

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046045.D
 Acq On : 02 Dec 2021 12:28
 Operator : SY/MD
 Sample : M4868-02
 Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKN9

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: VU046045.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	73	81	98	rVB	106515	160146	14.43%	1.820%
2	1.883	159	169	172	rBV	10791	14756	1.33%	0.168%
3	1.916	173	179	203	rVB	61613	124744	11.24%	1.418%
4	2.543	363	374	389	rBV	175955	284879	25.67%	3.237%
5	3.035	520	527	542	rVB5	2548	5654	0.51%	0.064%
6	3.179	557	572	593	rBV2	8312	23076	2.08%	0.262%
7	3.504	664	673	678	rBB	239	390	0.04%	0.004%
8	3.961	808	815	819	rBV2	297	468	0.04%	0.005%
9	4.488	976	979	987	rVB	169	270	0.02%	0.003%
10	4.661	1014	1033	1069	rBV	55491	266095	23.98%	3.024%
11	4.819	1072	1082	1125	rVB	52144	167398	15.08%	1.902%
12	5.067	1142	1159	1184	rBV	170783	431723	38.90%	4.906%
13	5.295	1229	1230	1236	rBV	343	306	0.03%	0.003%
14	5.723	1342	1363	1392	rBV2	437004	1109804	100.00%	12.612%
15	5.989	1433	1446	1459	rBV7	3561	9361	0.84%	0.106%
16	6.253	1512	1528	1554	rBV	218809	464283	41.83%	5.276%
17	6.533	1605	1615	1635	rBV3	7088	20127	1.81%	0.229%
18	6.694	1650	1665	1688	rBV	231108	499372	45.00%	5.675%
19	6.813	1699	1702	1708	rVB	555	546	0.05%	0.006%
20	7.189	1810	1819	1832	rVB5	1824	3520	0.32%	0.040%
21	7.378	1872	1878	1883	rVV3	380	567	0.05%	0.006%
22	7.571	1923	1938	1967	rBV	127237	251777	22.69%	2.861%
23	7.690	1967	1975	1979	rBV3	981	1260	0.11%	0.014%
24	7.796	2001	2008	2017	rBV5	1165	2077	0.19%	0.024%
25	7.903	2025	2041	2058	rBV	475250	912244	82.20%	10.367%
26	8.185	2117	2129	2158	rBV	75583	166951	15.04%	1.897%
27	8.475	2211	2219	2221	rBV2	501	638	0.06%	0.007%
28	8.584	2246	2253	2260	rBV	192	391	0.04%	0.004%
29	8.690	2260	2286	2319	rBV	158934	570222	51.38%	6.480%
30	8.838	2326	2332	2334	rBV3	765	799	0.07%	0.009%
31	8.964	2362	2371	2379	rBV2	653	1287	0.12%	0.015%
32	9.179	2429	2438	2443	rBV	168	386	0.03%	0.004%
33	9.333	2483	2486	2493	rVB	284	286	0.03%	0.003%
34	9.427	2501	2515	2540	rBV	242408	577936	52.08%	6.568%
35	9.578	2551	2562	2579	rVB	25787	50060	4.51%	0.569%
36	9.703	2587	2601	2625	rVB	73568	160477	14.46%	1.824%

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Integrator: RTE

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

37	10.111	2716	2728	2743	rBV3	21660	44093	3.97%	0.501%
38	10.256	2769	2773	2776	rVB2	511	371	0.03%	0.004%
39	10.369	2799	2808	2816	rBV7	1513	2539	0.23%	0.029%
40	10.497	2836	2848	2857	rBV3	2299	3814	0.34%	0.043%
41	10.674	2894	2903	2912	rVB4	3633	5815	0.52%	0.066%
42	10.777	2919	2935	2952	rBV	316153	541302	48.77%	6.151%
43	10.861	2957	2961	2962	rBV	433	255	0.02%	0.003%
44	10.912	2971	2977	2987	rVB3	2691	4636	0.42%	0.053%
45	11.009	2997	3007	3025	rBV2	8764	19541	1.76%	0.222%
46	11.102	3025	3036	3051	rBV2	7562	16048	1.45%	0.182%
47	11.208	3066	3069	3072	rVB	292	238	0.02%	0.003%
48	11.304	3088	3099	3108	rBV	3559	5485	0.49%	0.062%
49	11.375	3118	3121	3127	rVV2	580	604	0.05%	0.007%
50	11.420	3130	3135	3140	rVV2	832	1101	0.10%	0.013%
51	11.475	3140	3152	3164	rVB	27316	45519	4.10%	0.517%
52	11.581	3179	3185	3192	rBV3	868	1126	0.10%	0.013%
53	11.623	3192	3198	3201	rBV3	462	556	0.05%	0.006%
54	11.700	3213	3222	3231	rBV6	3346	5722	0.52%	0.065%
55	11.748	3231	3237	3247	rVB6	2115	3213	0.29%	0.037%
56	11.822	3247	3260	3274	rBV	352279	571520	51.50%	6.495%
57	11.906	3278	3286	3294	rVB	5658	8005	0.72%	0.091%
58	11.944	3295	3298	3302	rBV3	749	606	0.05%	0.007%
59	11.976	3303	3308	3325	rVB4	2824	4686	0.42%	0.053%
60	12.105	3337	3348	3352	rBV3	4270	6550	0.59%	0.074%
61	12.205	3363	3379	3394	rVB	506031	825439	74.38%	9.380%
62	12.275	3399	3401	3407	rBV2	261	250	0.02%	0.003%
63	12.327	3407	3417	3426	rBV4	4497	7355	0.66%	0.084%
64	12.385	3426	3435	3441	rBV2	1518	1921	0.17%	0.022%
65	12.471	3453	3462	3467	rBV	2029	2810	0.25%	0.032%
66	12.578	3486	3495	3505	rVB	3528	4482	0.40%	0.051%
67	12.645	3511	3516	3520	rBV2	287	271	0.02%	0.003%
68	12.716	3534	3538	3549	rVB5	1173	1725	0.16%	0.020%
69	12.893	3586	3593	3598	rVB3	961	1325	0.12%	0.015%
70	12.979	3612	3620	3628	rVV3	2483	3525	0.32%	0.040%
71	13.034	3628	3637	3644	rVB2	3715	5183	0.47%	0.059%
72	13.105	3655	3659	3667	rBV	234	305	0.03%	0.003%
73	13.147	3667	3672	3677	rBV3	443	629	0.06%	0.007%
74	13.172	3677	3680	3686	rVB	555	592	0.05%	0.007%
75	13.227	3692	3697	3703	rVB	1032	1029	0.09%	0.012%
76	13.291	3713	3717	3725	rVB3	900	1102	0.10%	0.013%

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 Title : VOC Analysis

77	13.414	3749	3755	3759	rVB3	441	582	0.05%	0.007%
78	13.459	3759	3769	3781	rBV5	2930	5009	0.45%	0.057%
79	13.568	3794	3803	3811	rVB2	558	859	0.08%	0.010%
80	13.626	3818	3821	3827	rBV2	478	510	0.05%	0.006%
81	13.844	3880	3889	3899	rBV5	6162	9814	0.88%	0.112%
82	14.092	3954	3966	3981	rBV	107708	171409	15.44%	1.948%
83	14.211	3994	4003	4013	rVB3	970	1633	0.15%	0.019%
84	14.336	4034	4042	4052	rVB4	3421	4729	0.43%	0.054%
85	14.487	4084	4089	4096	rBV3	500	709	0.06%	0.008%
86	14.581	4114	4118	4119	rBV2	755	525	0.05%	0.006%
87	14.674	4140	4147	4148	rBV2	1040	890	0.08%	0.010%
88	14.815	4185	4191	4198	rBV2	675	800	0.07%	0.009%
89	15.002	4242	4249	4253	rBV4	592	698	0.06%	0.008%
90	15.227	4308	4319	4331	rBV	54521	85285	7.68%	0.969%
91	15.413	4367	4377	4389	rVB	27021	39625	3.57%	0.450%
92	15.471	4389	4395	4397	rBV2	344	386	0.03%	0.004%
93	15.581	4425	4429	4432	rBV	332	265	0.02%	0.003%
94	15.761	4482	4485	4488	rBV	338	255	0.02%	0.003%
95	15.954	4539	4545	4559	rVB4	3488	5504	0.50%	0.063%
96	16.150	4599	4606	4613	rBV2	2376	3636	0.33%	0.041%
97	16.262	4633	4641	4652	rVB	8582	13600	1.23%	0.155%
98	16.413	4679	4688	4693	rBV4	6008	8598	0.77%	0.098%
99	16.449	4694	4699	4709	rVB5	4157	5933	0.53%	0.067%
100	16.635	4753	4757	4769	rVB6	1763	2808	0.25%	0.032%

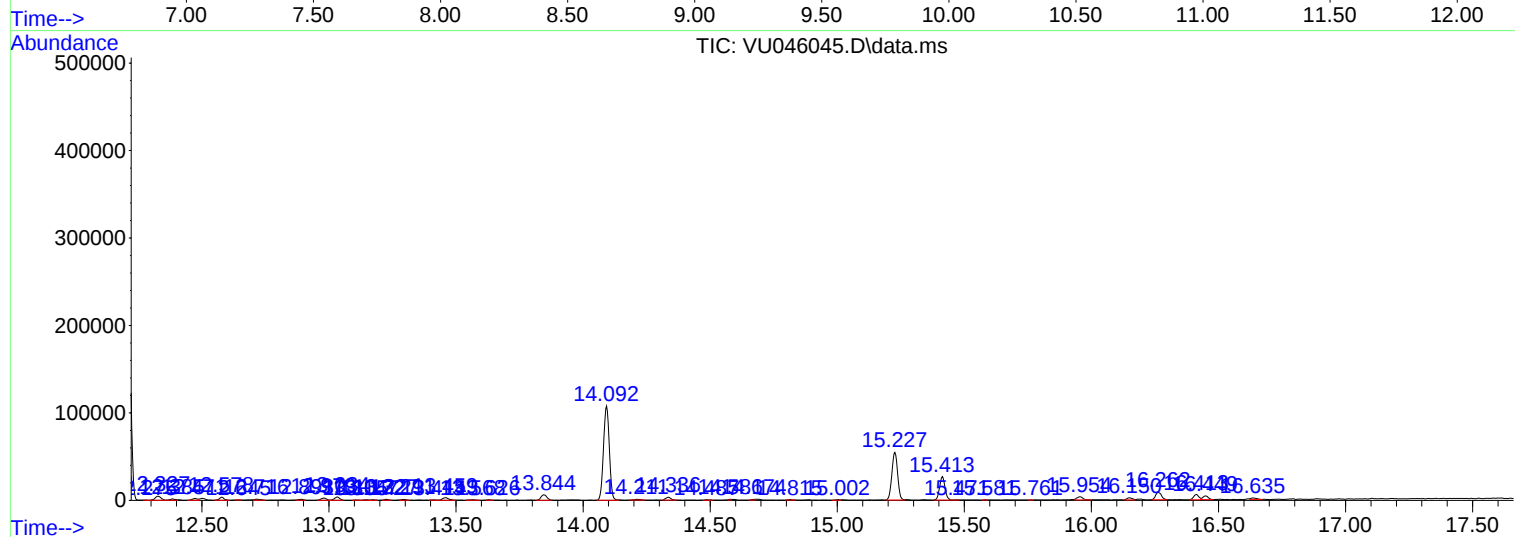
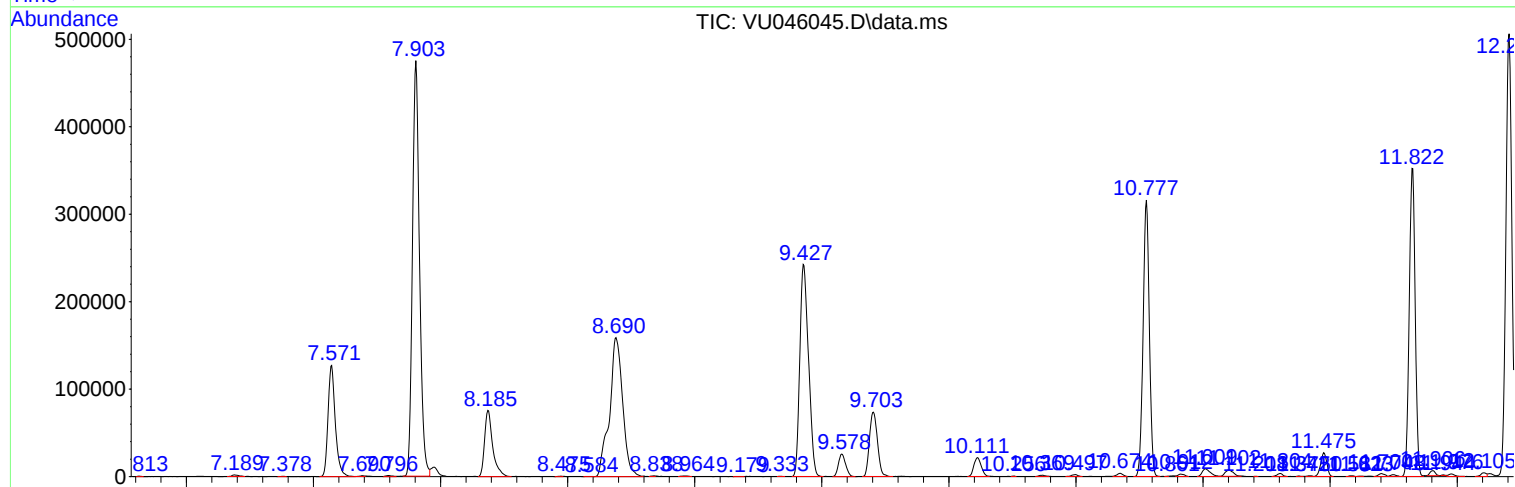
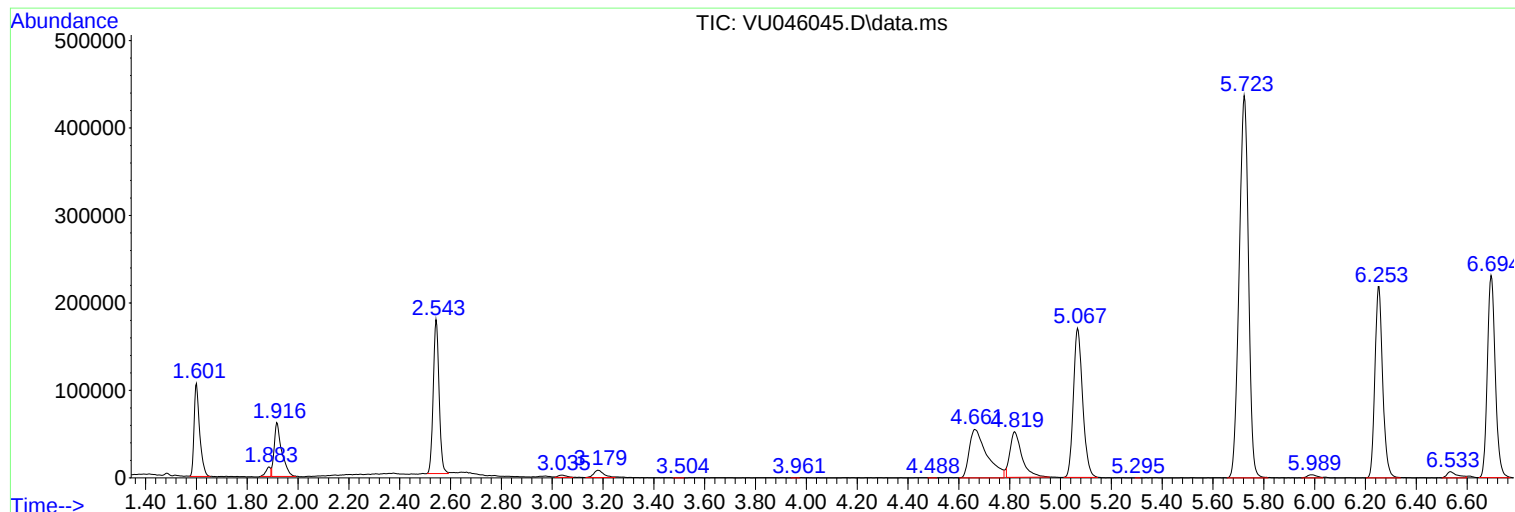
Sum of corrected areas: 8799626

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ALS Vial : 5 Sample Multiplier: 1

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



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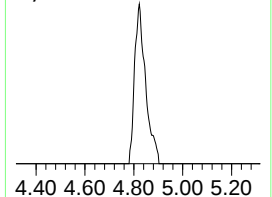
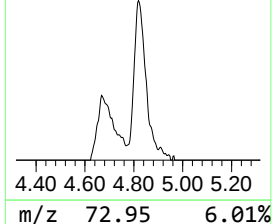
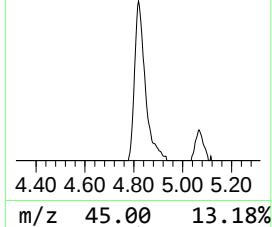
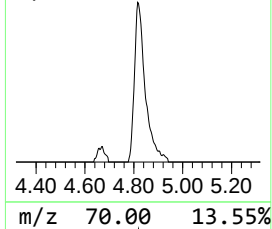
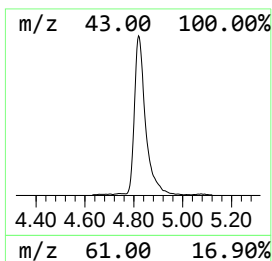
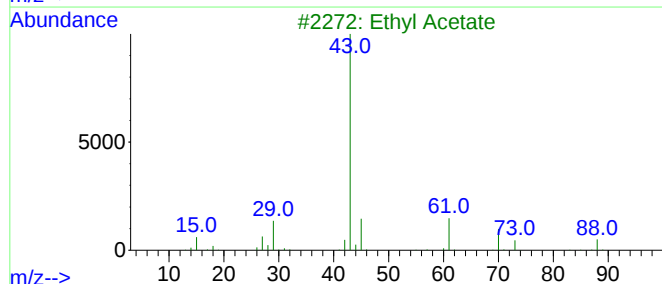
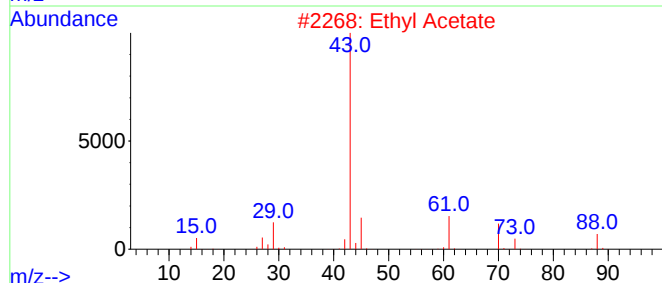
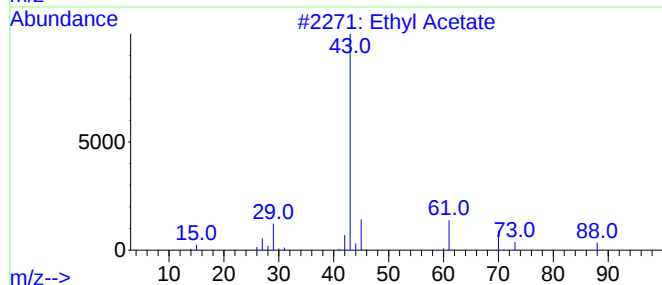
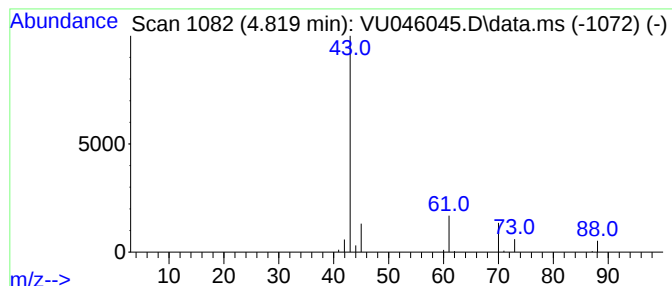
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.819	18.03 ug/L	167398	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	90
4			Ethyl Acetate	88	C4H8O2	000141-78-6	78
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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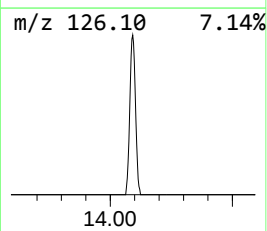
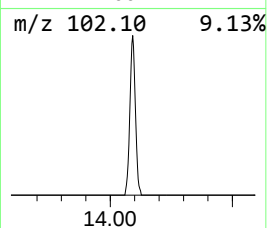
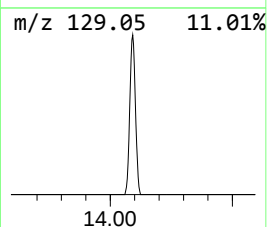
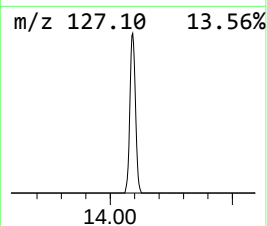
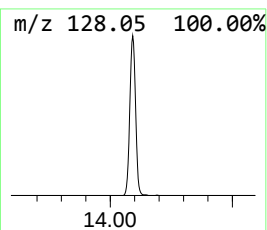
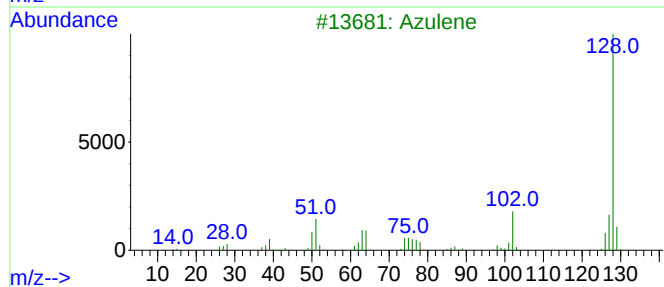
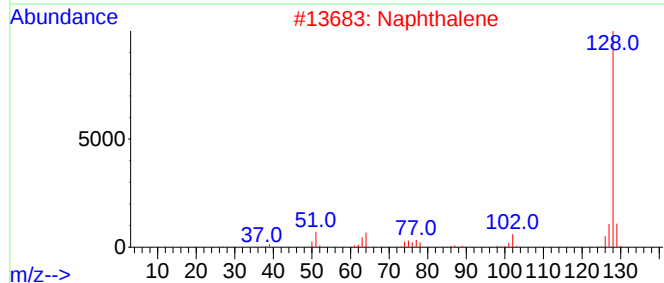
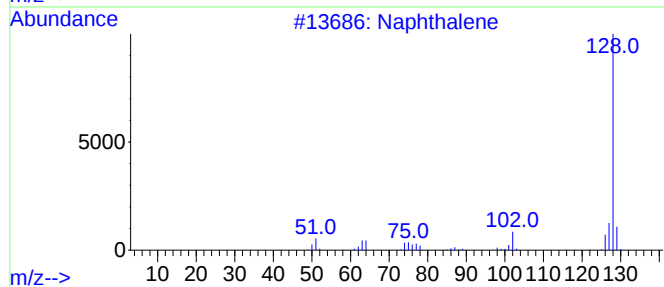
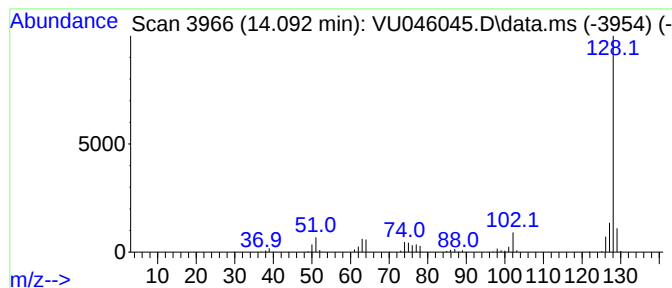
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	15.00 ug/L	171409	1,4-Dichlorobenzene-d4	11.825

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	94
4			Azulene	128	C10H8	000275-51-4	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
Ethyl Acetate	4.819	18.0	ug/L	167398	1	6.250	464283	50.0
Azulene	14.092	15.0	ug/L	171409	3	11.825	571520	50.0