

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
 Data File : VU057941.D
 Acq On : 23 Feb 2024 11:08
 Operator : MD/SY
 Sample : P1567-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JWAC2

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\SFAMULM021924WMA.M

Title : VOC Analysis

Signal : TIC: VU057941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	110	rVB	111887	127725	13.28%	1.509%
2	1.907	183	192	204	rBV	92147	118198	12.29%	1.397%
3	2.509	377	379	382	rVB	332	172	0.02%	0.002%
4	2.560	382	395	406	rBV	183874	303069	31.51%	3.581%
5	2.615	407	412	426	rVB	14829	24779	2.58%	0.293%
6	2.731	436	448	500	rBV	470101	961790	100.00%	11.364%
7	3.168	570	584	594	rBV5	3399	8362	0.87%	0.099%
8	3.251	608	610	612	rVB2	462	183	0.02%	0.002%
9	3.268	612	615	621	rBV2	330	326	0.03%	0.004%
10	3.345	635	639	644	rBV3	735	808	0.08%	0.010%
11	3.570	706	709	714	rBV3	321	339	0.04%	0.004%
12	3.602	714	719	724	rVV2	347	364	0.04%	0.004%
13	3.792	773	778	783	rVB2	308	392	0.04%	0.005%
14	3.846	790	795	798	rBV2	192	187	0.02%	0.002%
15	4.004	837	844	848	rBV2	240	390	0.04%	0.005%
16	4.107	874	876	880	rVB2	245	172	0.02%	0.002%
17	4.129	880	883	886	rBV	227	176	0.02%	0.002%
18	4.187	898	901	905	rBV2	300	294	0.03%	0.003%
19	4.396	963	966	971	rVB2	220	215	0.02%	0.003%
20	4.612	1021	1033	1062	rBV	60407	163406	16.99%	1.931%
21	4.821	1095	1098	1105	rVB3	533	563	0.06%	0.007%
22	4.965	1133	1143	1157	rBV	32618	81706	8.50%	0.965%
23	5.052	1158	1170	1195	rVB	164730	375076	39.00%	4.432%
24	5.464	1296	1298	1302	rVB2	257	178	0.02%	0.002%
25	5.486	1302	1305	1307	rBV	273	225	0.02%	0.003%
26	5.592	1334	1338	1341	rBV2	334	341	0.04%	0.004%
27	5.718	1357	1377	1408	rBV2	338369	923098	95.98%	10.906%
28	6.062	1481	1484	1492	rVB3	241	341	0.04%	0.004%
29	6.123	1501	1503	1507	rVB2	322	204	0.02%	0.002%
30	6.142	1507	1509	1512	rBV2	329	170	0.02%	0.002%
31	6.242	1527	1540	1567	rBV	362472	700928	72.88%	8.281%
32	6.480	1610	1614	1617	rBV	274	241	0.03%	0.003%
33	6.538	1623	1632	1634	rBV6	1533	1764	0.18%	0.021%
34	6.685	1664	1678	1704	rBV	203810	416658	43.32%	4.923%
35	7.004	1772	1777	1780	rBV2	194	182	0.02%	0.002%
36	7.052	1788	1792	1795	rBV2	227	171	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
 Data File : VU057941.D
 Acq On : 23 Feb 2024 11:08
 Operator : MD/SY
 Sample : P1567-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JWAC2

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\SFAMULM021924WMA.M
 Title : VOC Analysis

37	7.158	1820	1825	1831	rBV3	597	835	0.09%	0.010%
38	7.200	1836	1838	1841	rVB3	323	186	0.02%	0.002%
39	7.560	1936	1950	1978	rBV	113111	214173	22.27%	2.530%
40	7.711	1994	1997	2004	rVB4	969	944	0.10%	0.011%
41	7.798	2018	2024	2026	rBV2	450	415	0.04%	0.005%
42	7.891	2040	2053	2075	rBV	407384	723157	75.19%	8.544%
43	8.174	2129	2141	2165	rBV	78173	141929	14.76%	1.677%
44	8.335	2189	2191	2194	rVB2	275	179	0.02%	0.002%
45	8.364	2194	2200	2203	rBV2	348	368	0.04%	0.004%
46	8.435	2219	2222	2225	rVB	310	192	0.02%	0.002%
47	8.463	2225	2231	2236	rBV3	613	940	0.10%	0.011%
48	8.489	2236	2239	2242	rVB2	326	202	0.02%	0.002%
49	8.515	2242	2247	2249	rBV2	193	195	0.02%	0.002%
50	8.550	2249	2258	2271	rVB3	16049	26949	2.80%	0.318%
51	8.631	2271	2283	2315	rBV2	175583	395652	41.14%	4.675%
52	8.923	2370	2374	2380	rVB2	570	658	0.07%	0.008%
53	9.293	2485	2489	2495	rBV2	298	383	0.04%	0.005%
54	9.322	2495	2498	2502	rBV	228	185	0.02%	0.002%
55	9.412	2513	2526	2568	rVV	505502	863054	89.73%	10.197%
56	9.570	2568	2575	2579	rVB3	836	1082	0.11%	0.013%
57	9.698	2609	2615	2622	rVV2	739	1071	0.11%	0.013%
58	9.756	2630	2633	2635	rBV	240	173	0.02%	0.002%
59	9.971	2696	2700	2703	rVV	205	196	0.02%	0.002%
60	10.068	2726	2730	2734	rBV2	153	180	0.02%	0.002%
61	10.126	2743	2748	2754	rBV	656	821	0.09%	0.010%
62	10.235	2778	2782	2787	rBV2	242	253	0.03%	0.003%
63	10.367	2819	2823	2825	rBV	340	287	0.03%	0.003%
64	10.486	2855	2860	2862	rBV2	516	425	0.04%	0.005%
65	10.547	2876	2879	2882	rBV2	270	170	0.02%	0.002%
66	10.615	2896	2900	2904	rBV2	213	218	0.02%	0.003%
67	10.640	2904	2908	2912	rVB3	504	418	0.04%	0.005%
68	10.750	2928	2942	2965	rBV	250461	411837	42.82%	4.866%
69	10.888	2979	2985	2993	rVV	715	1046	0.11%	0.012%
70	10.952	3002	3005	3011	rBV	318	295	0.03%	0.003%
71	11.000	3016	3020	3027	rBV	258	302	0.03%	0.004%
72	11.090	3045	3048	3050	rBV2	274	210	0.02%	0.002%
73	11.184	3073	3077	3080	rBV2	295	301	0.03%	0.004%
74	11.335	3121	3124	3127	rBV	208	173	0.02%	0.002%
75	11.434	3150	3155	3156	rBV	232	203	0.02%	0.002%
76	11.576	3197	3199	3203	rVB2	262	176	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
 Data File : VU057941.D
 Acq On : 23 Feb 2024 11:08
 Operator : MD/SY
 Sample : P1567-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JWAC2

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\SFAMULM021924WMA.M
 Title : VOC Analysis

77	11.598	3203	3206	3209	rBV2	272	250	0.03%	0.003%
78	11.663	3223	3226	3229	rVB	360	229	0.02%	0.003%
79	11.705	3234	3239	3241	rBV2	156	175	0.02%	0.002%
80	11.750	3246	3253	3259	rBV4	1797	2469	0.26%	0.029%
81	11.807	3259	3271	3304	rVV	505629	823252	85.60%	9.727%
82	12.049	3341	3346	3348	rBV2	330	275	0.03%	0.003%
83	12.190	3377	3390	3422	rBV	373530	616828	64.13%	7.288%
84	12.389	3446	3452	3458	rBV2	276	422	0.04%	0.005%
85	12.557	3501	3504	3507	rBV2	224	176	0.02%	0.002%
86	12.602	3514	3518	3521	rBV2	182	172	0.02%	0.002%
87	12.669	3537	3539	3543	rVB	319	235	0.02%	0.003%
88	12.769	3566	3570	3577	rVB3	546	613	0.06%	0.007%
89	13.232	3707	3714	3720	rBV3	1046	1445	0.15%	0.017%
90	13.360	3750	3754	3762	rBV2	251	396	0.04%	0.005%
91	13.399	3763	3766	3773	rVB2	252	194	0.02%	0.002%
92	13.846	3899	3905	3906	rBV4	2397	1908	0.20%	0.023%
93	14.103	3978	3985	3997	rBV3	2686	4255	0.44%	0.050%
94	14.302	4044	4047	4050	rBV2	235	225	0.02%	0.003%
95	14.335	4050	4057	4068	rVB5	3160	5065	0.53%	0.060%
96	14.380	4068	4071	4077	rBV3	407	391	0.04%	0.005%
97	14.576	4129	4132	4135	rBV	284	197	0.02%	0.002%
98	14.865	4218	4222	4225	rBV2	381	389	0.04%	0.005%
99	15.759	4497	4500	4501	rBV3	361	217	0.02%	0.003%
100	16.605	4761	4763	4765	rBV2	774	400	0.04%	0.005%

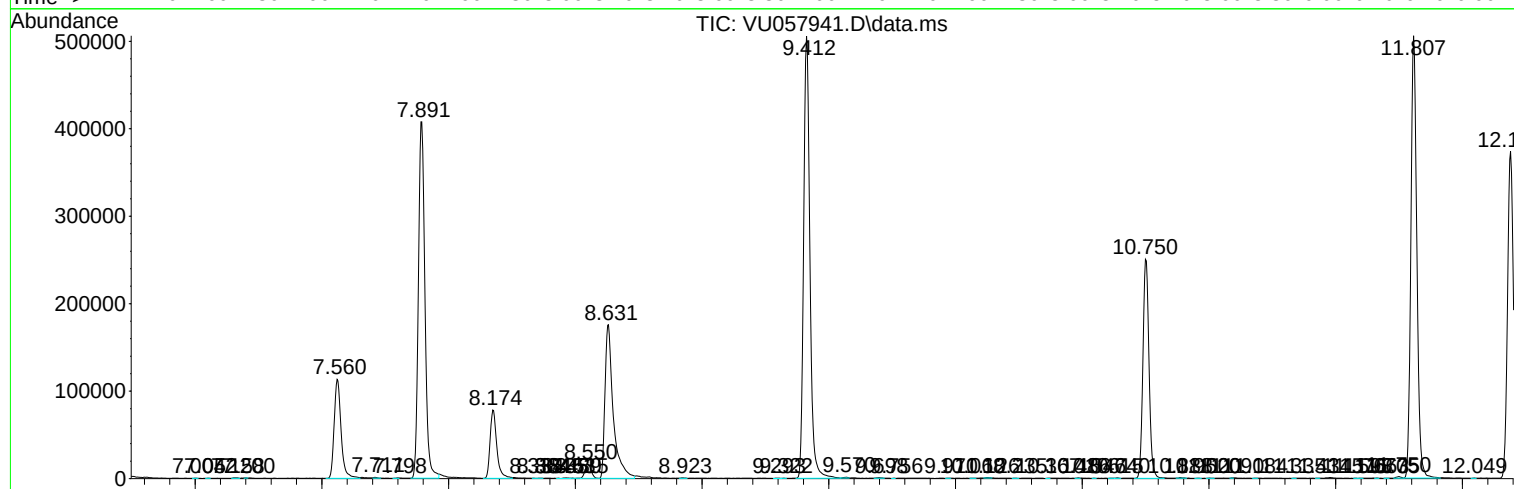
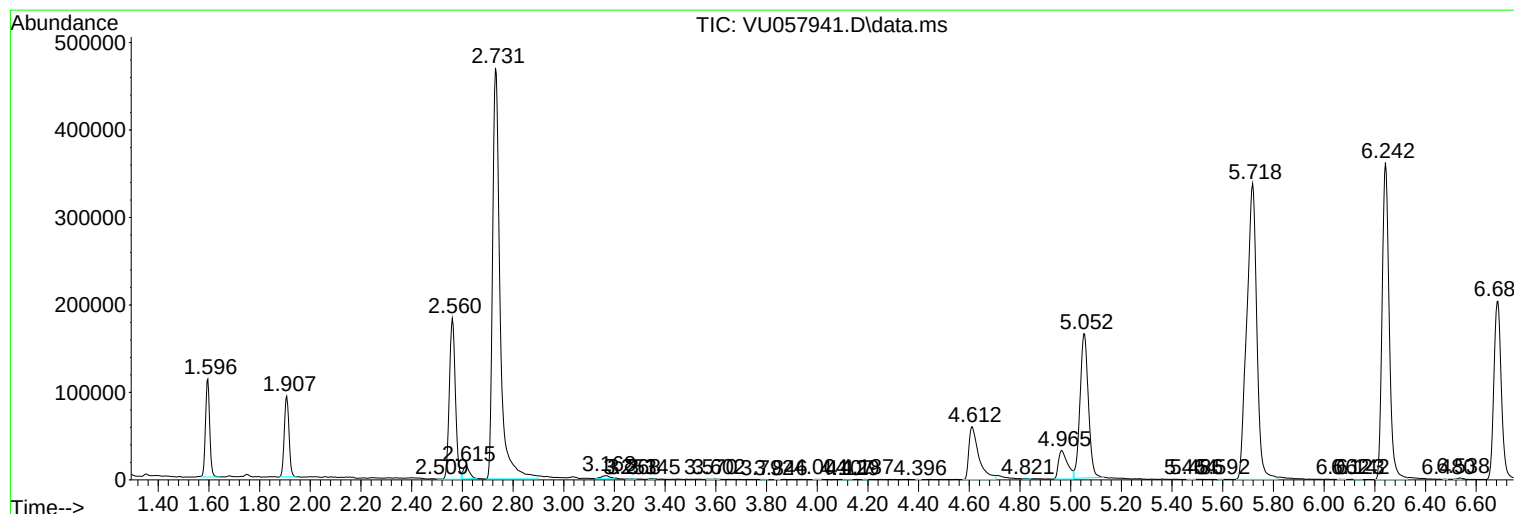
Sum of corrected areas: 8463804

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
Data File : VU057941.D
Acq On : 23 Feb 2024 11:08
Operator : MD/SY
Sample : P1567-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JWAC2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
Data File : VU057941.D
Acq On : 23 Feb 2024 11:08
Operator : MD/SY
Sample : P1567-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JWAC2

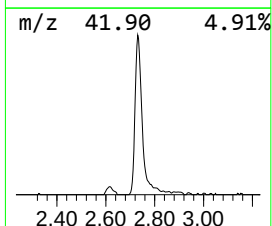
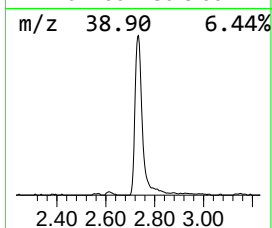
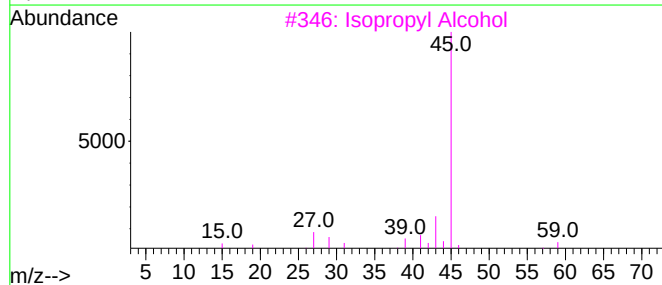
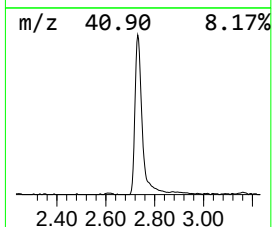
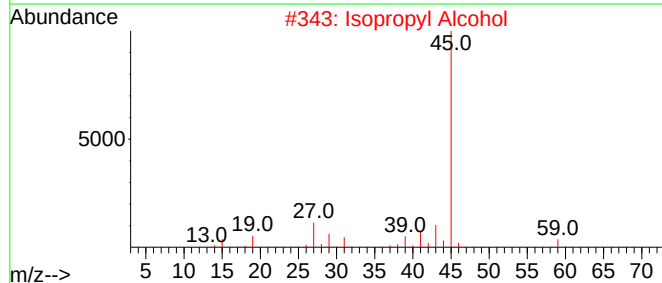
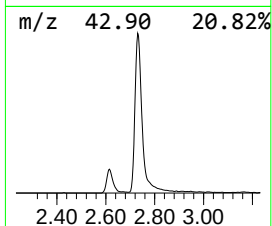
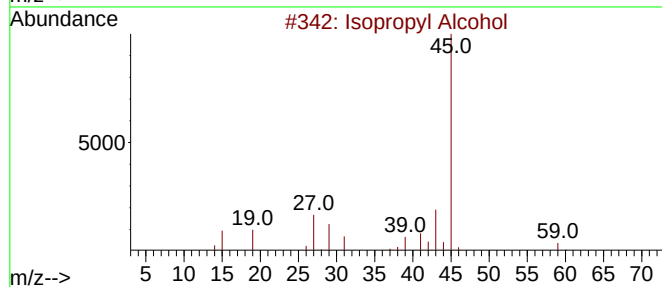
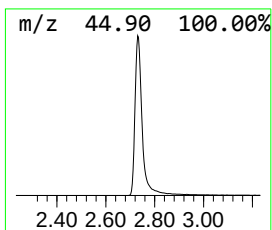
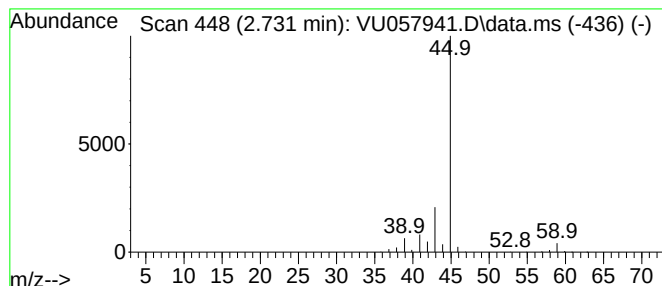
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.731	68.61 ug/L	961790	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
Data File : VU057941.D
Acq On : 23 Feb 2024 11:08
Operator : MD/SY
Sample : P1567-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JWAC2

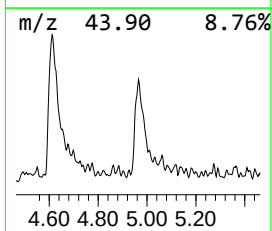
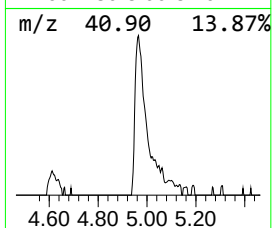
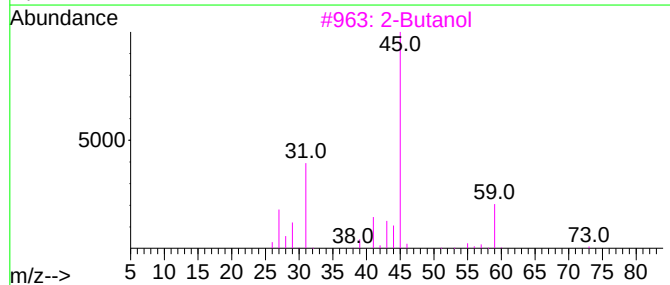
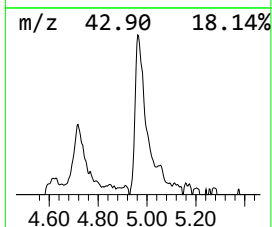
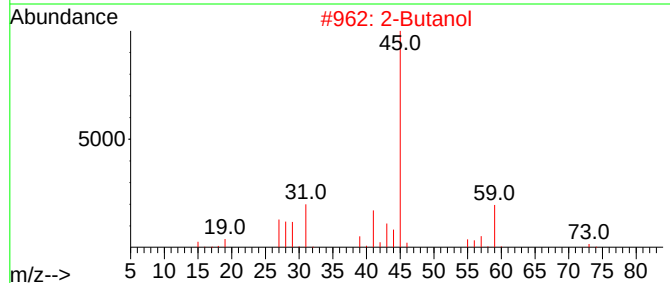
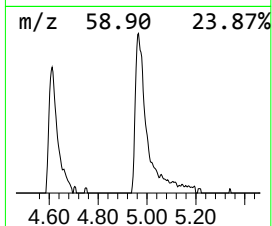
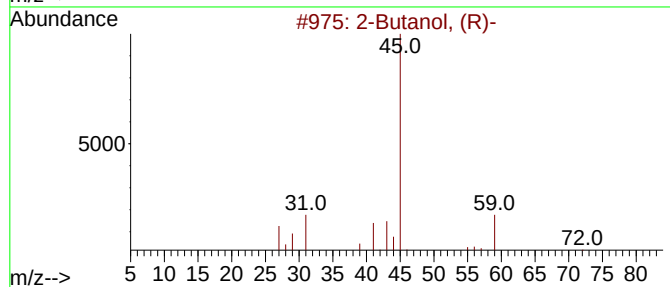
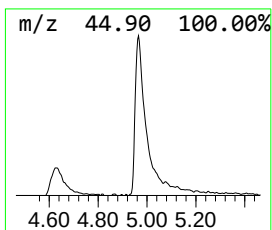
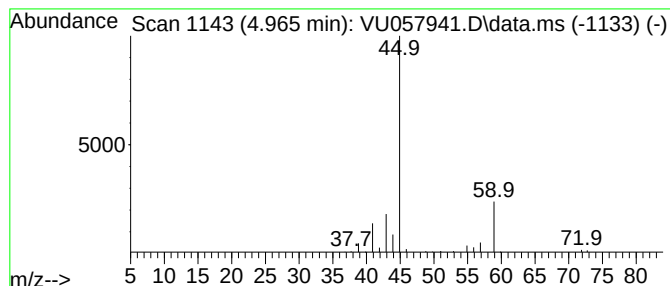
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Butanol, (R)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.965	5.83 ug/L	81706	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-			74	C4H10O	014898-79-4	83
2	2-Butanol			74	C4H10O	000078-92-2	83
3	2-Butanol			74	C4H10O	000078-92-2	83
4	2-Butanol, (R)-			74	C4H10O	014898-79-4	83
5	2-Butanol			74	C4H10O	000078-92-2	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022324\
Data File : VU057941.D
Acq On : 23 Feb 2024 11:08
Operator : MD/SY
Sample : P1567-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JWAC2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.731	68.6	ug/L	961790	1	6.242	700928	50.0
2-Butanol, (R)-	4.965	5.8	ug/L	81706	1	6.242	700928	50.0