

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046187.D
 Acq On : 08 Dec 2021 19:59
 Operator : SY/MD
 Sample : M4971-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046187.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	95	rVB	80226	90935	12.68%	1.483%
2	1.736	119	123	128	rVB2	2550	2119	0.30%	0.035%
3	1.919	171	180	192	rVB	63437	80469	11.22%	1.312%
4	2.031	212	215	223	rVB3	360	415	0.06%	0.007%
5	2.070	223	227	231	rBV3	657	584	0.08%	0.010%
6	2.163	253	256	263	rVB3	961	1078	0.15%	0.018%
7	2.398	323	329	335	rBV2	596	741	0.10%	0.012%
8	2.491	354	358	361	rBV	434	389	0.05%	0.006%
9	2.520	364	367	372	rBV2	477	458	0.06%	0.007%
10	2.572	372	383	401	rBV	143123	239955	33.47%	3.913%
11	2.793	447	452	453	rBV	685	562	0.08%	0.009%
12	2.809	454	457	461	rVV3	788	745	0.10%	0.012%
13	3.189	561	575	590	rBV	11604	25384	3.54%	0.414%
14	3.366	628	630	636	rBV2	439	387	0.05%	0.006%
15	3.443	651	654	658	rVB2	493	390	0.05%	0.006%
16	3.700	728	734	738	rBV2	333	413	0.06%	0.007%
17	3.893	790	794	798	rVB2	373	353	0.05%	0.006%
18	4.051	840	843	850	rVV2	492	526	0.07%	0.009%
19	4.112	858	862	866	rBV	349	366	0.05%	0.006%
20	4.385	944	947	952	rVB	359	341	0.05%	0.006%
21	4.469	968	973	976	rBV2	578	613	0.09%	0.010%
22	4.636	1009	1025	1065	rBV	83953	243543	33.97%	3.972%
23	4.903	1105	1108	1111	rBV	462	363	0.05%	0.006%
24	4.954	1119	1124	1126	rBV2	526	473	0.07%	0.008%
25	5.067	1143	1159	1180	rVV	128941	283370	39.53%	4.621%
26	5.369	1249	1253	1260	rVB2	534	679	0.09%	0.011%
27	5.517	1295	1299	1303	rVB	613	512	0.07%	0.008%
28	5.600	1322	1325	1330	rVB2	512	445	0.06%	0.007%
29	5.729	1342	1365	1383	rBV2	267810	716891	100.00%	11.692%
30	6.163	1496	1500	1502	rVV2	452	354	0.05%	0.006%
31	6.253	1507	1528	1546	rBV	242344	462781	64.55%	7.547%
32	6.417	1573	1579	1582	rBV2	339	431	0.06%	0.007%
33	6.546	1607	1619	1630	rBV3	10277	19099	2.66%	0.311%
34	6.694	1650	1665	1682	rBV	166898	321908	44.90%	5.250%
35	7.227	1823	1831	1834	rVB	510	639	0.09%	0.010%
36	7.295	1847	1852	1855	rVB2	431	398	0.06%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046187.D
 Acq On : 08 Dec 2021 19:59
 Operator : SY/MD
 Sample : M4971-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.324	1858	1861	1867	rVB2	337	335	0.05%	0.005%
38	7.436	1892	1896	1900	rBV	497	529	0.07%	0.009%
39	7.504	1911	1917	1919	rBV2	371	385	0.05%	0.006%
40	7.568	1923	1937	1959	rBV	94147	163773	22.84%	2.671%
41	7.677	1965	1971	1973	rBV	525	450	0.06%	0.007%
42	7.899	2026	2040	2056	rBV	336751	585458	81.67%	9.548%
43	8.115	2103	2107	2114	rVB2	416	518	0.07%	0.008%
44	8.182	2114	2128	2142	rBV	63479	107885	15.05%	1.759%
45	8.475	2210	2219	2231	rVB	2488	4245	0.59%	0.069%
46	8.632	2256	2268	2299	rBV	234184	419054	58.45%	6.834%
47	8.886	2341	2347	2349	rBV	408	419	0.06%	0.007%
48	9.041	2389	2395	2399	rVB2	390	396	0.06%	0.006%
49	9.163	2430	2433	2441	rVB2	632	786	0.11%	0.013%
50	9.263	2460	2464	2468	rBV2	414	359	0.05%	0.006%
51	9.417	2499	2512	2541	rVV	344757	582893	81.31%	9.506%
52	9.693	2593	2598	2612	rVB3	957	1932	0.27%	0.032%
53	10.230	2757	2765	2769	rVB2	441	547	0.08%	0.009%
54	10.259	2769	2774	2777	rBV2	488	580	0.08%	0.009%
55	10.491	2843	2846	2854	rVB2	628	517	0.07%	0.008%
56	10.674	2897	2903	2914	rVB2	1171	1616	0.23%	0.026%
57	10.758	2915	2929	2947	rBV	257553	415739	57.99%	6.780%
58	10.832	2950	2952	2960	rVB	489	473	0.07%	0.008%
59	10.896	2960	2972	2982	rBV2	2808	5072	0.71%	0.083%
60	11.459	3141	3147	3149	rBV2	1364	1292	0.18%	0.021%
61	11.510	3158	3163	3166	rBV	486	466	0.07%	0.008%
62	11.565	3175	3180	3183	rBV2	429	441	0.06%	0.007%
63	11.645	3201	3205	3207	rBV2	405	345	0.05%	0.006%
64	11.697	3212	3221	3226	rBV5	641	1059	0.15%	0.017%
65	11.812	3244	3257	3271	rBV	404070	636982	88.85%	10.388%
66	11.935	3291	3295	3297	rBV2	665	523	0.07%	0.009%
67	12.057	3330	3333	3335	rBV2	815	516	0.07%	0.008%
68	12.192	3362	3375	3389	rVB	367519	597503	83.35%	9.745%
69	12.327	3413	3417	3428	rVB3	1292	1851	0.26%	0.030%
70	12.774	3551	3556	3566	rVB4	1056	1672	0.23%	0.027%
71	13.021	3631	3633	3641	rVB3	528	559	0.08%	0.009%
72	13.060	3641	3645	3648	rBV3	640	452	0.06%	0.007%
73	13.137	3664	3669	3671	rBV	483	497	0.07%	0.008%
74	13.205	3684	3690	3692	rBV	327	355	0.05%	0.006%
75	13.237	3697	3700	3703	rVB2	627	334	0.05%	0.005%
76	13.336	3728	3731	3735	rVB	734	517	0.07%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046187.D
 Acq On : 08 Dec 2021 19:59
 Operator : SY/MD
 Sample : M4971-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	13.430	3756	3760	3767	rBV6	1309	2034	0.28%	0.033%
78	13.558	3796	3800	3803	rBV3	729	622	0.09%	0.010%
79	13.632	3820	3823	3826	rBV2	631	441	0.06%	0.007%
80	13.899	3903	3906	3908	rBV2	503	384	0.05%	0.006%
81	14.089	3957	3965	3977	rVB2	4658	7247	1.01%	0.118%
82	14.269	4019	4021	4025	rVB3	598	338	0.05%	0.006%
83	14.397	4057	4061	4064	rBV4	713	701	0.10%	0.011%
84	14.446	4073	4076	4082	rBV5	1122	1210	0.17%	0.020%
85	14.510	4093	4096	4097	rBV2	549	335	0.05%	0.005%
86	14.709	4155	4158	4160	rBV2	590	334	0.05%	0.005%
87	14.832	4193	4196	4199	rBV4	840	664	0.09%	0.011%
88	15.134	4288	4290	4296	rVB5	882	696	0.10%	0.011%
89	15.221	4309	4317	4329	rBV3	5060	9279	1.29%	0.151%
90	15.330	4348	4351	4353	rBV5	768	413	0.06%	0.007%
91	15.462	4389	4392	4400	rVB5	732	692	0.10%	0.011%
92	15.494	4400	4402	4407	rBV3	696	618	0.09%	0.010%
93	15.677	4454	4459	4461	rBV5	748	671	0.09%	0.011%
94	15.950	4539	4544	4549	rBV4	2424	3422	0.48%	0.056%
95	16.050	4570	4575	4580	rBV6	979	1296	0.18%	0.021%
96	16.262	4635	4641	4648	rBV2	4084	5530	0.77%	0.090%
97	16.410	4681	4687	4692	rBV4	4566	5531	0.77%	0.090%
98	16.880	4828	4833	4841	rBV6	4217	5488	0.77%	0.090%
99	17.095	4894	4900	4915	rVB4	11173	17385	2.43%	0.284%
100	17.407	4993	4997	5008	rVB	20157	27865	3.89%	0.454%

Sum of corrected areas: 6131630

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046187.D
Acq On : 08 Dec 2021 19:59
Operator : SY/MD
Sample : M4971-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D5

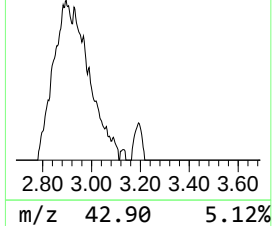
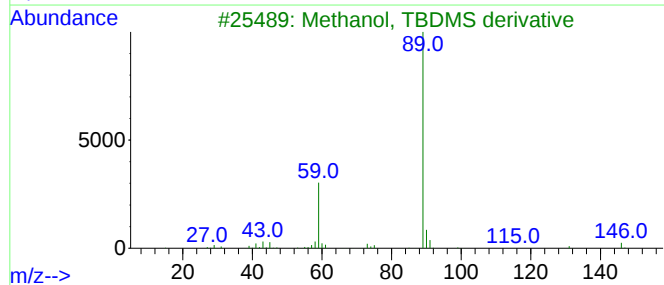
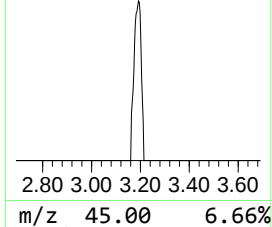
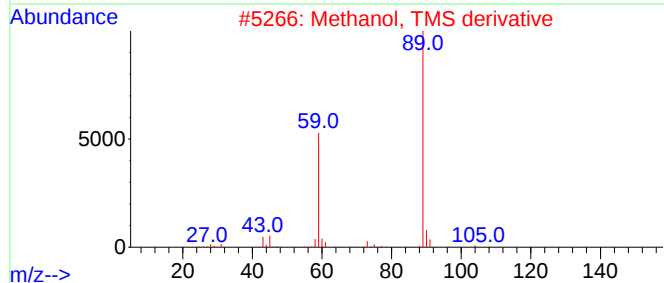
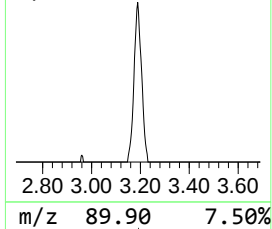
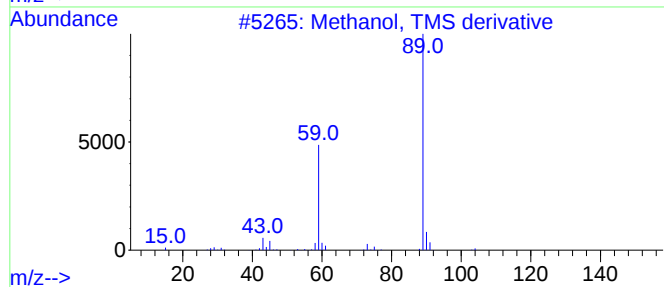
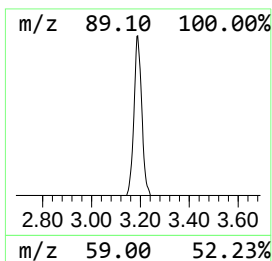
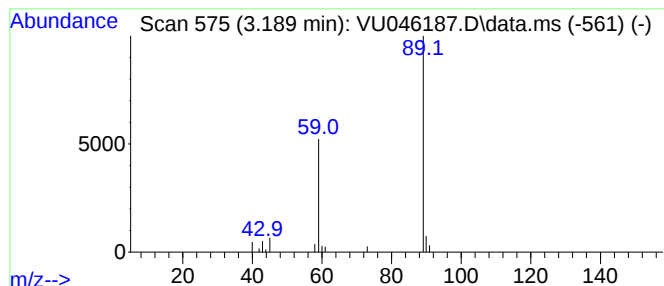
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	2.74 ug/L	25384	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64
5			Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046187.D
Acq On : 08 Dec 2021 19:59
Operator : SY/MD
Sample : M4971-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
Methanol, TMS d...	3.189	2.7	ug/L	25384	1	6.253	462781	50.0