

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071718\
 Data File : VU025473.D
 Acq On : 17 Jul 2018 22:06
 Operator : MD/SY
 Sample : J4024-03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB1P2

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071718WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	0.654	16	20	24	rVB3	481	488	0.04%	0.005%
2	0.735	43	45	48	rBV	359	250	0.02%	0.002%
3	0.767	52	55	56	rBV	347	228	0.02%	0.002%
4	0.812	65	69	75	rBV4	586	621	0.05%	0.006%
5	0.838	75	77	81	rBV2	243	211	0.02%	0.002%
6	0.857	81	83	91	rVB3	356	341	0.03%	0.003%
7	0.963	113	116	119	rBV3	365	220	0.02%	0.002%
8	1.088	146	155	177	rBV	1127175	1226695	100.00%	11.524%
9	1.404	246	253	265	rBV	115273	123483	10.07%	1.160%
10	1.683	333	340	356	rVB	100520	124174	10.12%	1.167%
11	2.275	515	524	536	rVB	224702	333986	27.23%	3.138%
12	2.764	673	676	678	rBV2	285	185	0.02%	0.002%
13	2.908	718	721	723	rBV3	436	221	0.02%	0.002%
14	3.227	818	820	824	rVB2	265	171	0.01%	0.002%
15	3.252	824	828	832	rVB3	584	525	0.04%	0.005%
16	3.275	832	835	837	rBV2	405	226	0.02%	0.002%
17	3.304	841	844	848	rBV3	453	306	0.02%	0.003%
18	3.329	848	852	856	rBV3	627	776	0.06%	0.007%
19	3.484	897	900	905	rBV2	371	335	0.03%	0.003%
20	3.764	982	987	988	rBV	683	524	0.04%	0.005%
21	3.793	994	996	998	rVB	395	172	0.01%	0.002%
22	3.860	1014	1017	1022	rBV3	525	586	0.05%	0.006%
23	3.940	1039	1042	1045	rVB3	531	363	0.03%	0.003%
24	3.963	1045	1049	1050	rBV	597	387	0.03%	0.004%
25	4.024	1063	1068	1071	rBV4	848	640	0.05%	0.006%
26	4.043	1071	1074	1077	rBV2	728	490	0.04%	0.005%
27	4.124	1093	1099	1100	rBV2	715	600	0.05%	0.006%
28	4.178	1101	1116	1154	rVV3	107547	311652	25.41%	2.928%
29	4.574	1237	1239	1241	rBV2	587	282	0.02%	0.003%
30	4.654	1247	1264	1286	rVB2	198705	473013	38.56%	4.444%
31	4.947	1353	1355	1359	rVB2	495	267	0.02%	0.003%
32	4.976	1361	1364	1367	rBV2	385	270	0.02%	0.003%
33	5.156	1418	1420	1426	rVB4	618	509	0.04%	0.005%
34	5.191	1426	1431	1433	rBV3	288	298	0.02%	0.003%

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 Title : VOC Analysis

35	5.346	1453	1479	1506	rBV2	380618	1136123	92.62%	10.673%
36	5.780	1611	1614	1618	rBV3	456	421	0.03%	0.004%
37	5.892	1633	1649	1666	rBV	397059	776873	63.33%	7.298%
38	6.046	1692	1697	1702	rBV6	702	905	0.07%	0.009%
39	6.101	1712	1714	1718	rBV3	444	353	0.03%	0.003%
40	6.146	1725	1728	1729	rBV	363	230	0.02%	0.002%
41	6.230	1751	1754	1756	rBV	378	244	0.02%	0.002%
42	6.281	1767	1770	1772	rBV2	361	201	0.02%	0.002%
43	6.336	1772	1787	1808	rVV	264200	522797	42.62%	4.911%
44	6.452	1821	1823	1824	rBV2	613	267	0.02%	0.003%
45	6.490	1833	1835	1837	rBV2	470	281	0.02%	0.003%
46	6.519	1841	1844	1846	rBV	474	367	0.03%	0.003%
47	6.567	1856	1859	1861	rBV3	452	291	0.02%	0.003%
48	6.616	1865	1874	1884	rBV2	5686	11188	0.91%	0.105%
49	6.712	1901	1904	1906	rVB2	704	479	0.04%	0.004%
50	6.728	1906	1909	1911	rBV2	589	427	0.03%	0.004%
51	6.773	1919	1923	1927	rBV4	1002	809	0.07%	0.008%
52	6.792	1927	1929	1932	rBV3	359	178	0.01%	0.002%
53	6.815	1934	1936	1940	rVB2	465	257	0.02%	0.002%
54	6.847	1940	1946	1949	rBV4	2282	2687	0.22%	0.025%
55	6.940	1972	1975	1978	rBV2	526	345	0.03%	0.003%
56	7.030	1999	2003	2006	rBV4	715	668	0.05%	0.006%
57	7.117	2027	2030	2033	rBV2	494	420	0.03%	0.004%
58	7.230	2052	2065	2084	rBV	150450	267206	21.78%	2.510%
59	7.445	2131	2132	2135	rBV2	539	205	0.02%	0.002%
60	7.567	2157	2170	2192	rBV	517666	914738	74.57%	8.593%
61	7.853	2247	2259	2276	rBV2	107238	181853	14.82%	1.708%
62	8.185	2349	2362	2376	rBV	109475	207554	16.92%	1.950%
63	8.313	2391	2402	2433	rVB	317275	546711	44.57%	5.136%
64	8.824	2558	2561	2564	rVB2	569	425	0.03%	0.004%
65	8.847	2564	2568	2571	rBV3	708	496	0.04%	0.005%
66	8.963	2602	2604	2609	rVB2	740	392	0.03%	0.004%
67	8.998	2610	2615	2616	rBV2	413	295	0.02%	0.003%
68	9.040	2625	2628	2630	rBV3	486	374	0.03%	0.004%
69	9.091	2631	2644	2667	rVV	547444	903549	73.66%	8.488%
70	9.242	2688	2691	2692	rBV	483	299	0.02%	0.003%
71	9.320	2712	2715	2716	rBV	452	185	0.02%	0.002%

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 Title : VOC Analysis

72	9.374	2726	2732	2742	rVB6	3596	6219	0.51%	0.058%
73	9.429	2747	2749	2753	rBV	372	227	0.02%	0.002%
74	9.451	2753	2756	2758	rBV	429	289	0.02%	0.003%
75	9.612	2800	2806	2807	rBV	512	430	0.04%	0.004%
76	9.734	2842	2844	2847	rVB3	430	184	0.01%	0.002%
77	9.857	2880	2882	2884	rBV	619	358	0.03%	0.003%
78	9.886	2889	2891	2894	rVV2	477	289	0.02%	0.003%
79	9.988	2920	2923	2928	rBV2	399	363	0.03%	0.003%
80	10.133	2964	2968	2971	rBV2	538	443	0.04%	0.004%
81	10.352	3033	3036	3040	rVB3	467	312	0.03%	0.003%
82	10.435	3049	3062	3079	rBV	364583	580578	47.33%	5.454%
83	10.538	3091	3094	3095	rBV	424	225	0.02%	0.002%
84	10.612	3105	3117	3135	rVB	114293	195123	15.91%	1.833%
85	10.683	3136	3139	3140	rBV	605	344	0.03%	0.003%
86	10.821	3180	3182	3184	rBV2	543	359	0.03%	0.003%
87	10.876	3195	3199	3202	rBV3	859	778	0.06%	0.007%
88	11.120	3272	3275	3277	rBV	623	443	0.04%	0.004%
89	11.223	3304	3307	3313	rBV2	379	471	0.04%	0.004%
90	11.310	3330	3334	3337	rBV3	796	645	0.05%	0.006%
91	11.416	3362	3367	3370	rBV3	577	597	0.05%	0.006%
92	11.487	3377	3389	3404	rBV	535067	843356	68.75%	7.923%
93	11.750	3469	3471	3474	rBV4	651	458	0.04%	0.004%
94	11.863	3494	3506	3523	rBV	533840	856041	69.78%	8.042%
95	12.181	3603	3605	3607	rBV	375	153	0.01%	0.001%
96	12.483	3688	3699	3713	rVB2	38911	67231	5.48%	0.632%
97	12.573	3722	3727	3734	rVB5	2821	3189	0.26%	0.030%
98	12.998	3856	3859	3862	rBV2	519	402	0.03%	0.004%
99	13.336	3962	3964	3966	rBV2	481	287	0.02%	0.003%
100	13.403	3982	3985	3987	rBV2	571	297	0.02%	0.003%

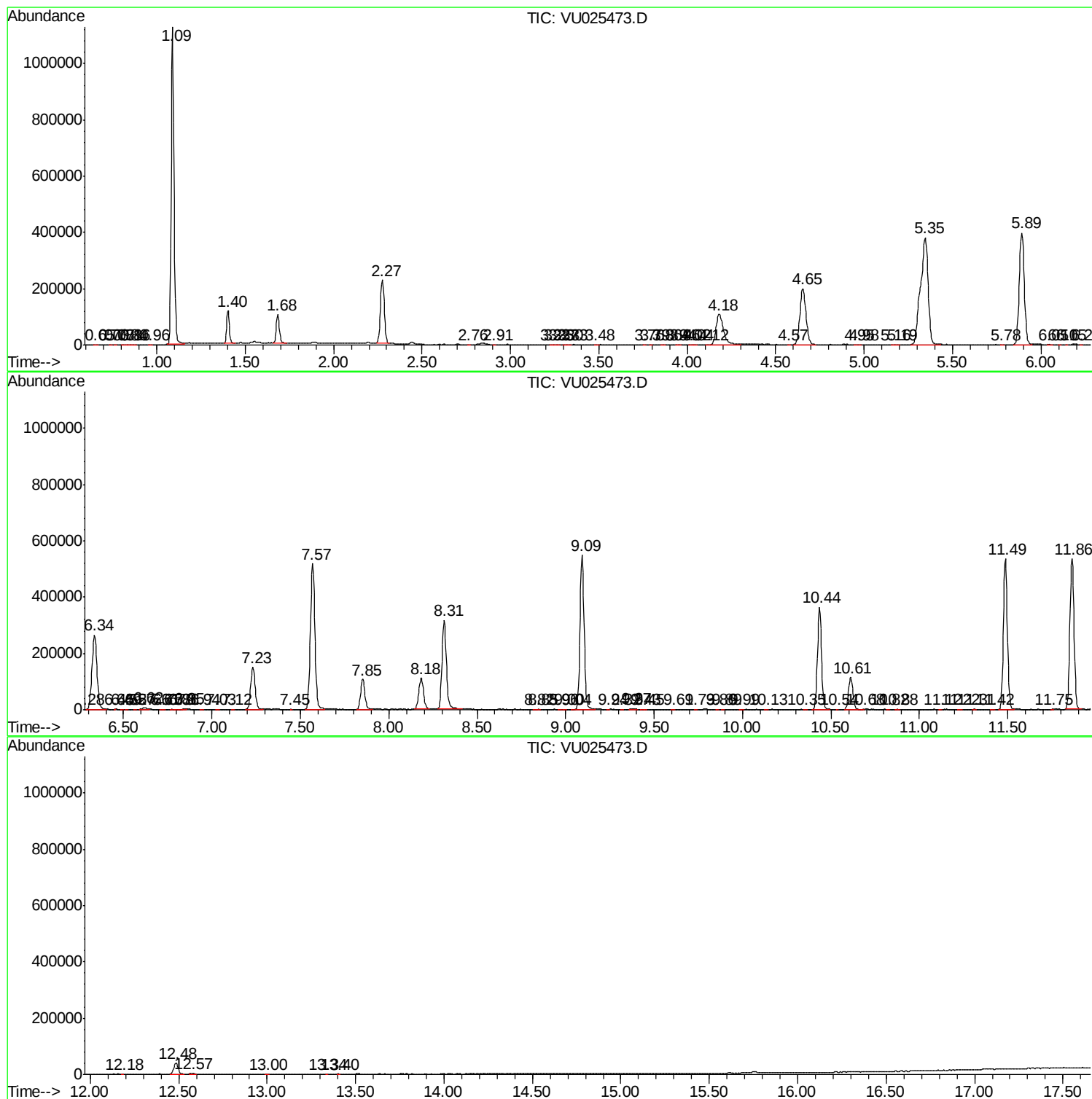
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071718WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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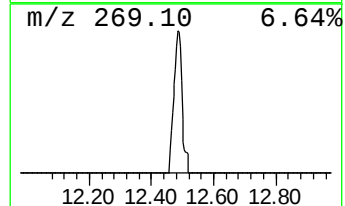
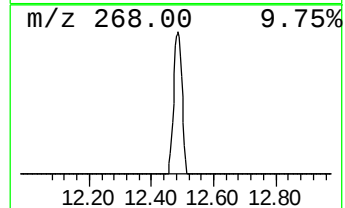
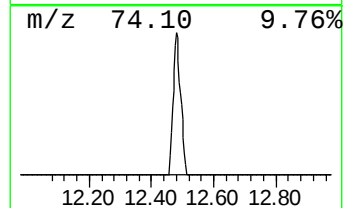
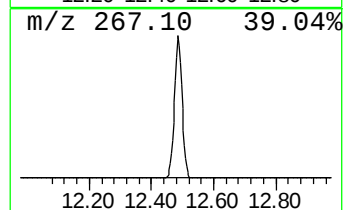
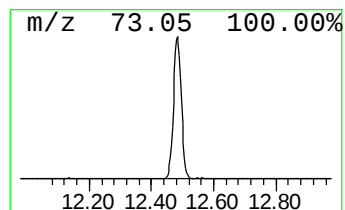
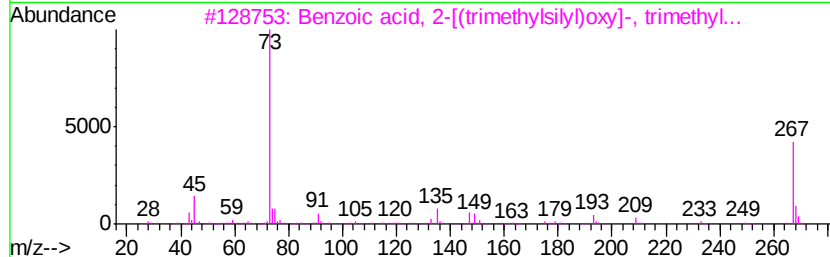
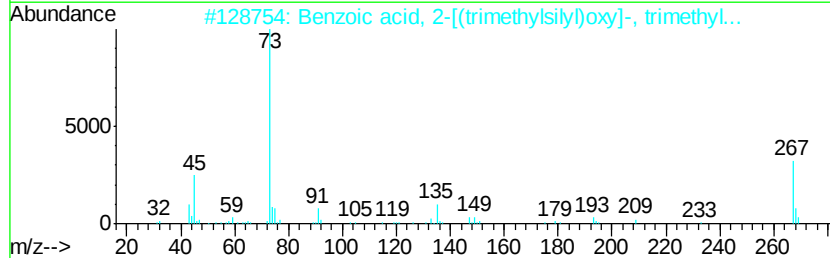
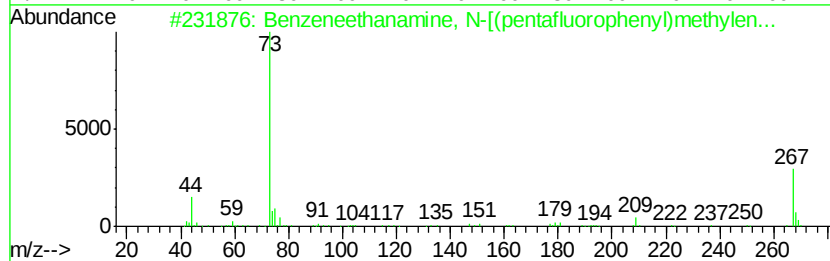
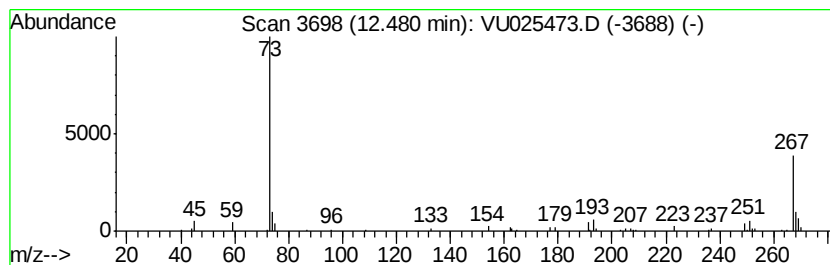
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071718WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzeneethanamine, N-[(pent... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.48	3.99 ug/L	67231	1,4-Dichlorobenzene-d4	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluoro-2-ylideneamino)dimethylsilyl]benzyl	475	C21H26F5N02Si2	055429-85-1	64
2	Benzoic acid, 2-[(trimethylsilyl)dimethylamino]benzyl	282	C13H22O3Si2	003789-85-3	59
3	Benzoic acid, 2-[(trimethylsilyl)dimethylamino]benzyl	282	C13H22O3Si2	003789-85-3	50
4	Benzoic acid, 2-[(trimethylsilyl)dimethylamino]benzyl	282	C13H22O3Si2	003789-85-3	45
5	11H-Dibenzo[b,e][1,4]diazepin-11-yl	267	C16H17N3O	013450-73-2	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzeneethanamine...	12.48	4.0	ug/L	67231	3	11.49	843356	50.0