

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053529.D
 Acq On : 03 Apr 2023 18:49
 Operator : JC/MD
 Sample : 02158-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-5(20230329)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053529.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	71	81	96	rBV2	449932	537252	0.20%	0.062%
2	1.909	169	177	197	rVB	109117	153088	0.06%	0.018%
3	2.568	368	382	410	rBV3	260662	528152	0.19%	0.061%
4	3.044	520	530	533	rBV7	2769	4195	0.00%	0.000%
5	3.353	612	626	645	rBV2	36339	87388	0.03%	0.010%
6	3.697	720	733	747	rVB4	8753	19875	0.01%	0.002%
7	3.903	794	797	803	rVB2	1474	1265	0.00%	0.000%
8	4.526	977	991	1008	rBV2	18791	44807	0.02%	0.005%
9	4.661	1008	1033	1067	rBV2	36482745	80242123	29.47%	9.229%
10	5.057	1143	1156	1174	rVB	183109	393828	0.14%	0.045%
11	5.382	1242	1257	1271	rBV5	59639	139283	0.05%	0.016%
12	5.587	1309	1321	1329	rBV2	17123	36333	0.01%	0.004%
13	5.719	1343	1362	1370	rBV2	353347	946535	0.35%	0.109%
14	5.986	1434	1445	1464	rVB5	27083	63805	0.02%	0.007%
15	6.131	1478	1490	1504	rVB3	23651	44961	0.02%	0.005%
16	6.243	1512	1525	1550	rBV	310567	594210	0.22%	0.068%
17	6.539	1598	1617	1651	rBV	9344499	17234270	6.33%	1.982%
18	6.684	1653	1662	1673	rVV	229783	465793	0.17%	0.054%
19	6.758	1674	1685	1709	rVB	341789	700840	0.26%	0.081%
20	6.976	1740	1753	1767	rVB3	19191	34803	0.01%	0.004%
21	7.063	1767	1780	1797	rVB5	5692	12698	0.00%	0.001%
22	7.234	1824	1833	1846	rVB8	5805	11506	0.00%	0.001%
23	7.407	1866	1887	1900	rBV8	9121	24849	0.01%	0.003%
24	7.494	1905	1914	1922	rBV3	9548	16096	0.01%	0.002%
25	7.562	1923	1935	1954	rVV	134691	250157	0.09%	0.029%
26	7.658	1958	1965	1972	rVB3	8088	11799	0.00%	0.001%
27	7.758	1989	1996	1997	rBV3	2000	1690	0.00%	0.000%
28	7.854	2012	2026	2029	rBV	63995	101197	0.04%	0.012%
29	7.896	2030	2039	2048	rVV	468188	860946	0.32%	0.099%
30	7.983	2048	2066	2104	rVB3	58348446	130723024	48.01%	15.035%
31	8.176	2119	2126	2136	rVB	103504	161286	0.06%	0.019%
32	8.240	2137	2146	2165	rVB4	68142	128731	0.05%	0.015%
33	8.365	2174	2185	2198	rVB	44257	76139	0.03%	0.009%
34	8.472	2212	2218	2227	rVB7	3836	6178	0.00%	0.001%
35	8.562	2227	2246	2261	rBV	55634655	99712331	36.62%	11.468%
36	8.806	2315	2322	2330	rBV3	25431	40480	0.01%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	8.861	2330	2339	2350	rVB	123294	196245	0.07%	0.023%
38	8.922	2350	2358	2367	rVB2	25504	37946	0.01%	0.004%
39	9.063	2395	2402	2405	rBV4	1881	2350	0.00%	0.000%
40	9.115	2411	2418	2424	rBV3	4137	6049	0.00%	0.001%
41	9.160	2424	2432	2441	rVV3	9523	16556	0.01%	0.002%
42	9.214	2441	2449	2455	rVB6	5280	9093	0.00%	0.001%
43	9.291	2469	2473	2479	rBV6	1093	1524	0.00%	0.000%
44	9.333	2479	2486	2493	rVB4	3254	4832	0.00%	0.001%
45	9.443	2497	2520	2534	rBV	4621408	8158483	3.00%	0.938%
46	9.565	2547	2558	2581	rVB	4548477	7516037	2.76%	0.864%
47	9.690	2582	2597	2629	rVB	18463642	29285628	10.76%	3.368%
48	9.886	2650	2658	2670	rVB3	9494	15746	0.01%	0.002%
49	10.095	2695	2723	2756	rVV	6211060	9754381	3.58%	1.122%
50	10.272	2771	2778	2787	rVB5	9230	13218	0.00%	0.002%
51	10.362	2792	2806	2815	rBV8	4594	8716	0.00%	0.001%
52	10.478	2830	2842	2865	rVB	644681	1015513	0.37%	0.117%
53	10.584	2865	2875	2889	rBV	6092	13299	0.00%	0.002%
54	10.658	2889	2898	2907	rBV4	11162	19509	0.01%	0.002%
55	10.751	2914	2927	2943	rVB	352423	561846	0.21%	0.065%
56	10.816	2943	2947	2955	rVB6	2356	3313	0.00%	0.000%
57	10.902	2955	2974	2989	rBV	910714	1454406	0.53%	0.167%
58	10.992	2989	3002	3021	rVV	2625647	5737854	2.11%	0.660%
59	11.086	3021	3031	3051	rVB	1465790	2255342	0.83%	0.259%
60	11.227	3064	3075	3083	rBV2	163023	247407	0.09%	0.028%
61	11.288	3083	3094	3112	rVB	1363952	2120128	0.78%	0.244%
62	11.414	3122	3133	3137	rBV2	22320	32416	0.01%	0.004%
63	11.465	3137	3149	3167	rVV	4106544	6326195	2.32%	0.728%
64	11.555	3168	3177	3185	rVV3	23288	37103	0.01%	0.004%
65	11.607	3187	3193	3198	rVV	23319	35990	0.01%	0.004%
66	11.642	3199	3204	3214	rVB	37308	54150	0.02%	0.006%
67	11.742	3221	3235	3247	rBV	7211888	11162224	4.10%	1.284%
68	11.838	3248	3265	3276	rVV2	40565020	66429840	24.40%	7.640%
69	11.893	3276	3282	3306	rVB	1498976	2263527	0.83%	0.260%
70	12.008	3313	3318	3325	rVB3	23058	30395	0.01%	0.003%
71	12.092	3325	3344	3352	rBV3	999758	2016868	0.74%	0.232%
72	12.211	3363	3381	3399	rVB	12678562	21286972	7.82%	2.448%
73	12.298	3402	3408	3420	rVB3	45272	73408	0.03%	0.008%
74	12.372	3422	3431	3448	rVB	189092	344455	0.13%	0.040%
75	12.462	3449	3459	3464	rBV	450162	712565	0.26%	0.082%
76	12.568	3481	3492	3501	rBV	852116	1313540	0.48%	0.151%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

77	12.680	3517	3527	3547	rVB3	214395	501598	0.18%	0.058%
78	12.873	3575	3587	3600	rVB	329108	559292	0.21%	0.064%
79	12.970	3600	3617	3625	rBV	541753	858358	0.32%	0.099%
80	13.024	3625	3634	3650	rVB	882892	1352034	0.50%	0.156%
81	13.102	3652	3658	3663	rBV3	14841	21955	0.01%	0.003%
82	13.137	3664	3669	3673	rBV3	14298	17018	0.01%	0.002%
83	13.217	3683	3694	3706	rVB	406288	637269	0.23%	0.073%
84	13.291	3706	3717	3729	rVB	376478	578520	0.21%	0.067%
85	13.452	3744	3767	3795	rBV3	893348	1567446	0.58%	0.180%
86	13.571	3796	3804	3810	rVV2	19233	32204	0.01%	0.004%
87	13.623	3811	3820	3837	rVB3	80785	139964	0.05%	0.016%
88	13.745	3843	3858	3870	rBV3	14510	34854	0.01%	0.004%
89	13.873	3871	3898	3918	rBV2	98397893	272285007	100.00%	31.317%
90	14.086	3952	3964	3989	rVB	2113864	3328130	1.22%	0.383%
91	14.336	4025	4042	4070	rVB	43669283	72125465	26.49%	8.296%
92	14.484	4082	4088	4100	rVB2	17062	26823	0.01%	0.003%
93	14.671	4138	4146	4159	rVB6	17662	32988	0.01%	0.004%
94	14.806	4181	4188	4199	rVB	13637	19384	0.01%	0.002%
95	14.876	4203	4210	4220	rVB5	10037	17533	0.01%	0.002%
96	15.221	4308	4317	4335	rVB	39363	65177	0.02%	0.007%
97	15.410	4361	4376	4389	rVB3	99328	179294	0.07%	0.021%
98	15.693	4460	4464	4467	rBV4	1262	1142	0.00%	0.000%
99	15.764	4484	4486	4488	rBV3	1702	1090	0.00%	0.000%
100	15.992	4549	4557	4571	rVB2	48906	78992	0.03%	0.009%

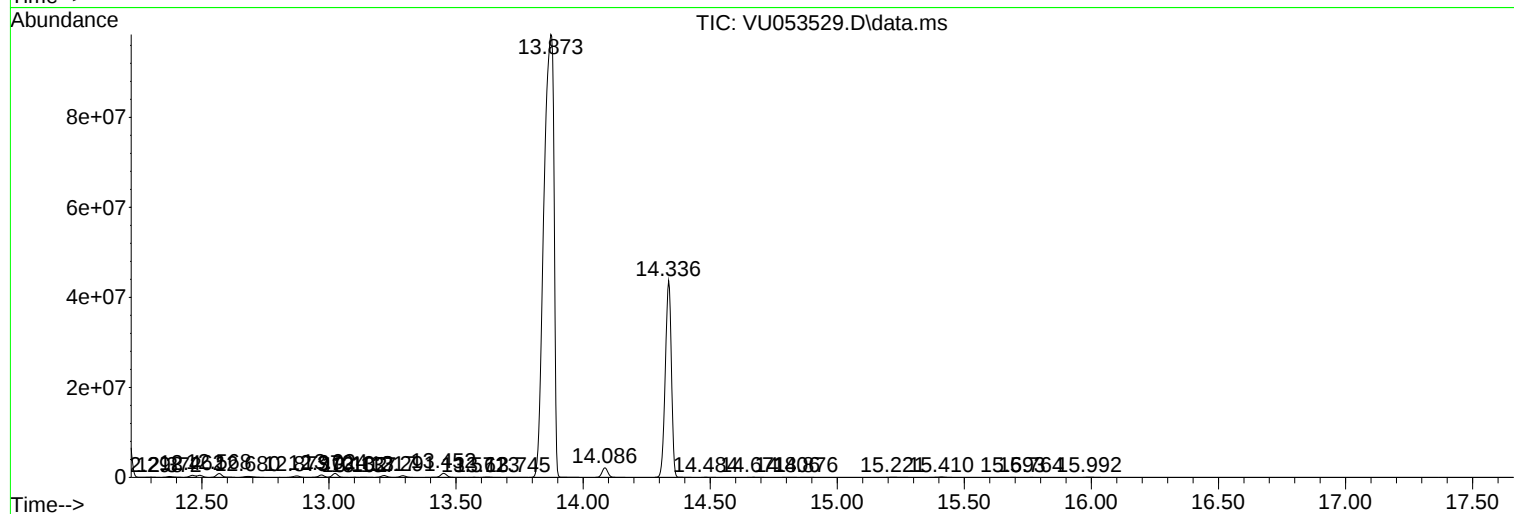
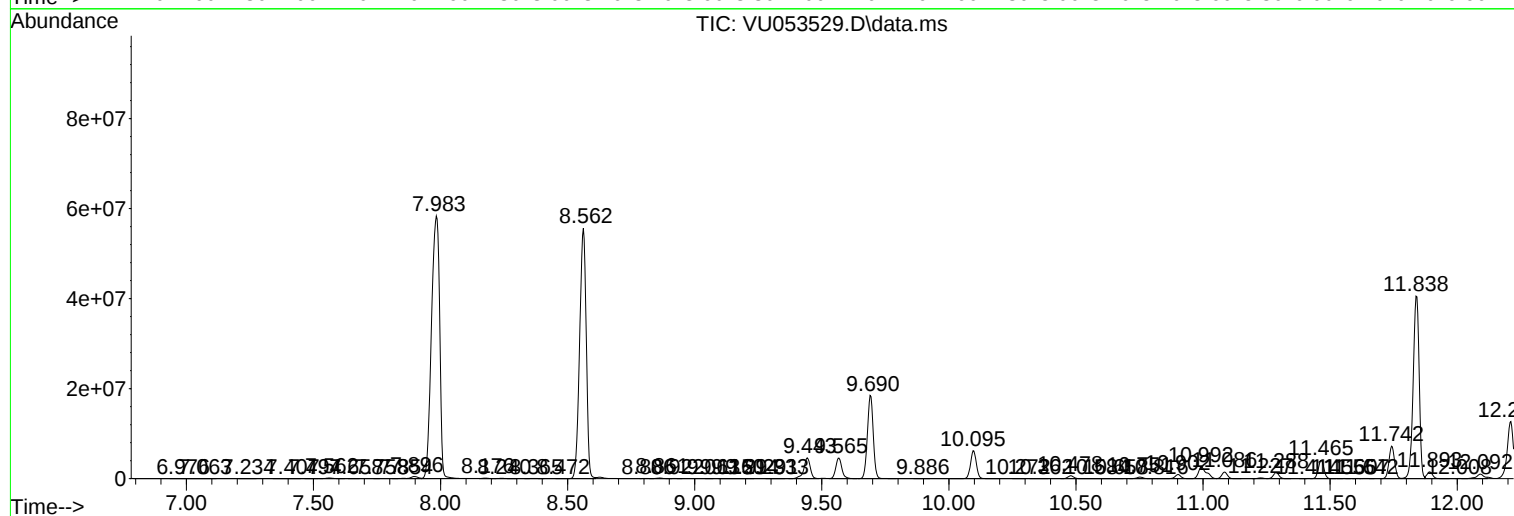
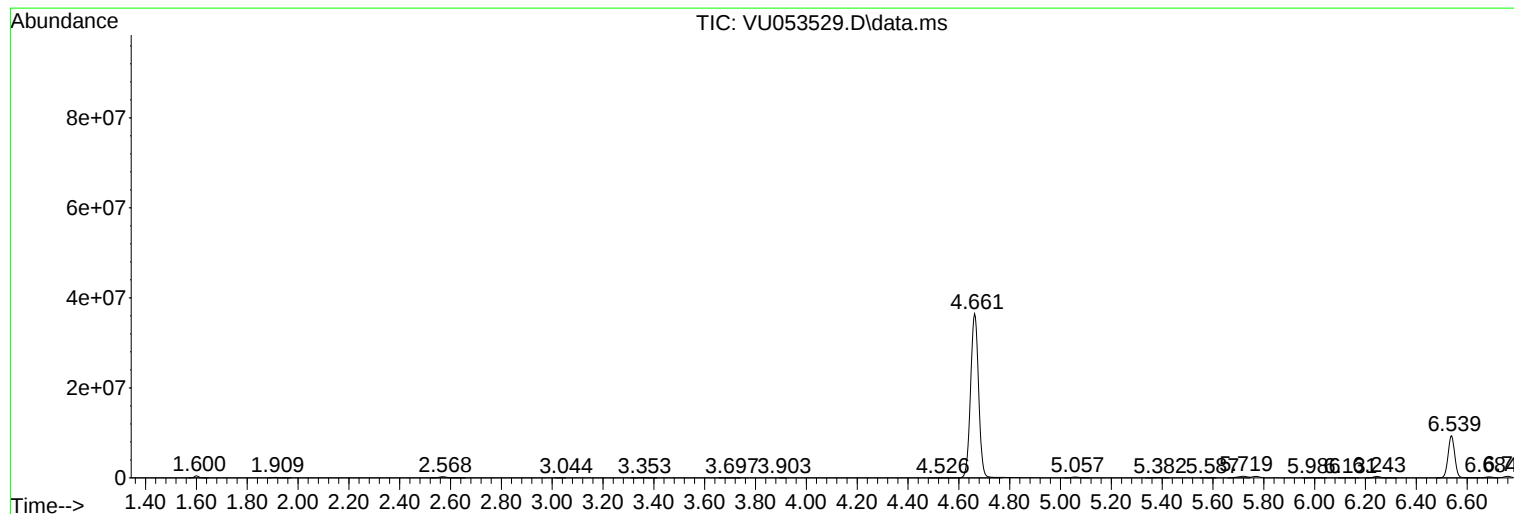
Sum of corrected areas: 869448519

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Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PMW-5(20230329)

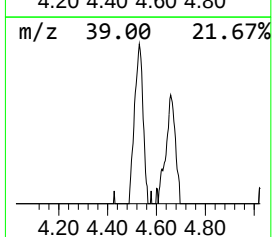
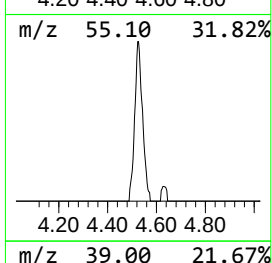
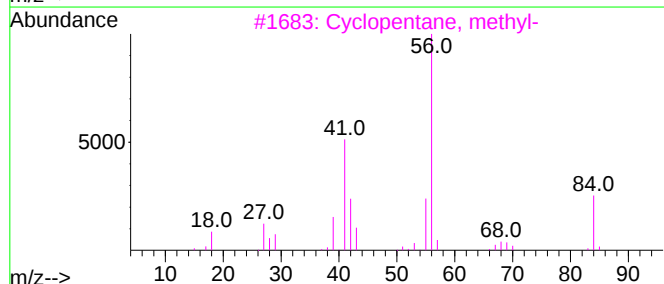
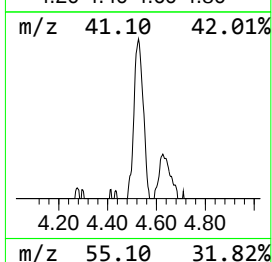
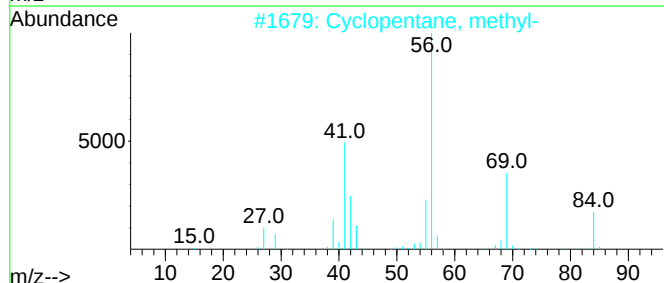
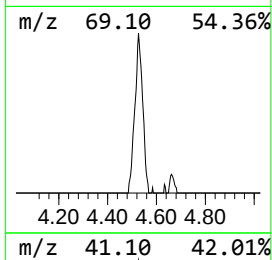
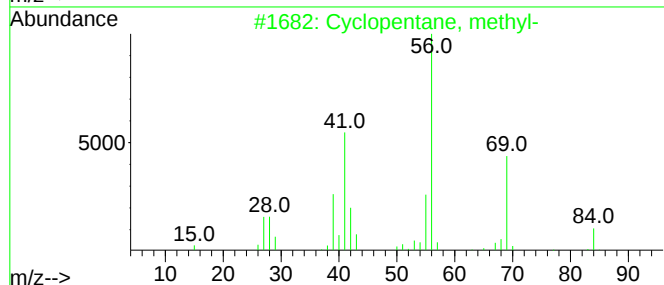
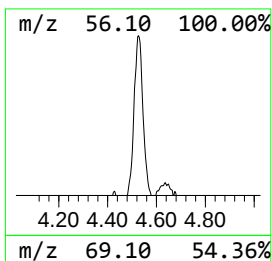
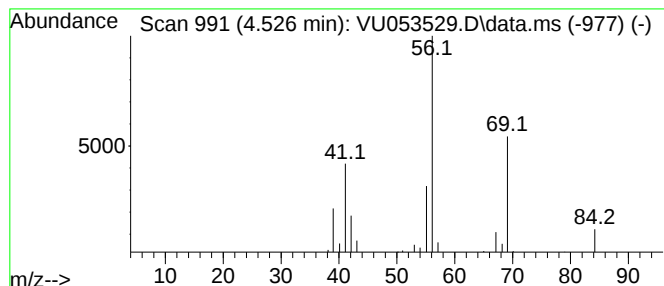
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.526 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.526	3.77 ug/L	44807	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



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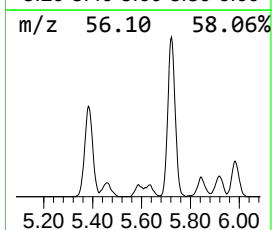
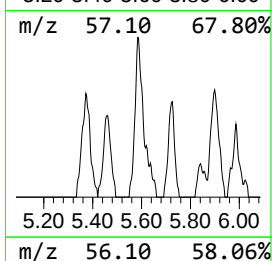
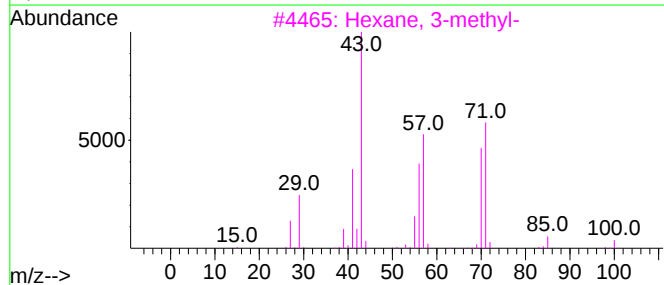
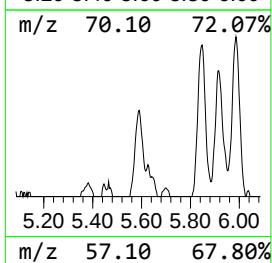
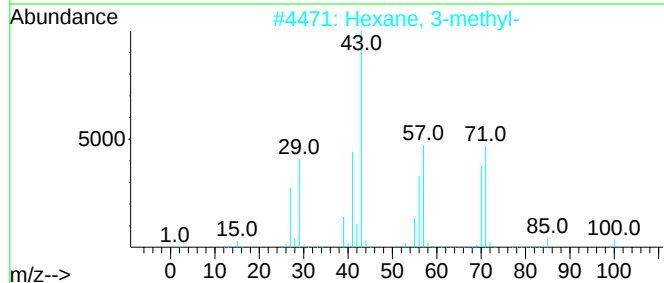
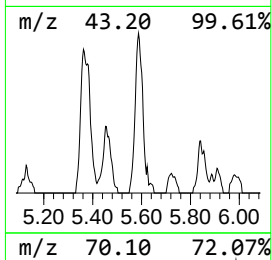
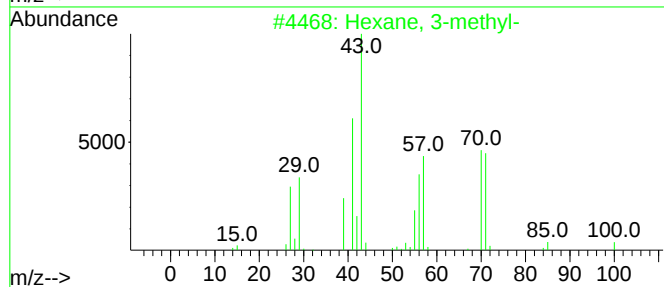
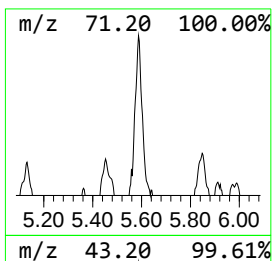
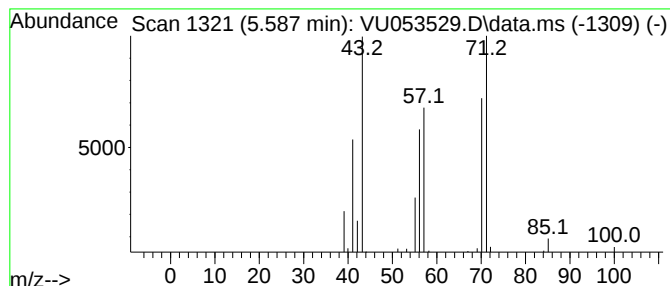
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.587	3.06 ug/L	36333	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	87
4			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	53



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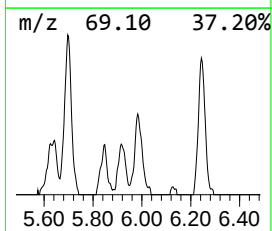
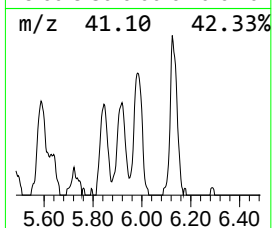
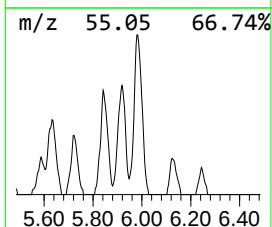
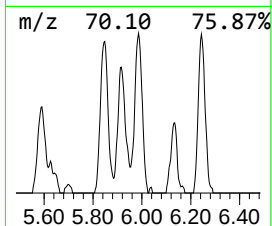
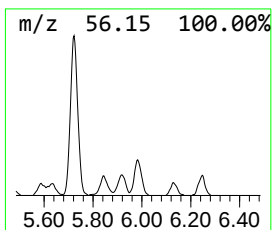
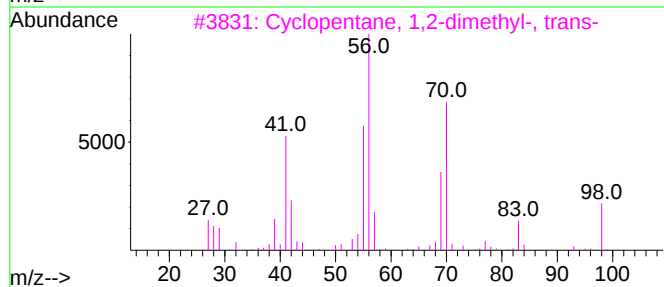
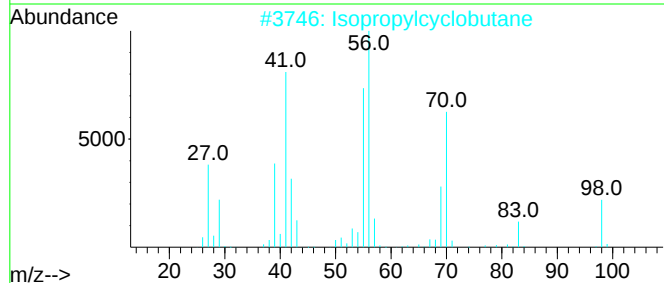
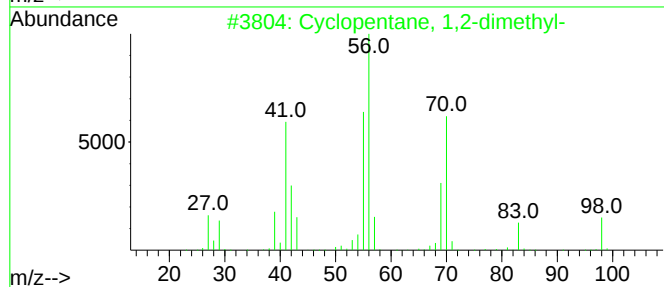
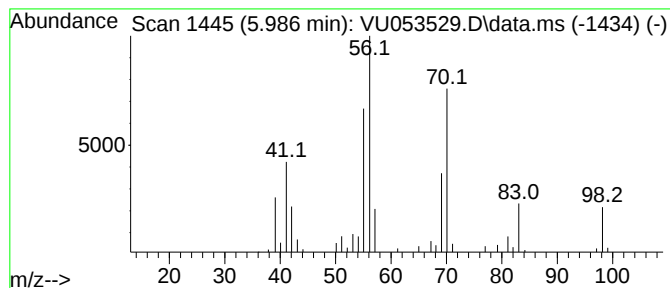
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic5.986 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.986	5.37 ug/L	63805	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
2			Isopropylcyclobutane	98	C7H14	000872-56-0	90
3			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	90
4			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	87
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053529.D
Acq On : 03 Apr 2023 18:49
Operator : JC/MD
Sample : 02158-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

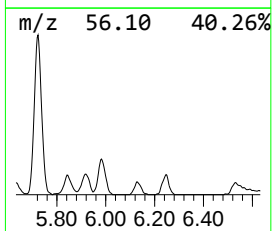
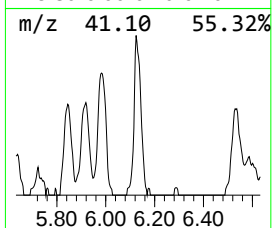
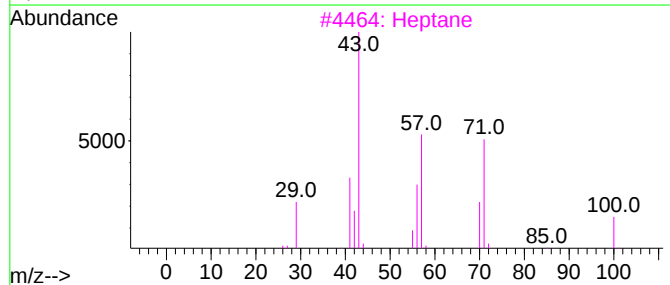
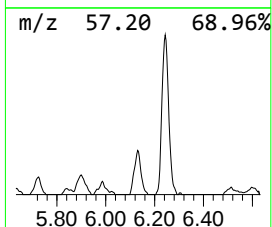
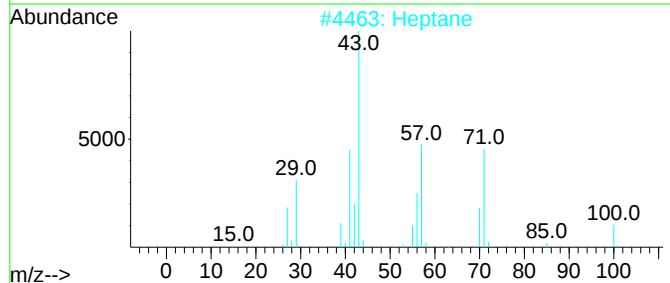
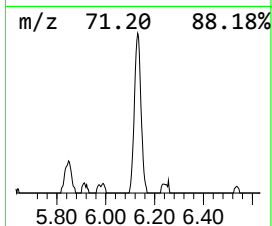
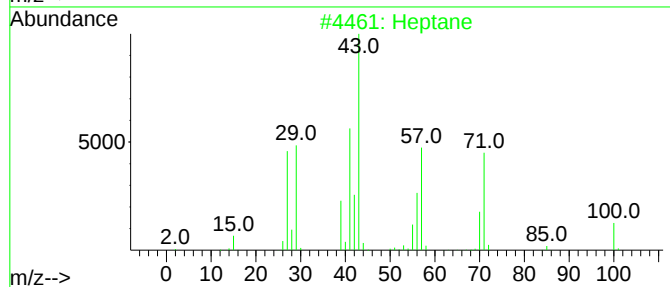
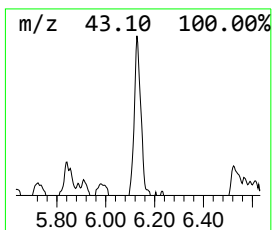
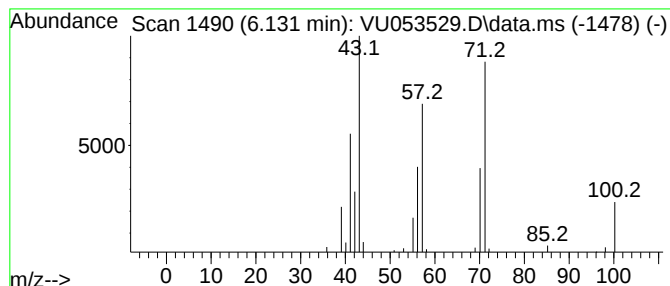
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.131	3.78 ug/L	44961	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane	100	C7H16	000142-82-5	91
2		Heptane	100	C7H16	000142-82-5	90
3		Heptane	100	C7H16	000142-82-5	87
4		Heptane	100	C7H16	000142-82-5	87
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053529.D
Acq On : 03 Apr 2023 18:49
Operator : JC/MD
Sample : 02158-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

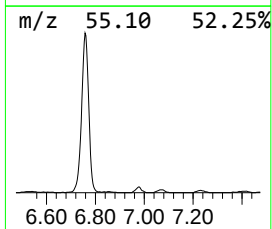
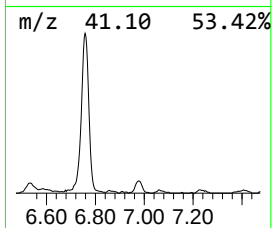
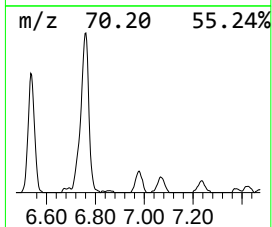
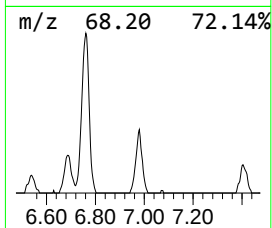
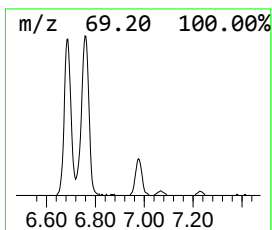
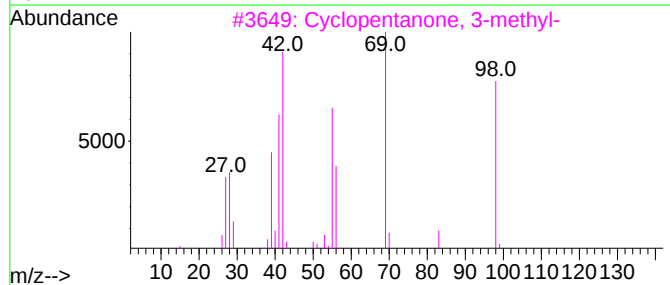
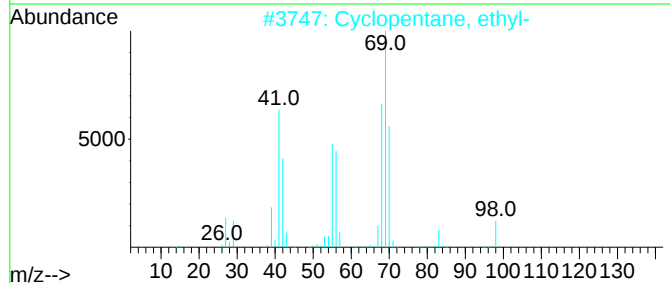
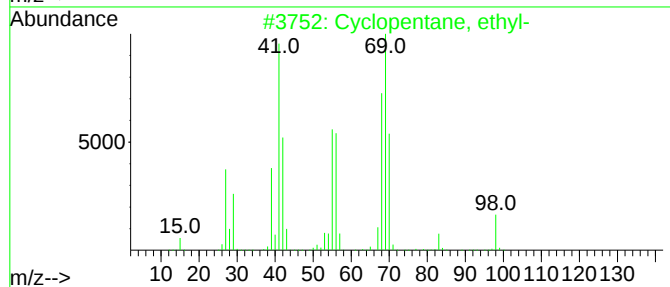
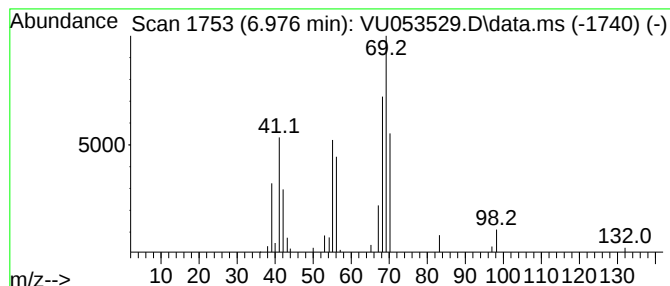
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic6.976 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.976	2.93 ug/L	34803	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, ethyl-	98	C7H14	001640-89-7	90
2			Cyclopentane, ethyl-	98	C7H14	001640-89-7	90
3			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	46
4			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	46
5			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053529.D
Acq On : 03 Apr 2023 18:49
Operator : JC/MD
Sample : 02158-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

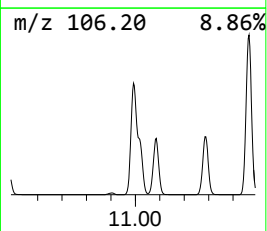
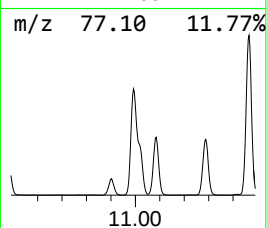
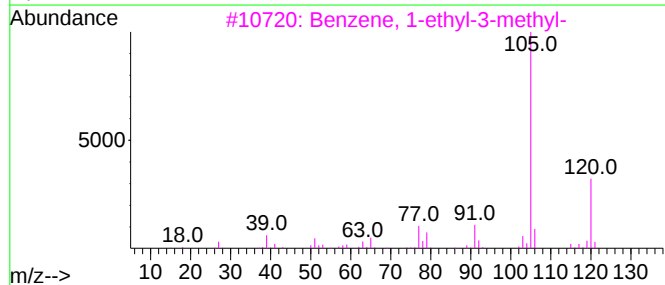
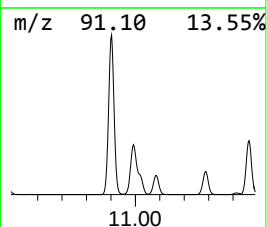
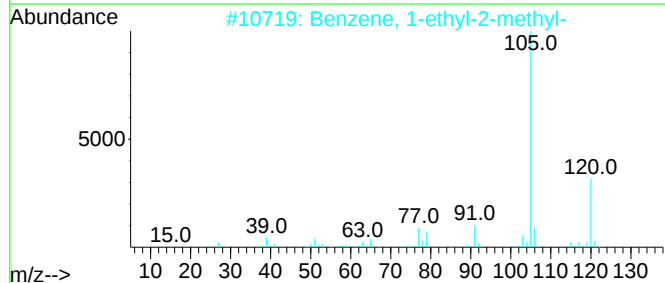
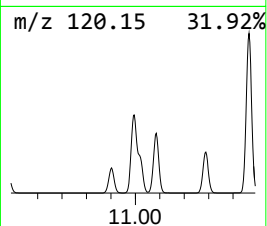
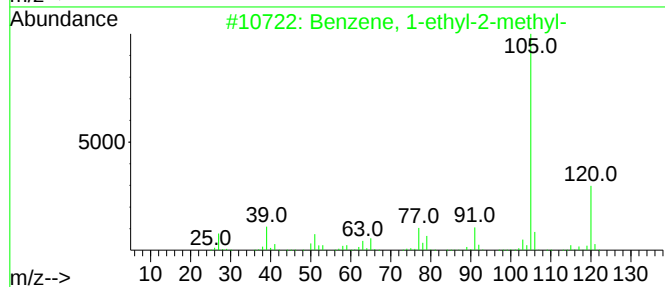
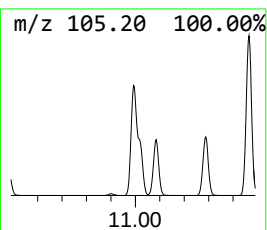
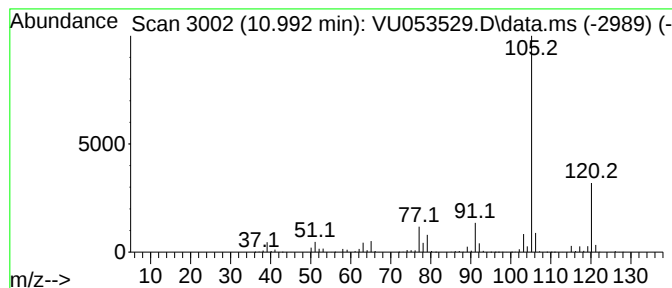
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Quant Title : VOC Analysis

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	4.32 ug/L	5737850	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053529.D
Acq On : 03 Apr 2023 18:49
Operator : JC/MD
Sample : 02158-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

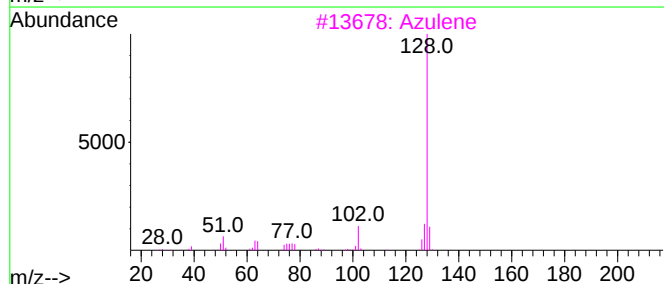
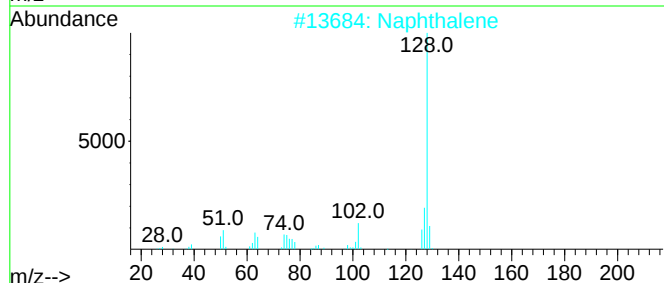
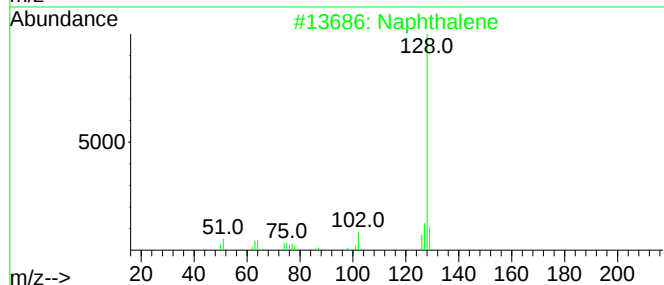
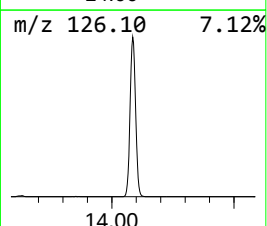
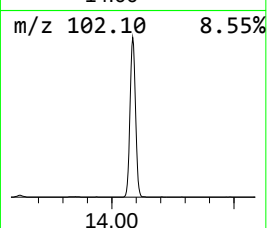
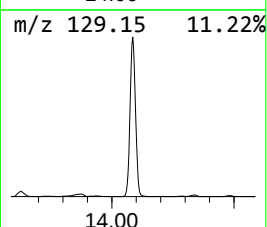
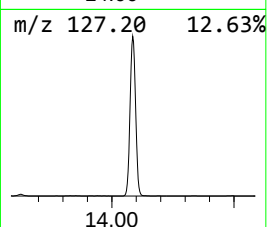
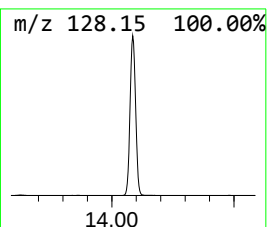
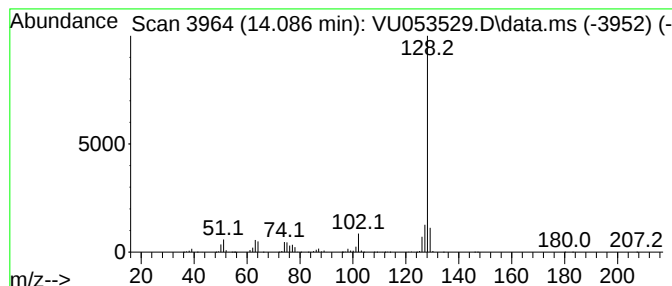
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Quant Title : VOC Analysis

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

Peak Number 9 Azulene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	2.50 ug/L	3328130	1,4-Dichlorobenzene-d4	11.812

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			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053529.D
Acq On : 03 Apr 2023 18:49
Operator : JC/MD
Sample : 02158-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-5(20230329)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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: C...	4.526	3.8	ug/L	44807	1	6.243	594210	50.0
(DEL) Alkane: S...	5.587	3.1	ug/L	36333	1	6.243	594210	50.0
(DEL) Alkane: C...	5.986	5.4	ug/L	63805	1	6.243	594210	50.0
(DEL) Alkane: S...	6.131	3.8	ug/L	44961	1	6.243	594210	50.0
(DEL) Alkane: C...	6.976	2.9	ug/L	34803	1	6.243	594210	50.0
Benzene, 1-ethy...	10.992	4.3	ug/L	5737850	3	11.812	66429800	50.0
Azulene	14.086	2.5	ug/L	3328130	3	11.812	66429800	50.0