

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041223\
 Data File : VY013277.D
 Acq On : 12 Apr 2023 19:19
 Operator : KP/MD
 Sample : 02283-07
 Misc : 3.77g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20230222-7-4

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: VY013277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.857	3	6	22	rVB2	41854	77420	8.00%	1.038%
2	2.211	60	64	65	rBV2	14823	16582	1.71%	0.222%
3	2.241	66	69	77	rVB	23673	38077	3.94%	0.511%
4	2.686	137	142	150	rVB	25591	48982	5.06%	0.657%
5	2.894	170	176	182	rBV6	4192	9884	1.02%	0.133%
6	3.247	226	234	246	rVB4	7334	21267	2.20%	0.285%
7	3.717	300	311	320	rVB7	4061	16765	1.73%	0.225%
8	3.948	338	349	355	rBV	75048	230321	23.81%	3.089%
9	4.021	355	361	376	rVV	113074	332621	34.39%	4.461%
10	4.186	379	388	399	rVB2	33445	93070	9.62%	1.248%
11	4.479	428	436	442	rBV	4584	14117	1.46%	0.189%
12	4.704	463	473	485	rBV2	37200	116123	12.01%	1.558%
13	5.747	634	644	651	rBV4	4000	11978	1.24%	0.161%
14	6.984	836	847	870	rBV2	42661	148842	15.39%	1.996%
15	7.710	955	966	972	rBV	142659	346655	35.84%	4.650%
16	7.783	972	978	989	rVB	227253	519776	53.74%	6.972%
17	8.130	1027	1035	1048	rBV	154670	359200	37.14%	4.818%
18	8.545	1095	1103	1112	rBV4	6711	15740	1.63%	0.211%
19	8.685	1116	1126	1139	rBV	356101	712708	73.69%	9.560%
20	9.179	1200	1207	1212	rVB8	4743	12426	1.28%	0.167%
21	10.173	1363	1370	1377	rBV	553765	967186	100.00%	12.973%
22	10.240	1377	1381	1388	rVB	42527	71260	7.37%	0.956%
23	10.368	1394	1402	1407	rVB4	7709	15732	1.63%	0.211%
24	11.484	1578	1585	1596	rBV	517523	850129	87.90%	11.403%
25	11.587	1596	1602	1611	rVV	7460	15720	1.63%	0.211%
26	11.697	1611	1620	1631	rVB	27583	60633	6.27%	0.813%
27	12.026	1664	1674	1681	rBV	57079	99714	10.31%	1.337%
28	12.111	1681	1688	1694	rVB5	4440	10135	1.05%	0.136%
29	12.325	1716	1723	1728	rBV	11701	19487	2.01%	0.261%
30	12.477	1742	1748	1760	rVV2	403333	668792	69.15%	8.971%
31	12.727	1784	1789	1792	rBV3	10492	17842	1.84%	0.239%
32	12.806	1797	1802	1814	rVB2	56981	108883	11.26%	1.460%
33	12.965	1822	1828	1835	rBV	30424	55114	5.70%	0.739%
34	13.038	1836	1840	1842	rVV4	8738	13323	1.38%	0.179%
35	13.069	1842	1845	1848	rVV	7819	10399	1.08%	0.139%
36	13.117	1848	1853	1859	rVV	56111	86941	8.99%	1.166%

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37	13.282	1872	1880	1883	rVV5	14712	27464	2.84%	0.368%
38	13.312	1883	1885	1889	rVV4	8381	11090	1.15%	0.149%
39	13.422	1896	1903	1919	rBV2	464665	851004	87.99%	11.415%
40	13.623	1931	1936	1939	rBV4	13120	22541	2.33%	0.302%
41	13.745	1952	1956	1960	rBV7	11375	18966	1.96%	0.254%
42	13.959	1986	1991	1998	rVB	90081	150351	15.55%	2.017%
43	14.142	2018	2021	2026	rVB6	6837	11584	1.20%	0.155%
44	14.203	2026	2031	2034	rBV5	6974	13805	1.43%	0.185%
45	14.251	2035	2039	2044	rVV8	7296	13652	1.41%	0.183%
46	14.379	2056	2060	2064	rBV6	10522	18594	1.92%	0.249%
47	14.678	2105	2109	2114	rVV8	6593	13183	1.36%	0.177%
48	14.727	2114	2117	2121	rVV4	10396	15522	1.60%	0.208%
49	14.794	2124	2128	2132	rBV3	10721	17393	1.80%	0.233%
50	14.934	2147	2151	2157	rBV9	6429	10581	1.09%	0.142%
51	15.215	2193	2197	2205	rBV8	7559	16577	1.71%	0.222%
52	15.605	2259	2261	2266	rVB5	12691	16715	1.73%	0.224%
53	16.153	2347	2351	2356	rVB6	8010	12519	1.29%	0.168%

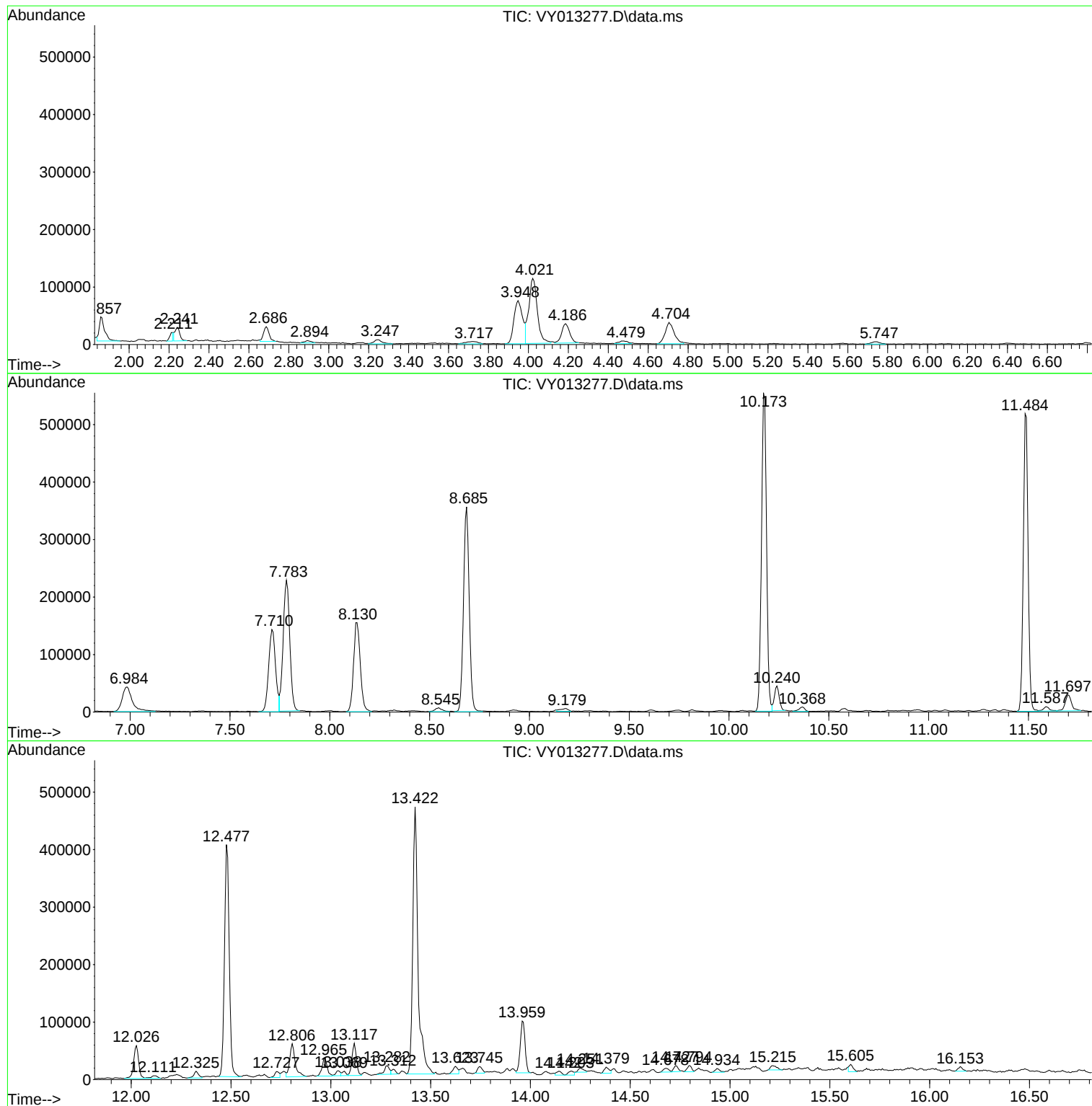
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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



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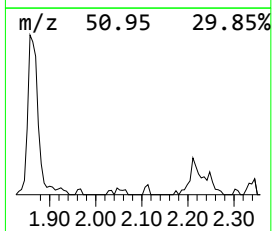
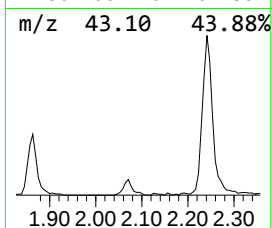
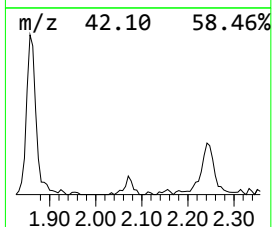
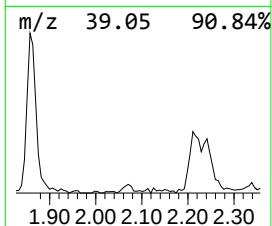
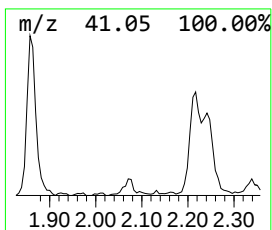
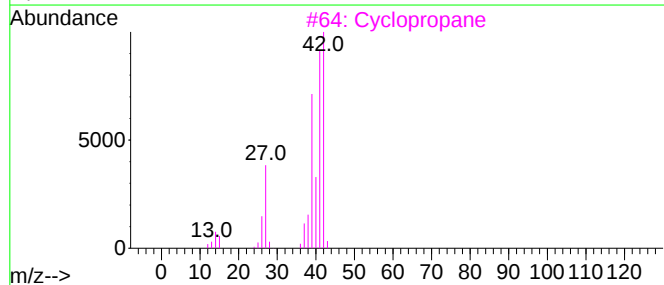
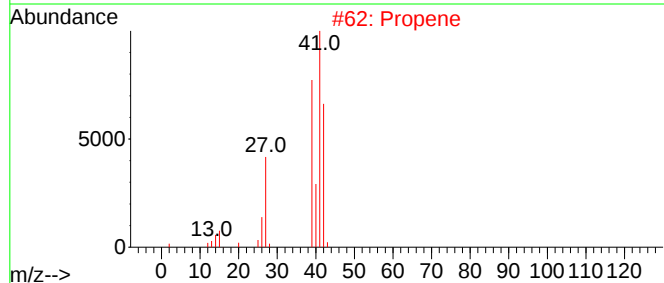
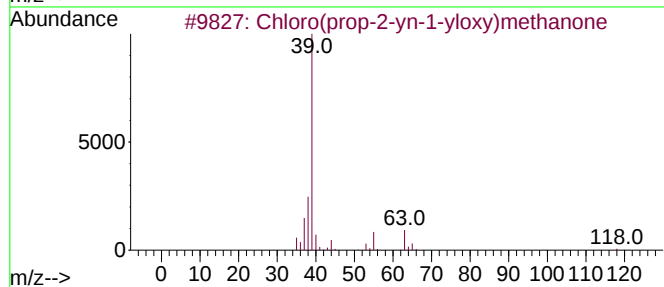
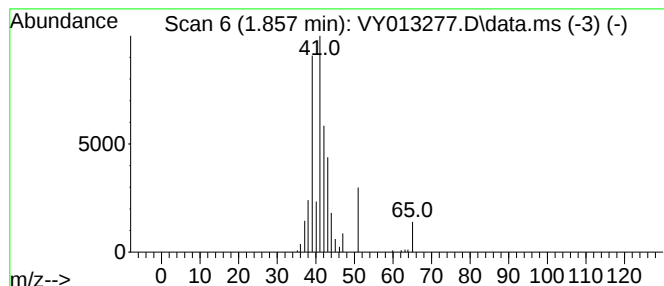
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 1 Chloro(prop-2-yn-1-yloxy)me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.857	7.45 ug/l	77420	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	50
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	40
4			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
5			Cyclopropene	40	C3H4	002781-85-3	4



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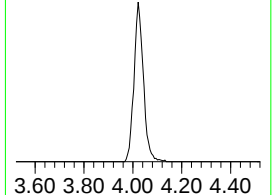
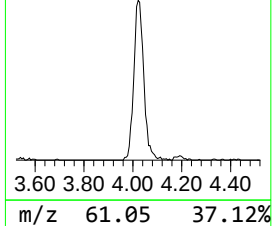
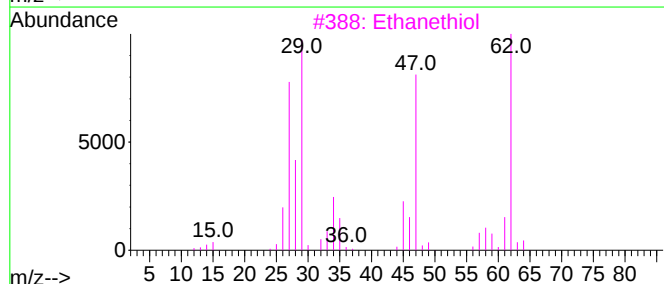
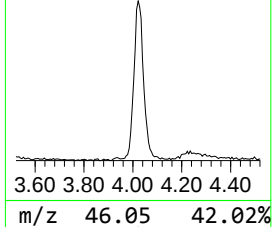
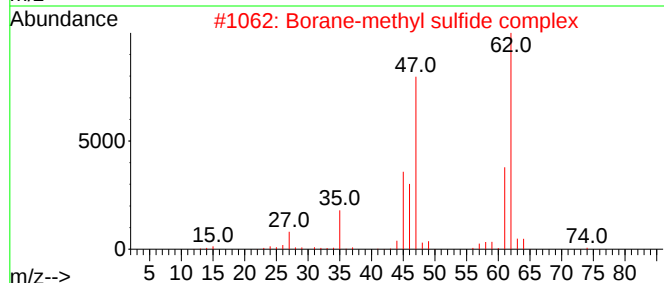
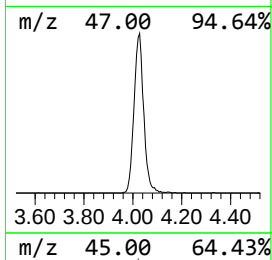
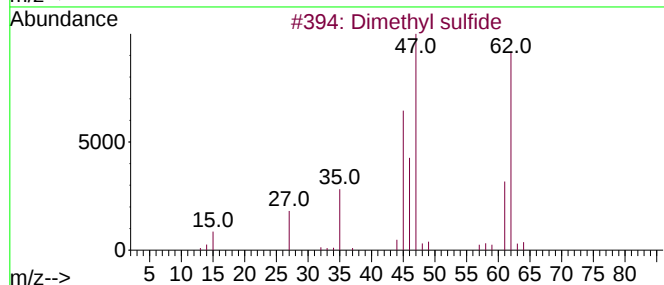
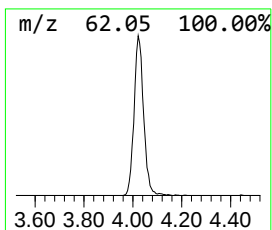
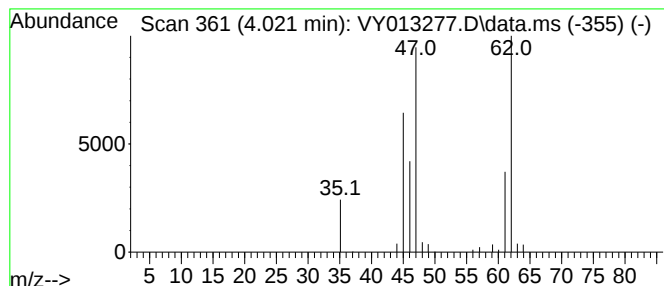
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041223S.M
Quant Title : SW846 8260

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

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.021	32.00 ug/l	332621	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	97
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83
3			Ethanethiol	62	C2H6S	000075-08-1	59
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	38
5			Boric acid	62	BH3O3	010043-35-3	9



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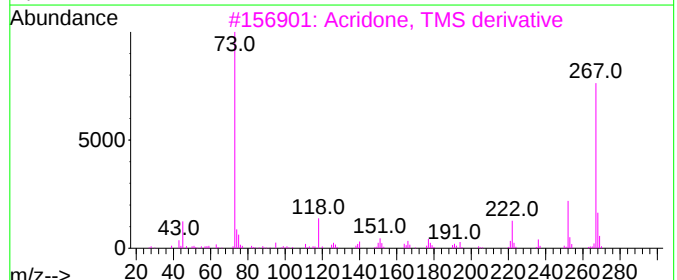
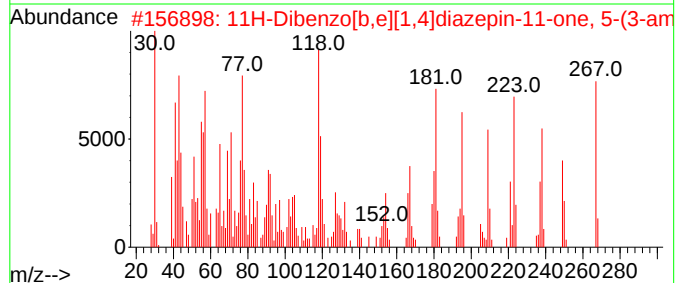
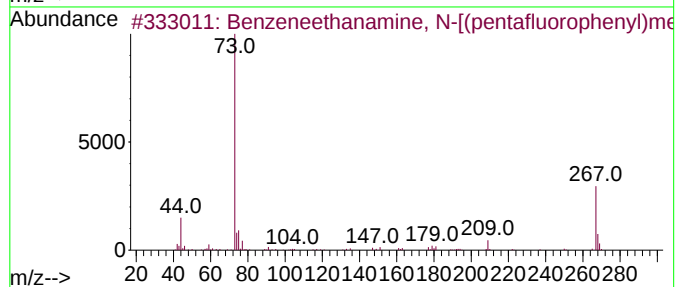
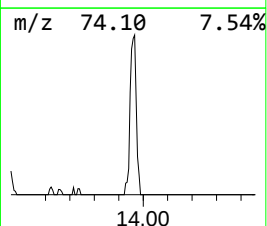
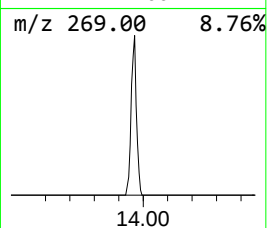
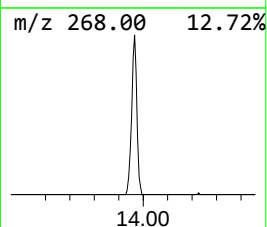
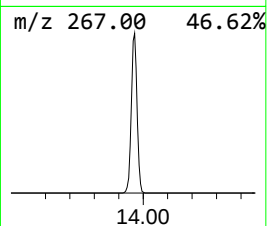
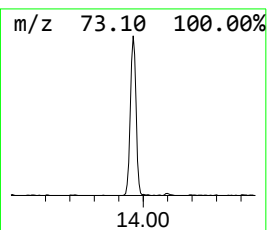
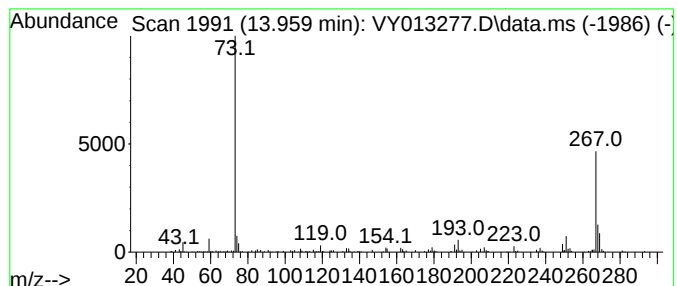
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzeneethanamine, N-[(pent... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	8.83 ug/l	150351	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanamine, N-[(pentafluoro...]	475	C21H26F5NO2Si2	055429-85-1	56
2			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	53
3			Acridone, TMS derivative	267	C16H17NO5i	1000478-16-0	50
4			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	45
5			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	45



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Chloro(prop-2-y...	1.857	7.5	ug/l	77420	1	7.783	519776	50.0
Dimethyl sulfide	4.021	32.0	ug/l	332621	1	7.783	519776	50.0
Benzeneethanami...	13.959	8.8	ug/l	150351	4	13.422	851004	50.0