

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046169.D
 Acq On : 08 Dec 2021 12:35
 Operator : SY/MD
 Sample : M4883-19ME
 Misc : 3.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW9H5ME

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: VU046169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	74	81	99	rVB	48258	63201	8.28%	1.186%
2	1.919	172	180	197	rVB	28250	46987	6.16%	0.882%
3	1.996	199	204	212	rVB3	1579	2122	0.28%	0.040%
4	2.549	366	376	390	rBV	65980	104943	13.76%	1.970%
5	3.179	558	572	598	rBV2	13809	38253	5.01%	0.718%
6	3.391	636	638	642	rVB2	382	197	0.03%	0.004%
7	3.440	650	653	659	rVB2	344	312	0.04%	0.006%
8	3.941	806	809	815	rBB	302	254	0.03%	0.005%
9	4.269	905	911	916	rBV	172	290	0.04%	0.005%
10	4.523	986	990	995	rBV3	286	232	0.03%	0.004%
11	4.661	1015	1033	1078	rBV	32097	150024	19.66%	2.816%
12	5.066	1142	1159	1186	rVB3	79599	218532	28.64%	4.102%
13	5.359	1245	1250	1252	rBV3	474	374	0.05%	0.007%
14	5.378	1252	1256	1265	rVB3	937	1315	0.17%	0.025%
15	5.607	1323	1327	1333	rBV	150	240	0.03%	0.005%
16	5.722	1342	1363	1395	rVV2	202644	530645	69.55%	9.960%
17	5.983	1432	1444	1462	rBV5	5374	13540	1.77%	0.254%
18	6.121	1483	1487	1491	rVV2	354	317	0.04%	0.006%
19	6.250	1511	1527	1560	rBV	261204	540413	70.83%	10.144%
20	6.542	1606	1618	1627	rBV8	4980	10747	1.41%	0.202%
21	6.607	1627	1638	1648	rBV5	1480	3186	0.42%	0.060%
22	6.690	1651	1664	1680	rBV	117073	242629	31.80%	4.554%
23	6.861	1714	1717	1723	rVB2	371	369	0.05%	0.007%
24	6.902	1726	1730	1733	rBV	185	213	0.03%	0.004%
25	7.060	1770	1779	1783	rBV2	332	556	0.07%	0.010%
26	7.089	1785	1788	1791	rVV	248	189	0.02%	0.004%
27	7.195	1818	1821	1825	rBV3	262	277	0.04%	0.005%
28	7.227	1825	1831	1835	rVV2	537	557	0.07%	0.010%
29	7.246	1835	1837	1845	rVB	308	319	0.04%	0.006%
30	7.295	1845	1852	1856	rBV2	435	568	0.07%	0.011%
31	7.311	1856	1857	1863	rVB2	260	196	0.03%	0.004%
32	7.568	1925	1937	1963	rBV2	62075	125360	16.43%	2.353%
33	7.697	1971	1977	1978	rBV	364	266	0.03%	0.005%
34	7.790	1997	2006	2022	rVB	2291	4168	0.55%	0.078%
35	7.851	2022	2025	2026	rBV	448	291	0.04%	0.005%
36	7.899	2026	2040	2056	rBV	222652	418426	54.84%	7.854%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	8.182	2115	2128	2157	rBV2	37063	83780	10.98%	1.573%
38	8.459	2209	2214	2215	rBV	559	316	0.04%	0.006%
39	8.471	2215	2218	2222	rVB	604	501	0.07%	0.009%
40	8.555	2235	2244	2252	rVB3	5035	7725	1.01%	0.145%
41	8.687	2260	2285	2312	rBV	92364	312080	40.91%	5.858%
42	8.867	2336	2341	2343	rBV3	381	363	0.05%	0.007%
43	8.957	2360	2369	2378	rVB2	872	1709	0.22%	0.032%
44	9.423	2499	2514	2541	rBV	293559	762926	100.00%	14.320%
45	9.574	2549	2561	2571	rBV3	1059	1813	0.24%	0.034%
46	9.697	2589	2599	2616	rVB3	3212	6307	0.83%	0.118%
47	9.918	2665	2668	2673	rVB2	194	195	0.03%	0.004%
48	10.118	2719	2730	2743	rVB7	2600	6086	0.80%	0.114%
49	10.320	2790	2793	2799	rVB2	202	183	0.02%	0.003%
50	10.484	2840	2844	2845	rBV2	364	224	0.03%	0.004%
51	10.536	2856	2860	2866	rBV	212	244	0.03%	0.005%
52	10.571	2866	2871	2877	rVB4	490	484	0.06%	0.009%
53	10.671	2894	2902	2908	rBV3	1170	1405	0.18%	0.026%
54	10.774	2917	2934	2951	rVB	193064	318320	41.72%	5.975%
55	10.896	2965	2972	2986	rVB3	923	1718	0.23%	0.032%
56	11.002	2998	3005	3008	rBV3	408	459	0.06%	0.009%
57	11.095	3026	3034	3035	rBV2	579	561	0.07%	0.011%
58	11.121	3040	3042	3045	rVB2	457	233	0.03%	0.004%
59	11.298	3093	3097	3103	rVB2	327	389	0.05%	0.007%
60	11.471	3136	3151	3160	rBV5	2106	3658	0.48%	0.069%
61	11.545	3167	3174	3180	rVB4	1410	1682	0.22%	0.032%
62	11.696	3216	3221	3226	rBV2	529	539	0.07%	0.010%
63	11.751	3234	3238	3241	rBV	207	187	0.02%	0.004%
64	11.819	3246	3259	3278	rBV	433671	708923	92.92%	13.306%
65	11.899	3278	3284	3290	rVV4	630	784	0.10%	0.015%
66	11.941	3293	3297	3300	rVV2	451	421	0.06%	0.008%
67	11.973	3303	3307	3317	rVB3	961	1104	0.14%	0.021%
68	12.073	3332	3338	3342	rBV2	967	923	0.12%	0.017%
69	12.201	3362	3378	3394	rVB	269300	436496	57.21%	8.193%
70	12.320	3407	3415	3417	rBV2	1533	1573	0.21%	0.030%
71	12.584	3493	3497	3500	rBV2	227	197	0.03%	0.004%
72	12.754	3546	3550	3552	rBV	408	246	0.03%	0.005%
73	12.770	3552	3555	3563	rVB2	785	1029	0.13%	0.019%
74	12.918	3596	3601	3606	rVB	232	275	0.04%	0.005%
75	13.426	3757	3759	3763	rBV2	406	262	0.03%	0.005%
76	13.449	3763	3766	3771	rVB	292	237	0.03%	0.004%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

77	13.629	3819	3822	3825	rBV	309	195	0.03%	0.004%
78	13.844	3884	3889	3895	rVB3	667	632	0.08%	0.012%
79	14.089	3953	3965	3980	rBV	28280	43664	5.72%	0.820%
80	14.146	3980	3983	3985	rBV2	296	195	0.03%	0.004%
81	14.192	3993	3997	4000	rBV3	385	385	0.05%	0.007%
82	14.336	4037	4042	4046	rBV3	453	458	0.06%	0.009%
83	14.449	4073	4077	4081	rBV4	528	511	0.07%	0.010%
84	14.581	4107	4118	4126	rBV2	1787	3181	0.42%	0.060%
85	14.767	4173	4176	4179	rVV2	319	188	0.02%	0.004%
86	14.812	4186	4190	4196	rVB2	358	390	0.05%	0.007%
87	14.838	4196	4198	4203	rVB	198	190	0.02%	0.004%
88	14.864	4203	4206	4209	rBV2	224	191	0.03%	0.004%
89	14.976	4235	4241	4242	rBV2	324	348	0.05%	0.007%
90	14.986	4242	4244	4247	rVB2	347	205	0.03%	0.004%
91	15.224	4308	4318	4330	rBV	13855	20685	2.71%	0.388%
92	15.407	4366	4375	4389	rVB2	8074	13311	1.74%	0.250%
93	15.953	4538	4545	4548	rBV4	1943	2132	0.28%	0.040%
94	16.259	4632	4640	4649	rBV2	6951	10822	1.42%	0.203%
95	16.410	4678	4687	4693	rBV	11851	18457	2.42%	0.346%
96	16.445	4694	4698	4707	rVB4	6515	8652	1.13%	0.162%
97	16.539	4725	4727	4731	rVB3	655	319	0.04%	0.006%
98	16.883	4828	4834	4842	rBV3	4329	5924	0.78%	0.111%
99	17.098	4896	4901	4908	rVB5	2777	3390	0.44%	0.064%
100	17.539	5032	5038	5045	rBV3	4896	6181	0.81%	0.116%

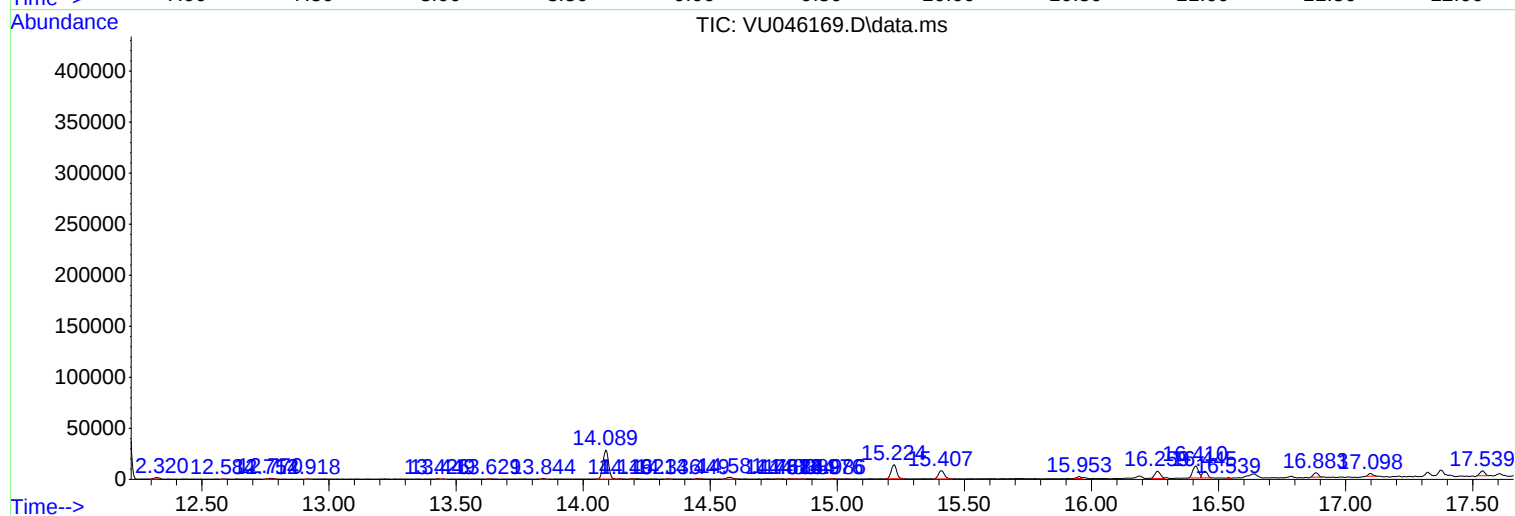
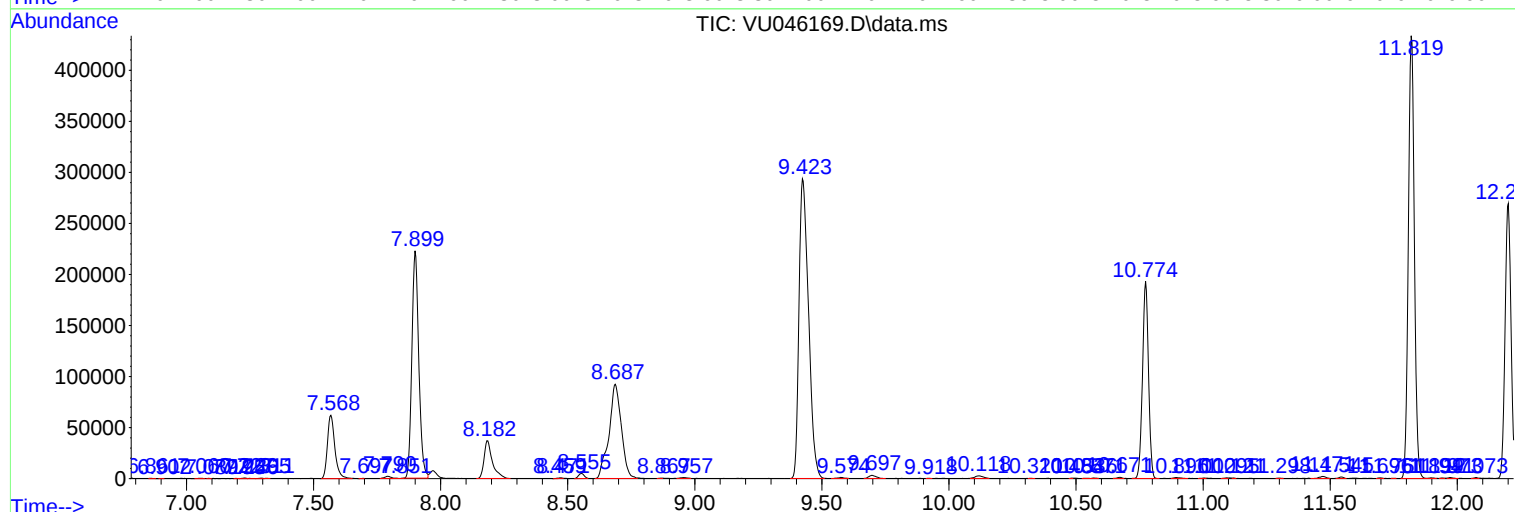
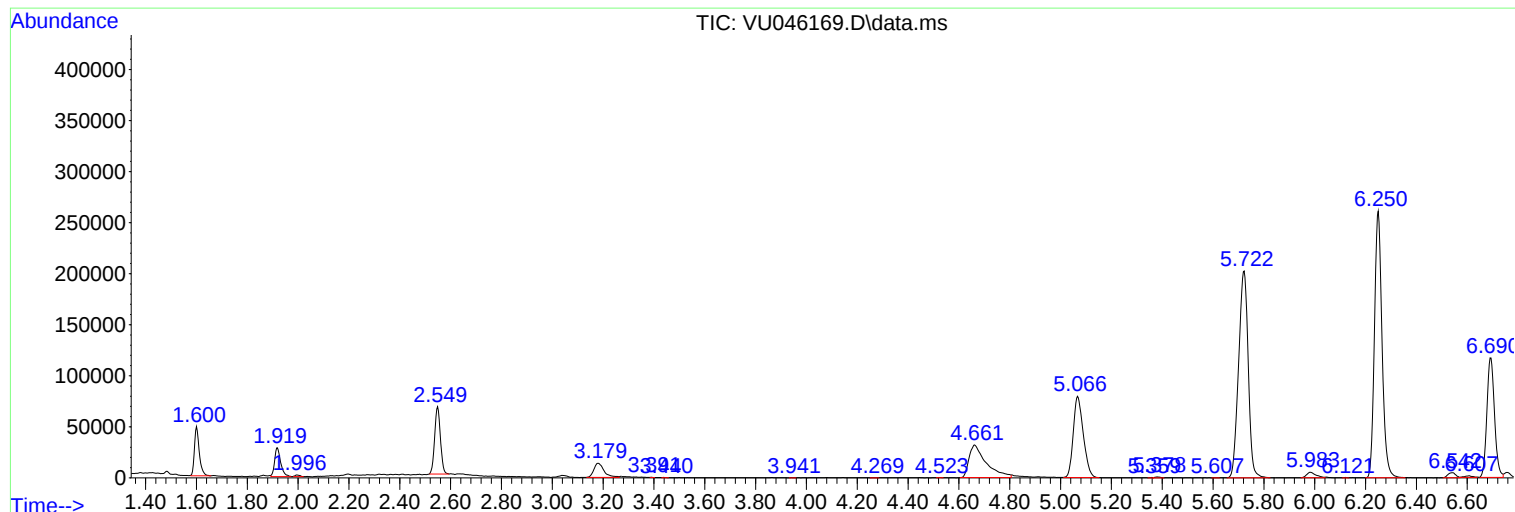
Sum of corrected areas: 5327671

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW9H5ME

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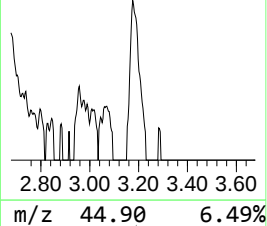
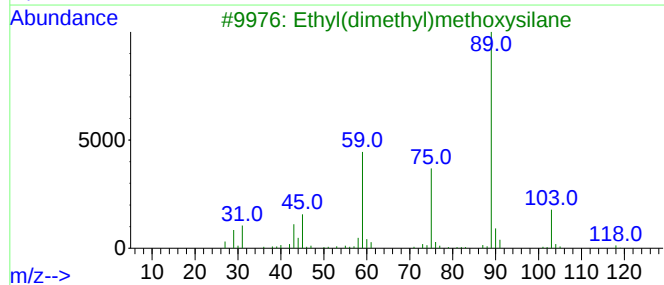
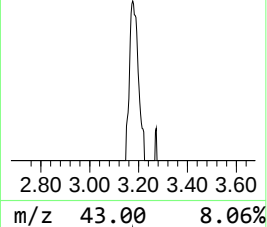
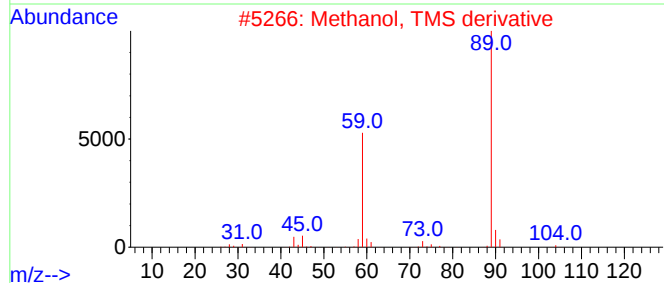
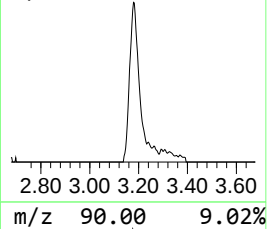
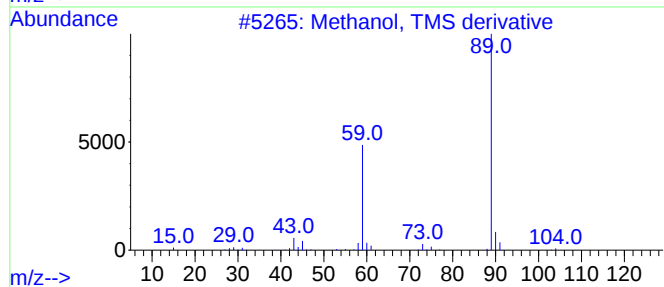
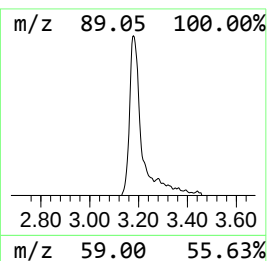
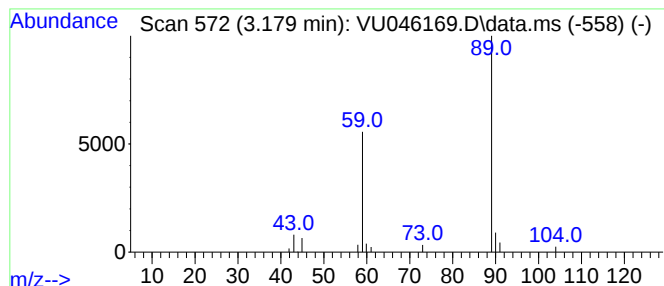
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.179	3.54 ug/L	38253	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			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74
5			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74



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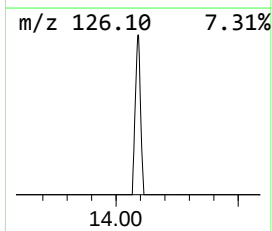
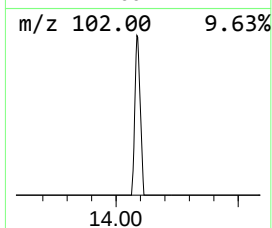
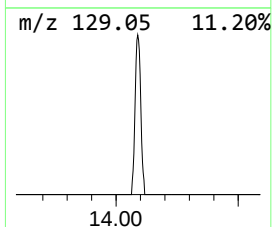
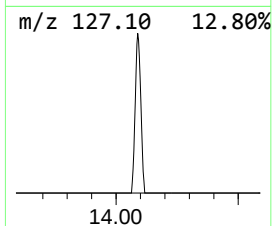
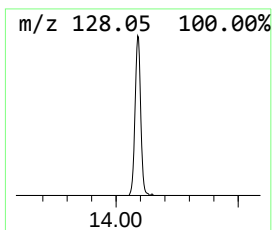
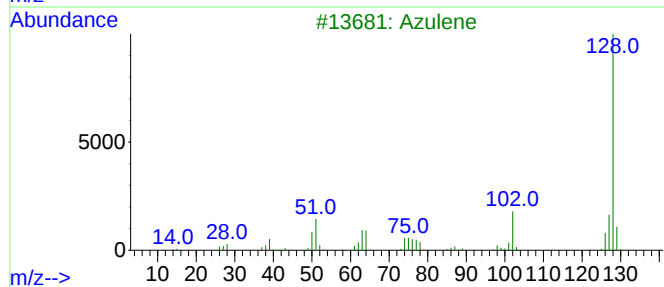
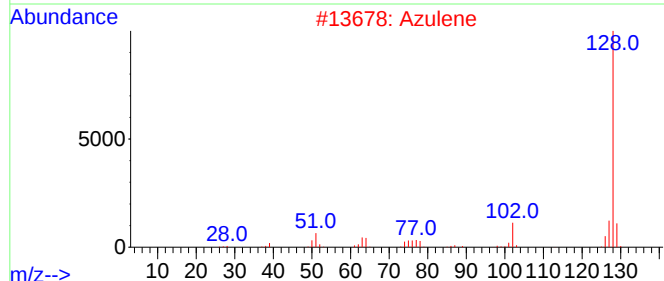
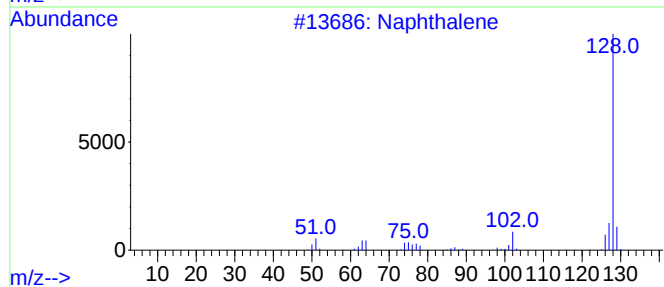
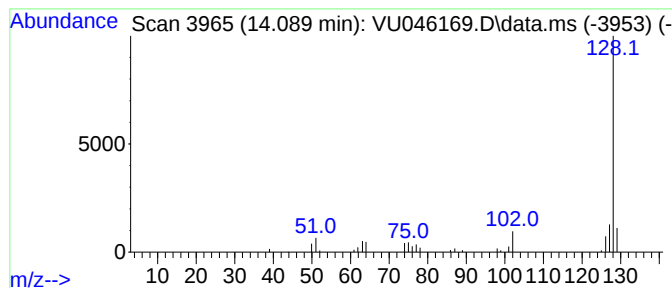
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Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	3.08 ug/L	43664	1,4-Dichlorobenzene-d4	11.819

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



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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...	3.179	3.5	ug/L	38253	1	6.250	540413	50.0
Azulene	14.089	3.1	ug/L	43664	3	11.819	708923	50.0