LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

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: VU055823.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.486	56	61	66	rBV3	6342	6891	0.01%	0.004%
2	1.602	87	97	115	rBV2	1037261	1290229	1.31%	0.699%
3	1.891	179	187	203	rVB	194373	283773	0.29%	0.154%
4	1.975	204	213	235	rVB	259183	380063	0.38%	0.206%
5	2.194	271	281	300	rVB	162163	238773	0.24%	0.129%
6	2.309	311	317	327	rVB	13180	18560	0.02%	0.010%
7	2.457	357	363	378	rVB5	12650	24517	0.02%	0.013%
8	2.560	382	395	426	rBV	449538	813977	0.82%	0.441%
9	2.959	512	519	520	rBV5	1843	1672	0.00%	0.001%
10	3.043	530	545	546	rBV2	44834	78267	0.08%	0.042%
11	3.290	616	622	625	rBV4	1376	1443	0.00%	0.001%
12	3.345	625	639	667	rVV2	581695	1219713	1.24%	0.660%
13	3.631	724	728	733	rVB4	666	633	0.00%	0.000%
14	3.692	733	747	768	rBV2	42220	94624	0.10%	0.051%
15	3.827	779	789	791	rBV5	3272	4472	0.00%	0.002%
16	3.907	802	814	815	rBV4	3667	4509	0.00%	0.002%
17	3.969	828	833	846	rVB4	6237	12129	0.01%	0.007%
18	4.084	855	869	884	rVB6	4533	10244	0.01%	0.006%
19	4.158	884	892	893	rBV3	630	720	0.00%	0.000%
20	4.174	893	897	902	rBV5	964	1128	0.00%	0.001%
21	4.287	919	932	938	rBV8	4392	10571	0.01%	0.006%
22	4.425	963	975	987	rBV5	7168	16483	0.02%	0.009%
23	4.525	989	1006	1023	rBV3	149771	368054	0.37%	0.199%
24	4.657	1023	1047	1083	rBV	16065759	36497464	36.97%	19.763%
25	5.055	1157	1171	1206	rVB	390707	885869	0.90%	0.480%
26	5.380	1255	1272	1286	rBV3	121620	294229	0.30%	0.159%
27	5.586	1323	1336	1346	rBV3	37603	87246	0.09%	0.047%
28	5.718	1358	1377	1405	rBV2	797121	2175898	2.20%	1.178%
29	5.843	1410	1416	1427	rVB3	32213	57206	0.06%	0.031%
30	5.985	1450	1460	1475	rVB3	45061	95672	0.10%	0.052%
31	6.132	1496	1506	1520	rBV7	8878	18316	0.02%	0.010%
32	6.190	1520	1524	1527	rVB3	1041	926	0.00%	0.001%
33	6.245	1527	1541	1577	rBV	591683	1174097	1.19%	0.636%
34	6.467	1603	1610	1615	rBV8	1706	2054	0.00%	0.001%
35	6.538	1615	1632	1667	rBV	15351285	28850362	29.22%	15.622%
36	6.685	1668	1678	1691	rVB	461151	852236	0.86%	0.461%

LSC Area Percent Report

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Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : E45J1

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	6.978	1759	1769	1781	rVB5	14063	28102	0.03%	0.015%
38	7.068	1788	1797	1811	rVB5	6850	14851	0.02%	0.008%
39	7.165	1813	1827	1828	rBV7	6008	8661	0.01%	0.005%
40	7.325	1872	1877	1882	rBV6	1254	1336	0.00%	0.001%
41	7.390	1888	1897	1903	rBV8	5467	10545	0.01%	0.006%
42	7.560	1939	1950	1972	rBV	270422	485405	0.49%	0.263%
43	7.853	2030	2041	2042	rBV3	13213	14280	0.01%	0.008%
44	7.894	2042	2054	2071	rVV	998602	1719818	1.74%	0.931%
45	8.174	2131	2141	2155	rBV	181579	316102	0.32%	0.171%
46	8.364	2190	2200	2202	rBV8	5873	8477	0.01%	0.005%
47	8.402	2209	2212	2213	rBV3	1568	1018	0.00%	0.001%
48	8.554	2241	2259	2276	rBV	55650633	98720422	100.00%	53.456%
49	8.634	2278	2284	2325	rVB2	482006	1234307	1.25%	0.668%
50	9.074	2414	2421	2427	rVB9	2771	4342	0.00%	0.002%
51	9.107	2429	2431	2435	rVB2	789	574	0.00%	0.000%
52	9.206	2460	2462	2468	rBV5	722	607	0.00%	0.000%
53	9.415	2513	2527	2550	rBV	879234	1484598	1.50%	0.804%
54	9.570	2566	2575	2592	rVB	34961	59424	0.06%	0.032%
55	9.692	2608	2613	2617	rBV7	2298	2878	0.00%	0.002%
56	10.033	2714	2719	2720	rBV2	1183	985	0.00%	0.001%
57	10.274	2785	2794	2803	rBV6	1867	3680	0.00%	0.002%
58	10.364	2815	2822	2824	rBV6	1433	1662	0.00%	0.001%
59	10.483	2851	2859	2872	rVB3	7126	12947	0.01%	0.007%
60	10.689	2920	2923	2931	rVV6	1770	1959	0.00%	0.001%
61	10.753	2931	2943	2973	rVV	763595	1255700	1.27%	0.680%
62	10.907	2981	2991	3003	rBV2	6188	10931	0.01%	0.006%
63	10.981	3011	3014	3018	rVB2	837	560	0.00%	0.000%
64	11.090	3043	3048	3051	rBV5	1383	1315	0.00%	0.001%
65	11.123	3054	3058	3062	rBV4	828	761	0.00%	0.000%
66	11.293	3102	3111	3122	rBV7	2043	4281	0.00%	0.002%
67	11.473	3161	3167	3174	rVB4	1705	2028	0.00%	0.001%
68	11.560	3187	3194	3200	rBV3	626	820	0.00%	0.000%
69	11.608	3205	3209	3210	rBV2	1556	1145	0.00%	0.001%
70	11.637	3215	3218	3228	rVV4	2567	3697	0.00%	0.002%
71	11.750	3249	3253	3259	rVB5	1562	1589	0.00%	0.001%
72	11.811	3259	3272	3291	rBV	922660	1511996	1.53%	0.819%
73	12.094	3349	3360	3371	rBV3	37690	61632	0.06%	0.033%
74	12.190	3377	3390	3410	rBV	1014621	1695366	1.72%	0.918%
75	12.463	3472	3475	3480	rVB4	1209	1096	0.00%	0.001%
76	12.563	3503	3506	3509	rBV2	667	634	0.00%	0.000%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
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Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

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

77	12.611	3514	3521	3531	rVB4	5757	8845	0.01%	0.005%
78	12.679	3532	3542	3560	rVB4	21501	37571	0.04%	0.020%
79	12.785	3572	3575	3580	rVB2	688	546	0.00%	0.000%
80	12.817	3583	3585	3590	rVB3	758	524	0.00%	0.000%
81	12.846	3590	3594	3595	rBV2	909	545	0.00%	0.000%
82	12.868	3598	3601	3602	rBV2	1354	806	0.00%	0.000%
83	12.936	3619	3622	3626	rBV2	715	707	0.00%	0.000%
84	13.110	3669	3676	3684	rBV8	1641	2375	0.00%	0.001%
85	13.222	3708	3711	3713	rBV	1140	770	0.00%	0.000%
86	13.296	3726	3734	3750	rVB5	6369	11379	0.01%	0.006%
87	13.373	3755	3758	3765	rBV5	492	639	0.00%	0.000%
88	13.457	3774	3784	3796	rBV4	9511	16291	0.02%	0.009%
89	13.566	3815	3818	3822	rBV2	690	524	0.00%	0.000%
90	13.791	3880	3888	3896	rVB7	3288	5302	0.01%	0.003%
91	13.849	3900	3906	3914	rBV8	4307	5823	0.01%	0.003%
92	13.942	3932	3935	3944	rVB5	3674	4021	0.00%	0.002%
93	14.103	3977	3985	3986	rBV4	3673	4017	0.00%	0.002%
94	14.335	4050	4057	4060	rBV5	2655	3328	0.00%	0.002%
95	14.466	4095	4098	4101	rBV3	693	595	0.00%	0.000%
96	14.531	4113	4118	4123	rBV3	1236	1476	0.00%	0.001%
97	14.627	4144	4148	4156	rVB6	929	1181	0.00%	0.001%
98	14.946	4244	4247	4249	rBV2	1198	708	0.00%	0.000%
99	14.991	4253	4261	4264	rBV6	1232	1915	0.00%	0.001%
100	15.495	4414	4418	4422	rBV4	1125	1150	0.00%	0.001%

Sum of corrected areas: 184674589

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
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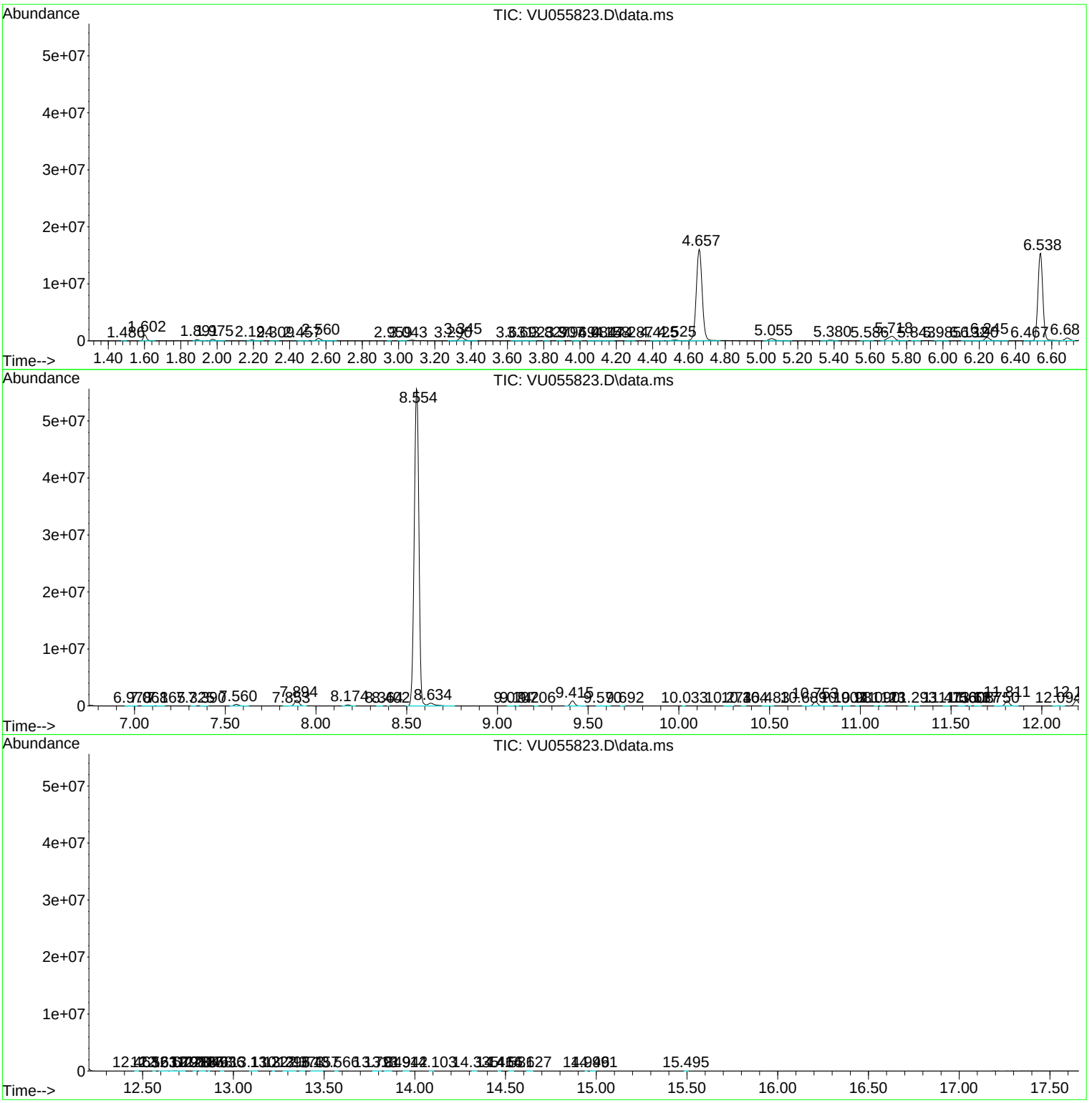
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

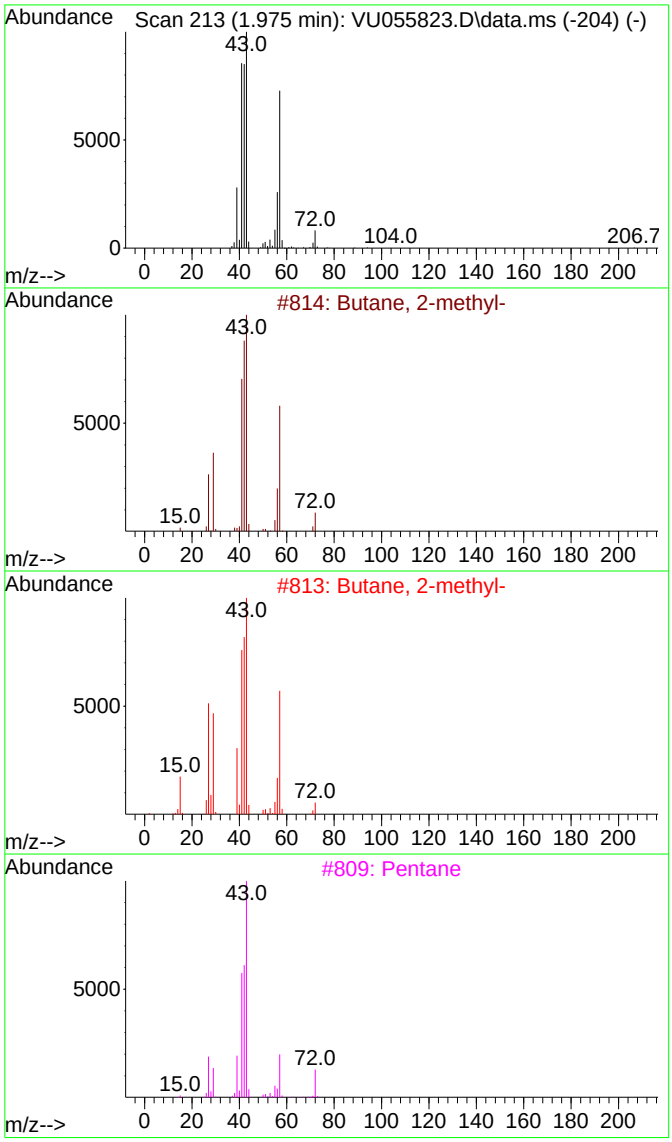
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

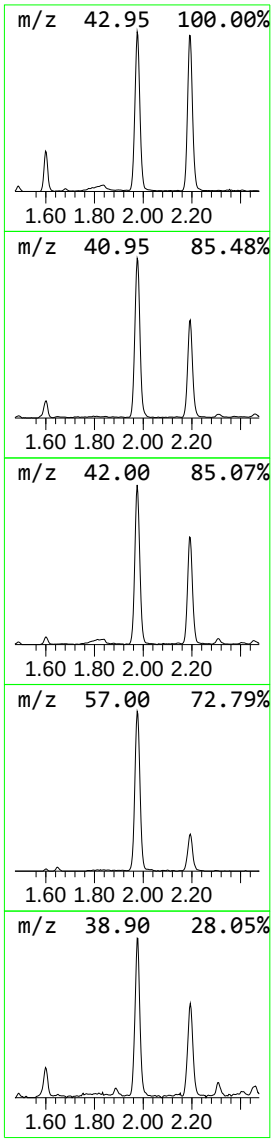
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.975	16.19 ug/L	380063	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	Pentane	72	C5H12	000109-66-0	50
4	3-Buten-1-ol	72	C4H8O	000627-27-0	47
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

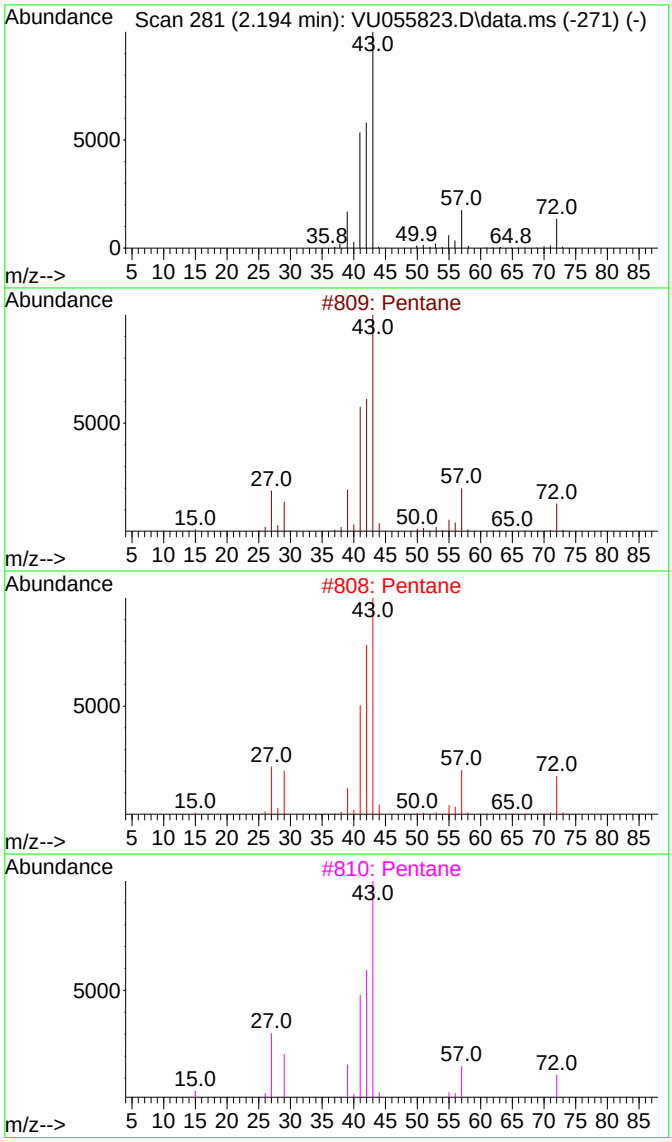
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

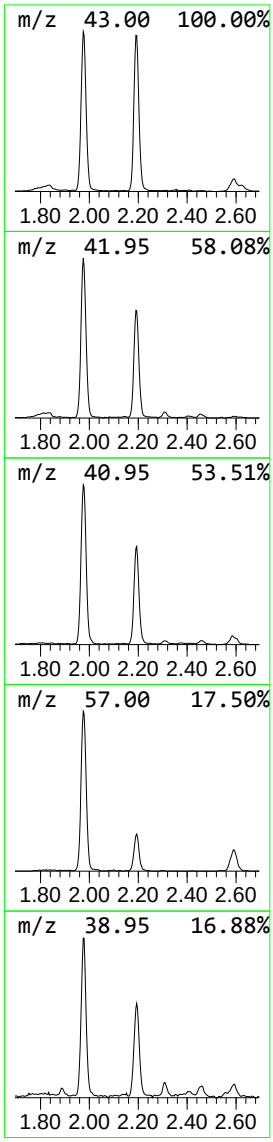
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.194	10.17 ug/L	238773	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Pentane	72	C5H12	000109-66-0	90
3	Pentane	72	C5H12	000109-66-0	90
4	Pentane	72	C5H12	000109-66-0	86
5	Pentane	72	C5H12	000109-66-0	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

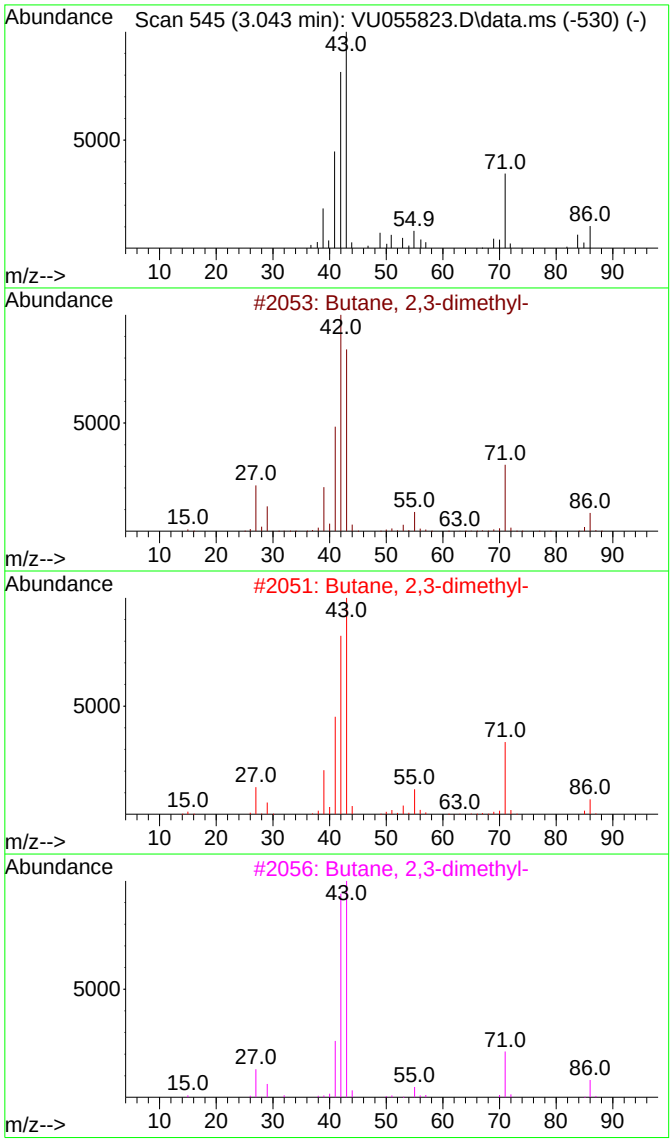
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

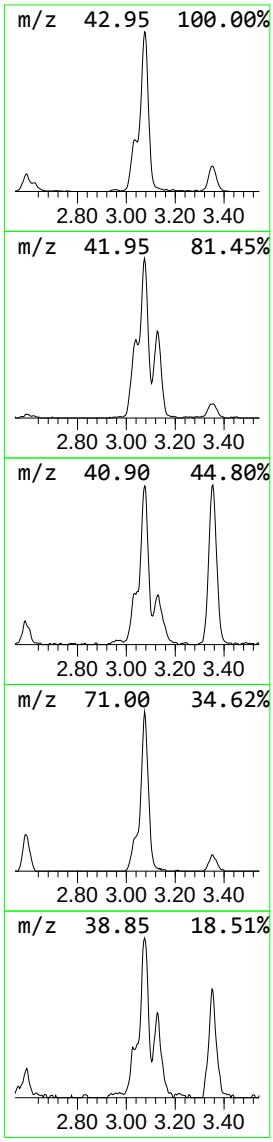
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	3.33 ug/L	78267	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	47
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

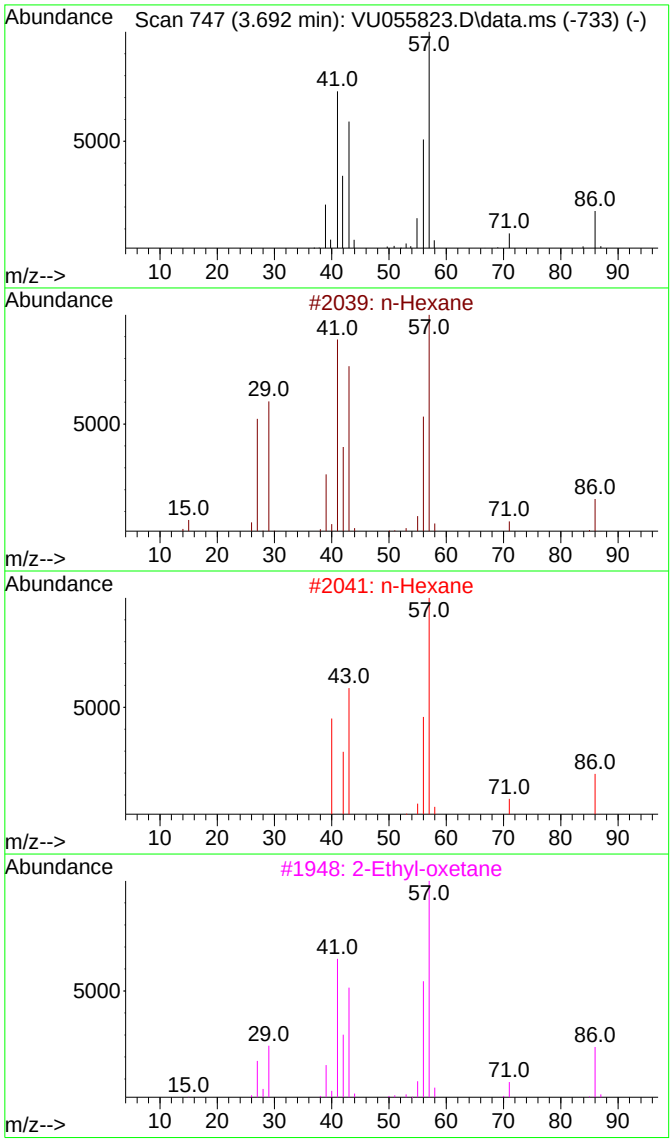
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

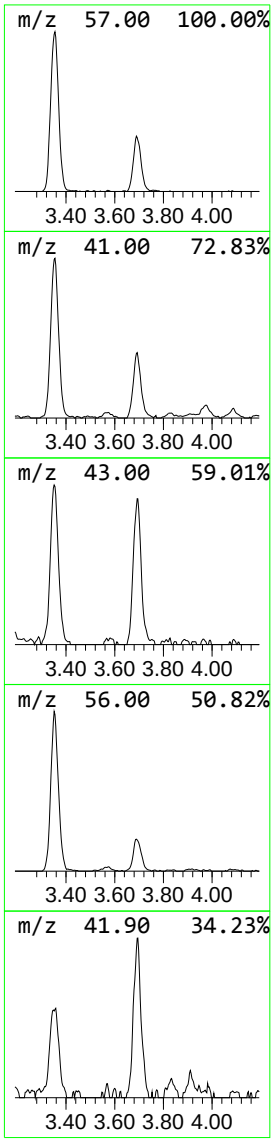
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.692	4.03 ug/L	94624	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	86
2	n-Hexane	86	C6H14	000110-54-3	86
3	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	86
4	n-Hexane	86	C6H14	000110-54-3	86
5	n-Hexane	86	C6H14	000110-54-3	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

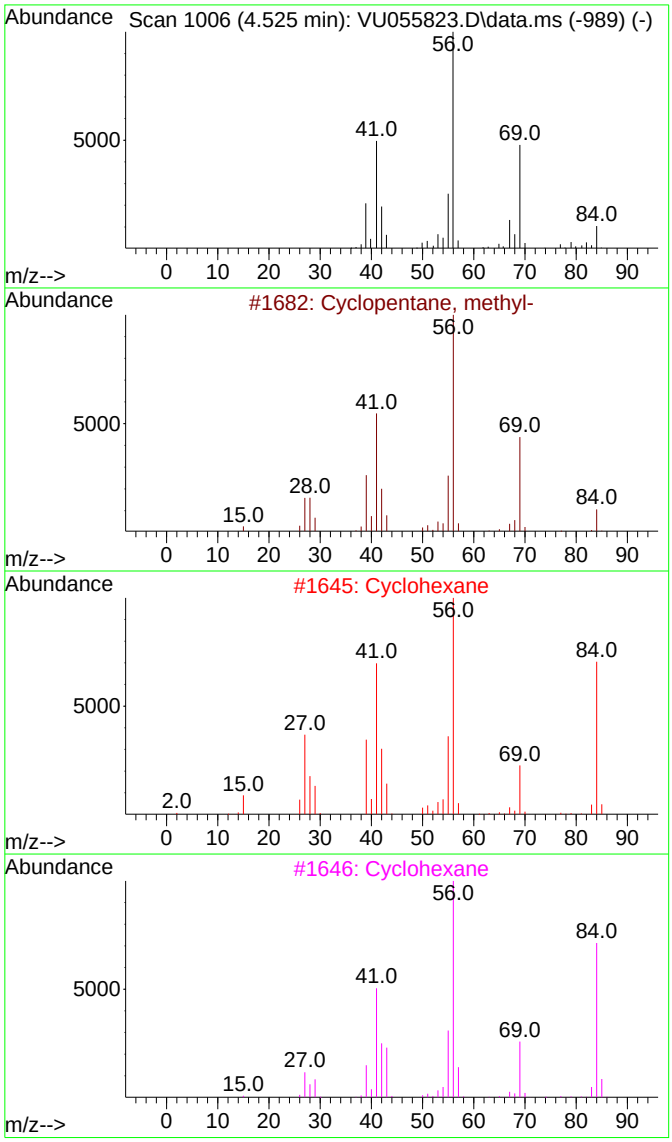
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

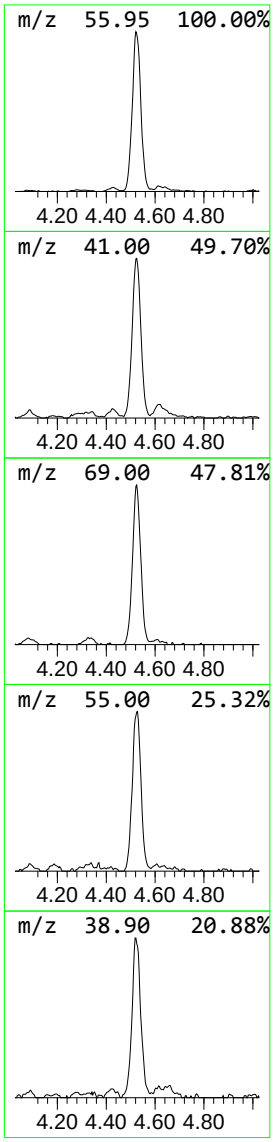
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic4.525 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.525	15.67 ug/L	368054	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclohexane	84	C6H12	000110-82-7	83
3	Cyclohexane	84	C6H12	000110-82-7	72
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





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Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

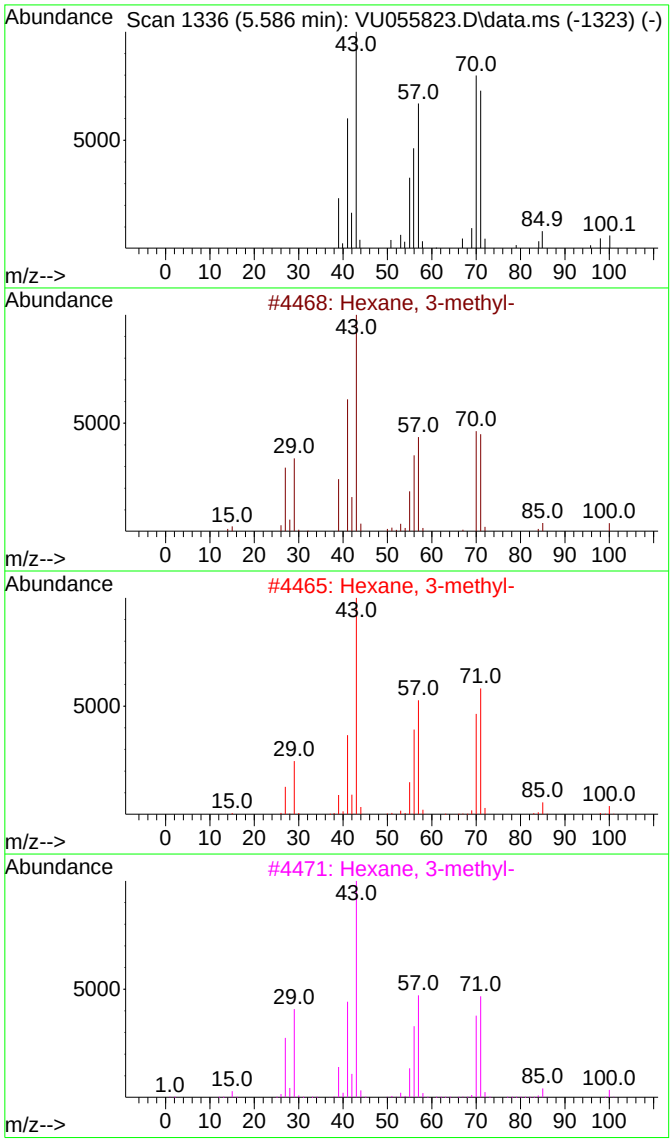
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

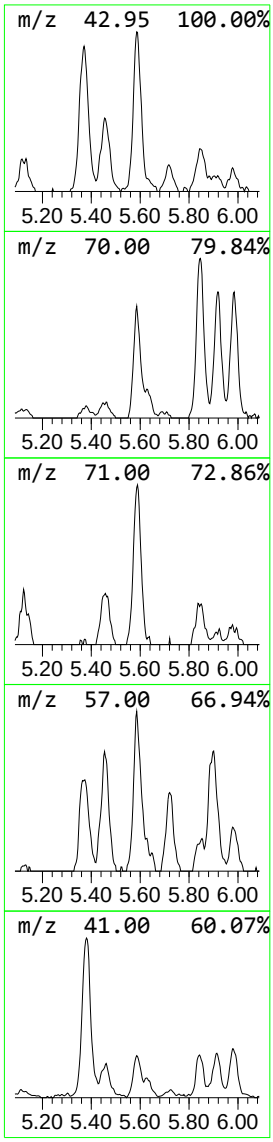
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.586	3.72 ug/L	87246	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	90
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	87
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

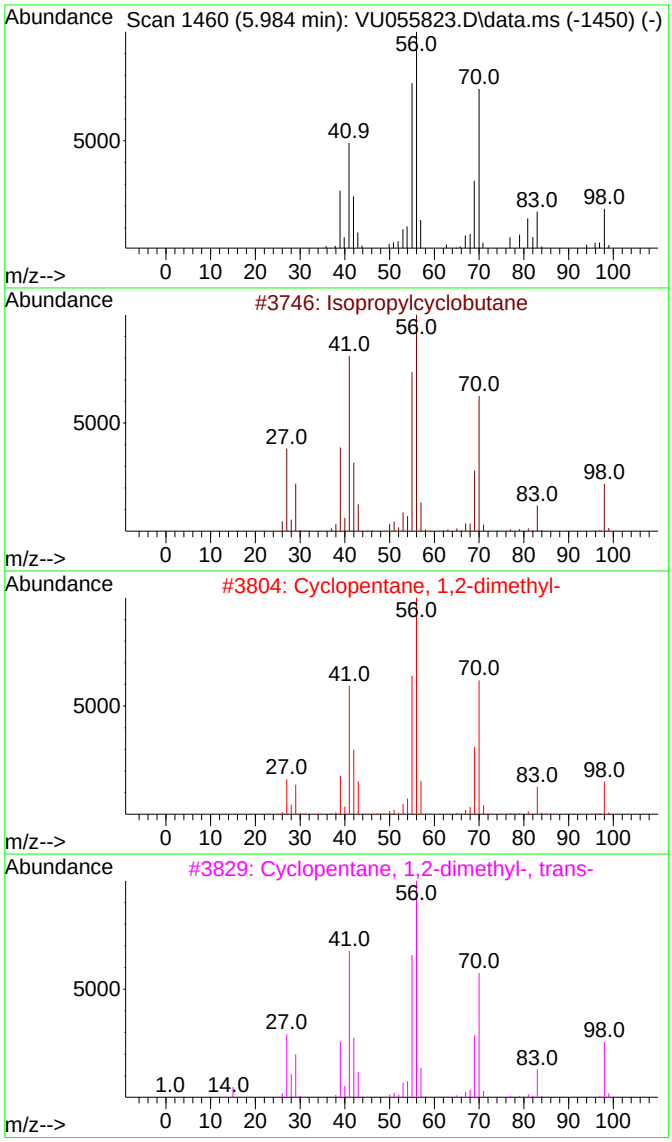
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

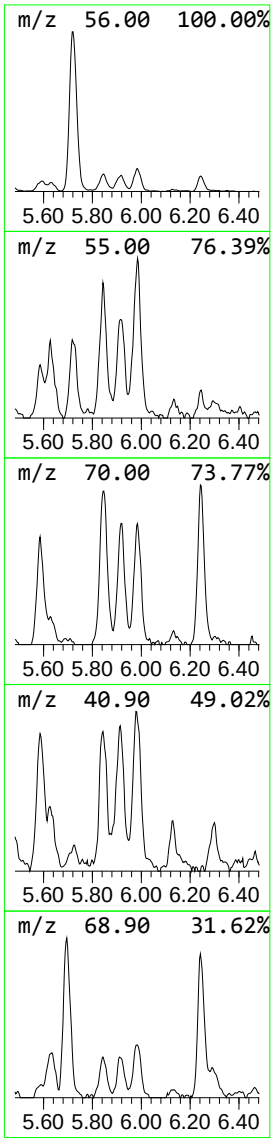
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Cyclic5.984 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.984	4.07 ug/L	95672	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	93
2	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	86
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
Data File : VU055823.D
Acq On : 20 Oct 2023 11:09
Operator : MD/SY
Sample : 04947-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45J1

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
(DEL) Alkane: S...	1.975	16.2	ug/L	380063	1	6.245	1174100	50.0
(DEL) Alkane: S...	2.194	10.2	ug/L	238773	1	6.245	1174100	50.0
(DEL) Alkane: S...	3.043	3.3	ug/L	78267	1	6.245	1174100	50.0
(DEL) Alkane: S...	3.692	4.0	ug/L	94624	1	6.245	1174100	50.0
(DEL) Alkane: C...	4.525	15.7	ug/L	368054	1	6.245	1174100	50.0
(DEL) Alkane: S...	5.586	3.7	ug/L	87246	1	6.245	1174100	50.0
(DEL) Alkane: C...	5.984	4.1	ug/L	95672	1	6.245	1174100	50.0