

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046180.D
 Acq On : 08 Dec 2021 16:56
 Operator : SY/MD
 Sample : M4887-15ME
 Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C9ME

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: VU046180.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	101	rVB	66912	88297	3.15%	0.927%
2	1.916	172	179	197	rVB	40969	68112	2.43%	0.715%
3	1.996	197	204	213	rVB3	4815	6913	0.25%	0.073%
4	2.096	230	235	237	rVV4	708	652	0.02%	0.007%
5	2.147	245	251	255	rBV5	783	812	0.03%	0.009%
6	2.195	261	266	267	rBV3	817	590	0.02%	0.006%
7	2.549	362	376	389	rBV	91882	150032	5.35%	1.575%
8	2.961	495	504	518	rBV3	2482	5913	0.21%	0.062%
9	3.182	559	573	590	rBV	8431	20418	0.73%	0.214%
10	3.678	724	727	733	rVB3	692	692	0.02%	0.007%
11	4.517	977	988	1002	rVB4	3503	7700	0.27%	0.081%
12	4.658	1016	1032	1074	rBV2	33694	158271	5.65%	1.661%
13	5.063	1142	1158	1182	rVB2	102187	260215	9.28%	2.731%
14	5.378	1247	1256	1271	rVB6	4525	10466	0.37%	0.110%
15	5.459	1271	1281	1289	rBV7	1406	2953	0.11%	0.031%
16	5.722	1339	1363	1388	rBV2	258346	665915	23.76%	6.990%
17	5.841	1397	1400	1410	rVB6	2172	2916	0.10%	0.031%
18	5.915	1413	1423	1432	rBV4	2360	3933	0.14%	0.041%
19	5.980	1433	1443	1465	rVV6	7388	18192	0.65%	0.191%
20	6.250	1512	1527	1550	rVB	267219	530128	18.91%	5.564%
21	6.539	1601	1617	1650	rBV	1472588	2802966	100.00%	29.421%
22	6.690	1651	1664	1677	rBV	144831	294316	10.50%	3.089%
23	6.980	1747	1754	1759	rBV4	1291	1832	0.07%	0.019%
24	7.234	1826	1833	1840	rVB5	2201	3293	0.12%	0.035%
25	7.568	1925	1937	1956	rBV	79265	155472	5.55%	1.632%
26	7.790	1997	2006	2017	rBV4	4022	7421	0.26%	0.078%
27	7.854	2017	2026	2027	rBV2	3503	3577	0.13%	0.038%
28	7.899	2028	2040	2056	rVV	293699	553369	19.74%	5.808%
29	7.970	2057	2062	2072	rVB	11987	19635	0.70%	0.206%
30	8.131	2107	2112	2116	rVB4	2044	2208	0.08%	0.023%
31	8.182	2117	2128	2153	rBV	46941	108749	3.88%	1.141%
32	8.407	2188	2198	2217	rBV5	10362	24607	0.88%	0.258%
33	8.555	2232	2244	2259	rVB2	58586	102774	3.67%	1.079%
34	8.681	2259	2283	2314	rBV2	108552	356271	12.71%	3.740%
35	8.809	2317	2323	2327	rBV4	885	1237	0.04%	0.013%
36	8.867	2331	2341	2350	rVB3	4450	7731	0.28%	0.081%

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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
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37	8.925	2350	2359	2370	rBV4	5162	10726	0.38%	0.113%
38	9.118	2411	2419	2428	rBV4	2742	4380	0.16%	0.046%
39	9.211	2445	2448	2454	rVB3	1231	975	0.03%	0.010%
40	9.269	2459	2466	2471	rBV	414	686	0.02%	0.007%
41	9.423	2497	2514	2532	rBV	312034	678030	24.19%	7.117%
42	9.578	2553	2562	2572	rBV	2912	4761	0.17%	0.050%
43	9.697	2586	2599	2610	rBV2	13049	26523	0.95%	0.278%
44	9.967	2679	2683	2689	rBV	610	651	0.02%	0.007%
45	10.021	2694	2700	2704	rBV3	859	968	0.03%	0.010%
46	10.108	2715	2727	2739	rVB2	12649	24450	0.87%	0.257%
47	10.243	2761	2769	2774	rBV6	3599	6266	0.22%	0.066%
48	10.324	2787	2794	2797	rVB4	645	710	0.03%	0.007%
49	10.359	2797	2805	2809	rBV7	2946	4399	0.16%	0.046%
50	10.478	2831	2842	2856	rBV4	5938	14188	0.51%	0.149%
51	10.552	2857	2865	2868	rBV5	1091	1286	0.05%	0.013%
52	10.700	2908	2911	2917	rVB4	1458	1559	0.06%	0.016%
53	10.771	2919	2933	2955	rVV	215870	369797	13.19%	3.882%
54	10.912	2970	2977	2985	rVB3	4121	6050	0.22%	0.064%
55	11.008	2999	3007	3019	rVB4	8084	14686	0.52%	0.154%
56	11.115	3028	3040	3054	rVB8	7724	18345	0.65%	0.193%
57	11.298	3089	3097	3106	rBV3	4376	7145	0.25%	0.075%
58	11.417	3126	3134	3141	rBV3	4848	6836	0.24%	0.072%
59	11.471	3141	3151	3164	rVB2	12017	22379	0.80%	0.235%
60	11.584	3180	3186	3188	rBV2	935	966	0.03%	0.010%
61	11.645	3200	3205	3214	rVB4	3401	5000	0.18%	0.052%
62	11.703	3214	3223	3226	rBV4	2431	3625	0.13%	0.038%
63	11.748	3232	3237	3245	rVB5	2395	3418	0.12%	0.036%
64	11.819	3245	3259	3271	rBV	460384	724975	25.86%	7.610%
65	11.899	3278	3284	3296	rVB2	7057	10855	0.39%	0.114%
66	11.976	3302	3308	3313	rBV5	1438	1967	0.07%	0.021%
67	12.131	3343	3356	3361	rBV5	2432	4587	0.16%	0.048%
68	12.198	3365	3377	3389	rBV	334925	546760	19.51%	5.739%
69	12.327	3408	3417	3428	rVB	25692	36854	1.31%	0.387%
70	12.381	3428	3434	3442	rBV6	2642	4299	0.15%	0.045%
71	12.446	3450	3454	3455	rBV2	871	613	0.02%	0.006%
72	12.468	3455	3461	3465	rVV4	1982	2488	0.09%	0.026%
73	12.629	3504	3511	3517	rBV2	869	1509	0.05%	0.016%
74	12.709	3528	3536	3549	rBV7	2304	5093	0.18%	0.053%
75	12.774	3551	3556	3560	rBV5	1356	1701	0.06%	0.018%
76	12.812	3560	3568	3582	rVB2	15861	22986	0.82%	0.241%

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 Title : VOC Analysis

77	12.880	3584	3589	3595	rBV4	1018	1514	0.05%	0.016%
78	13.037	3631	3638	3649	rVB8	3113	5847	0.21%	0.061%
79	13.137	3666	3669	3673	rVV4	1192	902	0.03%	0.009%
80	13.163	3673	3677	3686	rVB5	2901	3922	0.14%	0.041%
81	13.291	3710	3717	3721	rVB6	951	1313	0.05%	0.014%
82	13.433	3753	3761	3775	rBV6	6354	12948	0.46%	0.136%
83	13.513	3775	3786	3798	rVB2	170647	258586	9.23%	2.714%
84	13.587	3804	3809	3818	rVB5	2421	2786	0.10%	0.029%
85	13.703	3836	3845	3852	rBV4	8993	12487	0.45%	0.131%
86	13.741	3852	3857	3869	rVB7	4196	6515	0.23%	0.068%
87	13.838	3880	3887	3897	rBV10	2871	4617	0.16%	0.048%
88	14.089	3956	3965	3982	rVB2	25838	41580	1.48%	0.436%
89	14.188	3992	3996	4004	rVB5	3315	4431	0.16%	0.047%
90	14.449	4071	4077	4085	rVB2	5156	6188	0.22%	0.065%
91	14.574	4110	4116	4117	rBV5	1799	1588	0.06%	0.017%
92	14.944	4226	4231	4233	rBV4	656	662	0.02%	0.007%
93	15.224	4307	4318	4327	rBV	22770	36855	1.31%	0.387%
94	15.407	4367	4375	4386	rVB3	19676	30737	1.10%	0.323%
95	15.500	4398	4404	4413	rVB8	3712	4994	0.18%	0.052%
96	16.143	4598	4604	4605	rBV5	2094	1951	0.07%	0.020%
97	16.262	4634	4641	4650	rBV5	5754	8953	0.32%	0.094%
98	16.410	4679	4687	4693	rBV	9821	14369	0.51%	0.151%
99	16.449	4694	4699	4707	rVB5	6762	9632	0.34%	0.101%
100	16.722	4780	4784	4785	rBV3	2001	1552	0.06%	0.016%

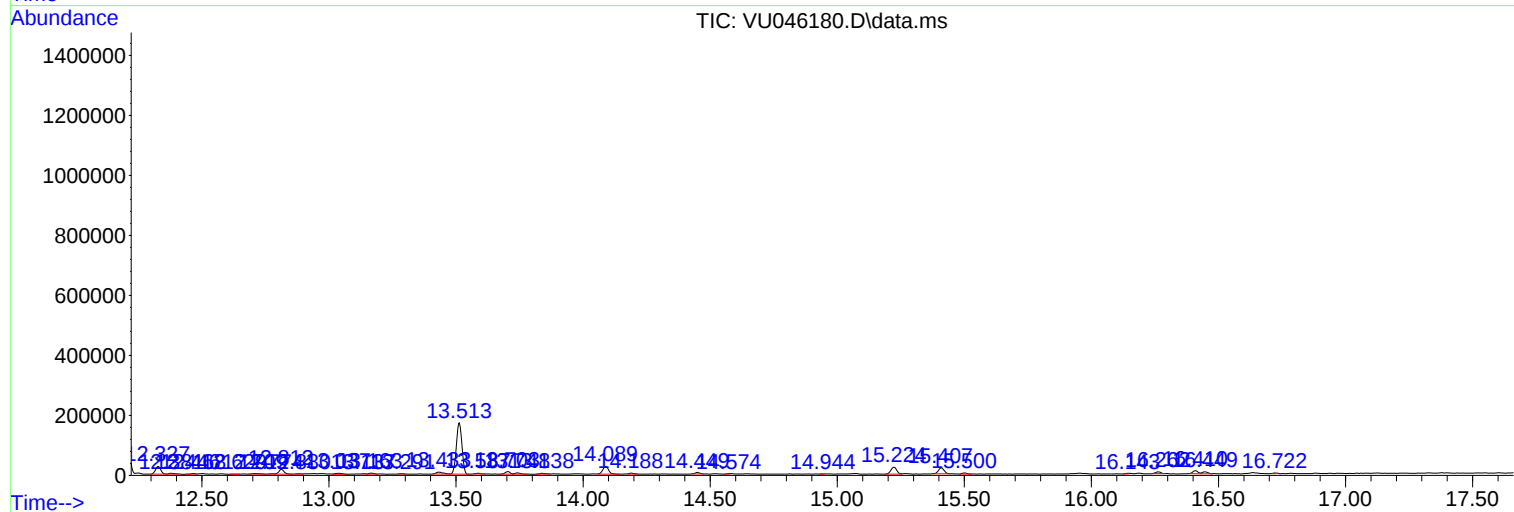
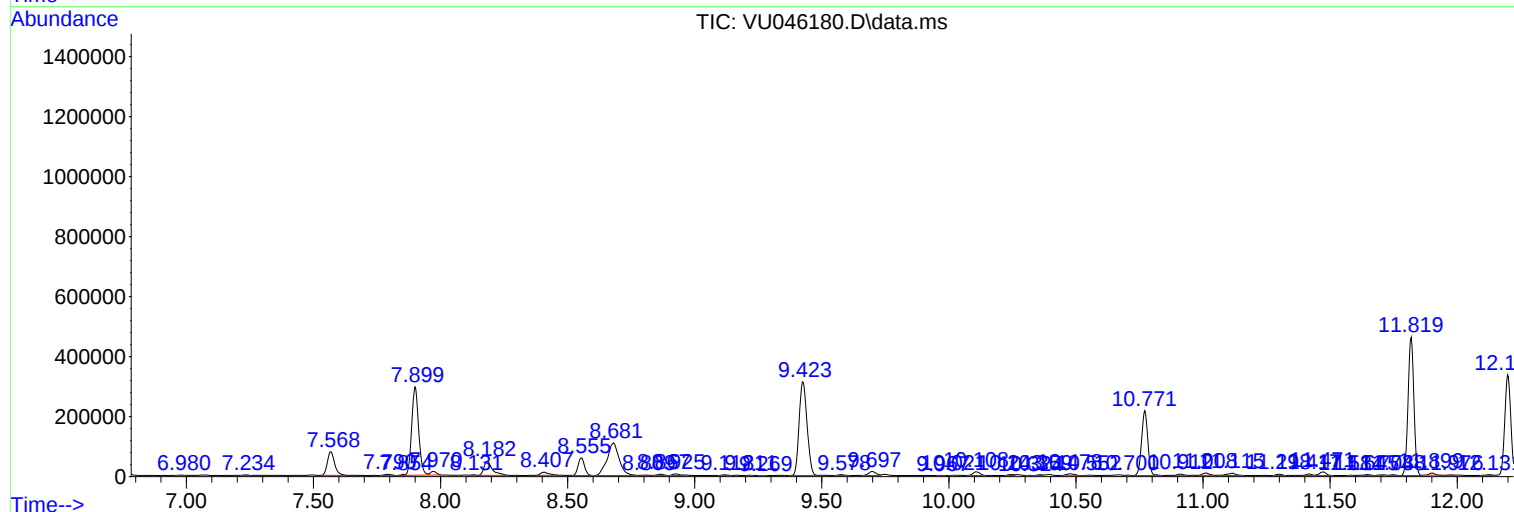
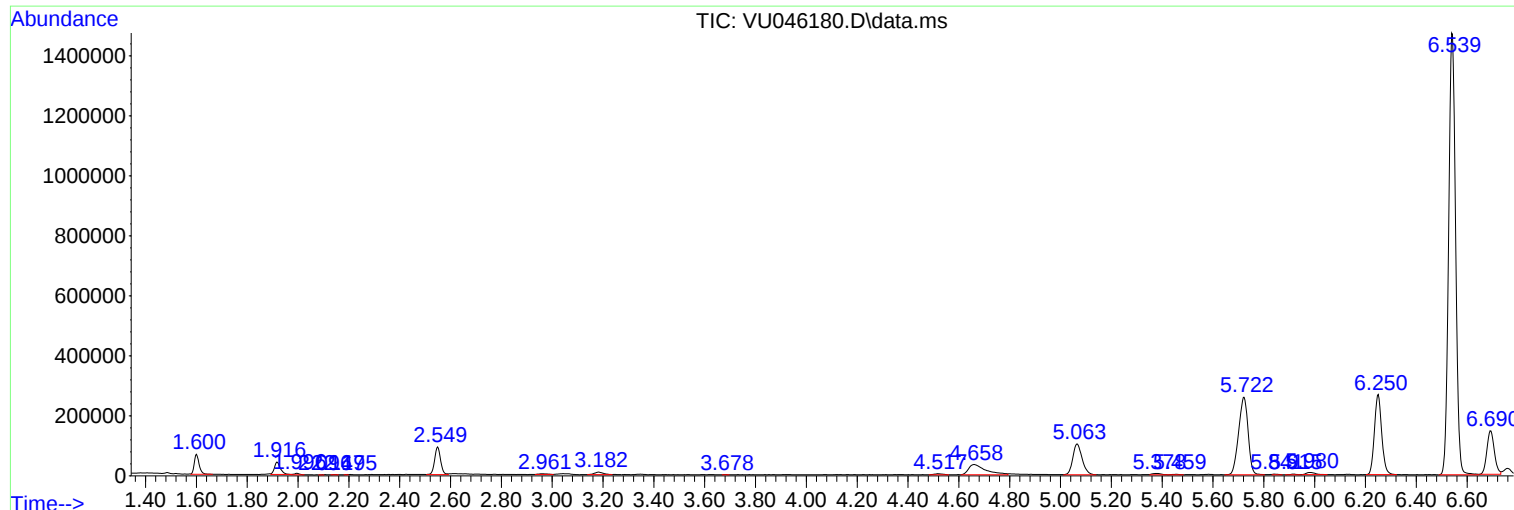
Sum of corrected areas: 9526999

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Instrument :
MSVOA_U
ClientSampleId :
EX8C9ME

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 :
EX8C9ME

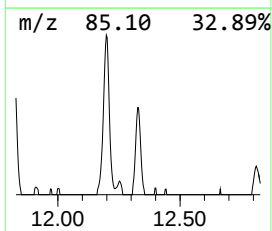
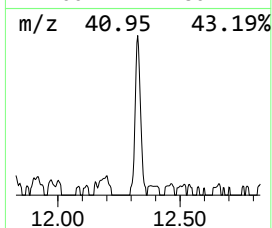
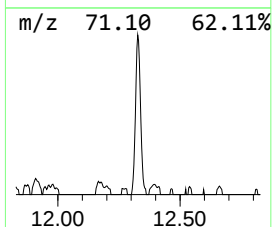
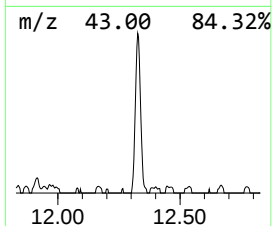
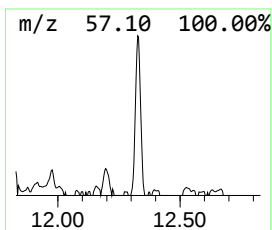
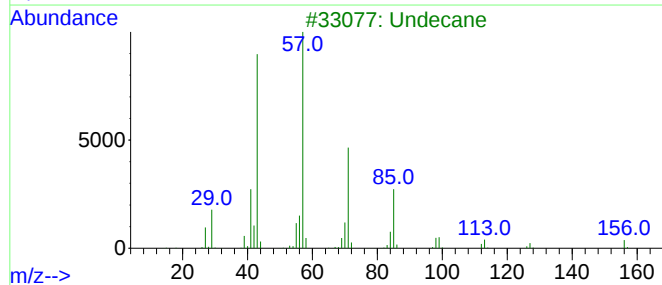
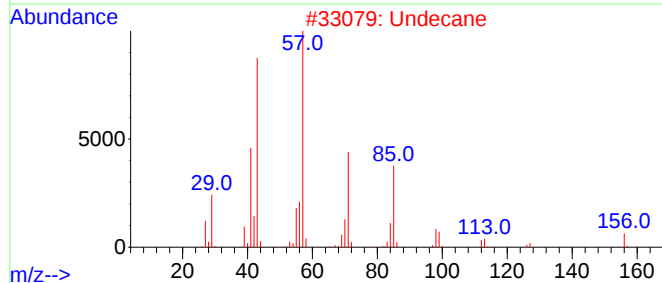
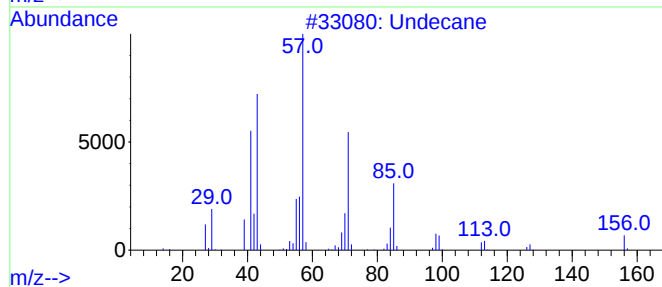
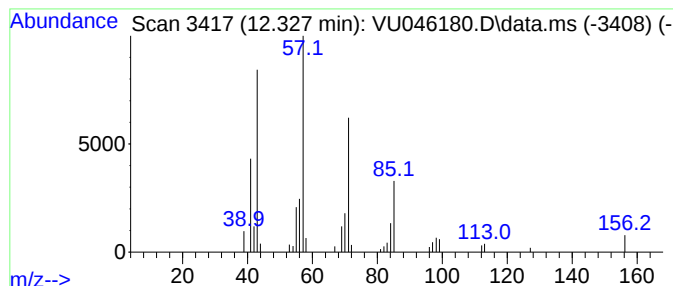
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	2.54 ug/L	36854	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	91
2	Undecane			156	C11H24	001120-21-4	81
3	Undecane			156	C11H24	001120-21-4	80
4	Undecane			156	C11H24	001120-21-4	74
5	Undecane			156	C11H24	001120-21-4	68



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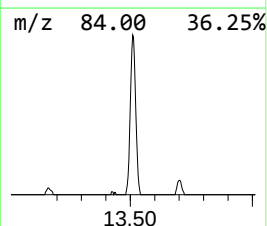
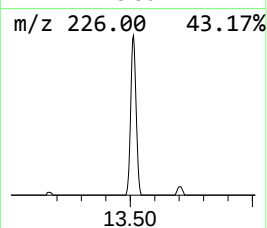
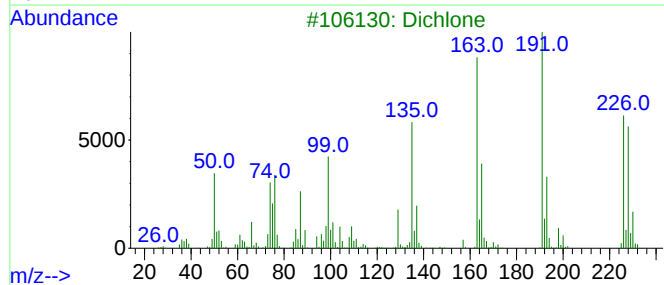
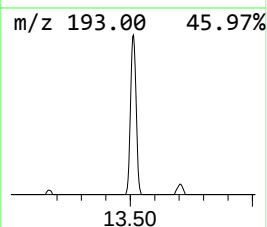
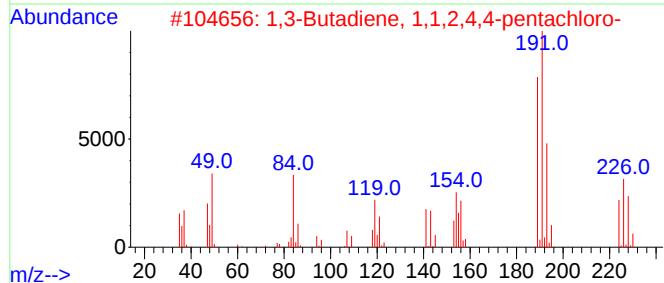
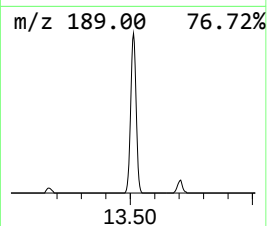
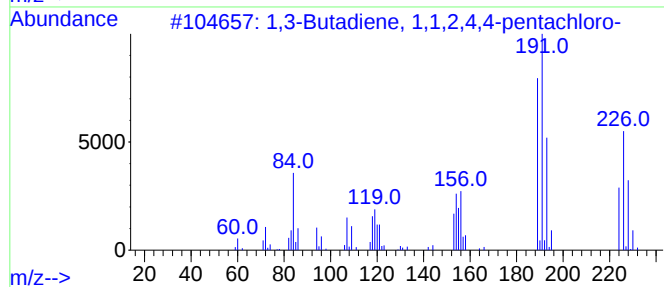
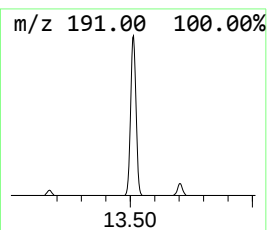
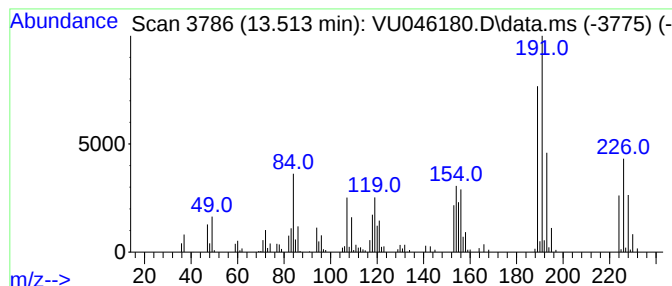
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Quant Title : VOC Analysis

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

Peak Number 3 1,3-Butadiene, 1,1,2,4,4-pe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	17.83 ug/L	258586	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99		
2	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	94		
3	Dichlone	226	C10H4Cl2O2	000117-80-6	38		
4	4-Bromo-2-furamide	189	C5H4BrN02	957345-95-8	35		
5	1,8-Bis(chloromethyl)naphthalene	224	C12H10Cl2	050585-29-0	35		



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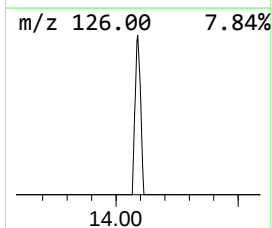
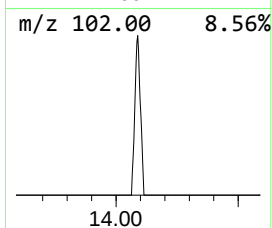
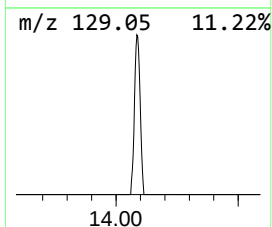
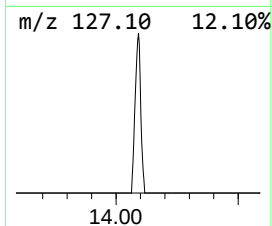
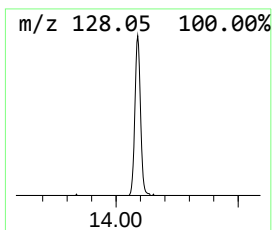
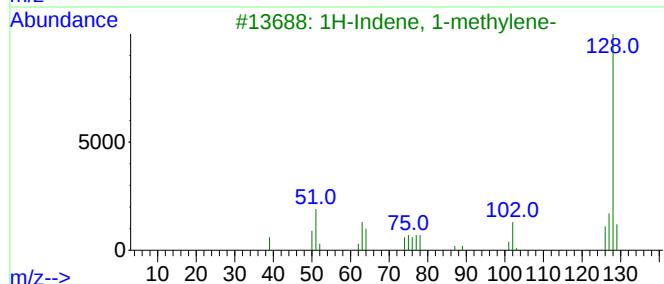
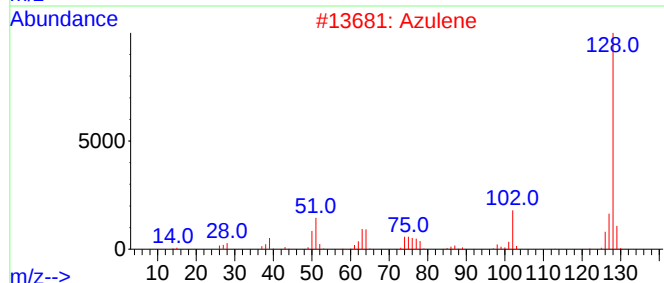
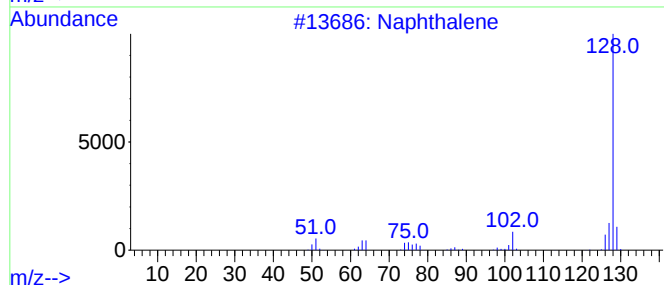
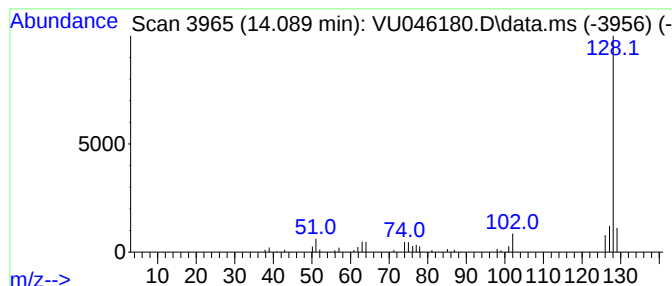
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1H-Indene, 1-methylene- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	2.87 ug/L	41580	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			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046180.D
Acq On : 08 Dec 2021 16:56
Operator : SY/MD
Sample : M4887-15ME
Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C9ME

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
(DEL) Alkane: S...	12.327	2.5	ug/L	36854	3	11.819	724975	50.0
1,3-Butadiene, ...	13.513	17.8	ug/L	258586	3	11.819	724975	50.0
1H-Indene, 1-me...	14.089	2.9	ug/L	41580	3	11.819	724975	50.0