

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY053025\
 Data File : VY022484.D
 Acq On : 30 May 2025 17:25
 Operator : SY/MD
 Sample : Q2161-01
 Misc : 5.18g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 B27-SOIL-SAMPLE

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\82Y052725S.M

Title : SW846 8260

Signal : TIC: VY022484.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.879	23	26	28	rBV2	687	782	2.13%	0.342%
2	2.117	49	65	66	rBV3	10533	36739	100.00%	16.073%
3	2.604	144	145	151	rVB5	793	784	2.13%	0.343%
4	2.763	170	171	175	rVV4	763	909	2.47%	0.398%
5	2.812	177	179	184	rVB4	628	736	2.00%	0.322%
6	2.982	201	207	209	rBV3	496	1053	2.87%	0.461%
7	3.190	238	241	245	rVB2	650	956	2.60%	0.418%
8	3.293	254	258	261	rVB2	532	860	2.34%	0.376%
9	3.330	261	264	269	rBV3	546	945	2.57%	0.413%
10	3.415	275	278	285	rBV2	469	1040	2.83%	0.455%
11	3.647	313	316	318	rBV2	699	764	2.08%	0.334%
12	3.714	326	327	331	rVB2	472	552	1.50%	0.242%
13	4.129	393	395	398	rVV2	474	551	1.50%	0.241%
14	4.263	416	417	420	rVB	823	572	1.56%	0.250%
15	4.470	448	451	454	rBV3	503	757	2.06%	0.331%
16	4.750	494	497	498	rBV2	461	559	1.52%	0.245%
17	4.939	524	528	531	rVB3	890	1501	4.09%	0.657%
18	5.043	543	545	548	rBV3	879	897	2.44%	0.392%
19	5.336	589	593	595	rBV2	474	674	1.83%	0.295%
20	5.366	597	598	601	rBV3	494	559	1.52%	0.245%
21	5.512	620	622	624	rBV2	502	597	1.62%	0.261%
22	5.738	656	659	662	rBV2	575	555	1.51%	0.243%
23	5.903	681	686	688	rBV	543	1081	2.94%	0.473%
24	6.134	719	724	725	rBV	534	678	1.85%	0.297%
25	6.433	771	773	779	rVB3	397	603	1.64%	0.264%
26	6.585	795	798	799	rBV2	669	640	1.74%	0.280%
27	7.067	875	877	881	rVB2	481	748	2.04%	0.327%
28	7.116	881	885	886	rVB2	719	823	2.24%	0.360%
29	7.158	888	892	897	rBV3	472	918	2.50%	0.402%
30	7.213	897	901	904	rBV3	439	645	1.76%	0.282%
31	7.299	911	915	918	rVB2	577	1119	3.05%	0.490%
32	7.341	918	922	923	rBV2	602	771	2.10%	0.337%
33	7.597	961	964	967	rBV3	723	951	2.59%	0.416%
34	7.640	967	971	975	rVV5	1338	2066	5.62%	0.904%
35	7.707	975	982	991	rVB2	8356	19767	53.80%	8.648%
36	7.914	1013	1016	1019	rBV3	549	696	1.89%	0.305%

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37	7.945	1019	1021	1023	rVB2	882	643	1.75%	0.281%
38	8.067	1034	1041	1048	rVB4	3630	9791	26.65%	4.284%
39	8.536	1114	1118	1120	rVB4	464	623	1.70%	0.273%
40	8.616	1125	1131	1139	rVV2	11867	25063	68.22%	10.965%
41	8.756	1150	1154	1155	rBV2	586	649	1.77%	0.284%
42	8.774	1155	1157	1160	rVB	735	827	2.25%	0.362%
43	8.963	1183	1188	1190	rBV3	476	722	1.97%	0.316%
44	9.006	1194	1195	1198	rBV2	635	594	1.62%	0.260%
45	9.079	1205	1207	1210	rBV	558	559	1.52%	0.245%
46	9.189	1223	1225	1229	rBV2	598	646	1.76%	0.283%
47	9.231	1229	1232	1237	rVV2	652	877	2.39%	0.384%
48	9.402	1258	1260	1264	rVB2	650	789	2.15%	0.345%
49	9.573	1283	1288	1291	rBV2	663	974	2.65%	0.426%
50	9.841	1328	1332	1335	rBV2	491	776	2.11%	0.340%
51	10.006	1356	1359	1363	rVB2	421	568	1.55%	0.249%
52	10.109	1369	1376	1382	rBV2	16629	29972	81.58%	13.113%
53	10.195	1389	1390	1395	rVB2	562	597	1.62%	0.261%
54	10.408	1422	1425	1427	rVB3	821	880	2.40%	0.385%
55	10.475	1433	1436	1439	rBV3	624	576	1.57%	0.252%
56	10.591	1450	1455	1457	rVB3	578	865	2.35%	0.378%
57	10.780	1485	1486	1489	rBV2	552	685	1.86%	0.300%
58	10.890	1500	1504	1508	rVB3	415	761	2.07%	0.333%
59	11.146	1541	1546	1547	rBV2	751	1195	3.25%	0.523%
60	11.182	1550	1552	1554	rVV3	558	631	1.72%	0.276%
61	11.219	1554	1558	1561	rVB3	376	697	1.90%	0.305%
62	11.414	1585	1590	1596	rBV2	12512	20966	57.07%	9.173%
63	11.597	1616	1620	1624	rVB3	532	970	2.64%	0.424%
64	11.633	1624	1626	1629	rBV2	449	576	1.57%	0.252%
65	12.017	1686	1689	1692	rBV2	445	604	1.64%	0.264%
66	12.127	1702	1707	1709	rBV2	624	941	2.56%	0.412%
67	12.231	1723	1724	1728	rBV3	547	903	2.46%	0.395%
68	12.408	1748	1753	1759	rVB2	5550	8882	24.18%	3.886%
69	12.792	1814	1816	1821	rBV3	402	597	1.62%	0.261%
70	12.840	1821	1824	1828	rBV2	771	1147	3.12%	0.502%
71	13.151	1873	1875	1878	rVB	732	622	1.69%	0.272%
72	13.194	1878	1882	1883	rBV2	540	697	1.90%	0.305%
73	13.346	1903	1907	1912	rVB5	3346	5673	15.44%	2.482%
74	13.535	1936	1938	1943	rVV3	384	571	1.55%	0.250%
75	13.578	1943	1945	1948	rVB2	586	598	1.63%	0.262%
76	13.834	1985	1987	1992	rVV2	486	770	2.10%	0.337%

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77	13.889	1994	1996	2000	rVB3	914	894	2.43%	0.391%
78	14.096	2027	2030	2033	rBV3	410	593	1.61%	0.259%
79	14.127	2033	2035	2037	rVB	977	628	1.71%	0.275%
80	14.169	2037	2042	2043	rBV2	442	652	1.77%	0.285%
81	14.456	2085	2089	2092	rBV4	697	1034	2.81%	0.452%
82	14.529	2096	2101	2102	rVV2	442	627	1.71%	0.274%
83	14.578	2106	2109	2112	rVV3	621	915	2.49%	0.400%
84	14.621	2112	2116	2118	rVB2	631	637	1.73%	0.279%
85	14.712	2127	2131	2134	rVB2	613	821	2.23%	0.359%
86	14.810	2144	2147	2150	rVB3	735	834	2.27%	0.365%
87	15.041	2182	2185	2187	rVB3	591	651	1.77%	0.285%
88	15.389	2239	2242	2243	rBV2	720	633	1.72%	0.277%
89	15.462	2249	2254	2256	rBV3	501	548	1.49%	0.240%
90	15.553	2266	2269	2270	rVB3	743	593	1.61%	0.259%
91	15.663	2284	2287	2290	rBV2	959	1170	3.18%	0.512%
92	15.742	2298	2300	2303	rVB2	624	680	1.85%	0.298%
93	15.803	2308	2310	2312	rBV2	560	619	1.68%	0.271%
94	15.840	2312	2316	2317	rBV3	599	664	1.81%	0.291%
95	15.907	2324	2327	2328	rBV2	729	725	1.97%	0.317%
96	15.956	2332	2335	2337	rVB3	822	607	1.65%	0.266%
97	16.291	2385	2390	2392	rVV3	731	1021	2.78%	0.447%
98	16.346	2396	2399	2402	rVB3	800	791	2.15%	0.346%
99	16.571	2434	2436	2439	rVB4	686	703	1.91%	0.308%
100	16.706	2455	2458	2462	rBV3	641	1206	3.28%	0.528%

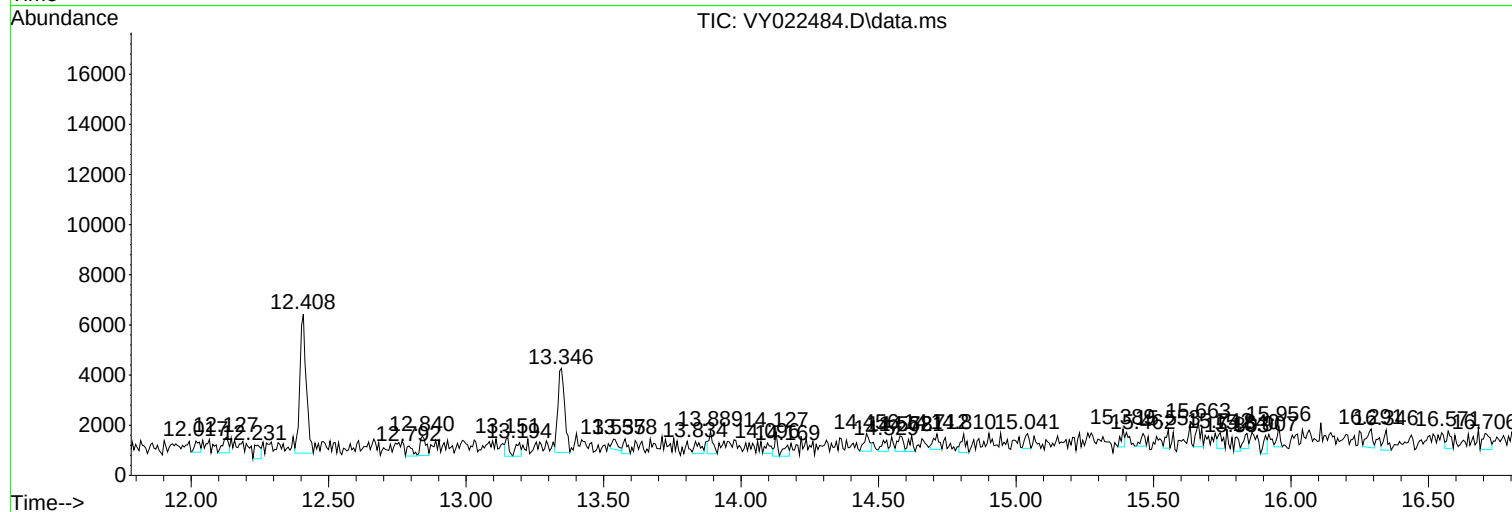
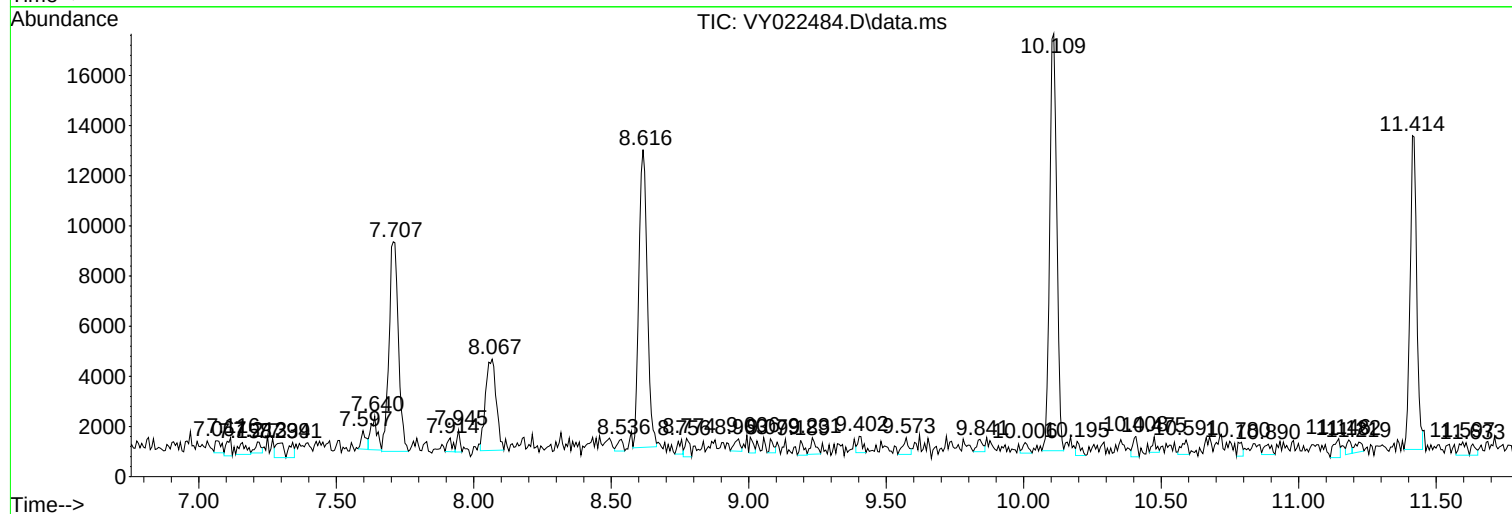
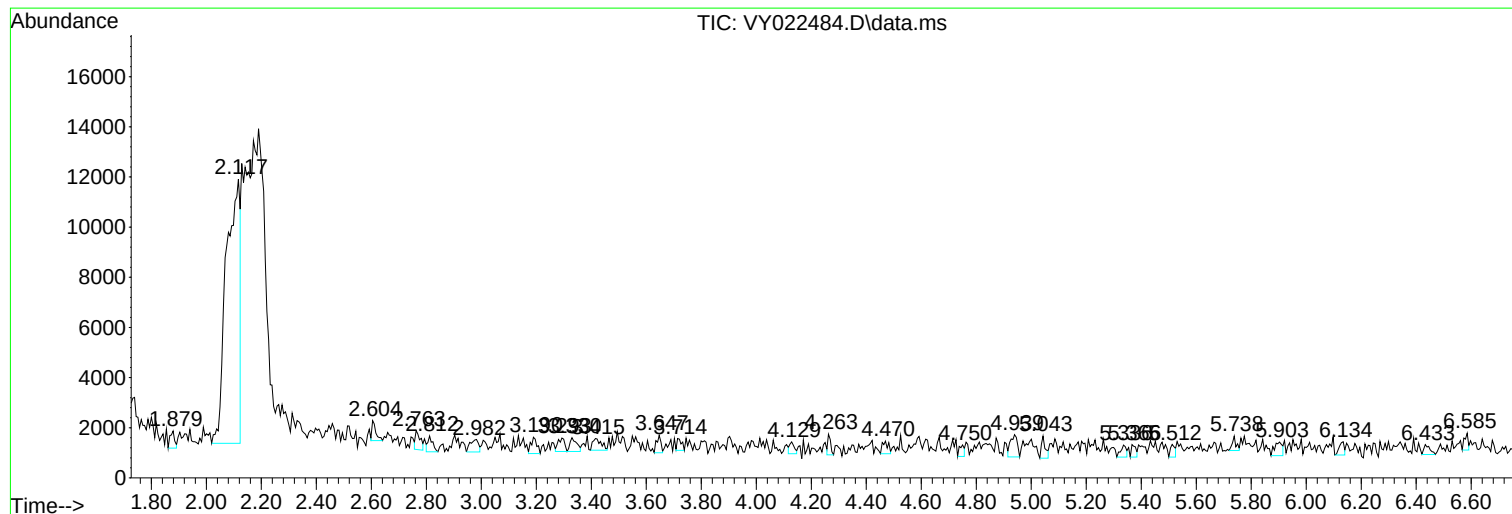
Sum of corrected areas: 228571

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052725S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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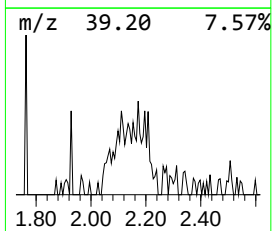
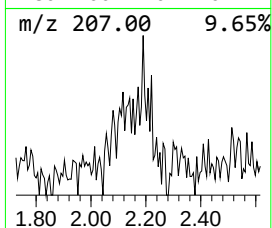
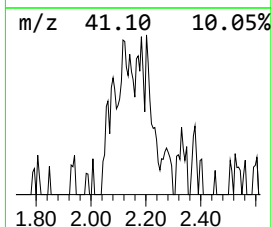
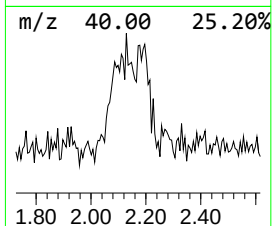
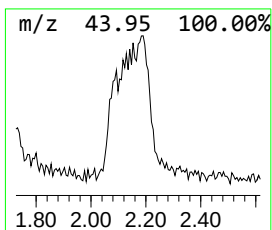
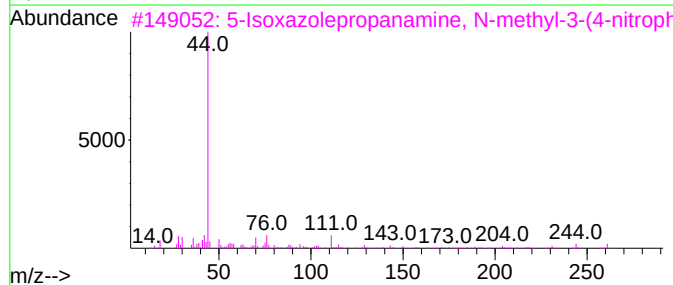
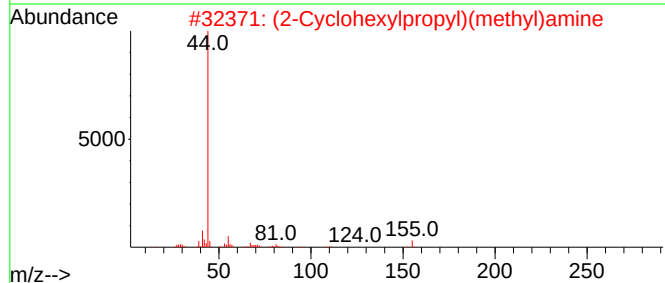
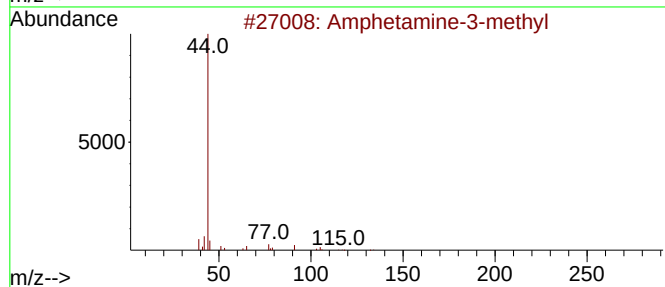
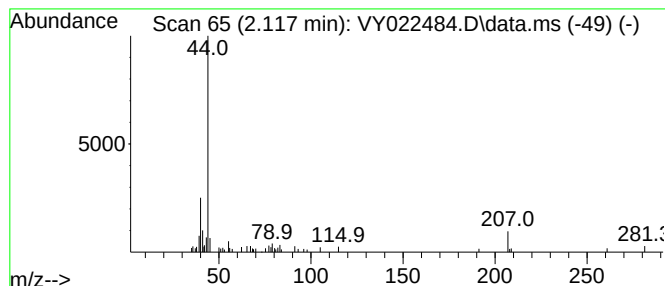
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052725S.M
Quant Title : SW846 8260

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

Peak Number 1 Amphetamine-3-methyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.117	92.93 ug/l	36739	Pentafluorobenzene	7.701

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amphetamine-3-methyl	149	C10H15N	000588-06-7	59
2			(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	53
3			5-Isoxazolepropanamine, N-methyl...	261	C13H15N3O3	157170-19-9	45
4			2-(Aminomethyl)-4-methylpentanoi...	173	C9H19NO2	1891247-86-1	42
5			n-Hexylmethylaniline	115	C7H17N	035161-70-7	42



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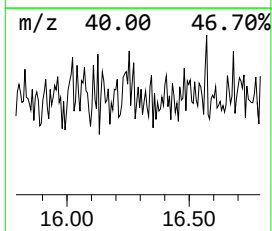
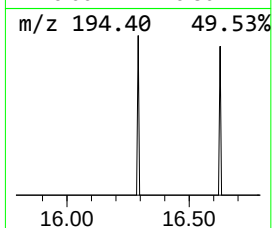
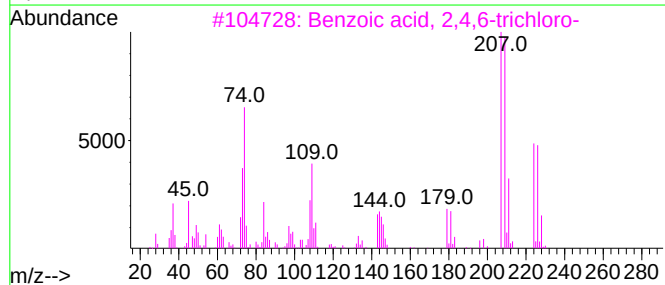
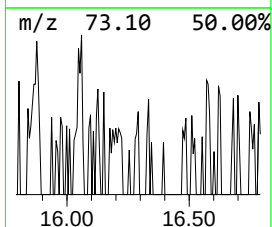
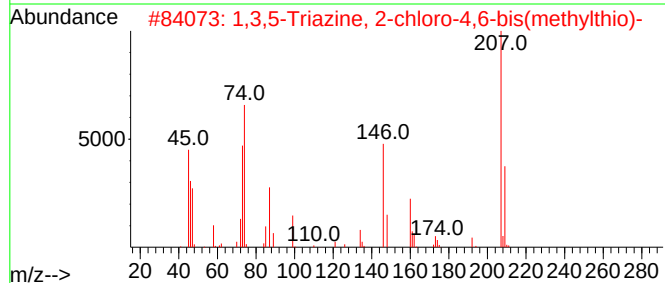
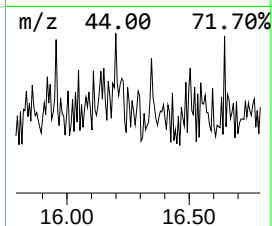
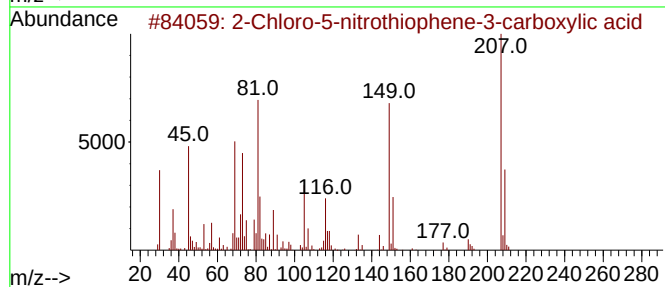
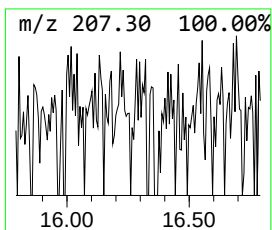
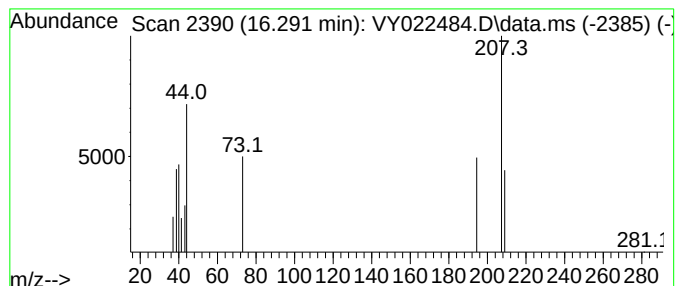
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2-Chloro-5-nitrothiophene-3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.291	9.00 ug/l	1021	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-5-nitrothiophene-3-carb...	207	C5H2ClNO4S	1000460-11-4	53
2			1,3,5-Triazine, 2-chloro-4,6-bis...	207	C5H6ClN3S2	004407-40-3	9
3			Benzoic acid, 2,4,6-trichloro-	224	C7H3Cl3O2	000050-43-1	9
4			N-(3-Phenylpropyl)thiourea	194	C10H14N2S	093168-20-8	5
5			7-Chloro-4-methoxy-3-methylquino...	207	C11H10ClNO	1000213-52-2	5



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amphetamine-3-m...	2.117	92.9	ug/l	36739	1	7.701	19767	50.0
2-Chloro-5-nitr...	16.291	9.0	ug/l	1021	4	13.352	5673	50.0