

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040623\
 Data File : VD075590.D
 Acq On : 06 Apr 2023 12:25
 Operator : KP/SY
 Sample : 02215-03
 Misc : 5.00G/10.00ml/MSVOA_D/SOIL
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 MDL-SOIL-QT2-2023-03

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\SFAMDLM033123SMA.M
 Title : SFAM01.0

Signal : TIC: VD075590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	11	26	39	rBV	564595	1118205	100.00%	12.110%
2	1.934	56	59	64	rVB2	5522	7253	0.65%	0.079%
3	2.152	92	96	102	rBV2	7264	12247	1.10%	0.133%
4	2.276	111	117	125	rBV	204511	299541	26.79%	3.244%
5	2.805	200	207	218	rVB	153750	292311	26.14%	3.166%
6	3.175	264	270	271	rBV2	5408	7822	0.70%	0.085%
7	3.611	341	344	345	rBV	909	707	0.06%	0.008%
8	3.740	364	366	368	rVB	719	336	0.03%	0.004%
9	3.923	387	397	414	rBV2	161999	457225	40.89%	4.952%
10	4.275	448	457	469	rBV2	5913	17563	1.57%	0.190%
11	4.393	475	477	478	rVB2	615	262	0.02%	0.003%
12	4.634	516	518	520	rVB	456	323	0.03%	0.003%
13	4.811	540	548	557	rVB5	11298	32970	2.95%	0.357%
14	4.964	572	574	576	rVB2	470	290	0.03%	0.003%
15	5.046	587	588	589	rBV	909	455	0.04%	0.005%
16	5.140	602	604	605	rBV	434	294	0.03%	0.003%
17	5.228	618	619	620	rVB	828	292	0.03%	0.003%
18	5.317	625	634	635	rBV5	7409	15259	1.36%	0.165%
19	5.411	646	650	651	rBV2	418	442	0.04%	0.005%
20	5.481	661	662	665	rBV2	671	412	0.04%	0.004%
21	5.699	697	699	700	rBV	880	683	0.06%	0.007%
22	5.975	744	746	751	rVB	518	681	0.06%	0.007%
23	6.046	756	758	760	rBV2	461	412	0.04%	0.004%
24	6.069	760	762	763	rBV	841	624	0.06%	0.007%
25	6.117	764	770	781	rVB5	4340	11195	1.00%	0.121%
26	6.311	801	803	805	rBV	510	326	0.03%	0.004%
27	6.369	811	813	814	rVB	535	275	0.02%	0.003%
28	6.593	849	851	854	rBV2	430	267	0.02%	0.003%
29	6.640	857	859	863	rVB2	447	334	0.03%	0.004%
30	6.681	863	866	868	rVB	760	563	0.05%	0.006%
31	6.699	868	869	870	rBV	555	296	0.03%	0.003%
32	6.828	889	891	894	rBV	454	334	0.03%	0.004%
33	6.993	910	919	926	rBV2	16225	47942	4.29%	0.519%
34	7.169	947	949	951	rBV2	765	926	0.08%	0.010%
35	7.258	960	964	966	rBV2	381	541	0.05%	0.006%
36	7.422	986	992	1000	rBV4	4996	10917	0.98%	0.118%

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 Title : SFAM01.0

37	7.569	1005	1017	1034	rBV2	174228	447302	40.00%	4.844%
38	7.787	1049	1054	1055	rBV	6632	7535	0.67%	0.082%
39	7.875	1064	1069	1078	rVB4	6921	16177	1.45%	0.175%
40	7.946	1078	1081	1082	rVV2	610	580	0.05%	0.006%
41	7.993	1083	1089	1099	rVB3	6305	14799	1.32%	0.160%
42	8.205	1115	1125	1141	rBV2	349367	1038744	92.89%	11.250%
43	8.334	1142	1147	1152	rVB4	4857	9317	0.83%	0.101%
44	8.475	1169	1171	1173	rVV2	695	417	0.04%	0.005%
45	8.540	1181	1182	1185	rBV	464	435	0.04%	0.005%
46	8.693	1206	1208	1211	rBV2	625	731	0.07%	0.008%
47	8.781	1214	1223	1232	rBV	321597	653472	58.44%	7.077%
48	9.028	1259	1265	1272	rVB4	11502	22872	2.05%	0.248%
49	9.210	1288	1296	1303	rBV	210937	432070	38.64%	4.679%
50	9.369	1321	1323	1325	rBV2	497	495	0.04%	0.005%
51	9.587	1355	1360	1366	rVB2	7436	13361	1.19%	0.145%
52	9.716	1381	1382	1384	rBV	820	528	0.05%	0.006%
53	9.810	1395	1398	1399	rBV	655	571	0.05%	0.006%
54	9.922	1415	1417	1420	rBV2	662	663	0.06%	0.007%
55	9.981	1420	1427	1438	rVV	109306	218273	19.52%	2.364%
56	10.157	1453	1457	1462	rVB3	4562	6498	0.58%	0.070%
57	10.269	1469	1476	1483	rBV	478447	861328	77.03%	9.328%
58	10.434	1502	1504	1505	rBV	661	323	0.03%	0.003%
59	10.528	1513	1520	1529	rBV	70885	135541	12.12%	1.468%
60	10.663	1537	1543	1550	rBV2	26969	47166	4.22%	0.511%
61	10.734	1550	1555	1560	rVB5	9879	16700	1.49%	0.181%
62	10.810	1563	1568	1574	rBV2	14530	23835	2.13%	0.258%
63	10.881	1574	1580	1595	rVB	63604	117093	10.47%	1.268%
64	11.028	1600	1605	1610	rBV2	25047	40602	3.63%	0.440%
65	11.122	1619	1621	1623	rBV	518	361	0.03%	0.004%
66	11.181	1625	1631	1638	rVB3	4308	7410	0.66%	0.080%
67	11.357	1658	1661	1663	rVB2	1495	1648	0.15%	0.018%
68	11.404	1663	1669	1675	rBV3	10558	15937	1.43%	0.173%
69	11.581	1692	1699	1710	rVB	453802	802512	71.77%	8.691%
70	11.687	1710	1717	1721	rBV	22007	34257	3.06%	0.371%
71	11.793	1730	1735	1742	rVB	16930	29262	2.62%	0.317%
72	11.904	1753	1754	1758	rBV2	710	599	0.05%	0.006%
73	12.128	1785	1792	1800	rBV2	25450	51990	4.65%	0.563%
74	12.299	1817	1821	1826	rVB3	4526	7057	0.63%	0.076%
75	12.381	1833	1835	1836	rBV	687	408	0.04%	0.004%
76	12.422	1837	1842	1847	rVV2	19792	30012	2.68%	0.325%

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 Title : SFAM01.0

77	12.581	1864	1869	1875	rBV2	10072	17019	1.52%	0.184%
78	12.651	1875	1881	1889	rVV	162176	274222	24.52%	2.970%
79	12.728	1889	1894	1898	rBV3	4848	6839	0.61%	0.074%
80	12.904	1919	1924	1932	rBV2	22132	33806	3.02%	0.366%
81	13.010	1939	1942	1945	rBV2	766	963	0.09%	0.010%
82	13.163	1966	1968	1972	rVB2	1073	820	0.07%	0.009%
83	13.216	1972	1977	1982	rBV	16295	23593	2.11%	0.256%
84	13.375	2003	2004	2006	rBV	1182	744	0.07%	0.008%
85	13.398	2006	2008	2011	rBV	596	472	0.04%	0.005%
86	13.463	2012	2019	2022	rBV	16529	25384	2.27%	0.275%
87	13.522	2022	2029	2037	rVB	403859	695419	62.19%	7.531%
88	13.628	2046	2047	2048	rBV	644	255	0.02%	0.003%
89	13.816	2072	2079	2089	rVB	375241	628962	56.25%	6.812%
90	13.946	2100	2101	2104	rVB	732	538	0.05%	0.006%
91	13.975	2104	2106	2107	rBV	564	347	0.03%	0.004%
92	14.045	2114	2118	2123	rVB2	6756	8857	0.79%	0.096%
93	14.363	2170	2172	2173	rBV	897	696	0.06%	0.008%
94	14.457	2182	2188	2189	rBV2	2050	2656	0.24%	0.029%
95	14.593	2206	2211	2218	rBV2	12992	20504	1.83%	0.222%
96	15.098	2292	2297	2303	rBV3	10223	15709	1.40%	0.170%
97	15.334	2332	2337	2343	rVB	7144	12006	1.07%	0.130%
98	15.522	2365	2369	2377	rVB3	8354	13449	1.20%	0.146%
99	16.198	2483	2484	2485	rBV	625	372	0.03%	0.004%
100	16.439	2524	2525	2526	rBV	914	459	0.04%	0.005%

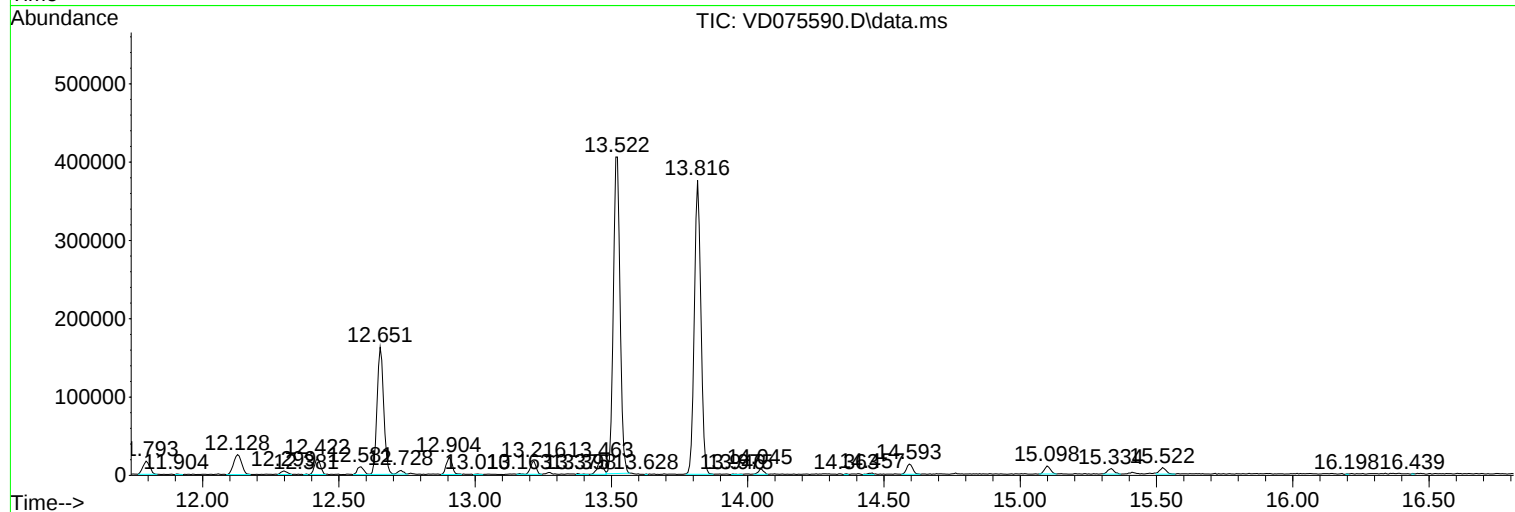
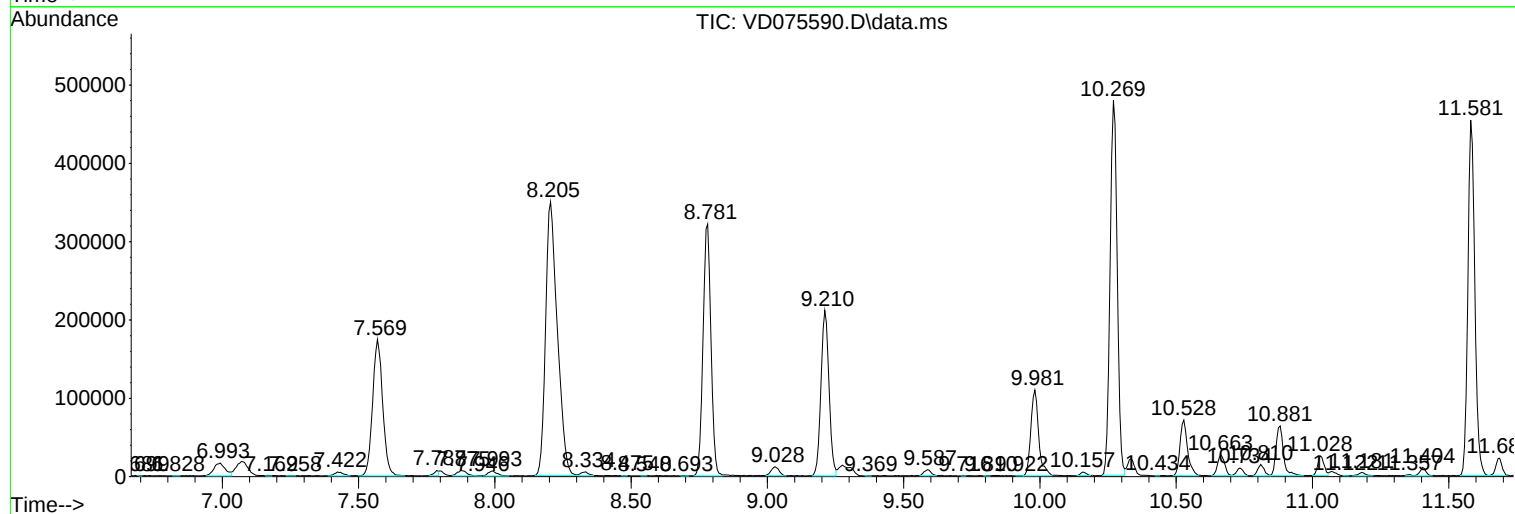
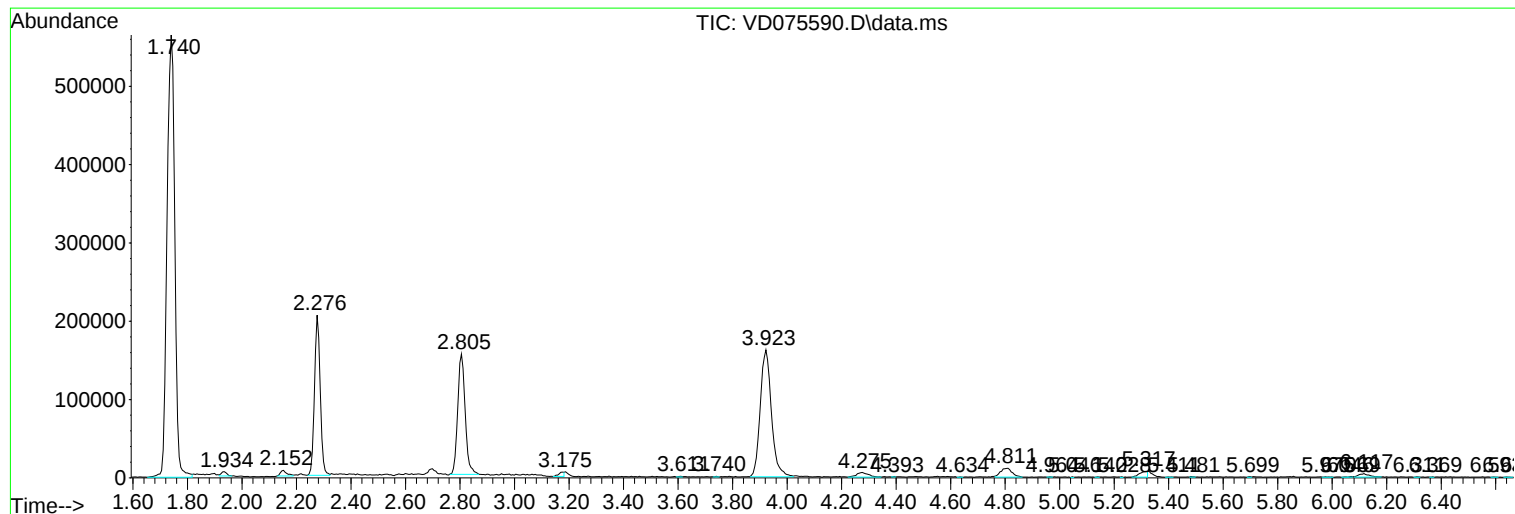
Sum of corrected areas: 9233497

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM033123SMA.M
Quant Title : SFAM01.0

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



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Instrument :
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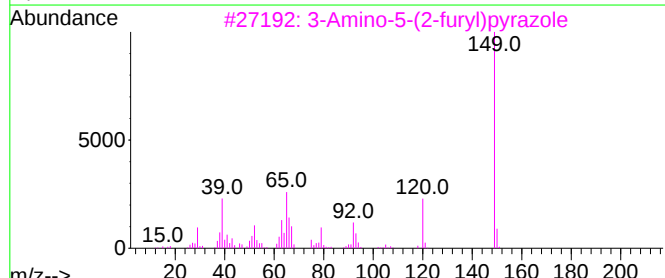
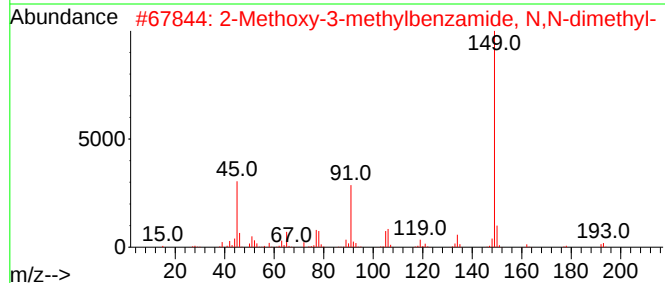
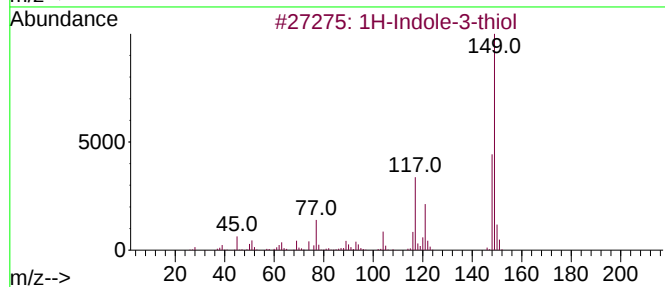
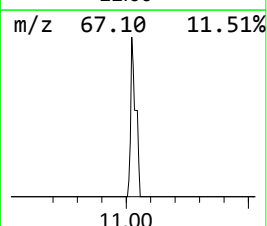
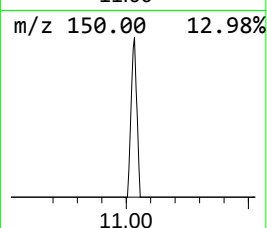
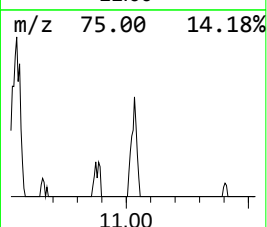
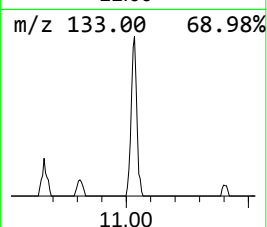
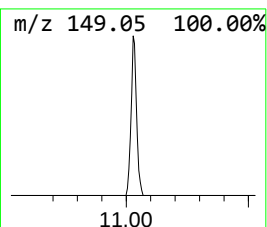
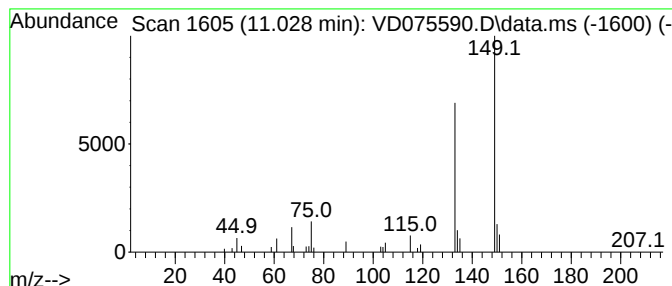
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM033123SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.028	1.26 ug/L	40602	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	43
2			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	38
3			3-Amino-5-(2-furyl)pyrazole	149	C7H7N3O	096799-02-9	37
4			4-(Methylthio)benzonitrile	149	C8H7NS	021382-98-9	37
5			Thioglycolic acid, tert-butyl dim...	206	C8H18O2SSi	1000476-01-2	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	11.028	1.3	ug/L	40602	2	11.581	802512	25.0