

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
 Data File : VW030182.D
 Acq On : 20 Sep 2024 18:02
 Operator : SY/MD
 Sample : P4109-18
 Misc : 5.51g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4EW0

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_W\Method\SFAMWLM091624SMA.M
 Title : SFAM01.0

Signal : TIC: VW030182.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	72	78	96	rVB	81921	199827	9.81%	1.327%
2	2.899	158	166	184	rBV	61497	185120	9.08%	1.229%
3	3.247	221	223	225	rVB2	493	403	0.02%	0.003%
4	3.289	228	230	231	rBV2	301	199	0.01%	0.001%
5	3.308	231	233	237	rVB2	484	705	0.03%	0.005%
6	3.350	237	240	242	rBV2	275	394	0.02%	0.003%
7	3.375	242	244	245	rVV	438	276	0.01%	0.002%
8	3.405	245	249	255	rVB4	773	1544	0.08%	0.010%
9	3.472	258	260	261	rBV2	403	321	0.02%	0.002%
10	3.552	270	273	275	rBV	405	442	0.02%	0.003%
11	3.576	275	277	279	rVB	399	323	0.02%	0.002%
12	3.661	290	291	293	rBV2	197	206	0.01%	0.001%
13	3.704	296	298	300	rBV2	241	258	0.01%	0.002%
14	3.765	307	308	311	rVB2	379	294	0.01%	0.002%
15	3.808	313	315	317	rBV	228	181	0.01%	0.001%
16	3.856	321	323	324	rBV2	244	249	0.01%	0.002%
17	4.021	339	350	363	rBV	206029	618781	30.36%	4.109%
18	4.393	402	411	416	rBV2	2244	6293	0.31%	0.042%
19	4.466	421	423	425	rVV	235	248	0.01%	0.002%
20	4.533	433	434	438	rVB2	229	239	0.01%	0.002%
21	4.564	438	439	442	rBV	291	287	0.01%	0.002%
22	4.679	456	458	461	rVV2	284	253	0.01%	0.002%
23	4.728	464	466	469	rVB2	274	272	0.01%	0.002%
24	4.765	469	472	474	rBV2	162	213	0.01%	0.001%
25	4.923	484	498	514	rBV3	7913	28099	1.38%	0.187%
26	5.118	526	530	531	rBV2	306	337	0.02%	0.002%
27	5.228	544	548	552	rVB2	210	391	0.02%	0.003%
28	5.332	560	565	567	rBV2	167	274	0.01%	0.002%
29	5.399	572	576	578	rBV2	174	223	0.01%	0.001%
30	5.557	599	602	603	rBV2	206	191	0.01%	0.001%
31	5.594	603	608	611	rVB2	129	214	0.01%	0.001%
32	5.679	617	622	623	rBV2	183	263	0.01%	0.002%
33	5.795	631	641	645	rBV5	818	2409	0.12%	0.016%
34	5.825	645	646	650	rVB2	440	453	0.02%	0.003%
35	5.947	657	666	673	rBV4	2340	6847	0.34%	0.045%
36	6.057	681	684	686	rBV2	285	283	0.01%	0.002%

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 Title : SFAM01.0

37	6.301	721	724	727	rVB2	424	438	0.02%	0.003%
38	6.472	747	752	757	rBV2	281	417	0.02%	0.003%
39	6.673	784	785	788	rVB2	329	246	0.01%	0.002%
40	6.838	808	812	813	rBV2	234	285	0.01%	0.002%
41	6.905	815	823	834	rBV4	1888	5950	0.29%	0.040%
42	7.075	842	851	868	rBV	43071	135741	6.66%	0.901%
43	7.337	891	894	896	rBV3	224	193	0.01%	0.001%
44	7.435	907	910	913	rBV2	182	263	0.01%	0.002%
45	7.539	921	927	933	rBV4	697	1687	0.08%	0.011%
46	7.648	933	945	958	rBV	324841	788809	38.71%	5.239%
47	7.734	958	959	960	rVV	537	329	0.02%	0.002%
48	7.770	960	965	971	rVV7	930	2218	0.11%	0.015%
49	7.941	990	993	995	rVB2	342	330	0.02%	0.002%
50	8.063	1009	1013	1018	rVB3	314	678	0.03%	0.005%
51	8.118	1018	1022	1023	rBV2	283	308	0.02%	0.002%
52	8.148	1023	1027	1028	rBV	155	226	0.01%	0.002%
53	8.276	1037	1048	1067	rBV2	663317	1885386	92.51%	12.521%
54	8.508	1084	1086	1088	rBV3	376	331	0.02%	0.002%
55	8.551	1090	1093	1094	rVV3	265	223	0.01%	0.001%
56	8.630	1100	1106	1111	rBV2	597	1142	0.06%	0.008%
57	8.697	1111	1117	1124	rBV4	1523	3376	0.17%	0.022%
58	8.843	1131	1141	1152	rBV	920246	1817151	89.16%	12.068%
59	9.044	1168	1174	1175	rBV5	1008	1593	0.08%	0.011%
60	9.081	1175	1180	1185	rVB6	1868	4511	0.22%	0.030%
61	9.215	1200	1202	1203	rBV2	254	188	0.01%	0.001%
62	9.276	1203	1212	1222	rBV	414354	847468	41.58%	5.628%
63	9.392	1230	1231	1234	rVB	459	268	0.01%	0.002%
64	9.489	1245	1247	1249	rVB	289	236	0.01%	0.002%
65	9.587	1257	1263	1265	rVB3	197	302	0.01%	0.002%
66	9.672	1270	1277	1279	rBV4	1102	2121	0.10%	0.014%
67	9.800	1297	1298	1300	rVB2	298	206	0.01%	0.001%
68	9.831	1300	1303	1304	rBV2	209	208	0.01%	0.001%
69	9.892	1309	1313	1317	rVB5	315	509	0.02%	0.003%
70	9.941	1320	1321	1323	rBV2	408	380	0.02%	0.003%
71	10.032	1327	1336	1346	rBV	219178	402260	19.74%	2.672%
72	10.130	1350	1352	1354	rVB2	526	466	0.02%	0.003%
73	10.215	1362	1366	1368	rVB5	547	603	0.03%	0.004%
74	10.319	1374	1383	1391	rBV	949026	1691723	83.01%	11.235%
75	10.459	1404	1406	1407	rVB2	414	261	0.01%	0.002%
76	10.501	1410	1413	1418	rVB4	981	1463	0.07%	0.010%

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 Title : SFAM01.0

77	10.575	1418	1425	1439	rVB	132201	236565	11.61%	1.571%
78	10.703	1439	1446	1454	rBV	7498	14755	0.72%	0.098%
79	10.782	1457	1459	1460	rVB	538	251	0.01%	0.002%
80	10.849	1466	1470	1475	rBV6	1571	3206	0.16%	0.021%
81	10.922	1475	1482	1497	rBV	196729	340265	16.70%	2.260%
82	11.154	1515	1520	1522	rBV4	1097	1735	0.09%	0.012%
83	11.404	1556	1561	1566	rBV6	2495	4567	0.22%	0.030%
84	11.471	1567	1572	1576	rVV3	2428	4854	0.24%	0.032%
85	11.629	1590	1598	1607	rBV	1220317	2037994	100.00%	13.535%
86	11.703	1608	1610	1619	rVB4	4411	9720	0.48%	0.065%
87	11.794	1624	1625	1626	rBV	1169	676	0.03%	0.004%
88	11.837	1627	1632	1641	rVB3	10495	19162	0.94%	0.127%
89	12.129	1673	1680	1683	rBV7	2432	5644	0.28%	0.037%
90	12.245	1697	1699	1704	rVB5	2231	2719	0.13%	0.018%
91	12.355	1715	1717	1720	rBV4	1592	1694	0.08%	0.011%
92	12.599	1754	1757	1762	rVB	6374	9585	0.47%	0.064%
93	12.690	1766	1772	1779	rVB	282839	465421	22.84%	3.091%
94	12.867	1797	1801	1804	rBV5	6065	11050	0.54%	0.073%
95	12.928	1807	1811	1819	rVV3	21293	47846	2.35%	0.318%
96	13.032	1823	1828	1833	rVB	33740	54350	2.67%	0.361%
97	13.275	1860	1868	1881	rVB2	93346	209984	10.30%	1.395%
98	13.556	1907	1914	1925	rBV	1065628	1733485	85.06%	11.513%
99	13.848	1955	1962	1974	rBV	657410	1096024	53.78%	7.279%
100	14.050	1991	1995	2009	rVB3	35115	88004	4.32%	0.584%

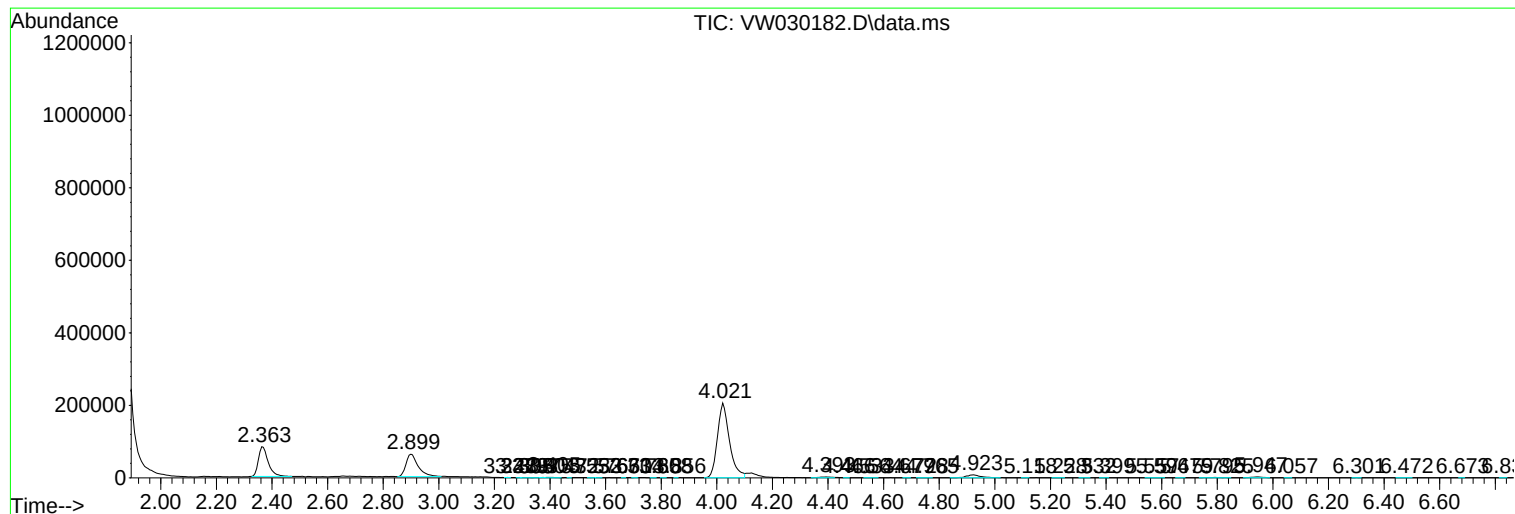
Sum of corrected areas: 15057361

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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



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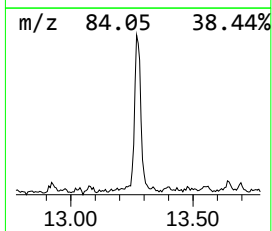
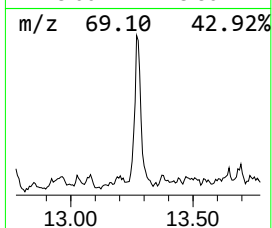
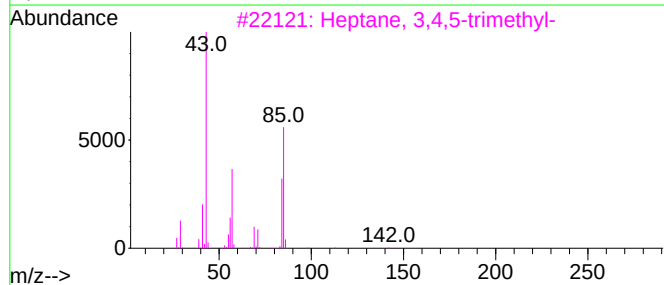
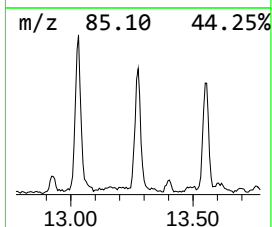
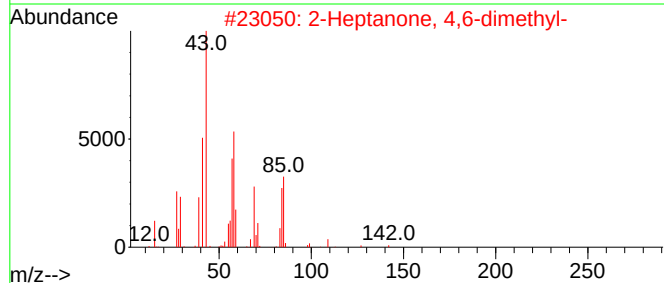
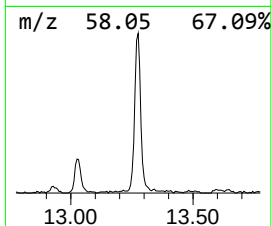
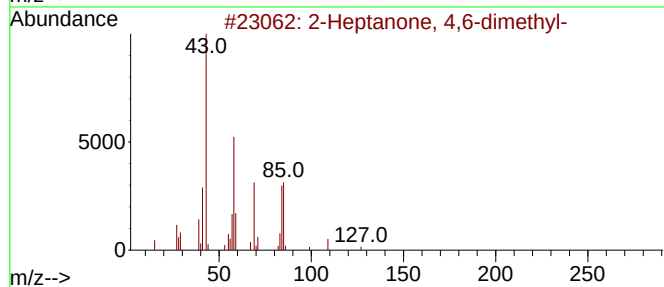
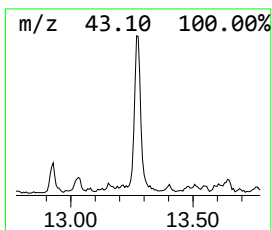
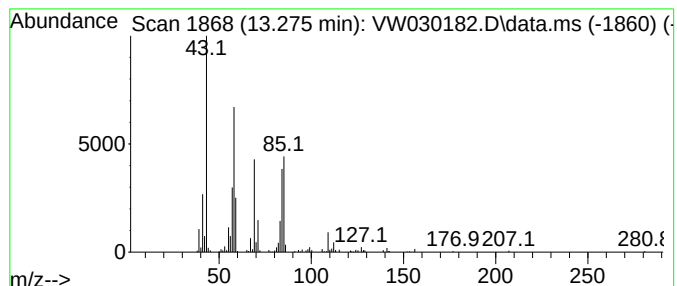
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 2-Heptanone, 4,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.275	3.03 ug/L	209984	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	86
2			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	78
3			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	43
4			2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	38
5			Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	27



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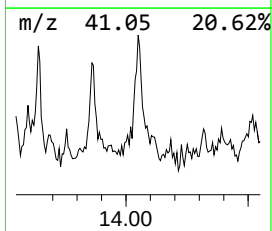
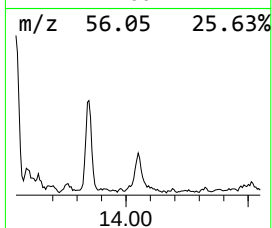
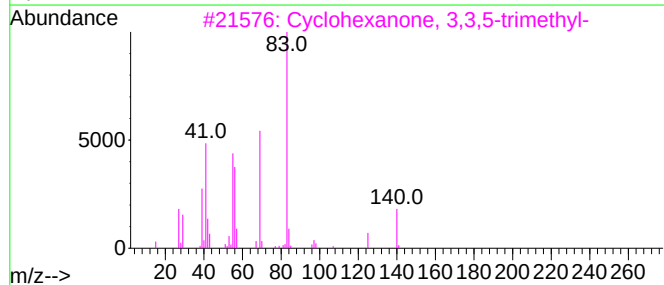
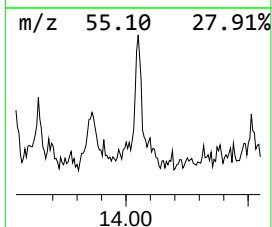
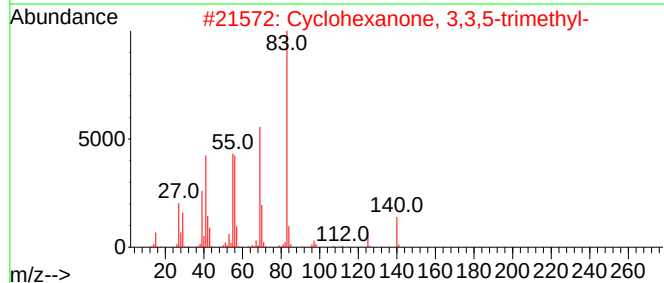
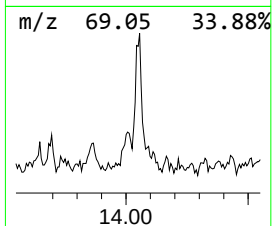
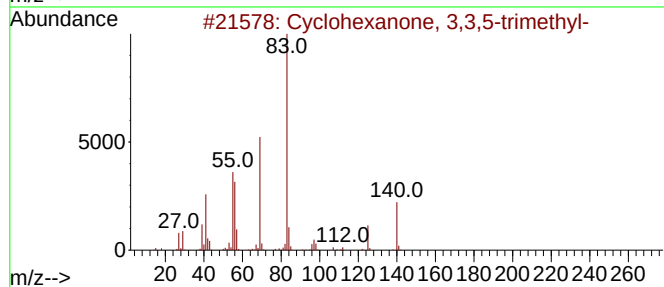
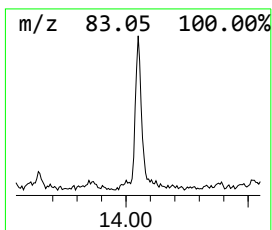
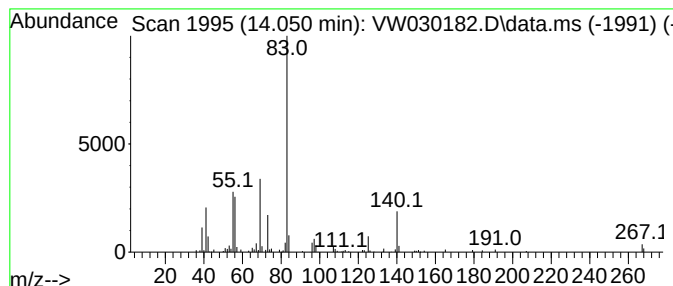
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Cyclohexanone, 3,3,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.050	1.27 ug/L	88004	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	80
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	72
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	72
4			1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	52
5			Cyclohexane, butyl-	140	C10H20	001678-93-9	42



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Heptanone, 4,...	13.275	3.0	ug/L	209984	3	13.556	1733490	25.0
Cyclohexanone, ...	14.050	1.3	ug/L	88004	3	13.556	1733490	25.0