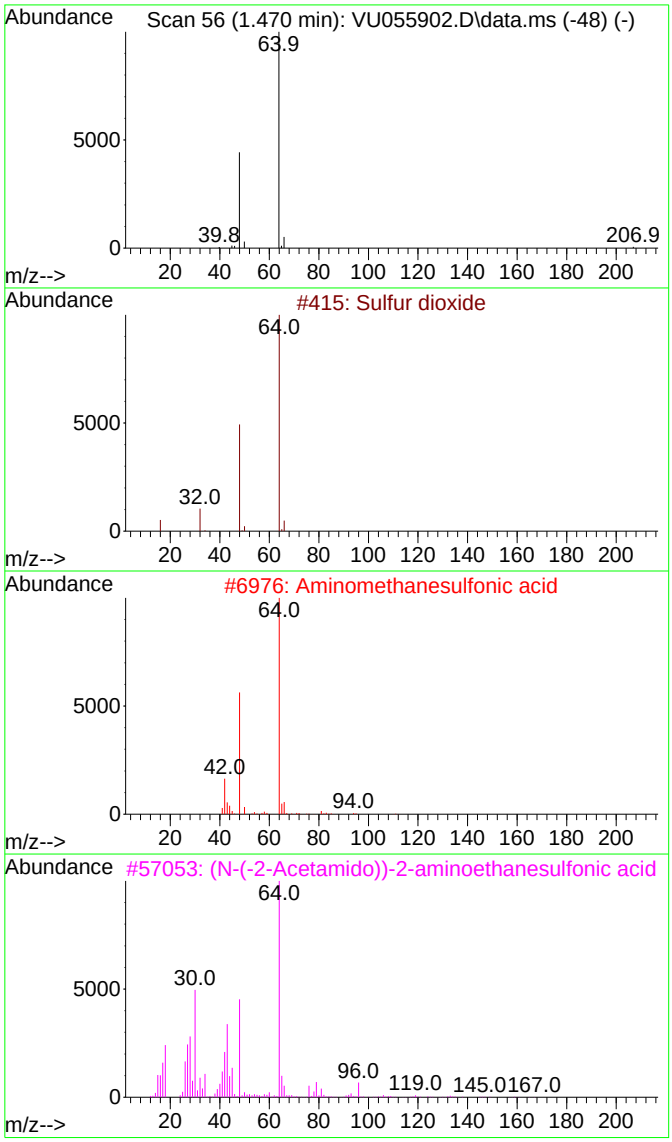
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

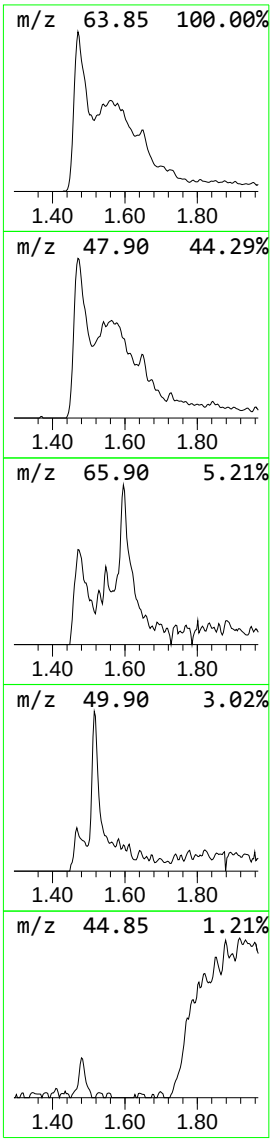
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	3.45 ug/L	88827	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5	N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0LJ2ME

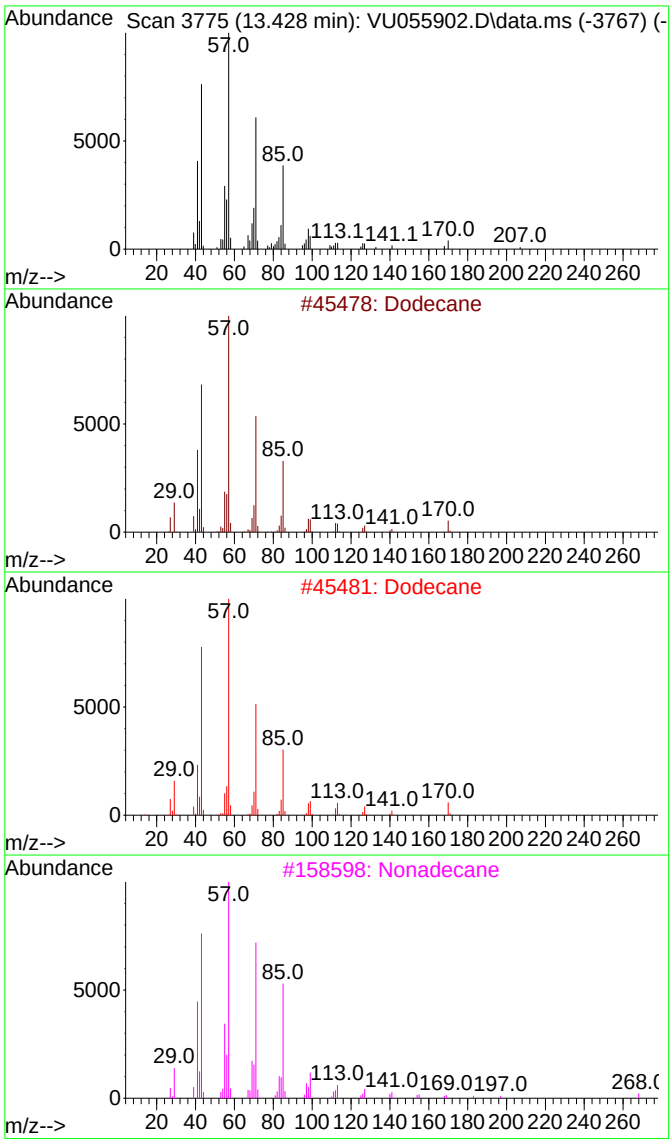
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

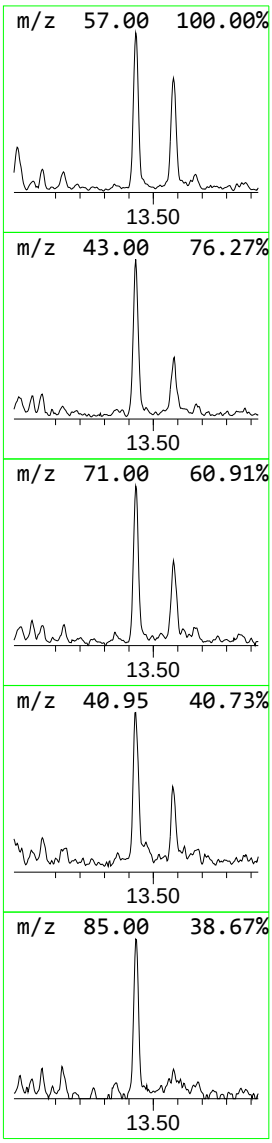
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.428	3.10 ug/L	107865	1,4-Dichlorobenzene-d4	11.814

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	87
2	Dodecane	170	C12H26	000112-40-3	83
3	Nonadecane	268	C19H40	000629-92-5	64
4	Tetradecane	198	C14H30	000629-59-4	59
5	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	59





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.470	3.5	ug/L	88827	1	6.245	1287930	50.0
(DEL) Alkane: S...	13.428	3.1	ug/L	107865	3	11.814	1741980	50.0