

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD020124\
 Data File : VD078307.D
 Acq On : 01 Feb 2024 16:14
 Operator : RP/MD
 Sample : P1329-05
 Misc : 4.58G/10ml/MSVOA_D/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 C0FL3

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\SFAMDLM020124SMA.M
 Title : SFAM01.0

Signal : TIC: VD078307.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.687	12	17	19	rBV	4773	6763	0.90%	0.178%
2	1.740	19	26	38	rVB	466368	752666	100.00%	19.799%
3	1.887	49	51	52	rBV	1128	625	0.08%	0.016%
4	2.276	111	117	125	rVB	103806	154637	20.55%	4.068%
5	2.799	200	206	216	rVB	72925	141224	18.76%	3.715%
6	3.346	298	299	302	rVB	1077	684	0.09%	0.018%
7	3.381	302	305	307	rVB	809	935	0.12%	0.025%
8	3.617	343	345	348	rVB	734	710	0.09%	0.019%
9	3.652	348	351	355	rVB3	605	925	0.12%	0.024%
10	3.775	370	372	379	rVB2	796	1224	0.16%	0.032%
11	3.917	387	396	408	rBV2	60939	165635	22.01%	4.357%
12	4.187	440	442	444	rVB	750	635	0.08%	0.017%
13	4.217	444	447	449	rBV	968	911	0.12%	0.024%
14	4.364	470	472	473	rBV	1101	637	0.08%	0.017%
15	4.440	484	485	489	rBV	776	763	0.10%	0.020%
16	4.546	500	503	506	rBV2	708	836	0.11%	0.022%
17	4.805	540	547	556	rVB3	11005	28968	3.85%	0.762%
18	5.081	590	594	597	rVB2	822	1253	0.17%	0.033%
19	5.134	597	603	604	rBV	1166	1538	0.20%	0.040%
20	5.181	610	611	614	rVB2	842	606	0.08%	0.016%
21	5.222	614	618	620	rBV2	719	842	0.11%	0.022%
22	5.581	677	679	682	rVB2	560	558	0.07%	0.015%
23	5.652	688	691	692	rBV	713	630	0.08%	0.017%
24	5.740	704	706	708	rVV2	552	570	0.08%	0.015%
25	5.846	718	724	727	rBV4	2570	5599	0.74%	0.147%
26	5.975	745	746	749	rVB	953	670	0.09%	0.018%
27	6.069	760	762	765	rVV	841	832	0.11%	0.022%
28	6.140	771	774	776	rVB	733	705	0.09%	0.019%
29	6.281	795	798	801	rBV2	894	1073	0.14%	0.028%
30	6.322	801	805	807	rBV2	592	871	0.12%	0.023%
31	6.464	828	829	832	rBV	693	683	0.09%	0.018%
32	6.728	872	874	877	rBV	972	839	0.11%	0.022%
33	6.993	910	919	929	rBV	25006	75493	10.03%	1.986%
34	7.458	996	998	1001	rBV2	968	681	0.09%	0.018%
35	7.569	1008	1017	1028	rBV	78269	203194	27.00%	5.345%
36	7.993	1086	1089	1090	rBV	1024	873	0.12%	0.023%

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 Title : SFAM01.0

37	8.122	1109	1111	1114	rVB2	972	1000	0.13%	0.026%
38	8.205	1114	1125	1141	rBV2	159256	483005	64.17%	12.706%
39	8.305	1141	1142	1145	rVV	900	695	0.09%	0.018%
40	8.434	1162	1164	1165	rBV	1278	867	0.12%	0.023%
41	8.452	1165	1167	1168	rVV2	1046	554	0.07%	0.015%
42	8.540	1180	1182	1184	rBV2	731	804	0.11%	0.021%
43	8.669	1201	1204	1206	rVB2	754	714	0.09%	0.019%
44	8.775	1213	1222	1229	rBV	54424	103044	13.69%	2.711%
45	9.005	1260	1261	1265	rVB	1050	809	0.11%	0.021%
46	9.046	1265	1268	1271	rBV2	657	1001	0.13%	0.026%
47	9.116	1277	1280	1282	rBV2	807	972	0.13%	0.026%
48	9.210	1288	1296	1305	rVB2	101718	210156	27.92%	5.528%
49	9.563	1354	1356	1357	rBV2	647	586	0.08%	0.015%
50	9.599	1359	1362	1363	rVV2	840	598	0.08%	0.016%
51	9.763	1389	1390	1393	rVV3	933	849	0.11%	0.022%
52	9.828	1396	1401	1405	rVB2	1057	1464	0.19%	0.039%
53	9.863	1405	1407	1410	rBV	762	803	0.11%	0.021%
54	9.910	1412	1415	1416	rBV	789	867	0.12%	0.023%
55	9.981	1420	1427	1435	rVV	59445	104435	13.88%	2.747%
56	10.269	1468	1476	1485	rBV	210925	369030	49.03%	9.708%
57	10.387	1493	1496	1497	rBV2	749	694	0.09%	0.018%
58	10.522	1512	1519	1527	rVV3	38813	71267	9.47%	1.875%
59	10.669	1538	1544	1549	rVB2	8197	14854	1.97%	0.391%
60	10.810	1565	1568	1569	rBV	1050	975	0.13%	0.026%
61	10.881	1572	1580	1587	rBV	91501	160640	21.34%	4.226%
62	10.952	1590	1592	1595	rVB	1597	1217	0.16%	0.032%
63	11.028	1600	1605	1610	rBV3	5543	8469	1.13%	0.223%
64	11.257	1640	1644	1649	rVB3	1086	1667	0.22%	0.044%
65	11.581	1693	1699	1708	rVV2	73580	127243	16.91%	3.347%
66	11.657	1710	1712	1714	rVB2	736	600	0.08%	0.016%
67	11.675	1714	1715	1718	rBV2	891	783	0.10%	0.021%
68	11.716	1718	1722	1723	rBV2	751	827	0.11%	0.022%
69	11.781	1731	1733	1736	rBV	532	578	0.08%	0.015%
70	11.993	1766	1769	1772	rVB	1059	1076	0.14%	0.028%
71	12.157	1795	1797	1801	rBV	1008	1317	0.17%	0.035%
72	12.275	1816	1817	1819	rBV	905	652	0.09%	0.017%
73	12.316	1822	1824	1827	rVV	923	910	0.12%	0.024%
74	12.575	1864	1868	1874	rVB2	4788	7611	1.01%	0.200%
75	12.651	1874	1881	1887	rBV	112901	183303	24.35%	4.822%
76	12.851	1912	1915	1922	rVB2	2401	3516	0.47%	0.092%

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 Title : SFAM01.0

77	12.946	1929	1931	1933	rBV	779	600	0.08%	0.016%
78	13.075	1949	1953	1956	rBV2	758	1217	0.16%	0.032%
79	13.134	1961	1963	1965	rVB	1096	899	0.12%	0.024%
80	13.516	2022	2028	2034	rVB2	60579	95915	12.74%	2.523%
81	13.581	2037	2039	2040	rVV	1260	719	0.10%	0.019%
82	13.610	2042	2044	2050	rVB5	3279	4526	0.60%	0.119%
83	13.722	2058	2063	2065	rBV2	920	1596	0.21%	0.042%
84	13.816	2072	2079	2087	rVB	151649	248550	33.02%	6.538%
85	14.016	2111	2113	2114	rVV	786	609	0.08%	0.016%
86	14.051	2114	2119	2124	rVB3	3583	5813	0.77%	0.153%
87	14.369	2172	2173	2175	rBV2	983	755	0.10%	0.020%
88	14.487	2191	2193	2196	rVB2	1140	779	0.10%	0.020%
89	14.663	2221	2223	2226	rVB	1066	818	0.11%	0.022%
90	14.804	2245	2247	2248	rBV2	970	708	0.09%	0.019%
91	14.828	2248	2251	2254	rVB2	1367	1472	0.20%	0.039%
92	14.881	2258	2260	2262	rBV	1278	767	0.10%	0.020%
93	15.034	2284	2286	2292	rBV2	816	1217	0.16%	0.032%
94	15.151	2304	2306	2308	rBV2	1002	595	0.08%	0.016%
95	15.598	2379	2382	2384	rBV3	1052	1581	0.21%	0.042%
96	15.998	2449	2450	2452	rVB	1325	717	0.10%	0.019%
97	16.045	2452	2458	2459	rBV2	1824	2363	0.31%	0.062%
98	16.216	2486	2487	2489	rBV	1313	795	0.11%	0.021%
99	16.416	2519	2521	2524	rBV3	977	874	0.12%	0.023%
100	16.545	2541	2543	2544	rBV	1509	818	0.11%	0.022%

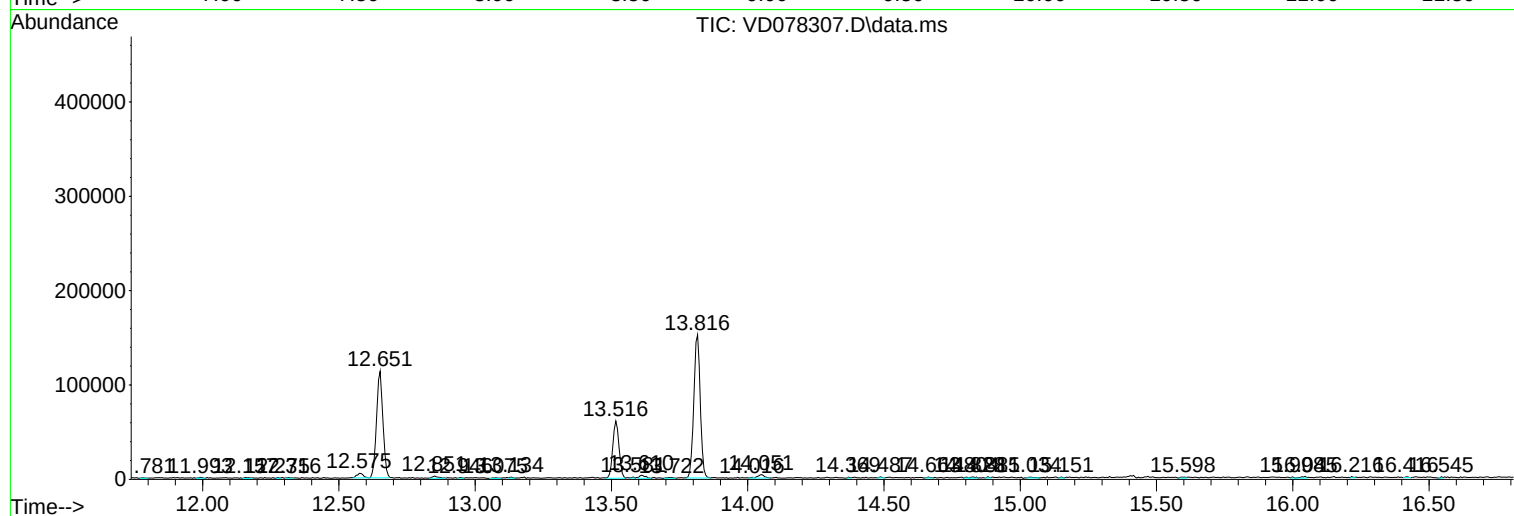
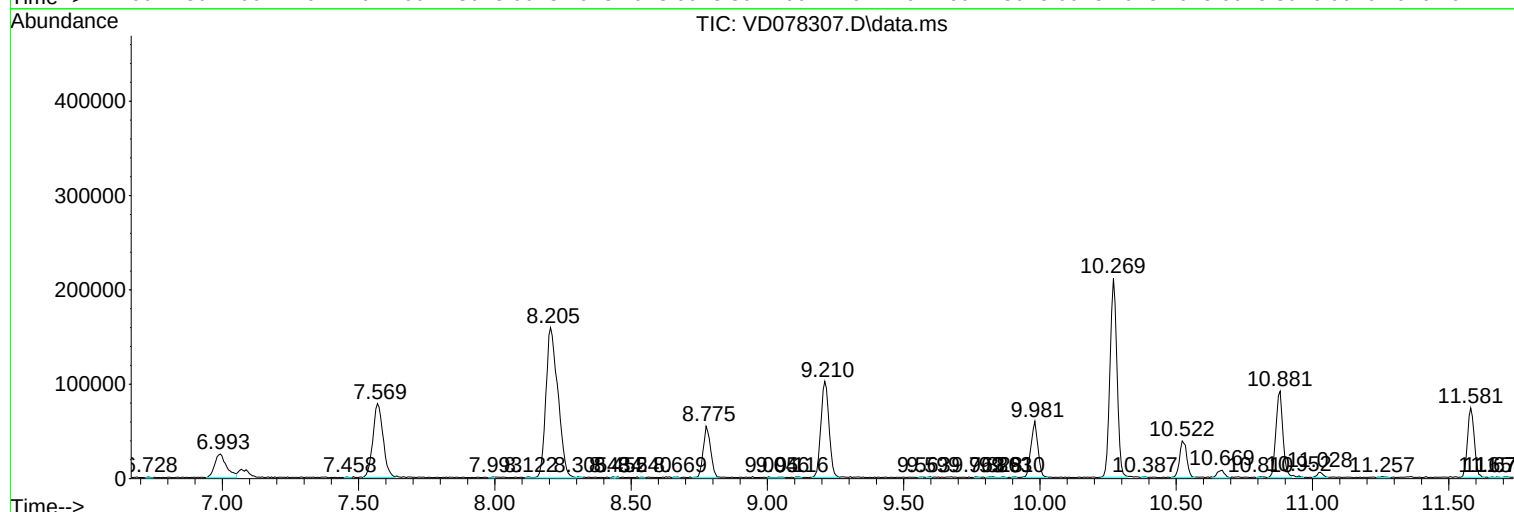
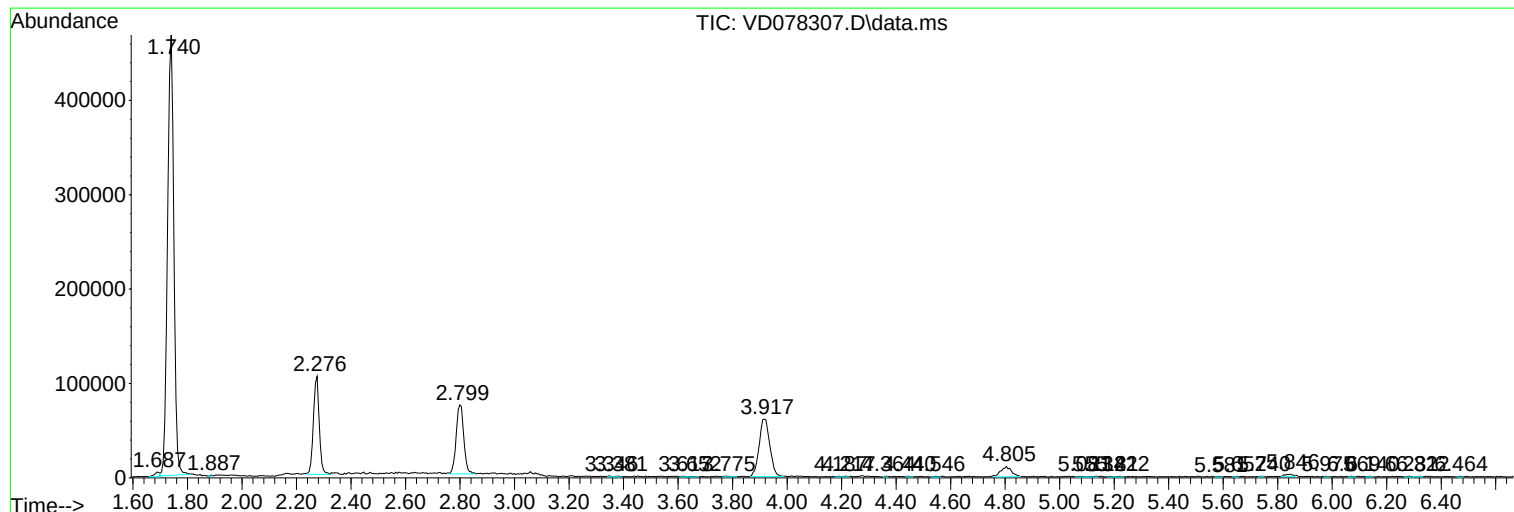
Sum of corrected areas: 3801443

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM020124SMA.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\SFAMDLM020124SMA.M
Quant Title : SFAM01.0

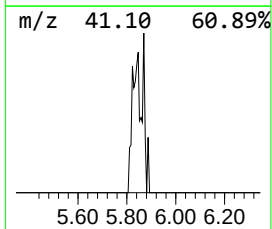
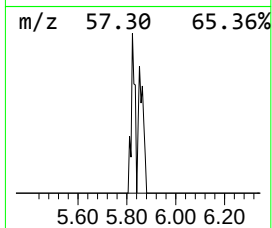
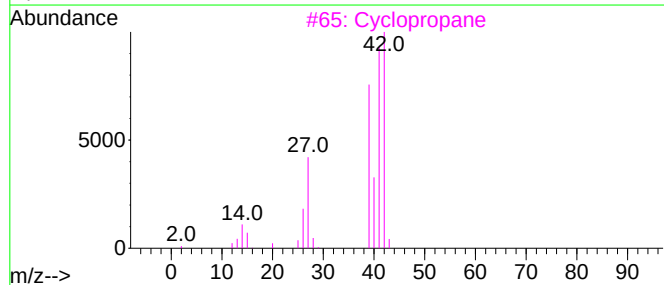
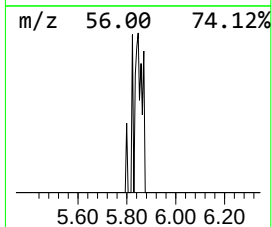
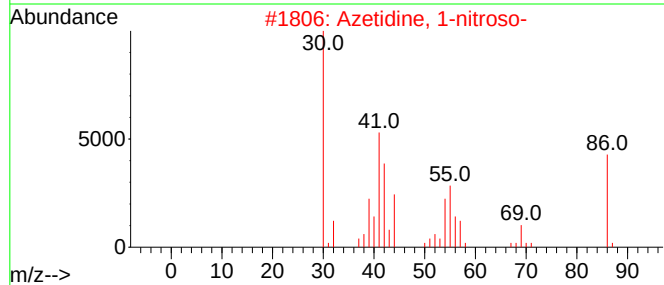
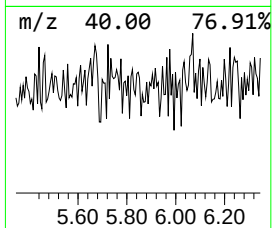
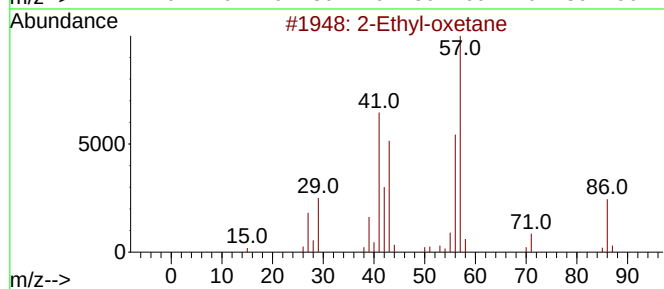
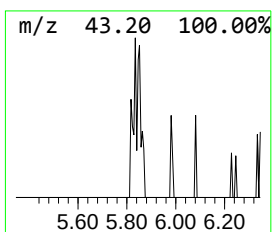
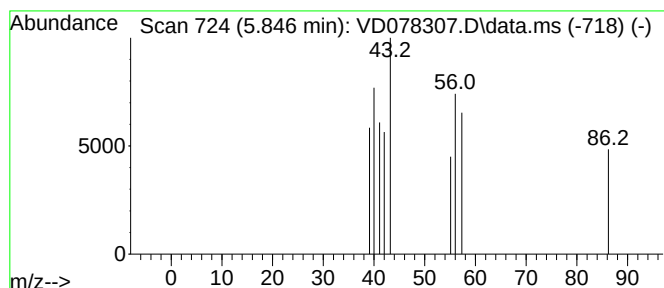
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Ethyl-oxetane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.846	1.36 ug/L	5599	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	53
2			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	32
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Propene	42	C3H6	000115-07-1	9
5			2H-Pyran-2-one, tetrahydro-3,6-d...	128	C7H12O2	003720-22-7	9



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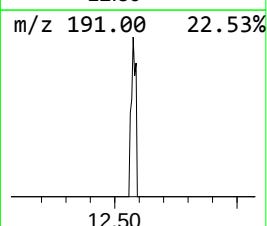
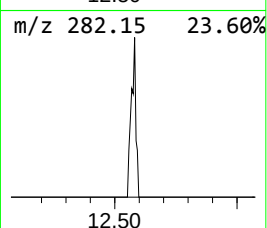
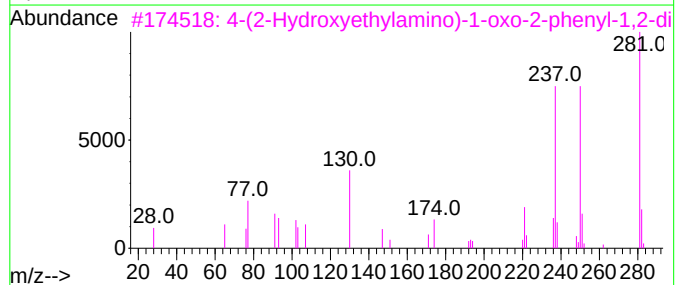
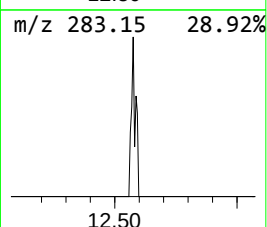
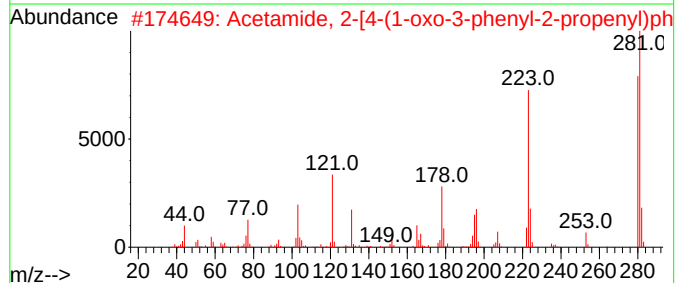
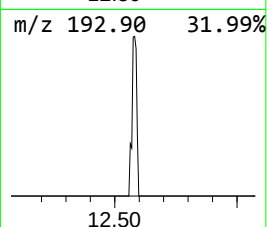
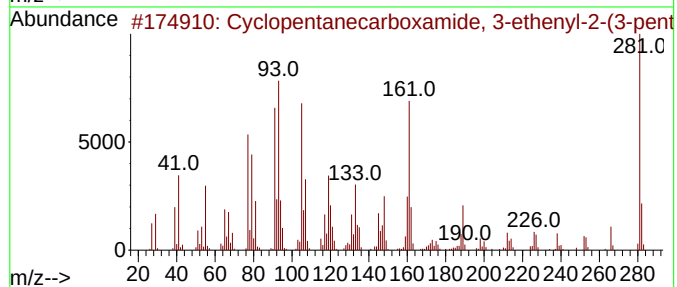
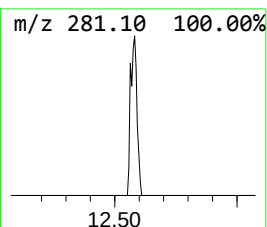
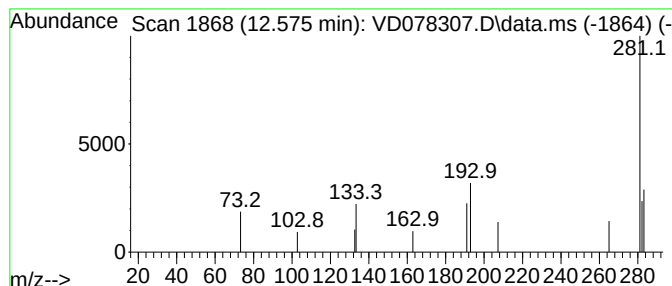
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM020124SMA.M
Quant Title : SFAM01.0

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

Peak Number 7 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	1.98 ug/L	7611	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanecarboxamide, 3-ethen...	281	C19H23NO	136091-23-1	38
2			Acetamide, 2-[4-(1-oxo-3-phenyl-...	281	C17H15NO3	019152-45-5	9
3			4-(2-Hydroxyethylamino)-1-oxo-2-...	281	C16H15N3O2	087365-21-7	9
4			4-[N-Methylpiperazino]-5-nitro v...	281	C13H19N3O4	030058-29-8	9
5			Ethyl 3-amino-4-(1,3-benzodiazol...	281	C16H15N3O2	1000444-00-5	9



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Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Ethyl-oxetane	5.846	1.4	ug/L	5599	1	8.775	103044	25.0
unknown-01	12.575	2.0	ug/L	7611	3	13.516	95915	25.0