

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041923\
 Data File : VY013345.D
 Acq On : 19 Apr 2023 15:08
 Operator : KP/MD
 Sample : 02371-09
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-20-8.0-8.5

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_Y\methods\82Y041223S.M
 Title : SW846 8260

Signal : TIC: VY013345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.912	13	15	16	rBV	898	661	1.17%	0.153%
2	2.070	38	41	43	rBV2	724	694	1.23%	0.161%
3	2.131	45	51	52	rBV4	959	1574	2.79%	0.365%
4	2.144	52	53	57	rVV3	524	607	1.08%	0.141%
5	2.223	61	66	70	rVV2	2345	3599	6.38%	0.834%
6	2.259	70	72	75	rVB2	995	990	1.76%	0.229%
7	2.296	75	78	79	rBV2	578	569	1.01%	0.132%
8	2.314	79	81	83	rVV3	758	644	1.14%	0.149%
9	2.516	113	114	116	rVV2	651	578	1.03%	0.134%
10	2.540	116	118	122	rVV3	1277	1300	2.31%	0.301%
11	2.674	138	140	142	rVB2	840	779	1.38%	0.180%
12	2.735	148	150	153	rVV3	916	787	1.40%	0.182%
13	2.765	153	155	157	rVV4	706	597	1.06%	0.138%
14	2.790	157	159	161	rVV2	646	636	1.13%	0.147%
15	2.875	171	173	176	rVB2	1029	848	1.50%	0.196%
16	2.918	179	180	183	rVB2	984	583	1.03%	0.135%
17	2.961	183	187	189	rBV5	892	903	1.60%	0.209%
18	3.003	191	194	197	rVB3	733	949	1.68%	0.220%
19	3.028	197	198	200	rBV	620	565	1.00%	0.131%
20	3.131	213	215	218	rVB2	559	609	1.08%	0.141%
21	3.211	225	228	232	rVV2	498	705	1.25%	0.163%
22	3.357	250	252	254	rBV2	694	579	1.03%	0.134%
23	3.381	254	256	260	rVB3	427	624	1.11%	0.145%
24	3.954	342	350	353	rVV5	1158	3432	6.09%	0.795%
25	4.198	383	390	393	rBV4	1678	3837	6.81%	0.889%
26	4.223	393	394	399	rVB	727	723	1.28%	0.167%
27	4.430	425	428	433	rBV	431	818	1.45%	0.189%
28	4.692	468	471	472	rBV2	756	849	1.51%	0.197%
29	4.716	472	475	481	rVB3	1168	2435	4.32%	0.564%
30	4.954	510	514	516	rVV2	377	564	1.00%	0.131%
31	5.747	636	644	649	rBV4	838	2356	4.18%	0.546%
32	5.844	655	660	663	rVB2	361	615	1.09%	0.142%
33	6.436	754	757	759	rVB2	637	619	1.10%	0.143%
34	6.460	759	761	764	rBV	415	654	1.16%	0.151%
35	6.966	835	844	857	rVV	9979	29805	52.86%	6.903%
36	7.057	857	859	862	rVV	583	647	1.15%	0.150%

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37	7.380	909	912	915	rVB2	443	589	1.04%	0.136%
38	7.716	956	967	973	rVV2	11266	27499	48.77%	6.369%
39	7.783	973	978	989	rVB3	14399	34172	60.61%	7.915%
40	8.015	1012	1016	1019	rBV3	606	686	1.22%	0.159%
41	8.136	1029	1036	1046	rVB3	11702	28970	51.38%	6.710%
42	8.374	1070	1075	1080	rVV2	401	758	1.34%	0.176%
43	8.460	1086	1089	1093	rBV2	476	666	1.18%	0.154%
44	8.575	1104	1108	1112	rVB2	533	690	1.22%	0.160%
45	8.685	1116	1126	1136	rVV	20695	44453	78.84%	10.296%
46	8.959	1168	1171	1175	rVB	405	600	1.06%	0.139%
47	9.088	1188	1192	1197	rVB3	420	704	1.25%	0.163%
48	9.697	1291	1292	1296	rVB2	685	735	1.30%	0.170%
49	10.063	1350	1352	1357	rVV4	892	1116	1.98%	0.258%
50	10.179	1362	1371	1380	rBV	32266	56384	100.00%	13.059%
51	10.569	1432	1435	1440	rBV2	731	1011	1.79%	0.234%
52	10.654	1447	1449	1452	rBV2	532	587	1.04%	0.136%
53	10.770	1464	1468	1471	rVB2	424	575	1.02%	0.133%
54	10.947	1494	1497	1501	rBV2	584	708	1.26%	0.164%
55	11.044	1509	1513	1516	rVB2	560	752	1.33%	0.174%
56	11.313	1553	1557	1562	rVB4	1067	1476	2.62%	0.342%
57	11.490	1579	1586	1594	rVB	30328	51316	91.01%	11.885%
58	11.947	1658	1661	1665	rBV2	568	645	1.14%	0.149%
59	12.270	1710	1714	1717	rVB2	397	726	1.29%	0.168%
60	12.434	1736	1741	1743	rVV2	590	906	1.61%	0.210%
61	12.483	1743	1749	1758	rVB3	24869	42873	76.04%	9.930%
62	12.556	1758	1761	1764	rBV2	488	806	1.43%	0.187%
63	12.599	1767	1768	1772	rVB2	597	692	1.23%	0.160%
64	12.825	1800	1805	1806	rVV2	1054	1150	2.04%	0.266%
65	12.837	1806	1807	1812	rVB2	549	726	1.29%	0.168%
66	13.178	1861	1863	1867	rVV2	688	961	1.70%	0.223%
67	13.318	1882	1886	1887	rVV2	722	647	1.15%	0.150%
68	13.337	1887	1889	1893	rVV3	1303	1857	3.29%	0.430%
69	13.379	1893	1896	1898	rVV2	872	937	1.66%	0.217%
70	13.422	1898	1903	1910	rVV2	21504	36085	64.00%	8.358%
71	13.489	1912	1914	1918	rVV2	816	1138	2.02%	0.264%
72	13.959	1987	1991	1995	rBV3	1526	2086	3.70%	0.483%
73	14.355	2052	2056	2057	rBV3	616	829	1.47%	0.192%
74	14.544	2084	2087	2090	rBV3	531	642	1.14%	0.149%
75	14.587	2090	2094	2097	rBV2	531	852	1.51%	0.197%
76	14.776	2122	2125	2128	rBV3	504	762	1.35%	0.176%

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77	15.245	2199	2202	2203	rBV2	594	623	1.10%	0.144%
78	15.306	2207	2212	2217	rBV5	998	2156	3.82%	0.499%
79	15.385	2222	2225	2227	rBV4	574	732	1.30%	0.170%
80	15.733	2281	2282	2287	rVB3	487	587	1.04%	0.136%
81	15.788	2289	2291	2293	rVV3	682	636	1.13%	0.147%
82	15.958	2316	2319	2321	rBV3	694	697	1.24%	0.161%
83	16.129	2343	2347	2349	rBV3	401	664	1.18%	0.154%
84	16.208	2359	2360	2365	rVB4	868	904	1.60%	0.209%
85	16.257	2365	2368	2370	rBV4	855	960	1.70%	0.222%
86	16.294	2372	2374	2378	rVB3	986	1231	2.18%	0.285%
87	16.330	2378	2380	2381	rBV	918	663	1.18%	0.154%
88	16.440	2395	2398	2399	rBV3	666	589	1.04%	0.136%
89	16.483	2401	2405	2409	rVB5	1272	1939	3.44%	0.449%
90	16.665	2432	2435	2436	rBV	824	842	1.49%	0.195%
91	16.751	2444	2449	2452	rVB4	641	1035	1.84%	0.240%

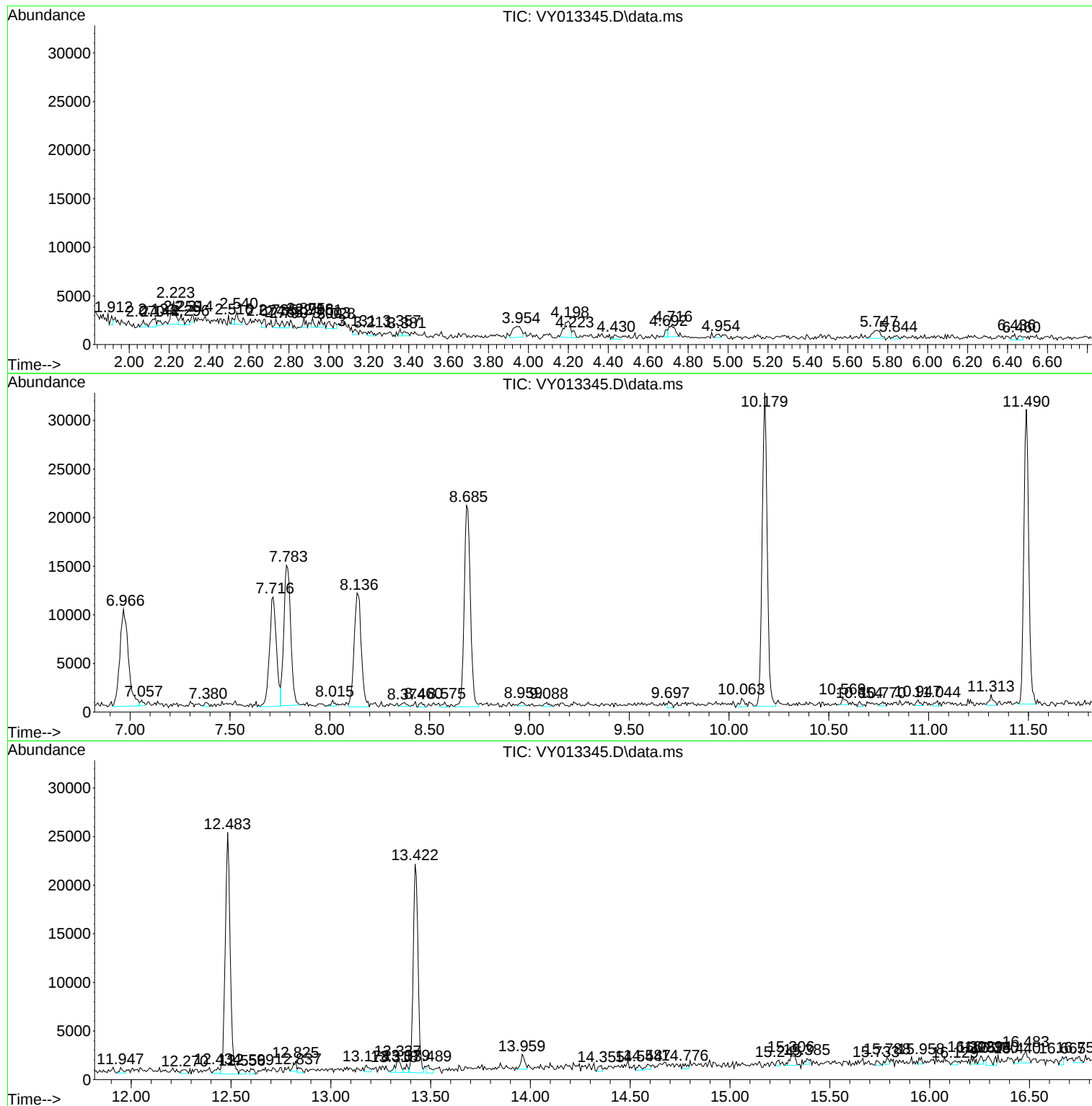
Sum of corrected areas: 431759

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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



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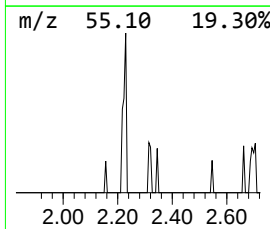
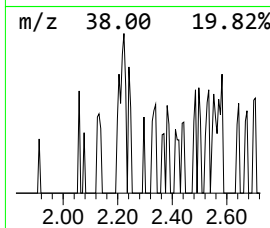
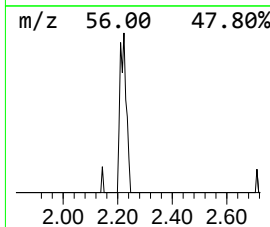
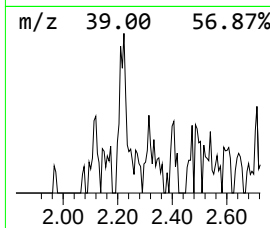
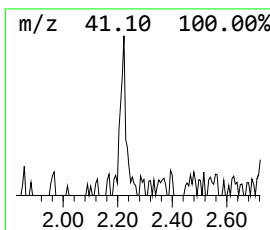
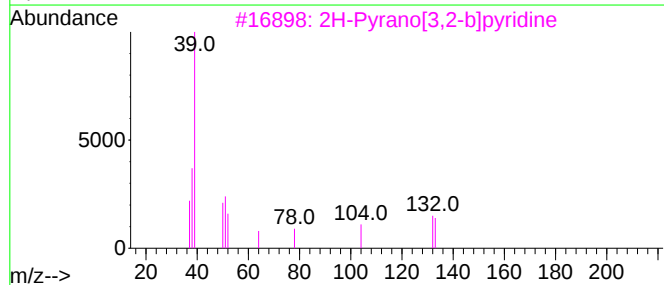
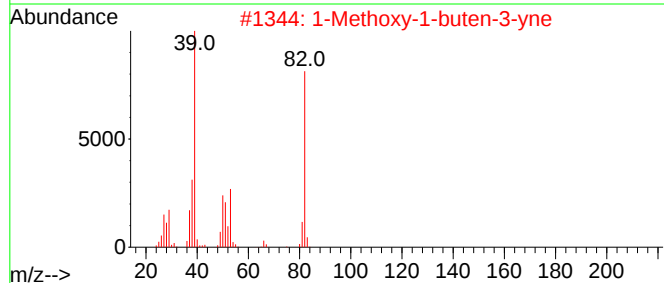
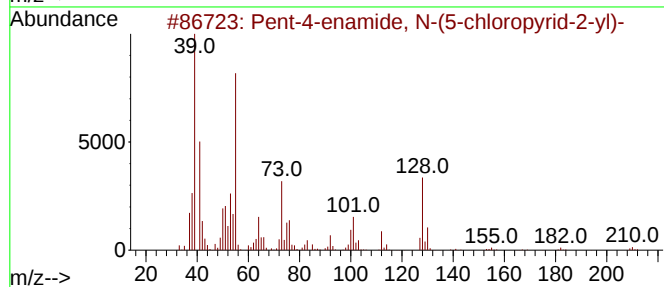
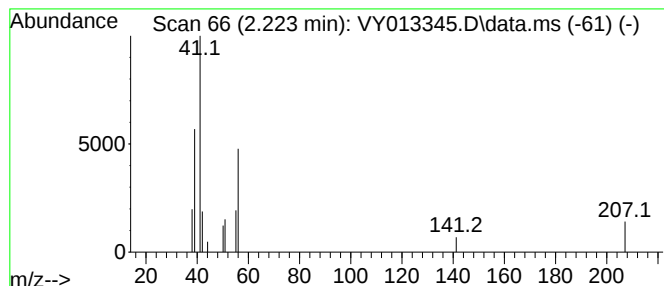
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.223 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.223	5.27 ug/l	3599	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pent-4-enamide, N-(5-chloropyrid-2-yl)-	210	C10H11ClN2O	306743-90-8	36
2			1-Methoxy-1-buten-3-yne	82	C5H6O	002798-73-4	36
3			2H-Pyrano[3,2-b]pyridine	133	C8H7NO	004767-91-3	36
4			Bis(3-methylbutyl) fluorene-2,7-diyl	466	C23H30O6S2	253664-95-8	36
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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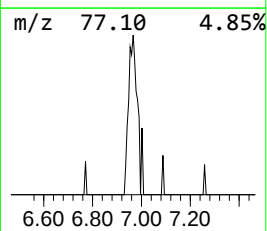
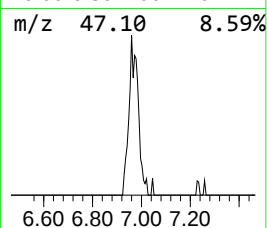
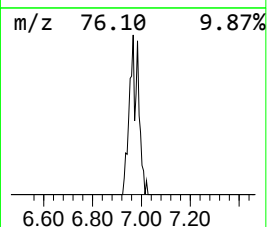
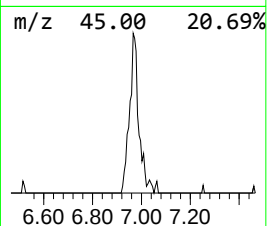
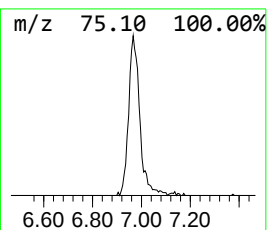
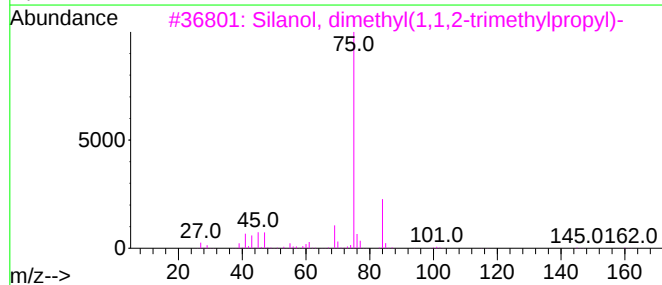
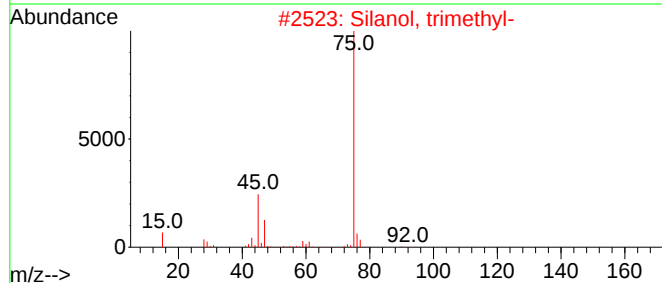
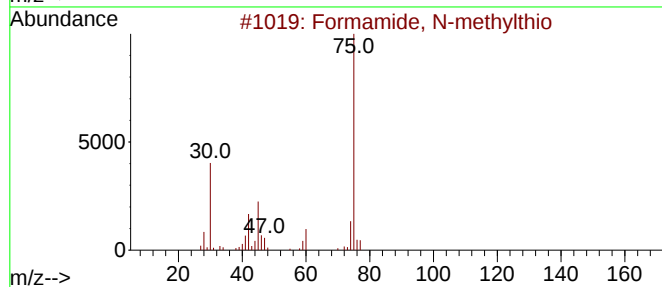
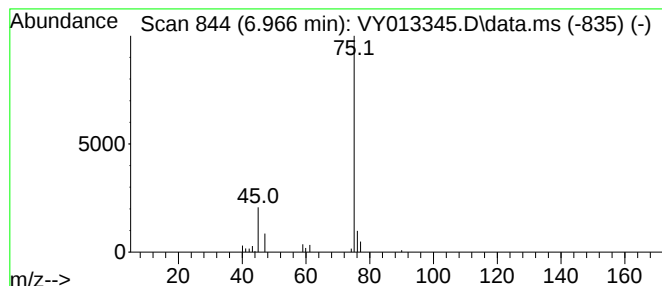
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Peak Number 3 Formamide, N-methylthio Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.966	43.61 ug/l	29805	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	72
2			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	72
3			Silanol, dimethyl(1,1,2-trimethyl...	160	C8H20OSi	055644-10-5	50
4			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	40
5			Silanol, ethyldimethyl-	104	C4H12OSi	005906-73-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.223	2.223	5.3	ug/l	3599	1	7.783	34172	50.0
Formamide, N-me...	6.966	43.6	ug/l	29805	1	7.783	34172	50.0