

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
 Data File : VV036977.D
 Acq On : 19 Aug 2024 14:56
 Operator : SY/MD
 Sample : P3593-02 10X
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCXW3

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\SFAMVLM080224WMA.M
 Title : VOC Analysis

Signal : TIC: VV036977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	92	rBV	341997	360846	13.63%	1.597%
2	1.532	146	153	172	rVB	290824	345049	13.03%	1.527%
3	2.060	307	317	326	rBV	599517	861426	32.53%	3.813%
4	2.111	326	333	359	rVB	451460	723488	27.32%	3.202%
5	2.442	430	436	451	rVB2	55713	89442	3.38%	0.396%
6	3.336	711	714	716	rBV4	1055	733	0.03%	0.003%
7	3.445	745	748	751	rVB5	1647	1102	0.04%	0.005%
8	3.462	751	753	756	rBV4	1555	1009	0.04%	0.004%
9	3.481	756	759	765	rVV6	1639	1601	0.06%	0.007%
10	3.507	765	767	770	rVV4	1422	1032	0.04%	0.005%
11	3.535	774	776	779	rVB3	1011	649	0.02%	0.003%
12	3.661	811	815	818	rBV6	1966	1334	0.05%	0.006%
13	3.764	844	847	848	rBV3	1988	1114	0.04%	0.005%
14	3.799	848	858	879	rBV	163655	437863	16.53%	1.938%
15	4.085	943	947	949	rBV5	1595	1059	0.04%	0.005%
16	4.117	955	957	960	rBV3	1358	618	0.02%	0.003%
17	4.179	971	976	978	rBV6	1686	1296	0.05%	0.006%
18	4.246	978	997	1021	rVV2	418512	1053238	39.77%	4.662%
19	4.362	1030	1033	1036	rBV4	1536	1172	0.04%	0.005%
20	4.478	1066	1069	1077	rVB8	1234	1526	0.06%	0.007%
21	4.516	1077	1081	1085	rBV6	2301	1816	0.07%	0.008%
22	4.535	1085	1087	1092	rVB5	884	725	0.03%	0.003%
23	4.596	1102	1106	1107	rBV3	984	673	0.03%	0.003%
24	4.625	1113	1115	1117	rBV3	1046	639	0.02%	0.003%
25	4.670	1124	1129	1133	rBV5	2062	1438	0.05%	0.006%
26	4.709	1138	1141	1146	rVB7	1532	1559	0.06%	0.007%
27	4.735	1146	1149	1152	rBV5	1872	1184	0.04%	0.005%
28	4.777	1158	1162	1164	rVB4	1022	651	0.02%	0.003%
29	4.950	1198	1216	1251	rBV2	1058470	2648376	100.00%	11.722%
30	5.162	1280	1282	1286	rVB4	1322	702	0.03%	0.003%
31	5.220	1292	1300	1318	rBV4	10834	26238	0.99%	0.116%
32	5.416	1358	1361	1363	rBV4	1063	746	0.03%	0.003%
33	5.429	1363	1365	1369	rVB4	1154	740	0.03%	0.003%
34	5.474	1371	1379	1383	rBV5	4511	6378	0.24%	0.028%
35	5.529	1386	1396	1419	rBV	735543	1499522	56.62%	6.637%
36	5.986	1527	1538	1559	rBV	599575	1188757	44.89%	5.261%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Title : VOC Analysis

37	6.268	1619	1626	1651	rVB	79759	182887	6.91%	0.809%
38	6.912	1815	1826	1857	rBV	341662	637790	24.08%	2.823%
39	7.117	1880	1890	1902	rBV	173514	305266	11.53%	1.351%
40	7.239	1917	1928	1953	rBV	1225134	2098441	79.24%	9.288%
41	7.551	2016	2025	2055	rBV	224454	407348	15.38%	1.803%
42	7.770	2091	2093	2099	rBV7	1389	1089	0.04%	0.005%
43	7.802	2101	2103	2106	rBV4	1620	768	0.03%	0.003%
44	7.857	2110	2120	2136	rBV	336145	564696	21.32%	2.499%
45	7.950	2142	2149	2159	rBV2	31030	57569	2.17%	0.255%
46	8.021	2159	2171	2203	rVV3	748429	1455429	54.96%	6.442%
47	8.616	2345	2356	2382	rBV	317996	516043	19.49%	2.284%
48	8.780	2395	2407	2438	rBV	1179419	1974857	74.57%	8.741%
49	9.156	2522	2524	2529	rBV6	1002	621	0.02%	0.003%
50	9.333	2568	2579	2591	rBV	14916	29622	1.12%	0.131%
51	9.481	2622	2625	2626	rBV2	1341	751	0.03%	0.003%
52	9.747	2705	2708	2711	rBV3	1598	1064	0.04%	0.005%
53	9.821	2728	2731	2733	rBV3	1807	1289	0.05%	0.006%
54	10.011	2786	2790	2791	rBV4	1010	728	0.03%	0.003%
55	10.149	2815	2833	2851	rBV	771837	1221125	46.11%	5.405%
56	10.284	2873	2875	2878	rBV3	1189	751	0.03%	0.003%
57	10.378	2900	2904	2906	rBV5	1014	770	0.03%	0.003%
58	10.503	2939	2943	2948	rBV6	2444	2213	0.08%	0.010%
59	10.545	2954	2956	2958	rBV3	1701	1000	0.04%	0.004%
60	10.632	2980	2983	2985	rBV4	1104	771	0.03%	0.003%
61	10.715	3006	3009	3013	rBV6	1426	1256	0.05%	0.006%
62	10.857	3045	3053	3055	rBV9	2205	3117	0.12%	0.014%
63	10.985	3090	3093	3095	rBV3	1190	742	0.03%	0.003%
64	11.120	3131	3135	3143	rBV9	3614	4588	0.17%	0.020%
65	11.181	3143	3154	3182	rBV	1203306	1902030	71.82%	8.418%
66	11.455	3237	3239	3242	rBV4	1764	941	0.04%	0.004%
67	11.500	3242	3253	3254	rBV9	5285	7096	0.27%	0.031%
68	11.554	3259	3270	3303	rVB	1176839	1892733	71.47%	8.377%
69	11.837	3353	3358	3360	rBV4	2046	1665	0.06%	0.007%
70	11.963	3391	3397	3401	rBV8	2257	2794	0.11%	0.012%
71	12.091	3435	3437	3440	rVB3	1369	759	0.03%	0.003%
72	12.117	3440	3445	3447	rBV6	1150	852	0.03%	0.004%
73	12.127	3447	3448	3454	rVB5	1386	968	0.04%	0.004%
74	12.159	3455	3458	3461	rBV5	895	639	0.02%	0.003%
75	12.188	3461	3467	3474	rBV7	4799	7614	0.29%	0.034%
76	12.252	3485	3487	3489	rBV3	1161	642	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
 Data File : VV036977.D
 Acq On : 19 Aug 2024 14:56
 Operator : SY/MD
 Sample : P3593-02 10X
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCXW3

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\SFAMVLM080224WMA.M
 Title : VOC Analysis

77	12.590	3588	3592	3596	rBV5	2115	2176	0.08%	0.010%
78	12.622	3599	3602	3606	rVV6	1606	1450	0.05%	0.006%
79	12.751	3639	3642	3647	rBV7	1079	944	0.04%	0.004%
80	12.779	3647	3651	3654	rVV5	1178	817	0.03%	0.004%
81	12.834	3657	3668	3671	rBV5	2521	3965	0.15%	0.018%
82	12.943	3699	3702	3704	rBV3	1514	979	0.04%	0.004%
83	13.050	3732	3735	3736	rBV3	1446	894	0.03%	0.004%
84	13.098	3744	3750	3756	rVB10	3046	4544	0.17%	0.020%
85	13.143	3759	3764	3765	rBV4	1646	1196	0.05%	0.005%
86	13.423	3848	3851	3853	rBV4	2101	1349	0.05%	0.006%
87	13.451	3858	3860	3861	rBV2	1574	632	0.02%	0.003%
88	13.577	3895	3899	3904	rBV8	2026	1973	0.07%	0.009%
89	13.648	3919	3921	3923	rBV3	933	615	0.02%	0.003%
90	13.757	3951	3955	3957	rBV3	1110	755	0.03%	0.003%
91	13.786	3961	3964	3966	rBV3	1324	794	0.03%	0.004%
92	13.876	3986	3992	3993	rBV6	1576	1340	0.05%	0.006%
93	13.985	4023	4026	4034	rVB5	4369	4602	0.17%	0.020%
94	14.114	4063	4066	4068	rBV3	1042	783	0.03%	0.003%
95	14.291	4119	4121	4125	rBV4	1248	692	0.03%	0.003%
96	14.342	4133	4137	4141	rBV6	2383	2245	0.08%	0.010%
97	14.406	4153	4157	4160	rBV5	1643	1299	0.05%	0.006%
98	14.847	4292	4294	4299	rVB5	1709	1115	0.04%	0.005%
99	14.947	4323	4325	4328	rBV3	1617	795	0.03%	0.004%
100	15.107	4373	4375	4376	rBV	1503	705	0.03%	0.003%

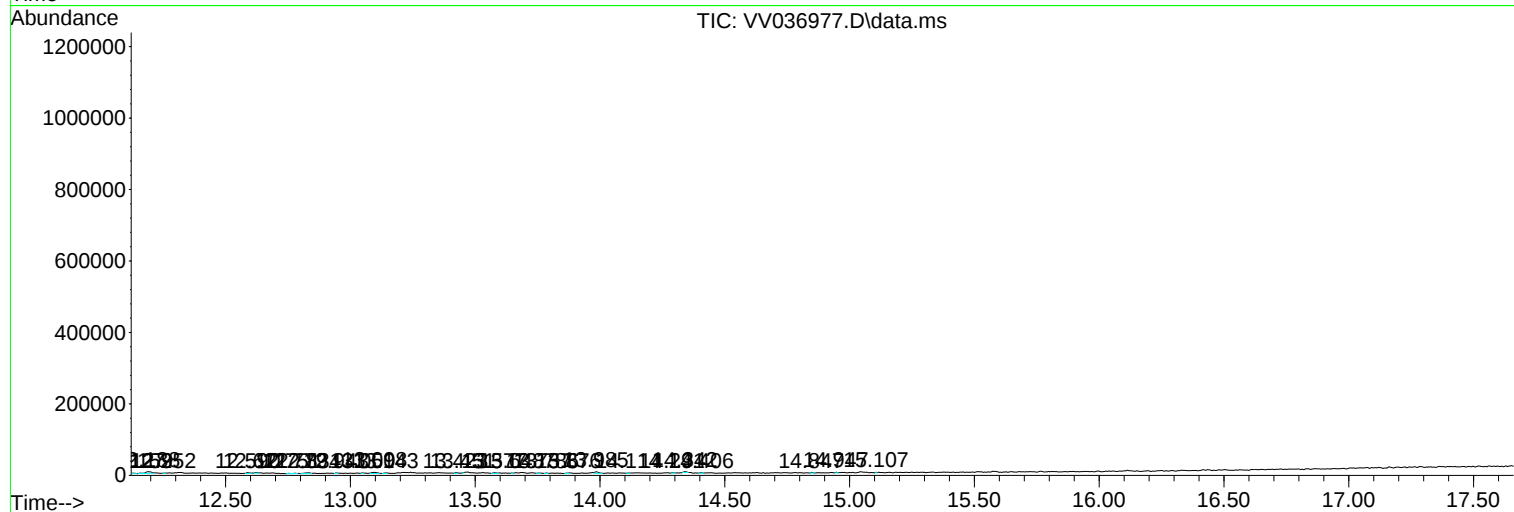
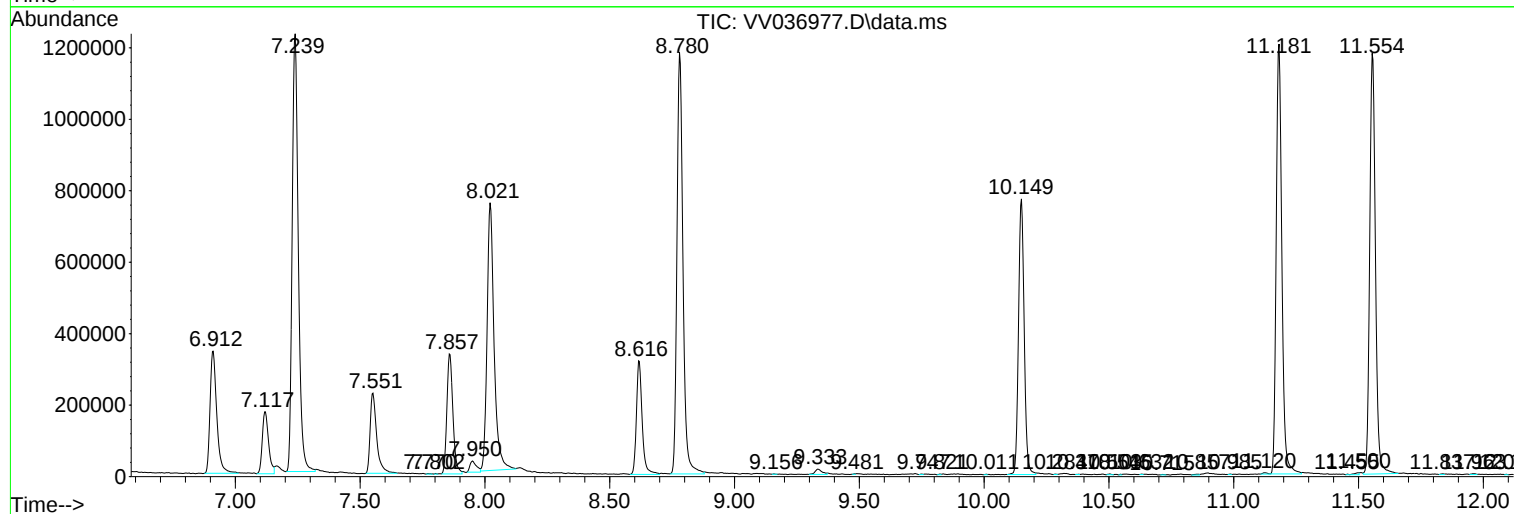
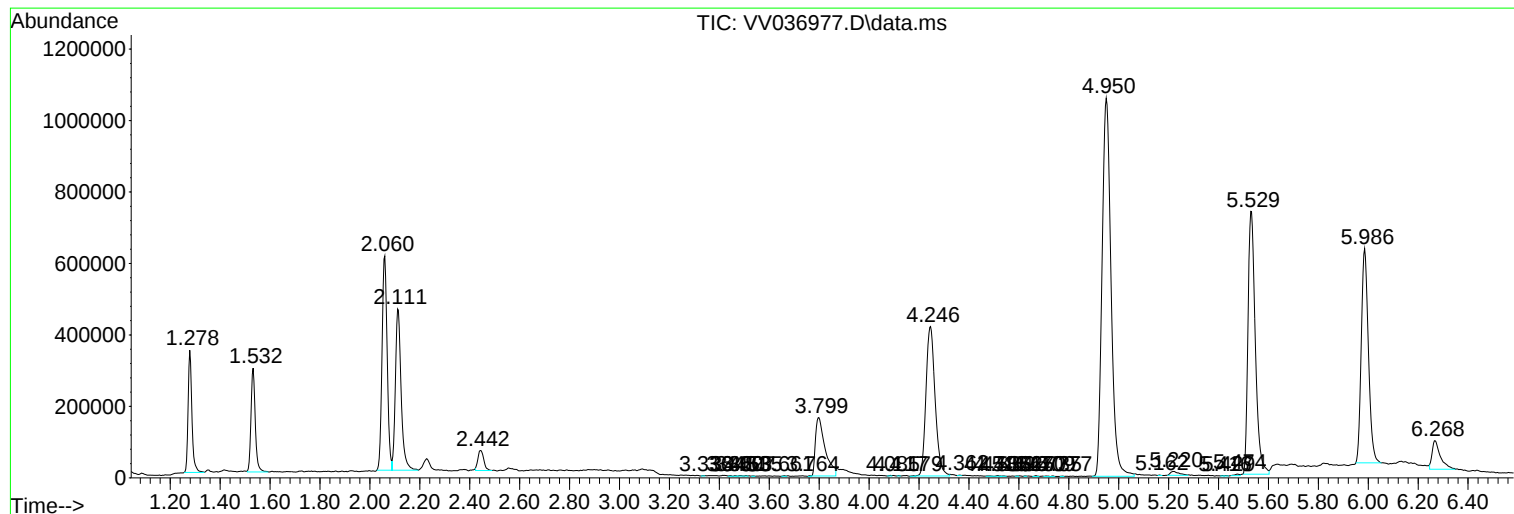
Sum of corrected areas: 22593724

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

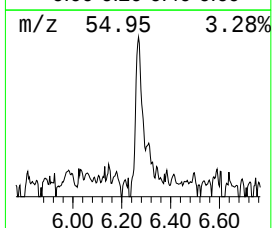
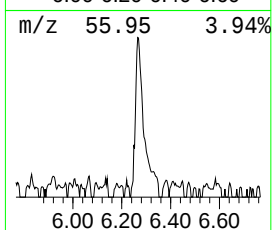
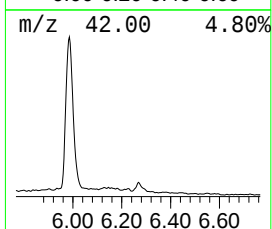
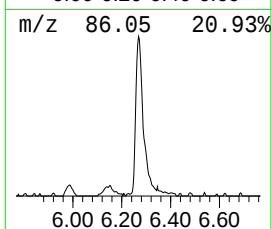
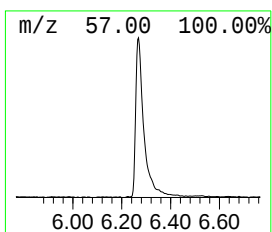
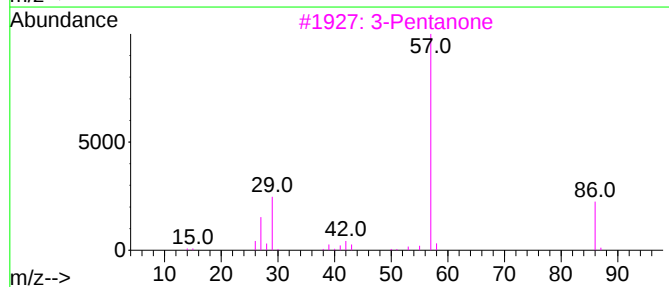
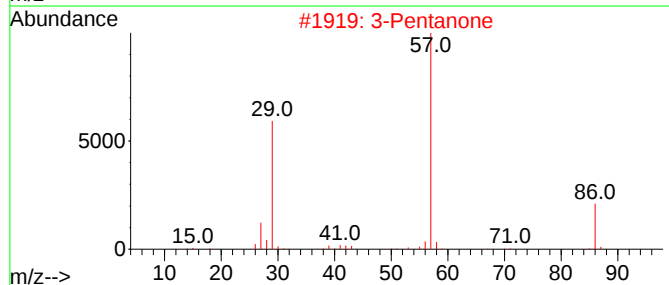
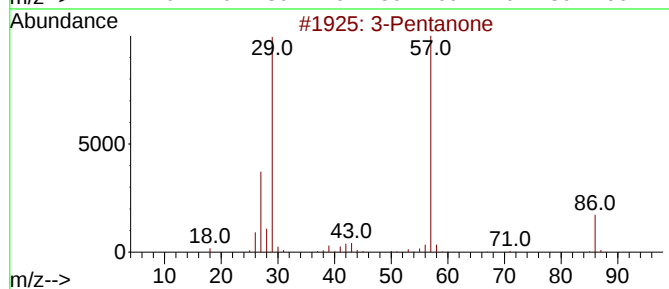
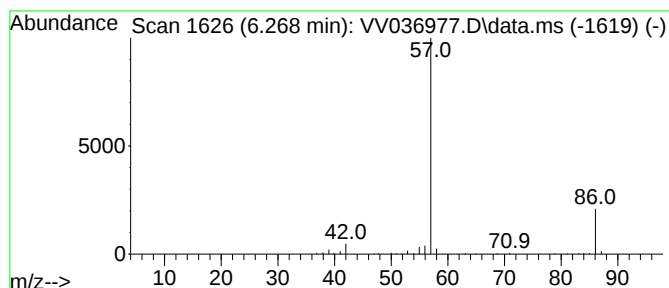
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 3-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.268	6.10 ug/L	182887	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone			86	C5H10O	000096-22-0	80
2	3-Pentanone			86	C5H10O	000096-22-0	72
3	3-Pentanone			86	C5H10O	000096-22-0	50
4	3-Pentanone			86	C5H10O	000096-22-0	9
5	2-Imidazolidinone			86	C3H6N2O	000120-93-4	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

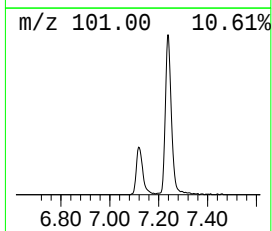
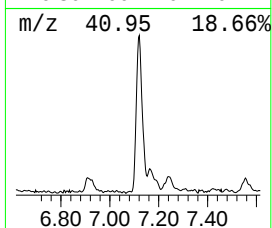
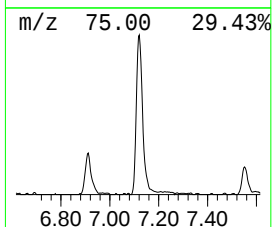
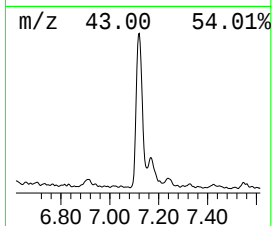
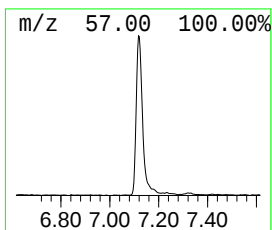
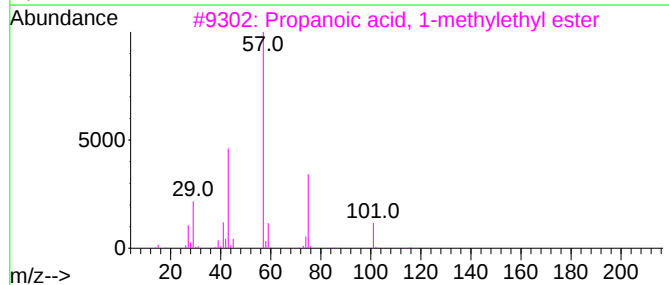
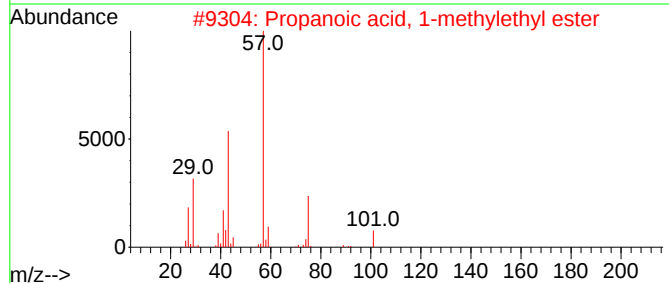
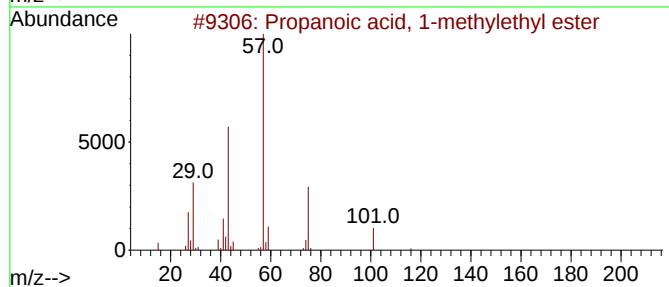
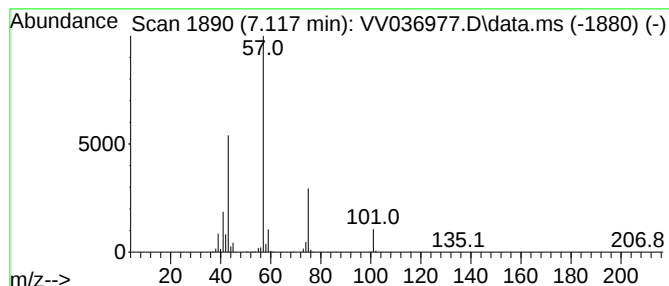
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.117	10.18 ug/L	305266	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

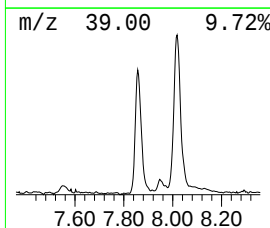
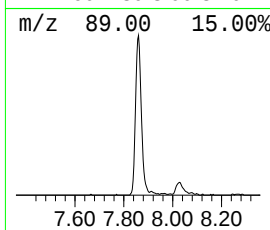
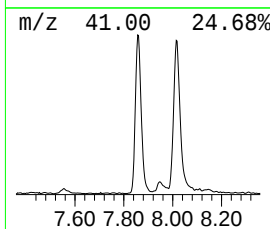
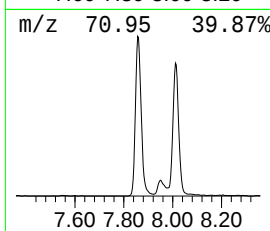
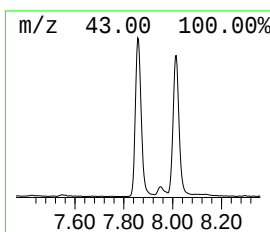
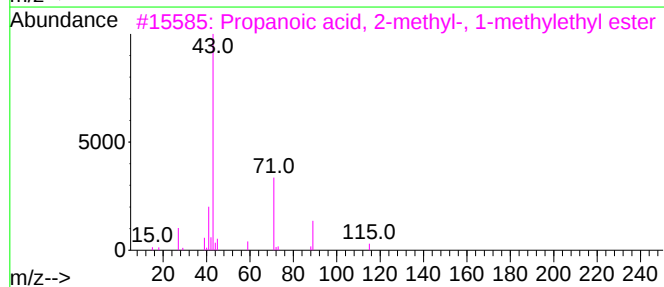
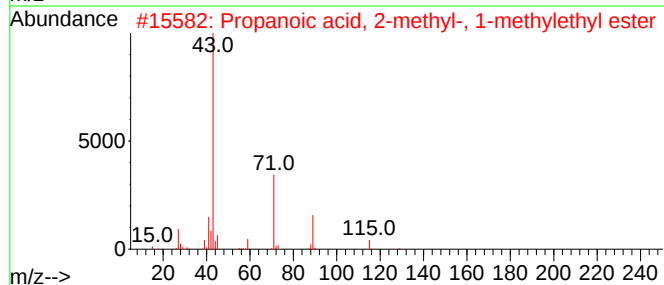
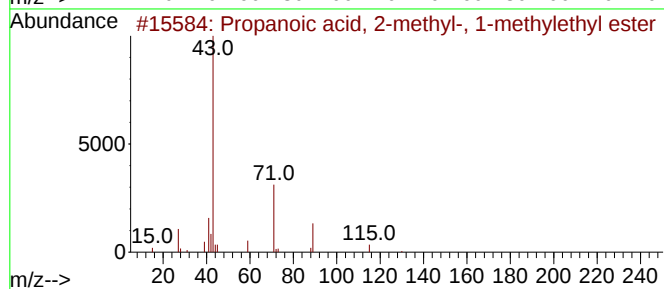
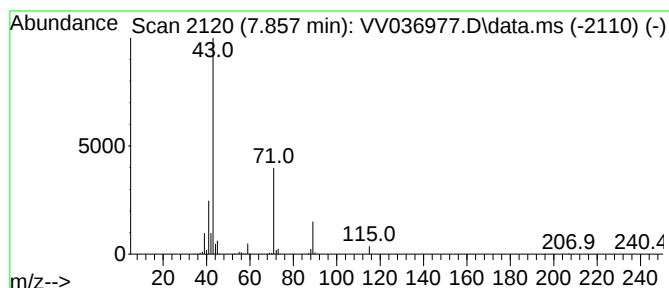
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.857	14.30 ug/L	564696	Chlorobenzene-d5	8.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

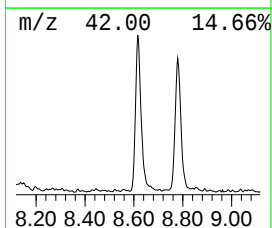
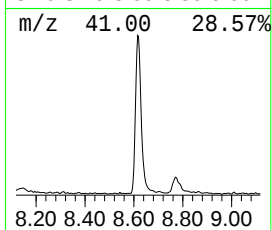
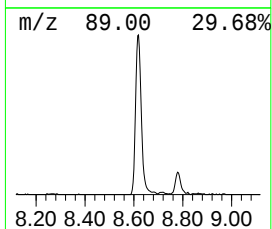
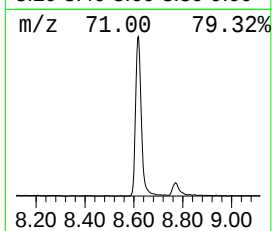
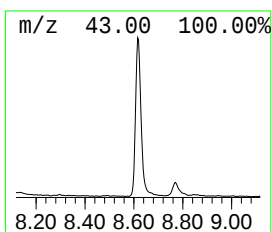
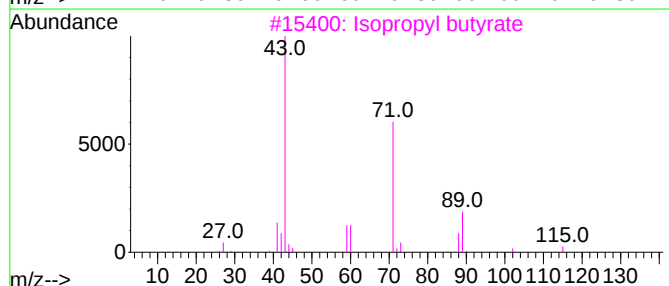
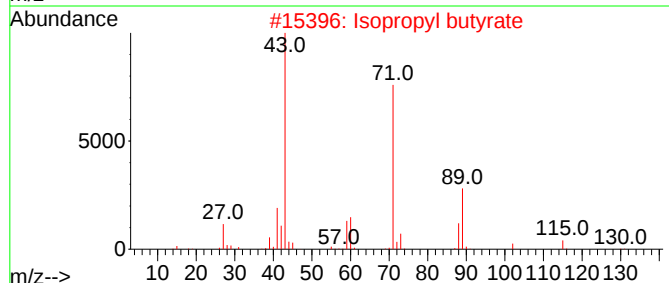
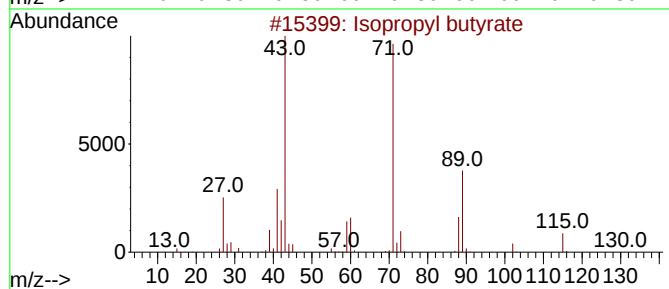
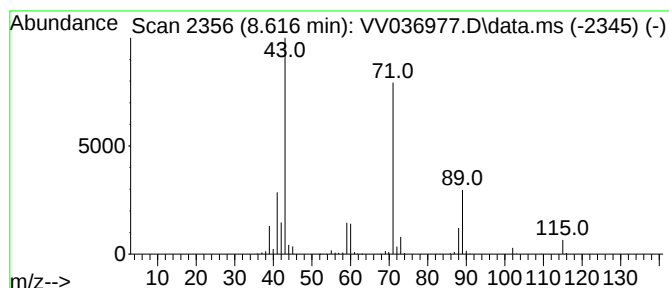
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	13.07 ug/L	516043	Chlorobenzene-d5	8.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
Data File : VV036977.D
Acq On : 19 Aug 2024 14:56
Operator : SY/MD
Sample : P3593-02 10X
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCXW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.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
3-Pentanone	6.268	6.1	ug/L	182887	1	5.532	1499520	50.0
Propanoic acid,...	7.117	10.2	ug/L	305266	1	5.532	1499520	50.0
Propanoic acid,...	7.857	14.3	ug/L	564696	2	8.780	1974860	50.0
Isopropyl butyrate	8.616	13.1	ug/L	516043	2	8.780	1974860	50.0