

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
 Data File : VV025873.D
 Acq On : 10 May 2022 20:19
 Operator : SY/MD
 Sample : N2746-06ME
 Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBSL2ME

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_V\Method\SFAMVLM051022WMA.M
 Title : VOC Analysis

Signal : TIC: VV025873.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	78	83	94	rVB	30897	36540	19.49%	4.197%
2	2.944	587	592	594	rBV3	420	361	0.19%	0.041%
3	2.976	599	602	604	rBV3	495	314	0.17%	0.036%
4	3.008	607	612	613	rBV3	338	258	0.14%	0.030%
5	3.079	632	634	637	rBV	285	154	0.08%	0.018%
6	3.117	644	646	652	rBV2	216	245	0.13%	0.028%
7	3.191	665	669	671	rVB3	289	175	0.09%	0.020%
8	3.211	671	675	678	rBV2	275	185	0.10%	0.021%
9	3.240	679	684	686	rBV2	345	264	0.14%	0.030%
10	3.288	692	699	702	rBV2	712	550	0.29%	0.063%
11	3.397	729	733	734	rVV2	398	276	0.15%	0.032%
12	3.436	739	745	747	rBV	395	335	0.18%	0.038%
13	3.455	747	751	752	rBV	278	156	0.08%	0.018%
14	3.793	850	856	860	rBV3	428	430	0.23%	0.049%
15	3.822	860	865	867	rBV2	290	241	0.13%	0.028%
16	3.966	896	910	912	rBV3	5685	9441	5.04%	1.084%
17	4.577	1098	1100	1102	rBV2	507	305	0.16%	0.035%
18	4.667	1126	1128	1130	rBV	360	159	0.08%	0.018%
19	4.709	1139	1141	1145	rBV2	463	256	0.14%	0.029%
20	4.757	1154	1156	1158	rBV	305	162	0.09%	0.019%
21	4.834	1177	1180	1182	rBV2	442	279	0.15%	0.032%
22	4.957	1212	1218	1222	rBV3	397	490	0.26%	0.056%
23	5.043	1231	1245	1273	rBV2	74448	187441	100.00%	21.528%
24	5.240	1303	1306	1309	rBV3	228	152	0.08%	0.017%
25	5.349	1329	1340	1343	rBV6	4512	8223	4.39%	0.944%
26	5.503	1387	1388	1392	rVB2	526	180	0.10%	0.021%
27	5.529	1393	1396	1398	rVV3	456	199	0.11%	0.023%
28	5.625	1417	1426	1441	rBV2	9330	20158	10.75%	2.315%
29	5.802	1478	1481	1483	rBV	265	178	0.09%	0.020%
30	5.883	1504	1506	1509	rVB3	442	205	0.11%	0.024%
31	5.912	1509	1515	1522	rBV5	2372	4566	2.44%	0.524%
32	6.005	1535	1544	1546	rBV7	1776	2724	1.45%	0.313%
33	6.072	1555	1565	1588	rVB2	35991	79747	42.55%	9.159%
34	6.201	1602	1605	1607	rBV3	628	324	0.17%	0.037%
35	6.214	1607	1609	1612	rVB2	338	201	0.11%	0.023%
36	6.249	1615	1620	1622	rBV3	346	304	0.16%	0.035%

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 ClientSampleId :
 DBSL2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
 Title : VOC Analysis

37	6.262	1622	1624	1630	rVB2	553	453	0.24%	0.052%
38	6.291	1630	1633	1636	rBV2	386	246	0.13%	0.028%
39	6.333	1643	1646	1651	rVB2	519	319	0.17%	0.037%
40	6.439	1673	1679	1680	rBV	238	163	0.09%	0.019%
41	6.468	1685	1688	1692	rBV	316	250	0.13%	0.029%
42	6.526	1702	1706	1709	rBV2	184	155	0.08%	0.018%
43	6.577	1720	1722	1725	rBV	296	188	0.10%	0.022%
44	6.590	1725	1726	1732	rVB	380	195	0.10%	0.022%
45	6.619	1732	1735	1737	rBV	369	205	0.11%	0.024%
46	6.641	1737	1742	1744	rBV3	1537	1197	0.64%	0.137%
47	6.744	1771	1774	1781	rVB4	658	618	0.33%	0.071%
48	6.789	1786	1788	1791	rBV3	369	211	0.11%	0.024%
49	6.876	1811	1815	1817	rBV2	392	309	0.16%	0.035%
50	6.947	1833	1837	1840	rBV2	328	213	0.11%	0.024%
51	6.995	1841	1852	1874	rBV2	15245	33674	17.97%	3.868%
52	7.133	1893	1895	1901	rVB3	303	230	0.12%	0.026%
53	7.162	1901	1904	1910	rVB2	359	264	0.14%	0.030%
54	7.220	1918	1922	1924	rBV2	422	241	0.13%	0.028%
55	7.236	1924	1927	1928	rBV2	536	276	0.15%	0.032%
56	7.317	1943	1952	1972	rBV2	62670	121582	64.86%	13.964%
57	7.551	2023	2025	2028	rBV	411	254	0.14%	0.029%
58	7.632	2040	2050	2071	rBV2	9641	21860	11.66%	2.511%
59	7.773	2092	2094	2098	rBV2	557	390	0.21%	0.045%
60	7.799	2098	2102	2104	rBV2	671	527	0.28%	0.061%
61	7.918	2135	2139	2141	rBV2	348	226	0.12%	0.026%
62	8.130	2192	2205	2234	rBV2	13415	50730	27.06%	5.827%
63	8.378	2279	2282	2288	rBV3	644	489	0.26%	0.056%
64	8.423	2293	2296	2299	rBV3	734	606	0.32%	0.070%
65	8.493	2314	2318	2321	rVB2	503	364	0.19%	0.042%
66	8.519	2321	2326	2329	rBV2	283	278	0.15%	0.032%
67	8.564	2338	2340	2343	rVB	264	155	0.08%	0.018%
68	8.632	2358	2361	2364	rBV2	220	176	0.09%	0.020%
69	8.712	2381	2386	2388	rBV2	288	262	0.14%	0.030%
70	8.751	2395	2398	2400	rBV2	353	213	0.11%	0.024%
71	8.792	2404	2411	2413	rBV2	237	248	0.13%	0.028%
72	8.863	2423	2433	2454	rBV	13822	28342	15.12%	3.255%
73	9.040	2486	2488	2492	rVB	494	262	0.14%	0.030%
74	9.111	2507	2510	2513	rBV2	221	158	0.08%	0.018%
75	9.400	2598	2600	2605	rVB2	395	180	0.10%	0.021%
76	9.526	2635	2639	2642	rBV2	322	288	0.15%	0.033%

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Instrument :
 MSVOA_V
 ClientSampleId :
 DBSL2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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_V\Method\SFAMVLM051022WMA.M
 Title : VOC Analysis

77	9.706	2693	2695	2699	rVB2	375	178	0.09%	0.020%
78	9.815	2725	2729	2730	rBV	224	152	0.08%	0.017%
79	9.863	2739	2744	2748	rVB3	464	387	0.21%	0.044%
80	9.972	2775	2778	2780	rBV	438	203	0.11%	0.023%
81	10.011	2786	2790	2794	rVB	228	169	0.09%	0.019%
82	10.223	2843	2856	2869	rBV	39694	70934	37.84%	8.147%
83	10.416	2911	2916	2919	rBV2	286	284	0.15%	0.033%
84	10.583	2960	2968	2972	rBV4	1671	2480	1.32%	0.285%
85	10.673	2994	2996	2998	rBV2	325	161	0.09%	0.018%
86	10.699	3001	3004	3009	rVV2	368	289	0.15%	0.033%
87	11.259	3169	3178	3194	rVB3	14848	24715	13.19%	2.839%
88	11.374	3212	3214	3215	rBV2	349	180	0.10%	0.021%
89	11.490	3247	3250	3254	rBV2	312	330	0.18%	0.038%
90	11.532	3256	3263	3273	rVB3	4465	6586	3.51%	0.756%
91	11.628	3282	3293	3313	rBV	57212	93409	49.83%	10.728%
92	11.812	3348	3350	3355	rVB	379	172	0.09%	0.020%
93	12.011	3408	3412	3413	rBV2	367	239	0.13%	0.027%
94	12.133	3447	3450	3451	rBV2	290	159	0.08%	0.018%
95	12.439	3541	3545	3546	rBV	298	207	0.11%	0.024%
96	12.545	3576	3578	3581	rBV2	504	230	0.12%	0.026%
97	12.966	3707	3709	3713	rVB2	409	190	0.10%	0.022%
98	13.056	3734	3737	3740	rVB2	570	302	0.16%	0.035%
99	13.503	3866	3876	3891	rBV	26683	45340	24.19%	5.208%
100	13.985	4024	4026	4027	rBV	486	195	0.10%	0.022%

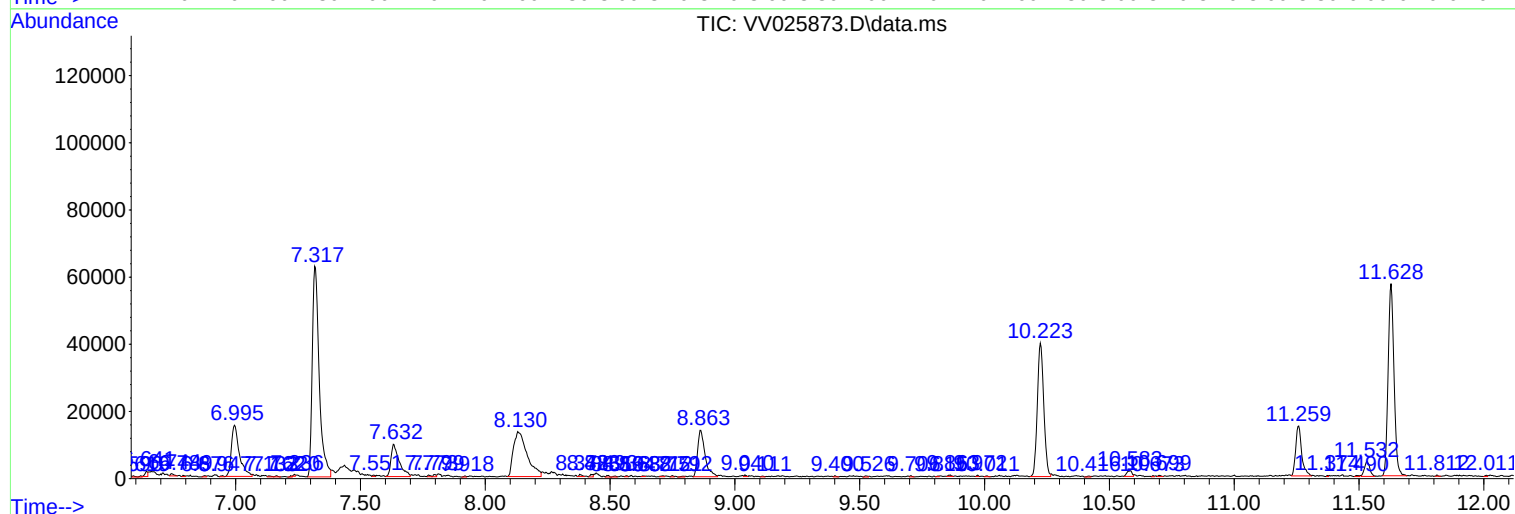
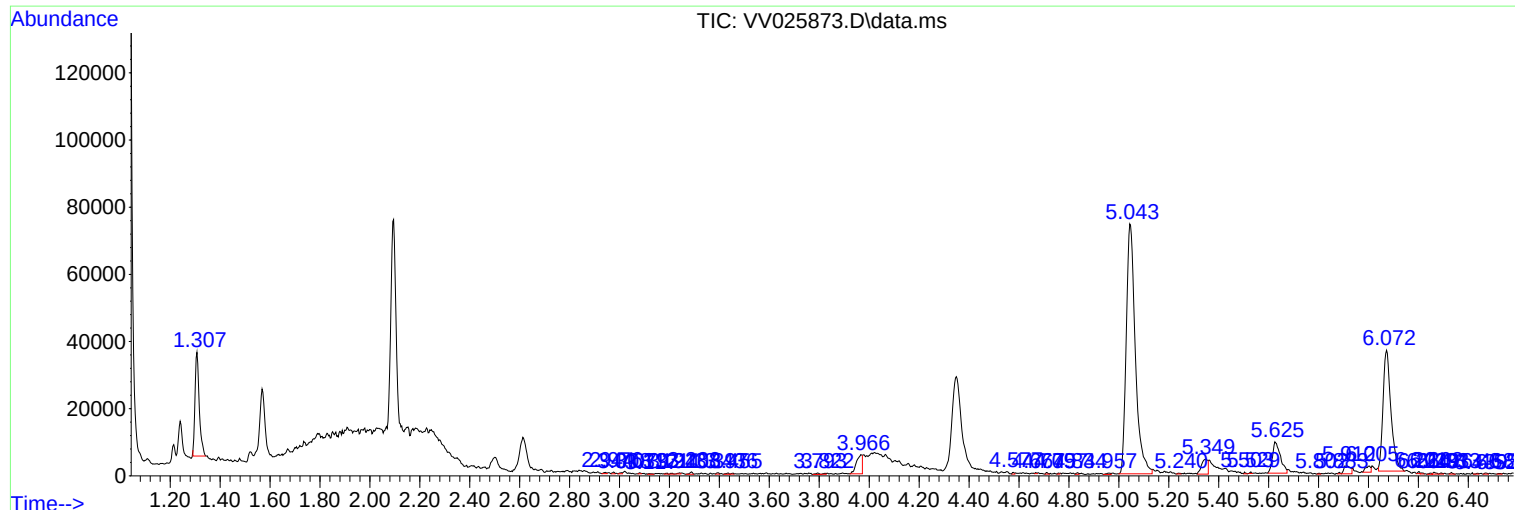
Sum of corrected areas: 870666

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBSL2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSL2ME

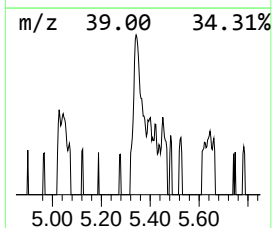
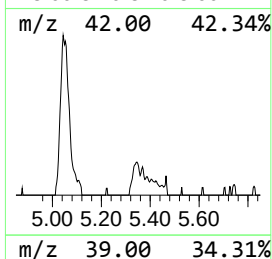
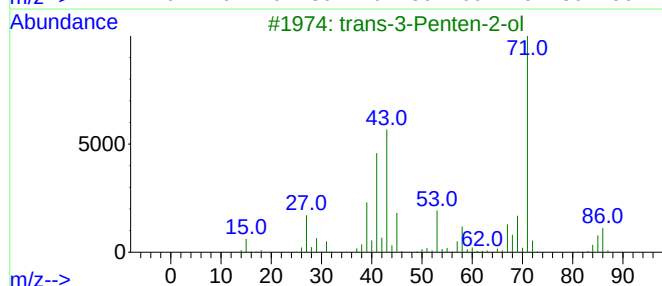
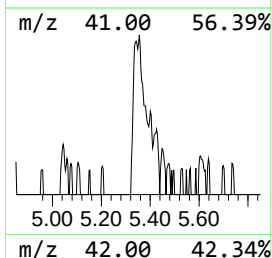
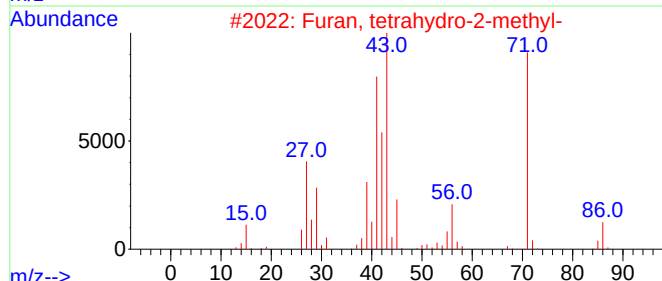
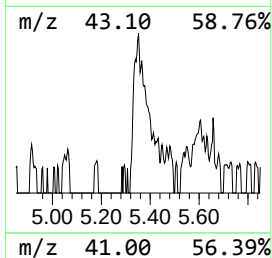
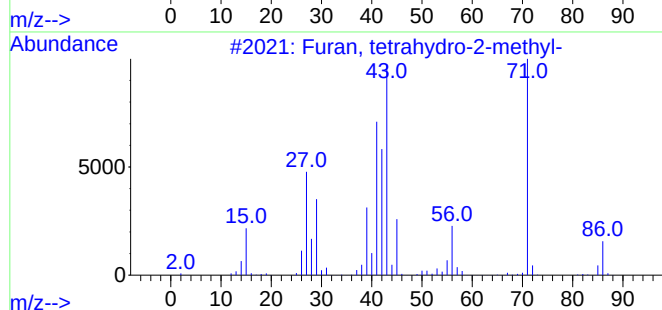
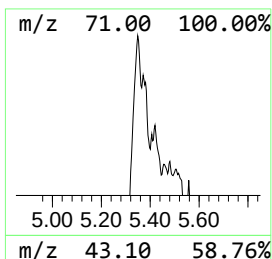
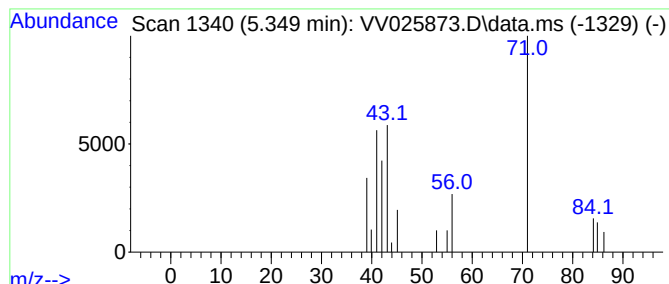
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Furan, tetrahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.349	20.40 ug/L	8223	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	58
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	49
3			trans-3-Penten-2-ol	86	C5H10O	003899-34-1	28
4			Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	27
5			3-Penten-2-ol	86	C5H10O	001569-50-2	23



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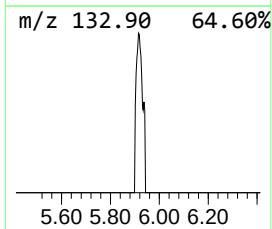
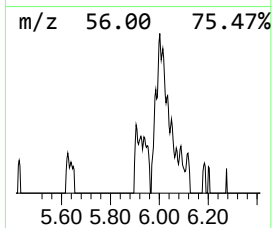
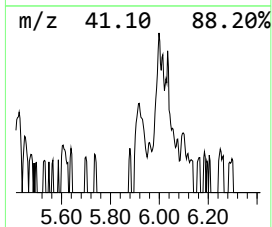
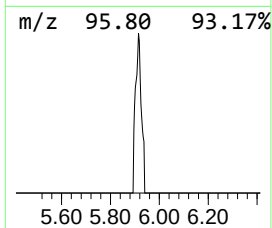
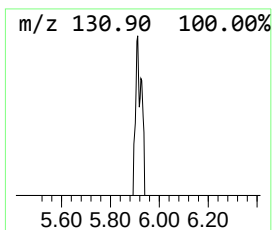
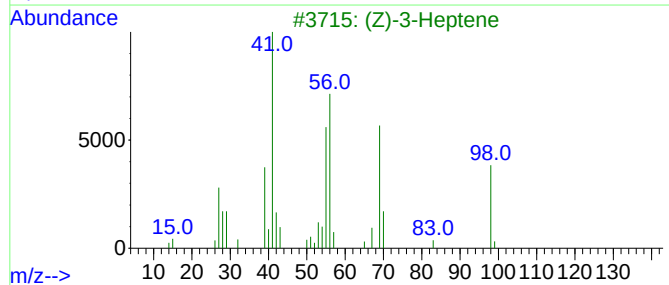
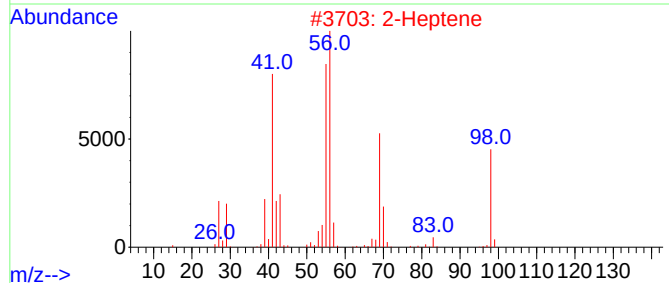
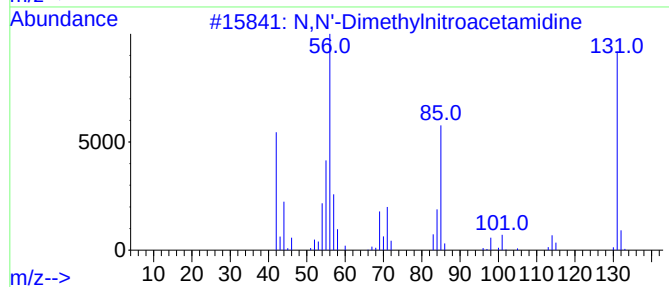
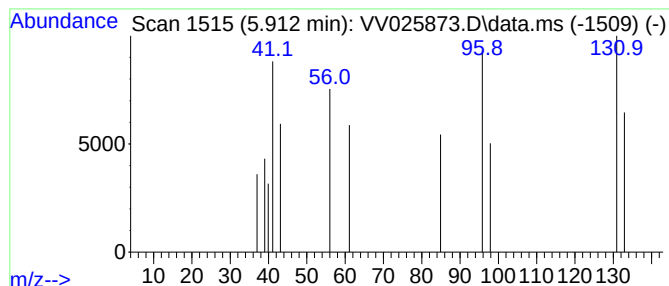
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.912	11.33 ug/L	4566	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N'-Dimethylnitroacetamide	131	C4H9N3O2	054252-45-8	32
2			2-Heptene	98	C7H14	000592-77-8	9
3			(Z)-3-Heptene	98	C7H14	007642-10-6	9
4			Propane, 1,2-bis(difluoroamino)-...	160	C4H8F4N2	016063-24-4	9
5			trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	9



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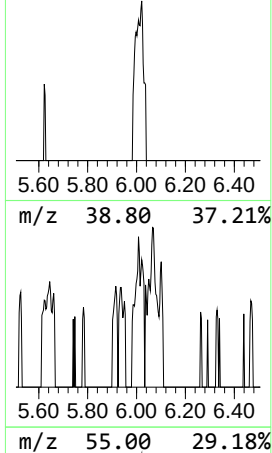
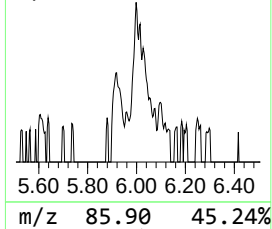
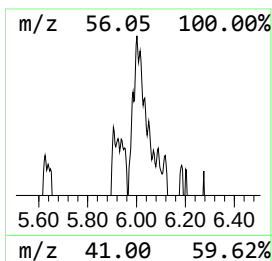
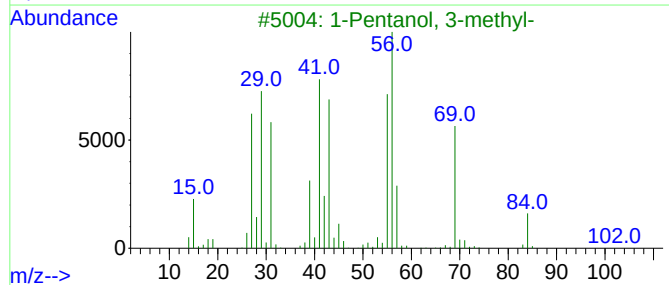
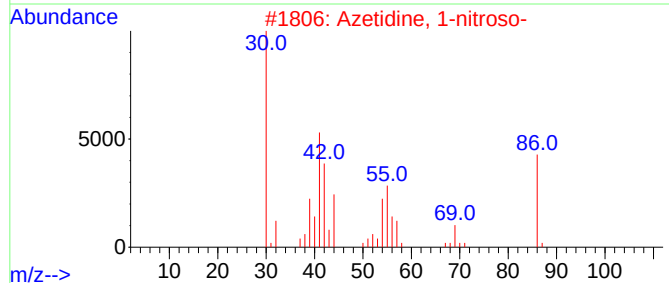
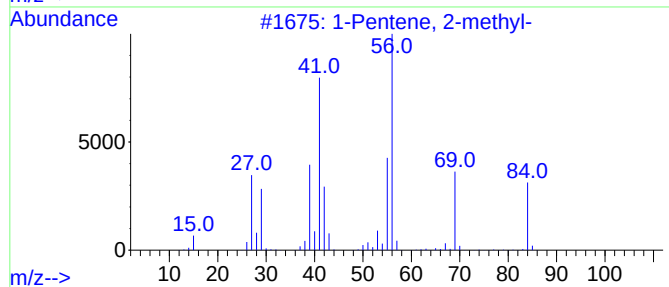
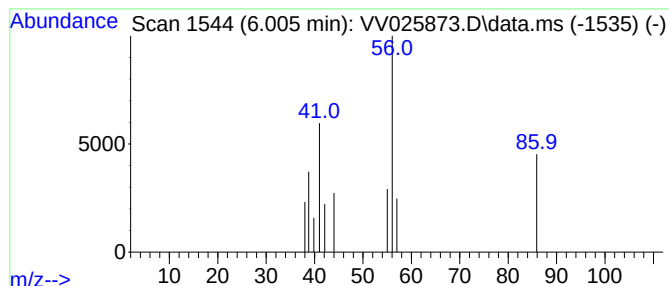
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.005	6.76 ug/L	2724	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	12
2			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
3			1-Pentanol, 3-methyl-	102	C6H14O	000589-35-5	9
4			Butyl aldoxime, 2-methyl-, syn-	101	C5H11NO	049805-56-3	9
5			2-Butenal, (E)-	70	C4H6O	000123-73-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025873.D
Acq On : 10 May 2022 20:19
Operator : SY/MD
Sample : N2746-06ME
Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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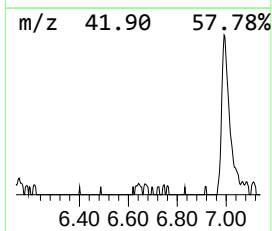
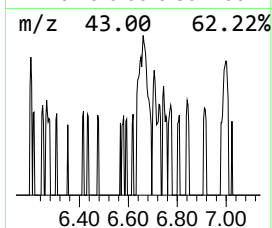
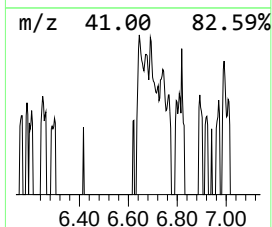
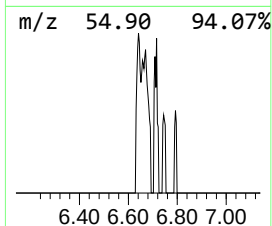
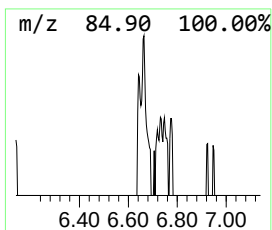
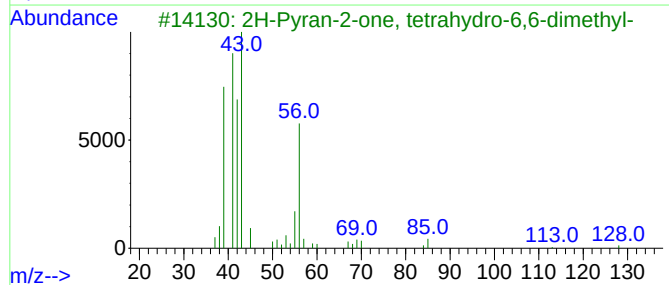
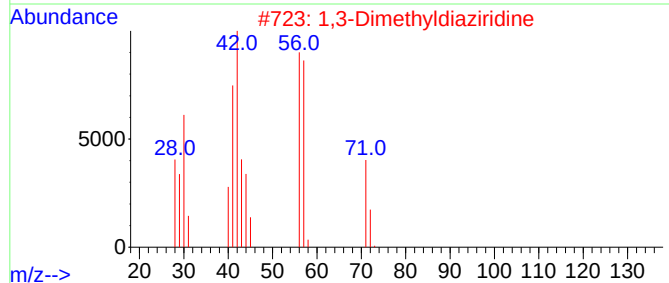
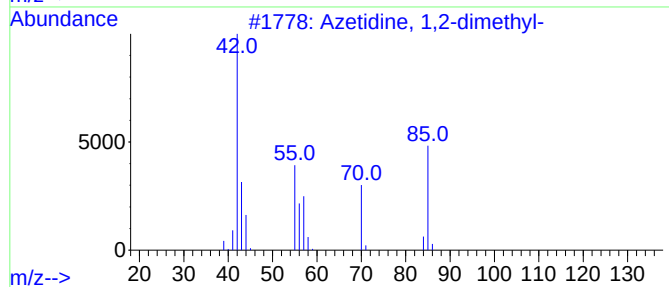
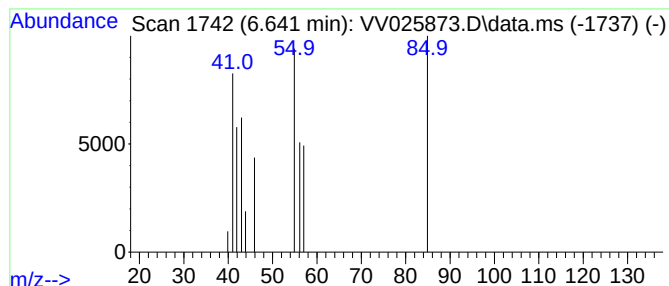
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Quant Title : VOC Analysis

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

Peak Number 4 Azetidine, 1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.641	2.97 ug/L	1197	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	50
2			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	12
3			2H-Pyran-2-one, tetrahydro-6,6-d...	128	C7H12O2	002610-95-9	9
4			Oxalic acid, isohexyl propyl ester	216	C11H20O4	1000309-32-6	9
5			1,5-Pentanediol, 3-methyl-	118	C6H14O2	004457-71-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025873.D
Acq On : 10 May 2022 20:19
Operator : SY/MD
Sample : N2746-06ME
Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSL2ME

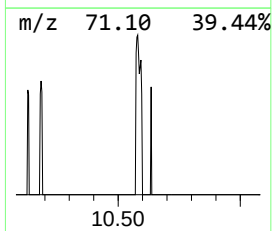
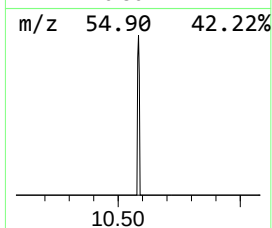
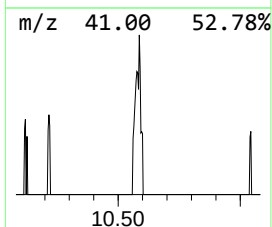
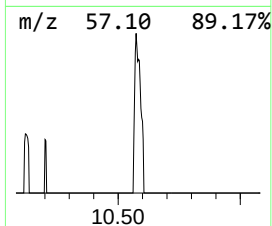
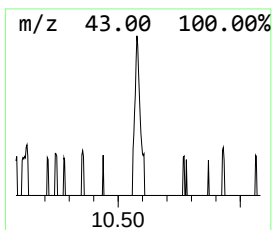
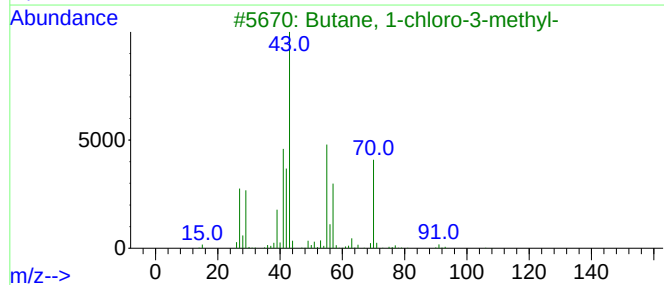
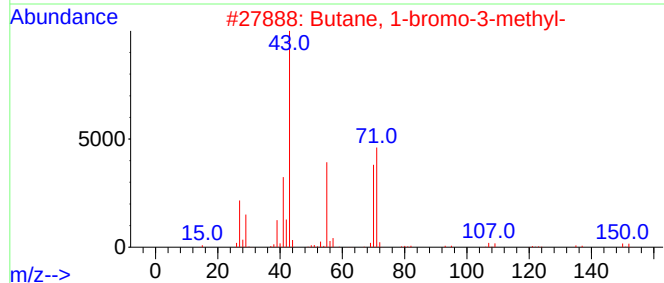
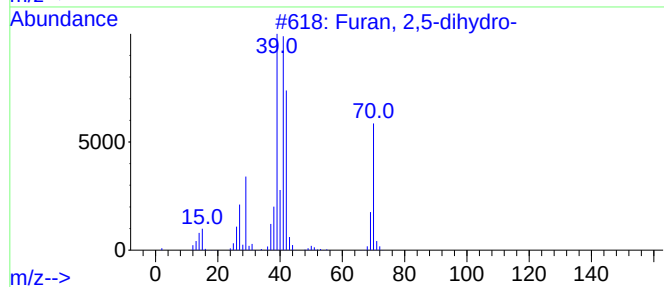
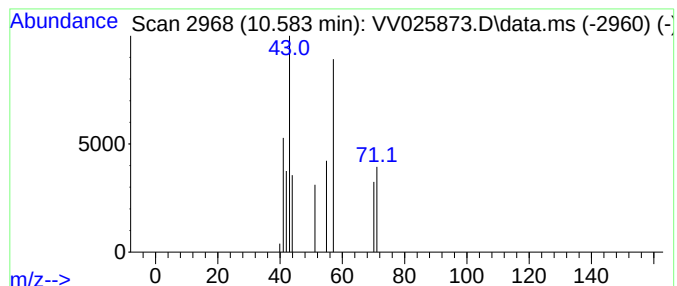
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.583	5.02 ug/L	2480	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	9
2			Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	9
3			Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	8
4			Ethoxyacetylene	70	C4H6O	000927-80-0	7
5			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025873.D
Acq On : 10 May 2022 20:19
Operator : SY/MD
Sample : N2746-06ME
Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSL2ME

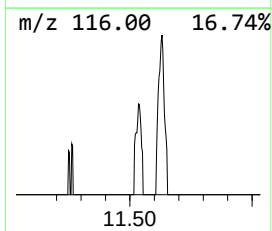
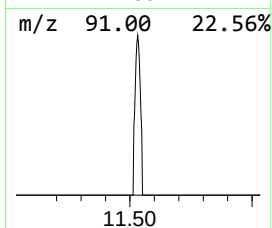
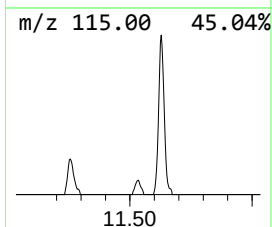
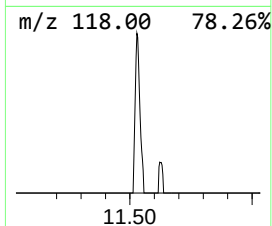
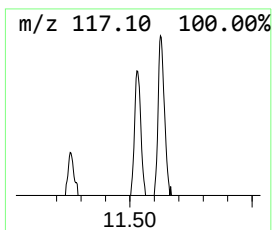
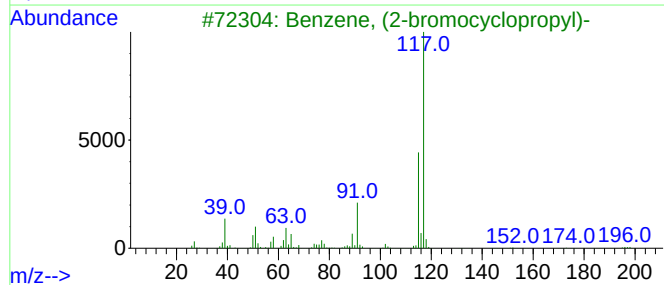
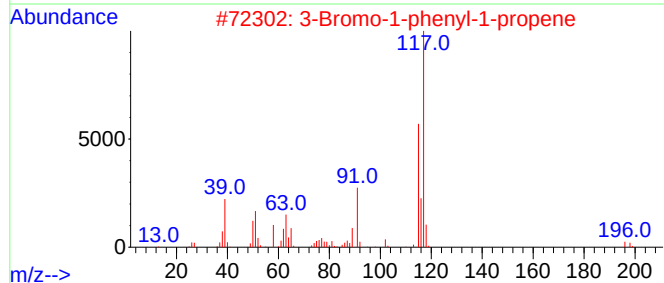
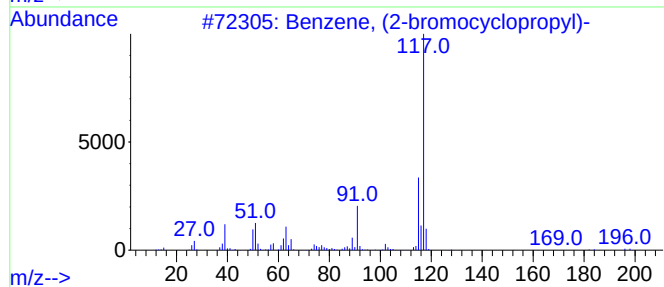
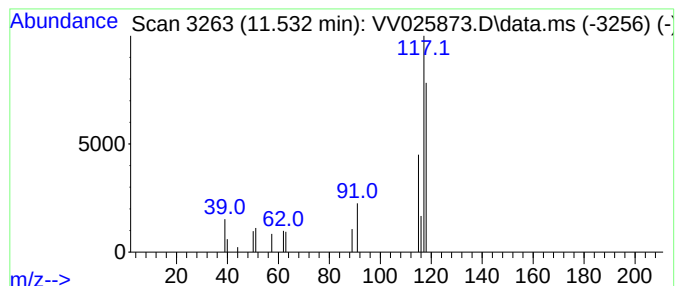
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Quant Title : VOC Analysis

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

Peak Number 7 Benzene, (2-bromocyclopropyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.532	13.32 ug/L	6586	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
2			3-Bromo-1-phenyl-1-propene	196	C9H9Br	004392-24-9	47
3			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43
4			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	43
5			1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025873.D
Acq On : 10 May 2022 20:19
Operator : SY/MD
Sample : N2746-06ME
Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSL2ME

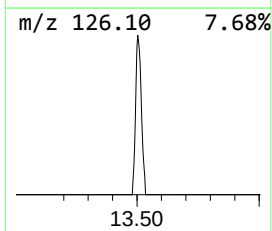
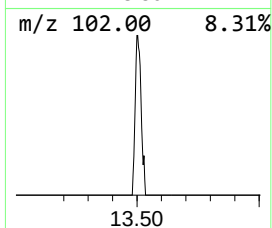
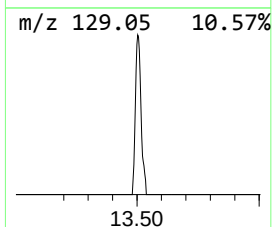
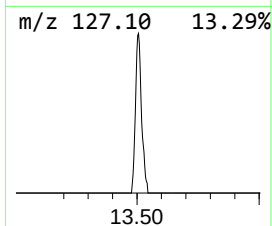
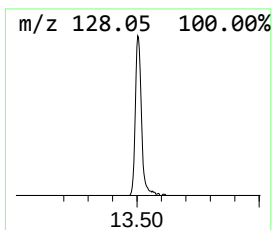
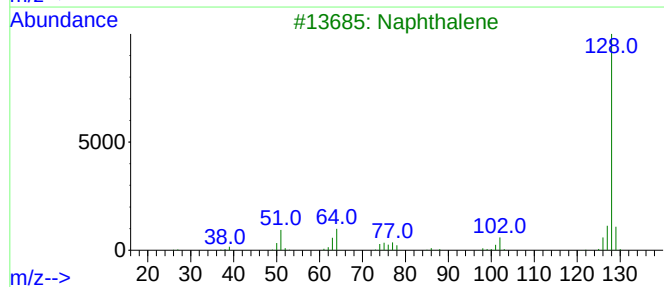
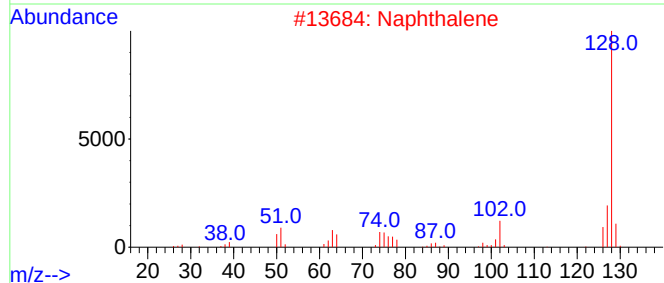
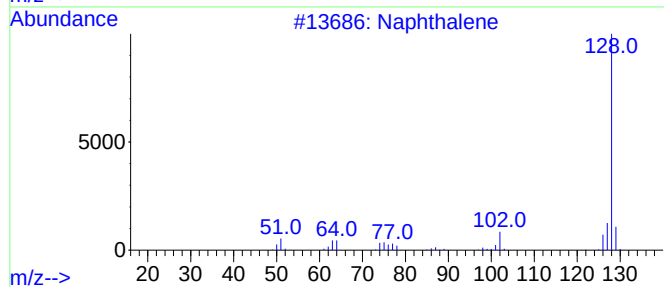
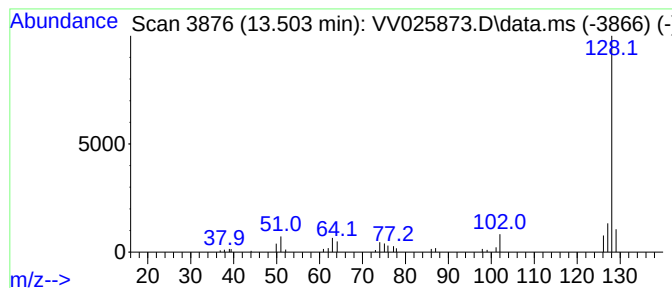
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Quant Title : VOC Analysis

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

Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.503	91.73 ug/L	45340	1,4-Dichlorobenzene-d4	11.259

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			Naphthalene	128	C10H8	000091-20-3	93
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025873.D
Acq On : 10 May 2022 20:19
Operator : SY/MD
Sample : N2746-06ME
Misc : 5.56g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSL2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Furan, tetrahyd...	5.349	20.4	ug/L	8223	1	5.629	20158	50.0
unknown-01	5.912	11.3	ug/L	4566	1	5.629	20158	50.0
(DEL) Alkane: S...	6.005	6.8	ug/L	2724	1	5.629	20158	50.0
Azetidine, 1,2-...	6.641	3.0	ug/L	1197	1	5.629	20158	50.0
unknown-02	10.583	5.0	ug/L	2480	3	11.259	24715	50.0
Benzene, (2-bro...	11.532	13.3	ug/L	6586	3	11.259	24715	50.0
Azulene	13.503	91.7	ug/L	45340	3	11.259	24715	50.0