

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD111423\
 Data File : VD077562.D
 Acq On : 14 Nov 2023 13:49
 Operator : JC/SY
 Sample : 05296-15
 Misc : 6.61G/10ml/MSVOA_D/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BH3T1

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_D\Method\SFAMDLM110923SMA.M
 Title : SFAM01.0

Signal : TIC: VD077562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	19	27	39	rBV	2915367	4474093	100.00%	28.957%
2	2.281	112	118	126	rVB	201660	301426	6.74%	1.951%
3	2.805	201	207	216	rVB	167716	303724	6.79%	1.966%
4	3.405	308	309	310	rVB	1899	670	0.01%	0.004%
5	3.422	310	312	314	rBV	1334	1281	0.03%	0.008%
6	3.499	324	325	330	rBV2	1340	1450	0.03%	0.009%
7	3.546	330	333	335	rVV2	993	1169	0.03%	0.008%
8	3.593	339	341	344	rVB	1596	1168	0.03%	0.008%
9	3.622	344	346	349	rBV	1351	1472	0.03%	0.010%
10	3.693	356	358	360	rBV2	1238	831	0.02%	0.005%
11	3.922	387	397	408	rBV	193811	516384	11.54%	3.342%
12	4.281	456	458	459	rVB	1346	765	0.02%	0.005%
13	4.299	459	461	462	rBV	1374	760	0.02%	0.005%
14	4.387	474	476	480	rVB2	953	1254	0.03%	0.008%
15	4.458	486	488	489	rBV	1273	796	0.02%	0.005%
16	4.622	515	516	518	rBV	881	699	0.02%	0.005%
17	4.687	525	527	530	rBV2	1219	1265	0.03%	0.008%
18	4.799	538	546	548	rBV4	11997	23491	0.53%	0.152%
19	4.893	559	562	563	rBV2	1078	1058	0.02%	0.007%
20	4.916	563	566	569	rVV2	1219	1603	0.04%	0.010%
21	4.952	571	572	575	rVB2	1496	1064	0.02%	0.007%
22	5.058	586	590	592	rBV2	1352	1699	0.04%	0.011%
23	5.099	595	597	599	rVV	1013	808	0.02%	0.005%
24	5.128	599	602	603	rVB2	944	801	0.02%	0.005%
25	5.146	603	605	609	rBV2	1065	1308	0.03%	0.008%
26	5.528	668	670	671	rVB2	1521	800	0.02%	0.005%
27	5.581	676	679	681	rBV2	742	858	0.02%	0.006%
28	5.746	705	707	708	rBV	1012	712	0.02%	0.005%
29	5.799	713	716	717	rBV	1263	1123	0.03%	0.007%
30	5.834	719	722	724	rBV	2520	3037	0.07%	0.020%
31	5.987	747	748	753	rVB2	1377	962	0.02%	0.006%
32	6.116	768	770	773	rVB2	1209	1101	0.02%	0.007%
33	6.146	773	775	776	rBV2	1061	669	0.01%	0.004%
34	6.157	776	777	780	rVB2	1715	1189	0.03%	0.008%
35	6.205	780	785	788	rBV	1184	2536	0.06%	0.016%
36	6.334	806	807	810	rVB2	1267	832	0.02%	0.005%

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 Title : SFAM01.0

37	6.375	813	814	817	rVB	1010	899	0.02%	0.006%
38	6.416	820	821	824	rVB	1049	781	0.02%	0.005%
39	6.481	828	832	833	rBV	1238	1518	0.03%	0.010%
40	6.634	856	858	861	rVB	1134	734	0.02%	0.005%

41	6.704	868	870	873	rVB2	1327	1323	0.03%	0.009%
42	6.746	873	877	881	rBV2	1484	2856	0.06%	0.018%
43	6.840	891	893	896	rBV2	1283	965	0.02%	0.006%
44	6.922	905	907	910	rVB2	865	928	0.02%	0.006%
45	6.981	910	917	925	rBV	32851	96191	2.15%	0.623%

46	7.140	941	944	945	rVB	1367	953	0.02%	0.006%
47	7.463	997	999	1001	rBV2	1595	1056	0.02%	0.007%
48	7.569	1006	1017	1028	rBV	238664	607154	13.57%	3.930%
49	7.816	1057	1059	1060	rBV	797	736	0.02%	0.005%
50	7.857	1063	1066	1068	rBV2	1396	1669	0.04%	0.011%

51	7.969	1082	1085	1088	rBV	1675	1735	0.04%	0.011%
52	8.128	1110	1112	1113	rBV	1668	959	0.02%	0.006%
53	8.204	1113	1125	1143	rVV2	507824	1489893	33.30%	9.643%
54	8.493	1172	1174	1179	rBV2	1185	1377	0.03%	0.009%
55	8.557	1182	1185	1186	rBV2	1767	1287	0.03%	0.008%

56	8.781	1213	1223	1233	rBV	496650	1026334	22.94%	6.643%
57	8.940	1248	1250	1253	rBV	1268	1125	0.03%	0.007%
58	9.034	1259	1266	1274	rVB3	31865	71889	1.61%	0.465%
59	9.210	1287	1296	1307	rBV	331167	693301	15.50%	4.487%
60	9.446	1334	1336	1338	rVV	889	870	0.02%	0.006%

61	9.475	1339	1341	1345	rVB2	1509	1627	0.04%	0.011%
62	9.616	1364	1365	1368	rVB	965	761	0.02%	0.005%
63	9.663	1371	1373	1375	rVB2	1174	1004	0.02%	0.006%
64	9.981	1419	1427	1435	rBV	185693	351123	7.85%	2.273%
65	10.181	1460	1461	1463	rBV	1480	718	0.02%	0.005%

66	10.269	1468	1476	1485	rBV	661435	1173907	26.24%	7.598%
67	10.528	1513	1520	1531	rBV	116428	209399	4.68%	1.355%
68	10.669	1539	1544	1549	rVB3	5132	7716	0.17%	0.050%
69	10.810	1560	1568	1574	rBV	556479	978980	21.88%	6.336%
70	10.875	1574	1579	1587	rVB	141453	239307	5.35%	1.549%

71	10.975	1593	1596	1597	rVB2	1686	1339	0.03%	0.009%
72	11.028	1603	1605	1608	rBV2	1568	1816	0.04%	0.012%
73	11.087	1614	1615	1618	rBV2	1519	1399	0.03%	0.009%
74	11.263	1644	1645	1649	rVB	1291	1109	0.02%	0.007%
75	11.298	1649	1651	1652	rVB	1084	754	0.02%	0.005%

76	11.316	1652	1654	1657	rBV2	1661	2180	0.05%	0.014%
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 Title : SFAM01.0

77	11.410	1668	1670	1671	rBV	1745	1013	0.02%	0.007%
78	11.581	1689	1699	1709	rBV	634419	1098697	24.56%	7.111%
79	11.792	1731	1735	1740	rVB4	5544	10665	0.24%	0.069%
80	11.881	1748	1750	1752	rBV2	1644	1429	0.03%	0.009%
81	12.022	1773	1774	1776	rBV	1296	845	0.02%	0.005%
82	12.122	1788	1791	1796	rVV3	3131	4711	0.11%	0.030%
83	12.187	1800	1802	1803	rBV2	1058	730	0.02%	0.005%
84	12.204	1803	1805	1808	rVB2	1341	1419	0.03%	0.009%
85	12.575	1860	1868	1874	rVB6	7508	15023	0.34%	0.097%
86	12.651	1874	1881	1888	rBV	179335	298078	6.66%	1.929%
87	12.745	1895	1897	1898	rBV	1181	702	0.02%	0.005%
88	12.804	1905	1907	1908	rBV	1540	847	0.02%	0.005%
89	12.910	1924	1925	1926	rBV	2261	976	0.02%	0.006%
90	12.975	1935	1936	1938	rBV2	1556	1204	0.03%	0.008%
91	13.198	1972	1974	1975	rBV2	1566	1122	0.03%	0.007%
92	13.457	2015	2018	2019	rBV	2009	1850	0.04%	0.012%
93	13.516	2022	2028	2036	rVB	464985	745794	16.67%	4.827%
94	13.639	2048	2049	2052	rVB	1954	974	0.02%	0.006%
95	13.816	2072	2079	2086	rBV	333260	560910	12.54%	3.630%
96	13.928	2095	2098	2100	rBV3	1685	2067	0.05%	0.013%
97	14.045	2114	2118	2123	rVB	12678	17505	0.39%	0.113%
98	14.151	2134	2136	2137	rVB	1814	801	0.02%	0.005%
99	14.292	2157	2160	2165	rBV2	1876	2840	0.06%	0.018%
100	14.786	2240	2244	2250	rVB3	30437	46097	1.03%	0.298%

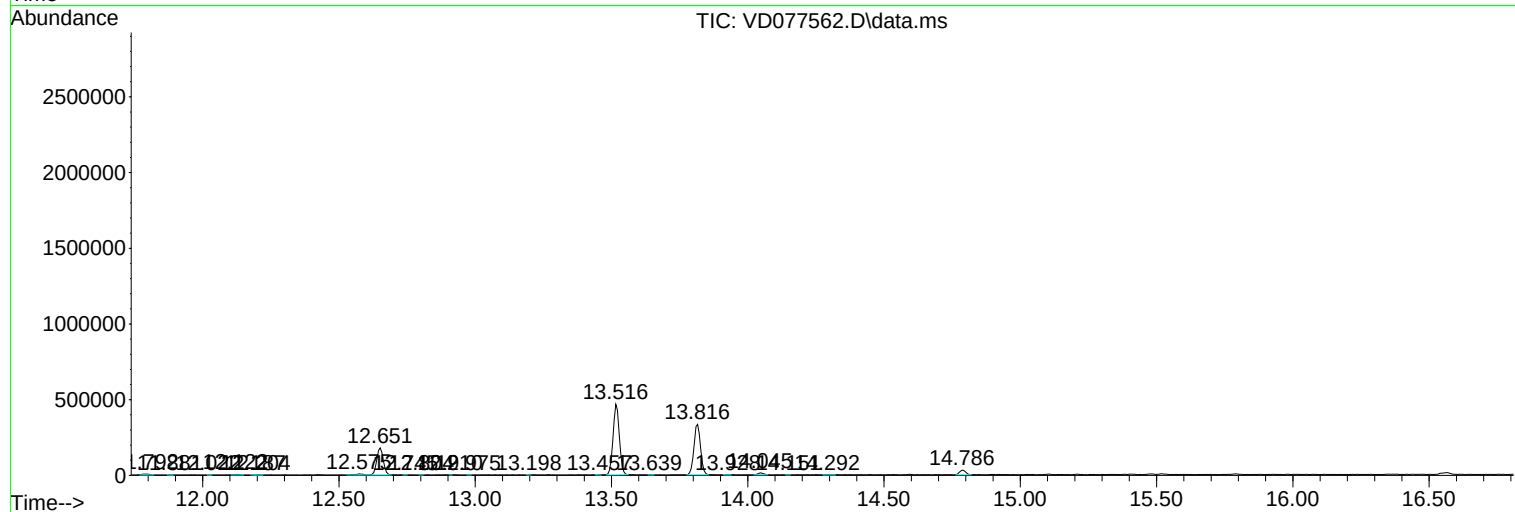
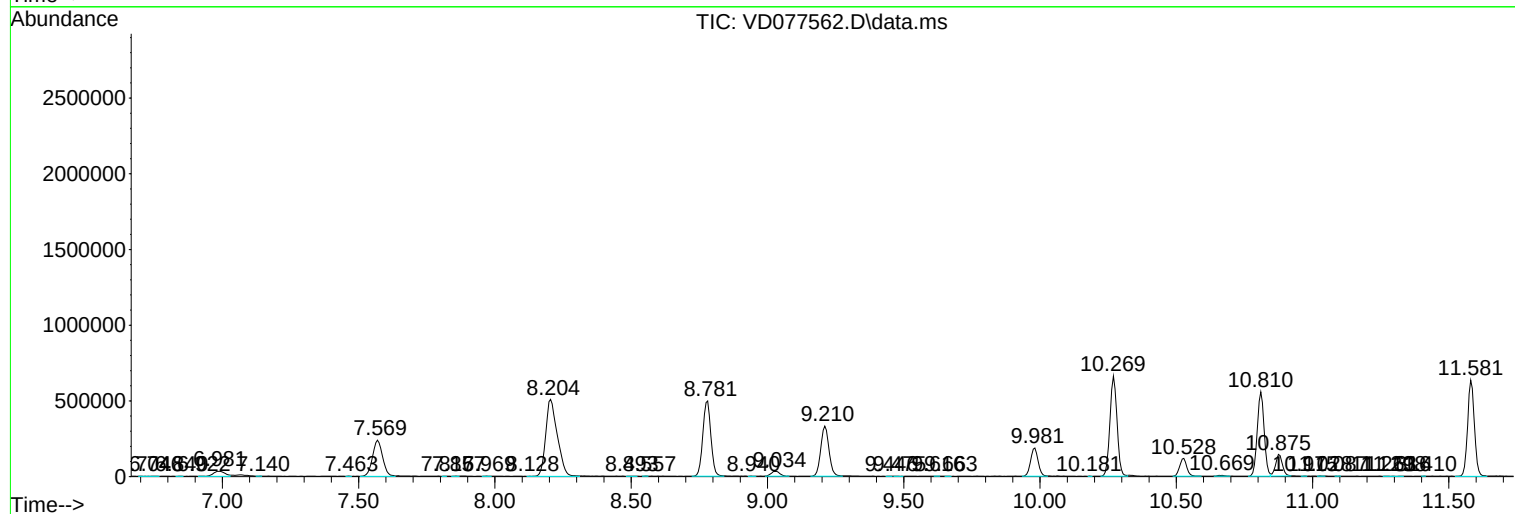
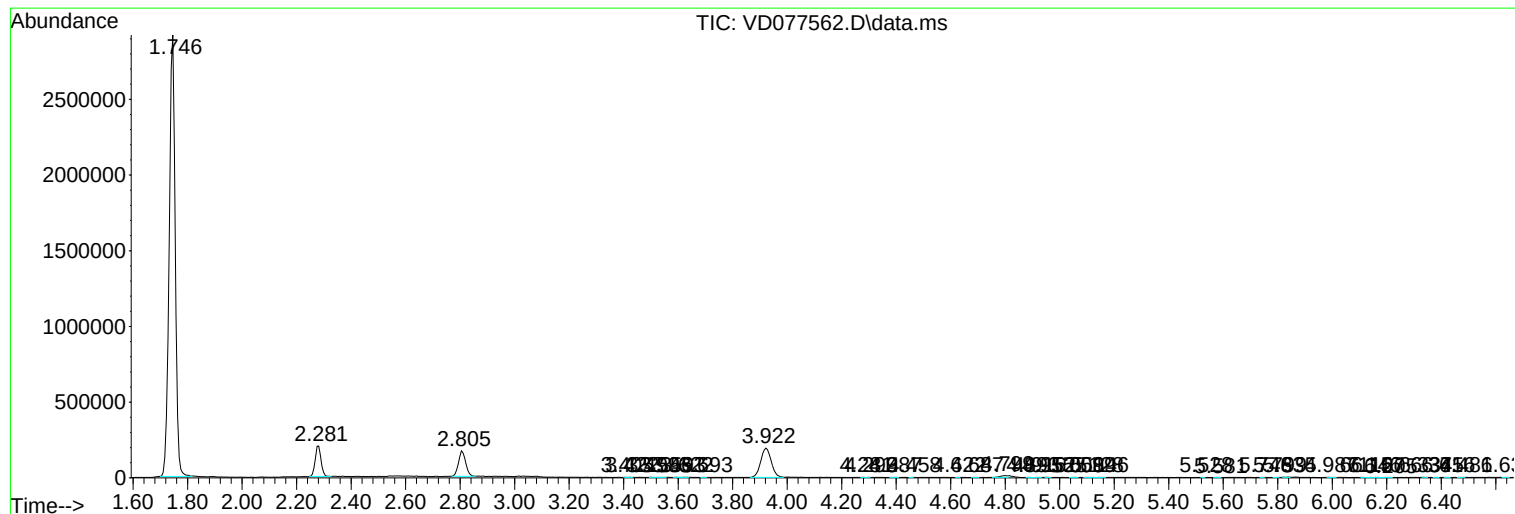
Sum of corrected areas: 15450829

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
Quant Title : SFAM01.0

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



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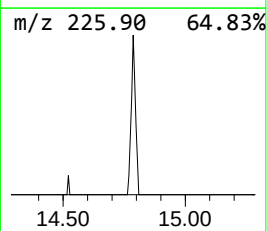
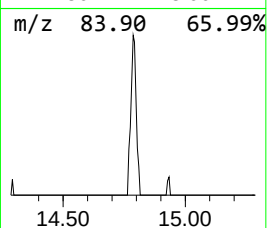
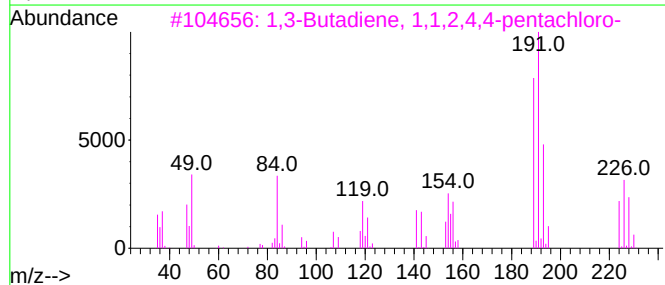
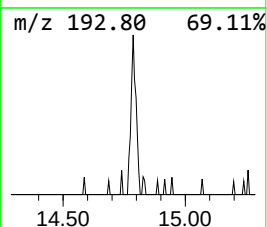
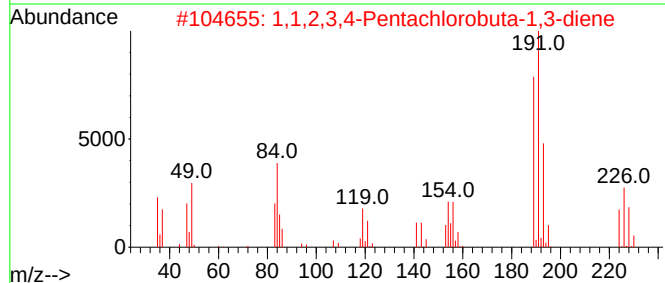
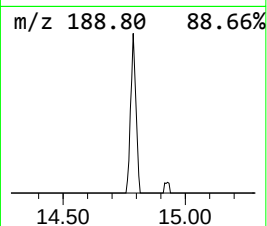
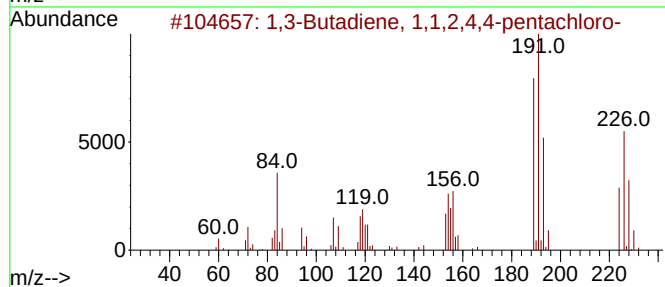
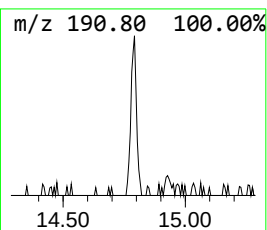
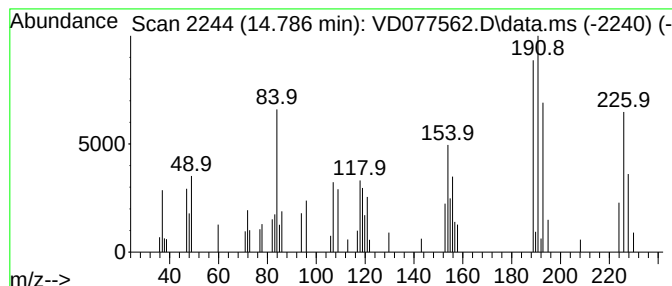
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
Quant Title : SFAM01.0

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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	1.55 ug/L	46097	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	97
2			1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HCl5	1010487-10-4	80
3			1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	72
4			2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClOS	031555-60-9	38
5			2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClOS	031555-60-9	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	14.786	1.6	ug/L	46097	3	13.516	745794	25.0