

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046173.D
 Acq On : 08 Dec 2021 14:20
 Operator : SY/MD
 Sample : M4887-05ME
 Misc : 5.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A2ME

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: VU046173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	98	rVB	90525	118138	4.30%	1.052%
2	1.919	171	180	198	rVV	55026	93198	3.39%	0.830%
3	1.993	198	203	212	rVB4	2348	3574	0.13%	0.032%
4	2.144	247	250	254	rBV5	871	675	0.02%	0.006%
5	2.549	364	376	389	rBV	129265	209761	7.63%	1.869%
6	3.182	559	573	590	rVV2	11835	31544	1.15%	0.281%
7	3.909	795	799	805	rVB2	608	671	0.02%	0.006%
8	4.401	944	952	956	rBV2	691	1181	0.04%	0.011%
9	4.520	985	989	991	rBV2	1057	989	0.04%	0.009%
10	4.662	1014	1033	1076	rBV2	43779	206715	7.52%	1.841%
11	5.067	1142	1159	1184	rVB	133892	339313	12.35%	3.023%
12	5.382	1246	1257	1270	rVB5	3457	7860	0.29%	0.070%
13	5.584	1316	1320	1326	rVB4	877	997	0.04%	0.009%
14	5.639	1331	1337	1342	rBV2	537	679	0.02%	0.006%
15	5.723	1342	1363	1390	rBV2	346244	885596	32.22%	7.889%
16	5.845	1397	1401	1409	rVB3	1217	1886	0.07%	0.017%
17	5.916	1415	1423	1432	rBV3	1343	2163	0.08%	0.019%
18	5.983	1432	1444	1465	rBV4	6942	18051	0.66%	0.161%
19	6.131	1477	1490	1498	rBV6	1590	2919	0.11%	0.026%
20	6.250	1511	1527	1558	rBV	283897	576415	20.97%	5.135%
21	6.539	1602	1617	1633	rBV	346194	653772	23.79%	5.824%
22	6.690	1650	1664	1678	rBV	189924	388522	14.14%	3.461%
23	6.809	1698	1701	1709	rVB3	1049	1295	0.05%	0.012%
24	7.067	1775	1781	1783	rBV3	844	871	0.03%	0.008%
25	7.224	1826	1830	1831	rBV3	1370	1036	0.04%	0.009%
26	7.494	1905	1914	1923	rBV6	1957	2986	0.11%	0.027%
27	7.568	1923	1937	1965	rVV	105418	208772	7.60%	1.860%
28	7.716	1980	1983	1989	rVB2	672	730	0.03%	0.007%
29	7.790	1997	2006	2014	rBV5	3479	6469	0.24%	0.058%
30	7.899	2020	2040	2056	rBV	393035	747392	27.19%	6.658%
31	8.092	2097	2100	2106	rVV4	665	756	0.03%	0.007%
32	8.128	2106	2111	2117	rVV4	2252	2524	0.09%	0.022%
33	8.182	2117	2128	2156	rVB	62361	143254	5.21%	1.276%
34	8.475	2207	2219	2227	rVV4	1825	3434	0.12%	0.031%
35	8.552	2230	2243	2262	rVV	1569804	2748271	100.00%	24.481%
36	8.684	2263	2284	2315	rVB	145097	454610	16.54%	4.050%

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Integrator: RTE

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	8.861	2329	2339	2340	rBV	2699	2742	0.10%	0.024%
38	8.928	2350	2360	2363	rBV5	2157	3315	0.12%	0.030%
39	8.960	2367	2370	2379	rVB4	1377	1690	0.06%	0.015%
40	9.121	2415	2420	2428	rVB5	1501	1937	0.07%	0.017%
41	9.427	2494	2515	2537	rBV	314522	729554	26.55%	6.499%
42	9.581	2553	2563	2572	rVB2	1783	3327	0.12%	0.030%
43	9.697	2587	2599	2609	rBV3	9969	19961	0.73%	0.178%
44	9.922	2663	2669	2674	rBV2	477	681	0.02%	0.006%
45	10.111	2715	2728	2741	rVB	8705	16022	0.58%	0.143%
46	10.250	2760	2771	2775	rBV5	1915	3456	0.13%	0.031%
47	10.356	2799	2804	2810	rVV5	1453	2204	0.08%	0.020%
48	10.394	2811	2816	2824	rVB4	2320	3488	0.13%	0.031%
49	10.491	2837	2846	2856	rVB4	1730	2717	0.10%	0.024%
50	10.613	2878	2884	2888	rBV2	884	1091	0.04%	0.010%
51	10.652	2888	2896	2897	rBV2	2065	1731	0.06%	0.015%
52	10.774	2920	2934	2955	rVB	272605	456219	16.60%	4.064%
53	10.899	2961	2973	2986	rVV7	3375	7864	0.29%	0.070%
54	11.005	2999	3006	3018	rVV7	2853	5010	0.18%	0.045%
55	11.115	3027	3040	3049	rVB6	6519	12519	0.46%	0.112%
56	11.208	3062	3069	3073	rBV3	593	739	0.03%	0.007%
57	11.295	3087	3096	3097	rBV4	2355	2238	0.08%	0.020%
58	11.417	3125	3134	3140	rBV4	3443	5228	0.19%	0.047%
59	11.468	3141	3150	3162	rVB2	9621	17540	0.64%	0.156%
60	11.578	3179	3184	3190	rBV6	1103	1547	0.06%	0.014%
61	11.645	3199	3205	3207	rBV5	941	909	0.03%	0.008%
62	11.687	3215	3218	3219	rBV2	1378	734	0.03%	0.007%
63	11.819	3246	3259	3273	rBV	480563	766464	27.89%	6.828%
64	11.902	3279	3285	3293	rBV4	3190	4532	0.16%	0.040%
65	11.976	3302	3308	3315	rBV6	1671	1887	0.07%	0.017%
66	12.073	3329	3338	3342	rBV5	2056	3059	0.11%	0.027%
67	12.198	3364	3377	3394	rVB	428204	706466	25.71%	6.293%
68	12.266	3394	3398	3402	rBV4	808	844	0.03%	0.008%
69	12.327	3408	3417	3428	rBV3	10790	16899	0.61%	0.151%
70	12.381	3430	3434	3436	rBV3	958	783	0.03%	0.007%
71	12.475	3454	3463	3467	rBV7	1527	2434	0.09%	0.022%
72	12.645	3511	3516	3519	rBV5	639	794	0.03%	0.007%
73	12.703	3530	3534	3539	rBV4	959	958	0.03%	0.009%
74	12.771	3549	3555	3561	rVB4	1388	1560	0.06%	0.014%
75	12.915	3597	3600	3602	rBV3	853	692	0.03%	0.006%
76	13.034	3631	3637	3638	rBV3	2345	1947	0.07%	0.017%

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 ClientSampleId :
 EX8A2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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

77	13.144	3663	3671	3676	rVB5	1764	2776	0.10%	0.025%
78	13.298	3716	3719	3725	rVB5	1143	997	0.04%	0.009%
79	13.353	3732	3736	3742	rBV7	1315	1686	0.06%	0.015%
80	13.433	3753	3761	3767	rBV3	10724	16415	0.60%	0.146%
81	13.587	3797	3809	3817	rBV3	6333	10939	0.40%	0.097%
82	13.838	3879	3887	3893	rBV4	2490	3451	0.13%	0.031%
83	13.967	3921	3927	3928	rBV6	1346	1336	0.05%	0.012%
84	14.089	3955	3965	3980	rVB	41648	66354	2.41%	0.591%
85	14.192	3986	3997	4009	rVB3	9116	15458	0.56%	0.138%
86	14.417	4062	4067	4069	rBV6	2289	2373	0.09%	0.021%
87	14.449	4071	4077	4086	rVB2	13296	18919	0.69%	0.169%
88	14.574	4108	4116	4120	rBV5	2443	3757	0.14%	0.033%
89	15.140	4287	4292	4296	rBV4	2405	2701	0.10%	0.024%
90	15.224	4306	4318	4329	rBV	42479	74717	2.72%	0.666%
91	15.378	4360	4366	4367	rBV3	6656	6810	0.25%	0.061%
92	15.407	4368	4375	4387	rVB2	42236	68698	2.50%	0.612%
93	16.147	4599	4605	4612	rBV5	7747	11458	0.42%	0.102%
94	16.259	4633	4640	4649	rBV	25336	42647	1.55%	0.380%
95	16.407	4678	4686	4693	rBV	54190	85406	3.11%	0.761%
96	16.510	4715	4718	4719	rBV3	1849	1017	0.04%	0.009%
97	16.610	4743	4749	4752	rBV4	12235	15766	0.57%	0.140%
98	16.876	4828	4832	4841	rVB3	8421	10549	0.38%	0.094%
99	17.375	4981	4987	4996	rBV2	23838	32587	1.19%	0.290%
100	17.539	5031	5038	5050	rVB2	31603	48440	1.76%	0.431%

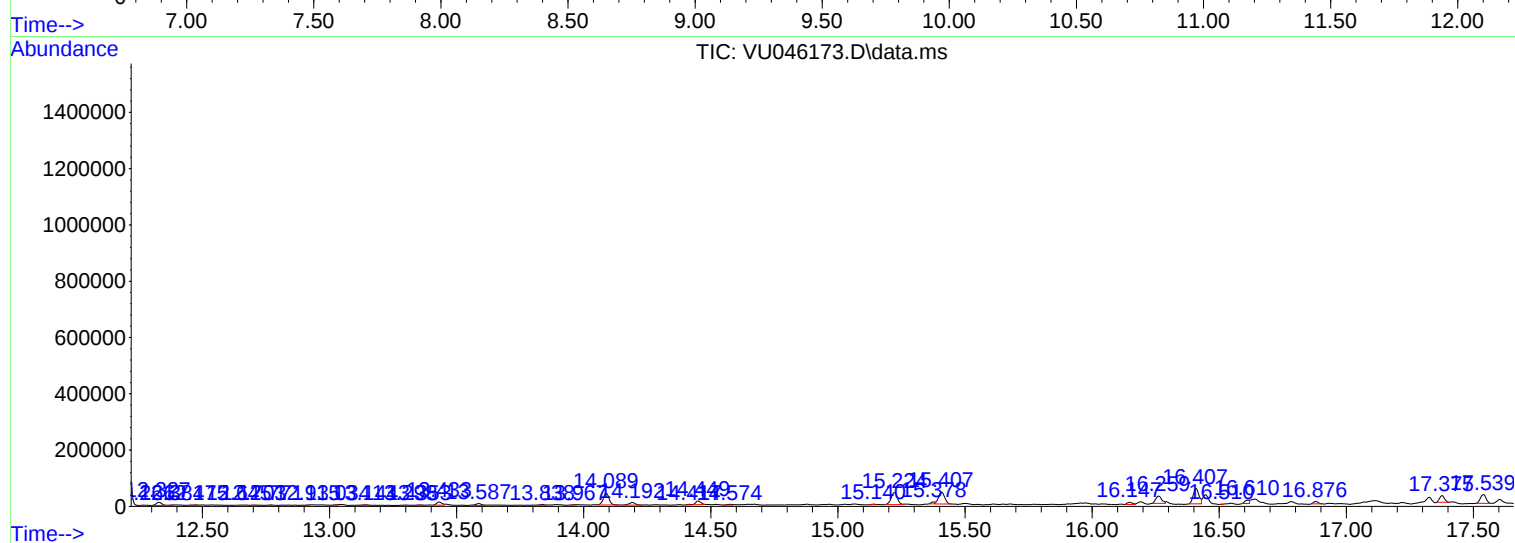
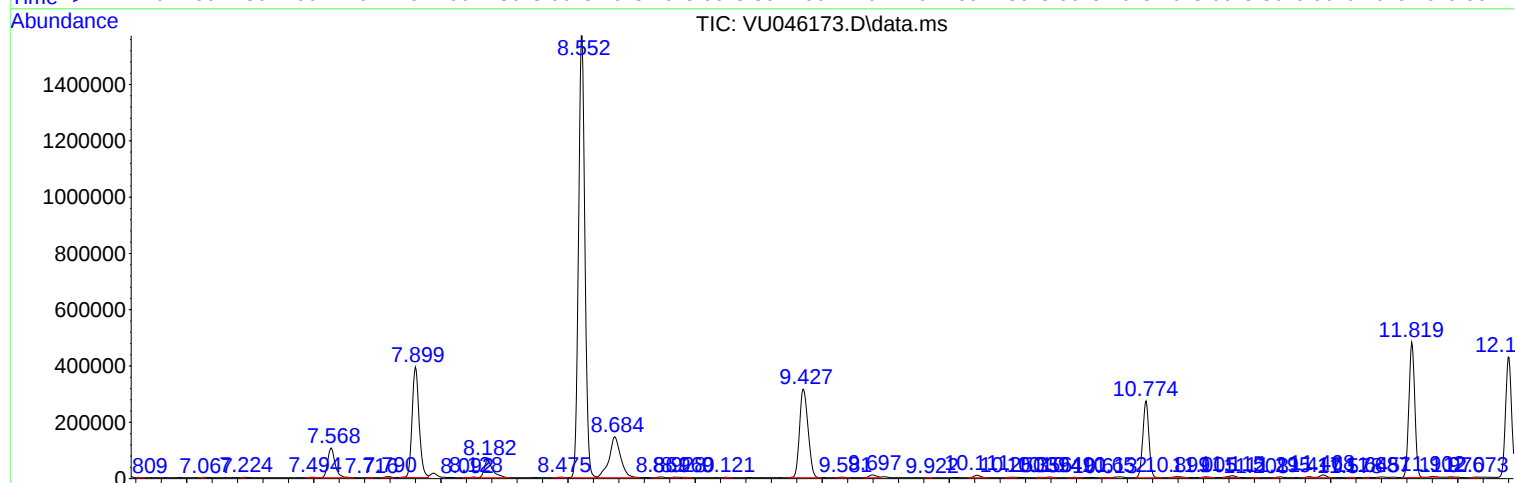
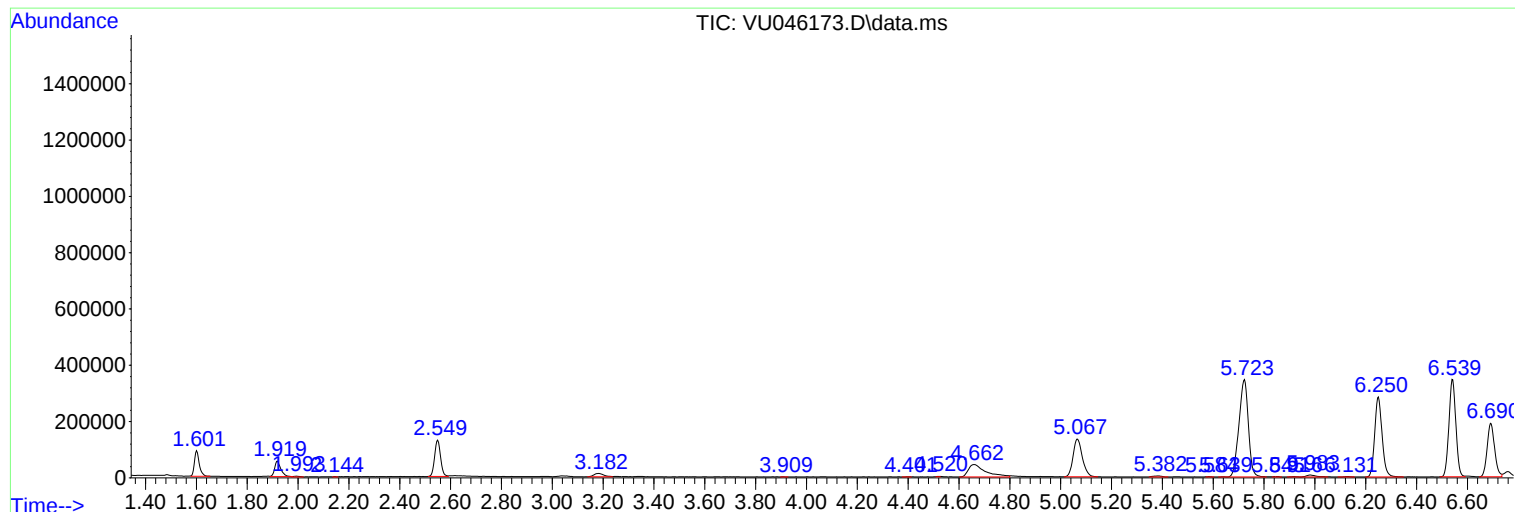
Sum of corrected areas: 11226058

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A2ME

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



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Instrument :
MSVOA_U
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EX8A2ME

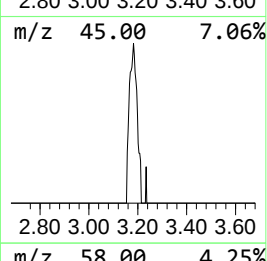
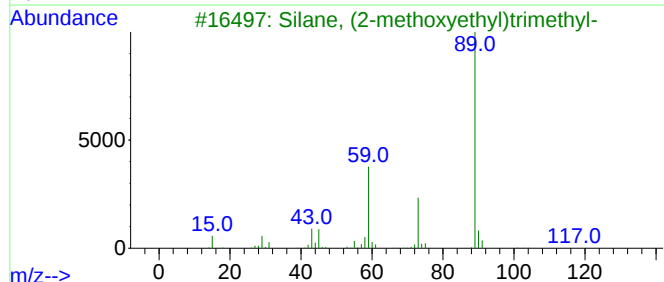
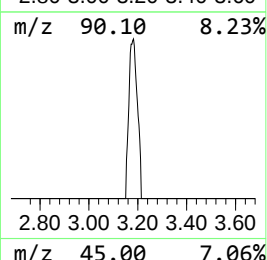
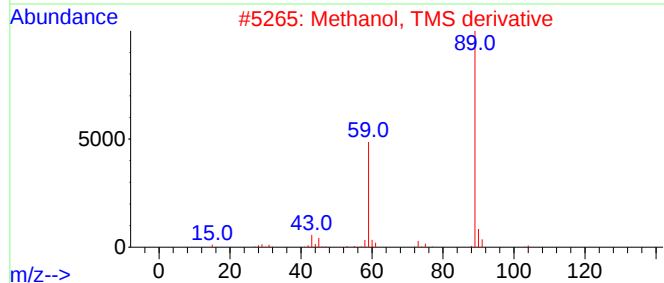
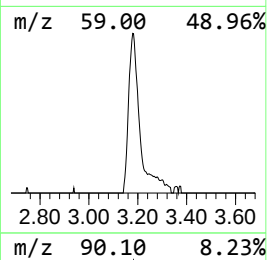
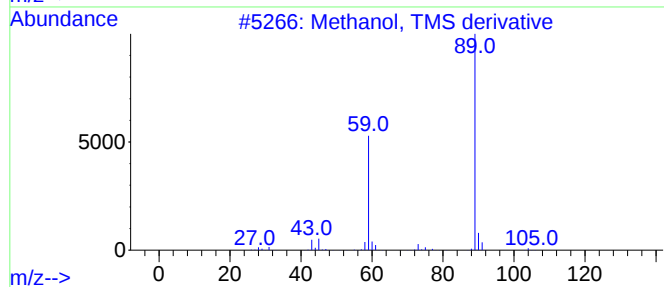
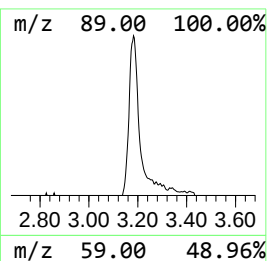
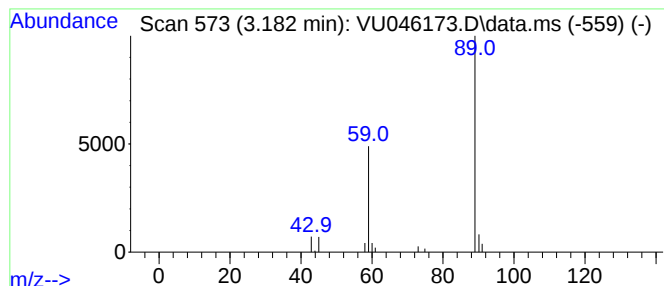
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.182	2.74 ug/L	31544	1,4-Difluorobenzene	6.250

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			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	83
4			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	83
5			2-Cyclopentene, 1,4-bis(methoxye...	276	C13H24O6	1000156-00-3	9



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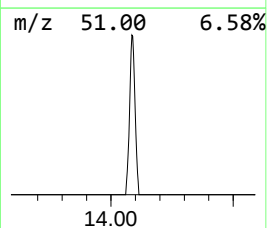
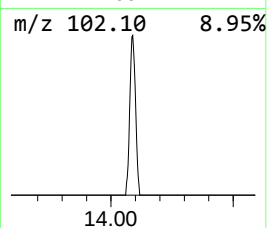
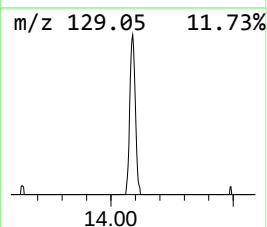
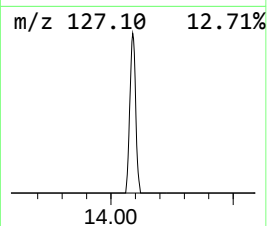
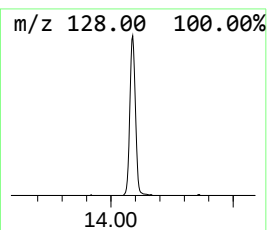
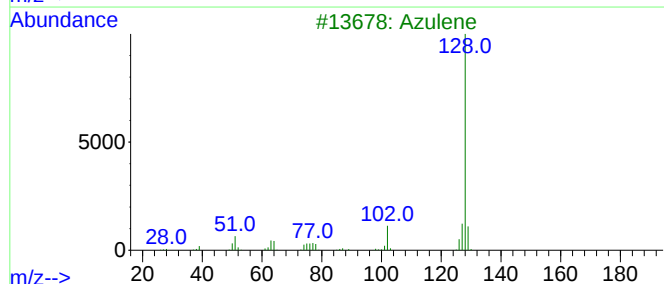
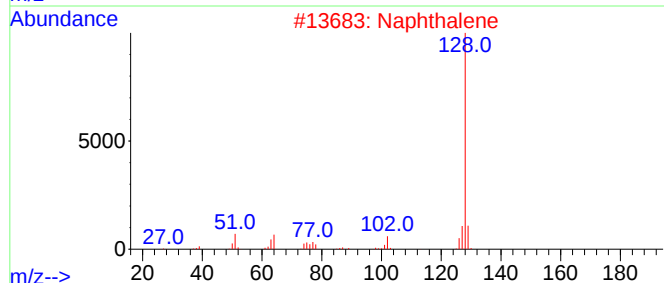
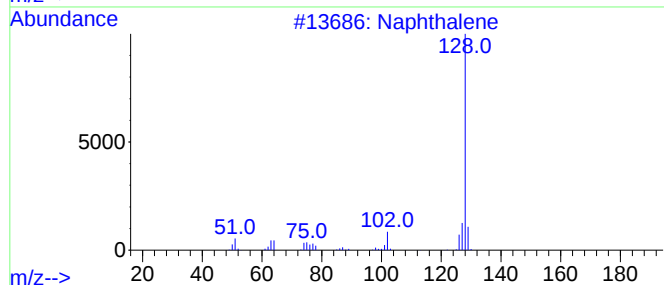
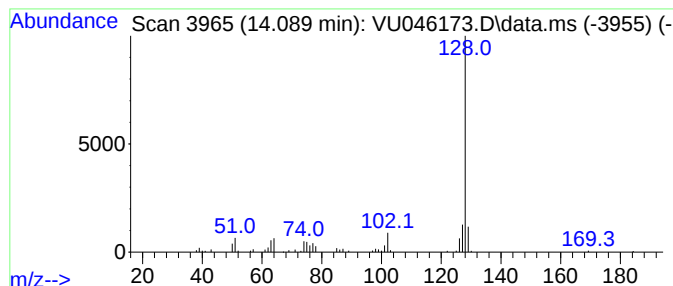
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	4.33 ug/L	66354	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Azulene	128	C10H8	000275-51-4	93
4			Naphthalene	128	C10H8	000091-20-3	91
5			Azulene	128	C10H8	000275-51-4	91



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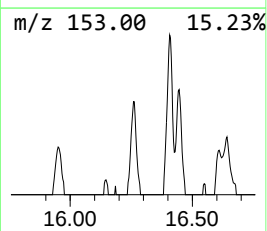
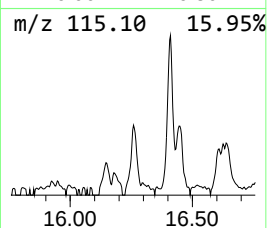
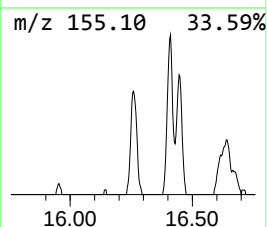
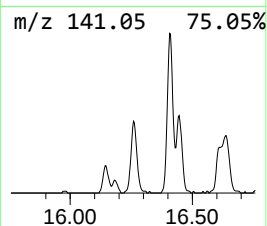
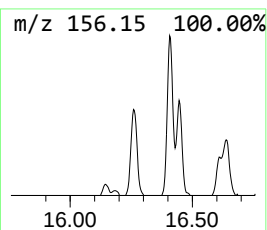
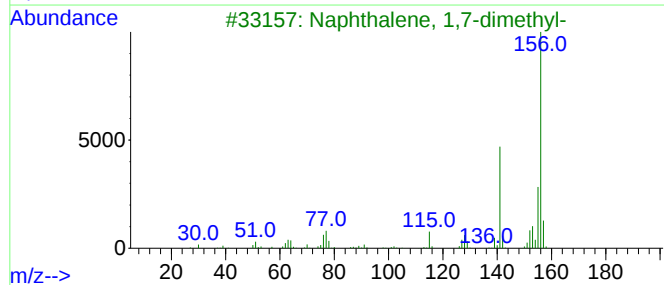
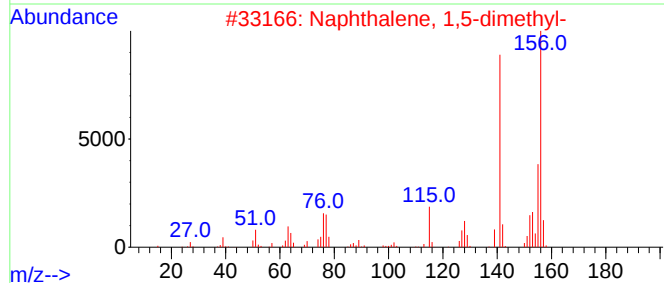
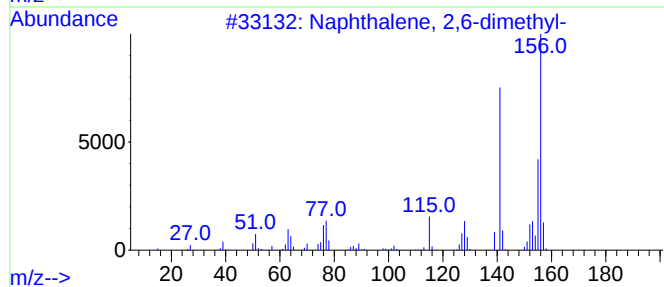
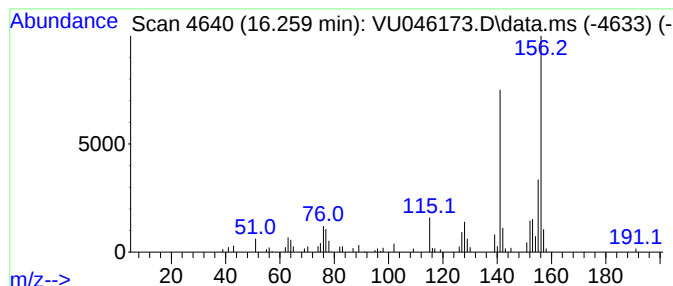
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Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.259	2.78 ug/L	42647	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046173.D
Acq On : 08 Dec 2021 14:20
Operator : SY/MD
Sample : M4887-05ME
Misc : 5.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A2ME

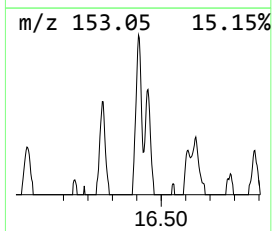
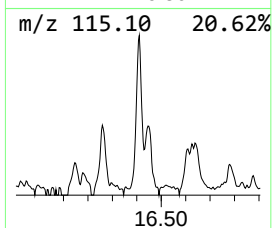
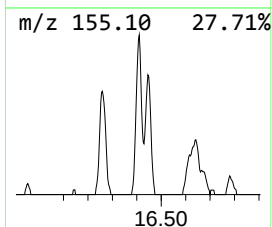
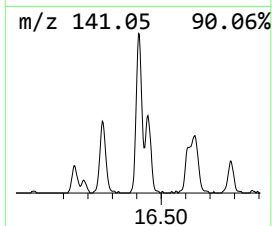
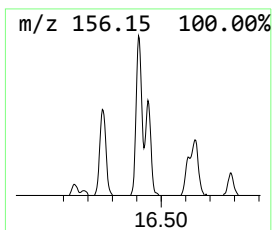
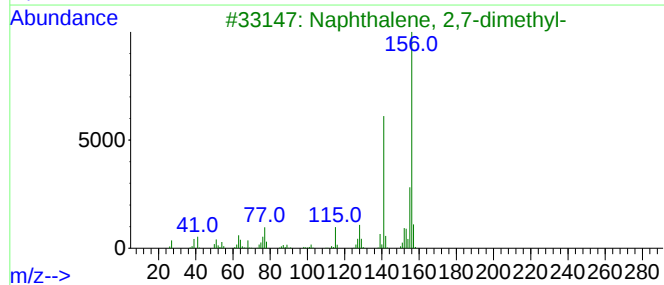
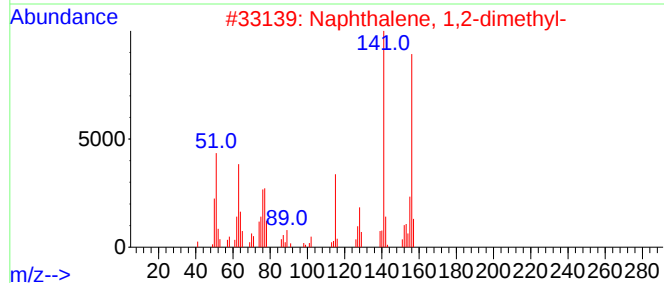
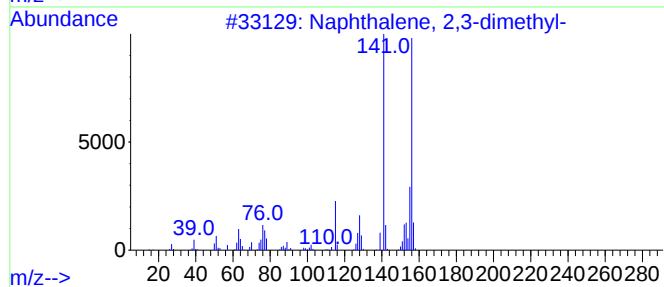
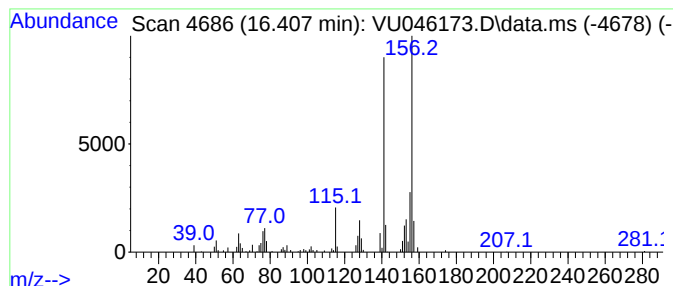
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	5.57 ug/L	85406	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046173.D
Acq On : 08 Dec 2021 14:20
Operator : SY/MD
Sample : M4887-05ME
Misc : 5.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A2ME

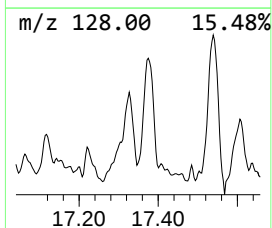
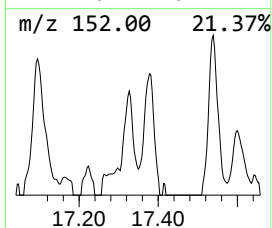
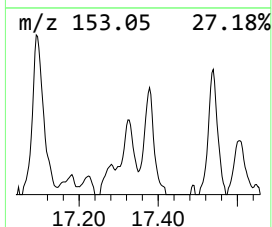
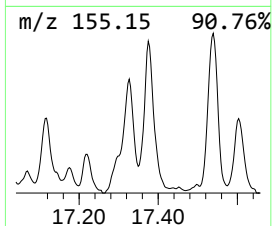
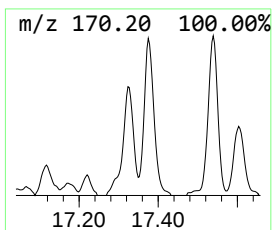
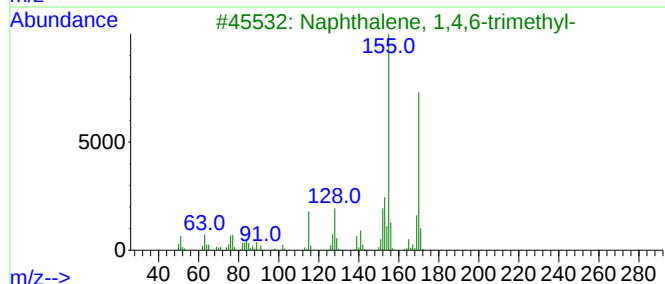
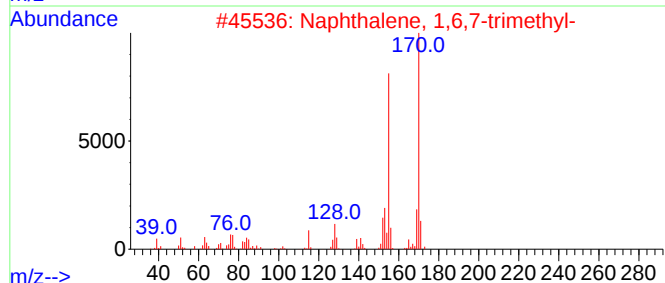
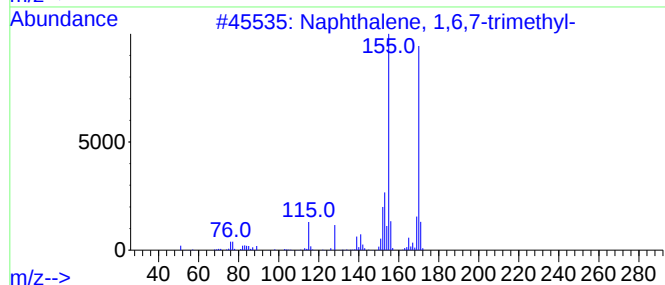
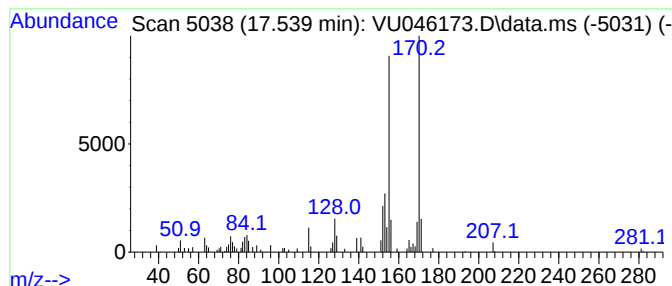
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Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1,6,7-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.539	3.16 ug/L	48440	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	98
2			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	94
3			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	94
4			4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94
5			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046173.D
Acq On : 08 Dec 2021 14:20
Operator : SY/MD
Sample : M4887-05ME
Misc : 5.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A2ME

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...	3.182	2.7	ug/L	31544	1	6.250	576415	50.0
Azulene	14.089	4.3	ug/L	66354	3	11.819	766464	50.0
Naphthalene, 2,...	16.259	2.8	ug/L	42647	3	11.819	766464	50.0
Naphthalene, 2,...	16.407	5.6	ug/L	85406	3	11.819	766464	50.0
Naphthalene, 1,...	17.539	3.2	ug/L	48440	3	11.819	766464	50.0