

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
 Data File : VY013480.D
 Acq On : 26 Apr 2023 17:50
 Operator : KP/MD
 Sample : 02448-01
 Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20230283-23-1

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\82Y042423S.M
 Title : SW846 8260

Signal : TIC: VY013480.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	15	rVB2	38878	59427	8.36%	1.243%
2	2.071	34	41	45	rBV2	7642	13166	1.85%	0.275%
3	2.223	59	66	68	rBV	23130	40695	5.72%	0.851%
4	2.247	68	70	77	rVB2	20159	27280	3.84%	0.571%
5	2.906	169	178	184	rBV5	7754	16744	2.36%	0.350%
6	3.253	229	235	247	rVB5	5226	14528	2.04%	0.304%
7	3.948	339	349	359	rBV	53226	174695	24.58%	3.654%
8	4.192	380	389	398	rBV	31567	86095	12.11%	1.801%
9	4.710	463	474	483	rBV4	15344	49265	6.93%	1.030%
10	5.741	635	643	646	rBV4	3584	8540	1.20%	0.179%
11	6.990	836	848	860	rBV2	23342	76599	10.78%	1.602%
12	7.716	952	967	972	rBV	107792	256050	36.02%	5.355%
13	7.789	972	979	990	rVB	165168	385751	54.27%	8.068%
14	8.143	1025	1037	1048	rBV	122093	264940	37.27%	5.541%
15	8.551	1095	1104	1113	rBV5	4118	10161	1.43%	0.213%
16	8.685	1116	1126	1139	rBV	265356	525245	73.89%	10.985%
17	10.179	1364	1371	1380	rBV	415169	710833	100.00%	14.867%
18	11.490	1578	1586	1595	rBV	386946	640225	90.07%	13.390%
19	12.209	1695	1704	1705	rBV7	4607	8812	1.24%	0.184%
20	12.227	1705	1707	1714	rVB7	5965	10749	1.51%	0.225%
21	12.477	1740	1748	1759	rBV2	301853	514345	72.36%	10.757%
22	12.630	1768	1773	1782	rVB7	6677	16919	2.38%	0.354%
23	12.806	1797	1802	1805	rBV7	9198	19323	2.72%	0.404%
24	13.069	1841	1845	1851	rVB2	11349	18107	2.55%	0.379%
25	13.172	1858	1862	1869	rVB6	5319	11402	1.60%	0.238%
26	13.282	1872	1880	1885	rBV2	32127	58959	8.29%	1.233%
27	13.337	1885	1889	1896	rVB4	18477	31517	4.43%	0.659%
28	13.422	1896	1903	1908	rBV	361360	553086	77.81%	11.568%
29	13.471	1908	1911	1918	rVB	25378	47669	6.71%	0.997%
30	13.642	1931	1939	1944	rBV9	8636	20777	2.92%	0.435%
31	13.739	1952	1955	1960	rVB5	6983	8570	1.21%	0.179%
32	13.959	1985	1991	1999	rVB2	31266	53561	7.53%	1.120%
33	14.385	2056	2061	2062	rBV3	5789	7673	1.08%	0.160%
34	14.733	2113	2118	2122	rVB9	3917	8004	1.13%	0.167%
35	14.849	2132	2137	2145	rVB9	3840	10498	1.48%	0.220%
36	15.123	2179	2182	2191	rVB8	5047	9666	1.36%	0.202%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

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\82Y042423S.M
Title : SW846 8260

37	15.605	2257	2261	2267	rVB7	6131	11499	1.62%	0.240%
----	--------	------	------	------	------	------	-------	-------	--------

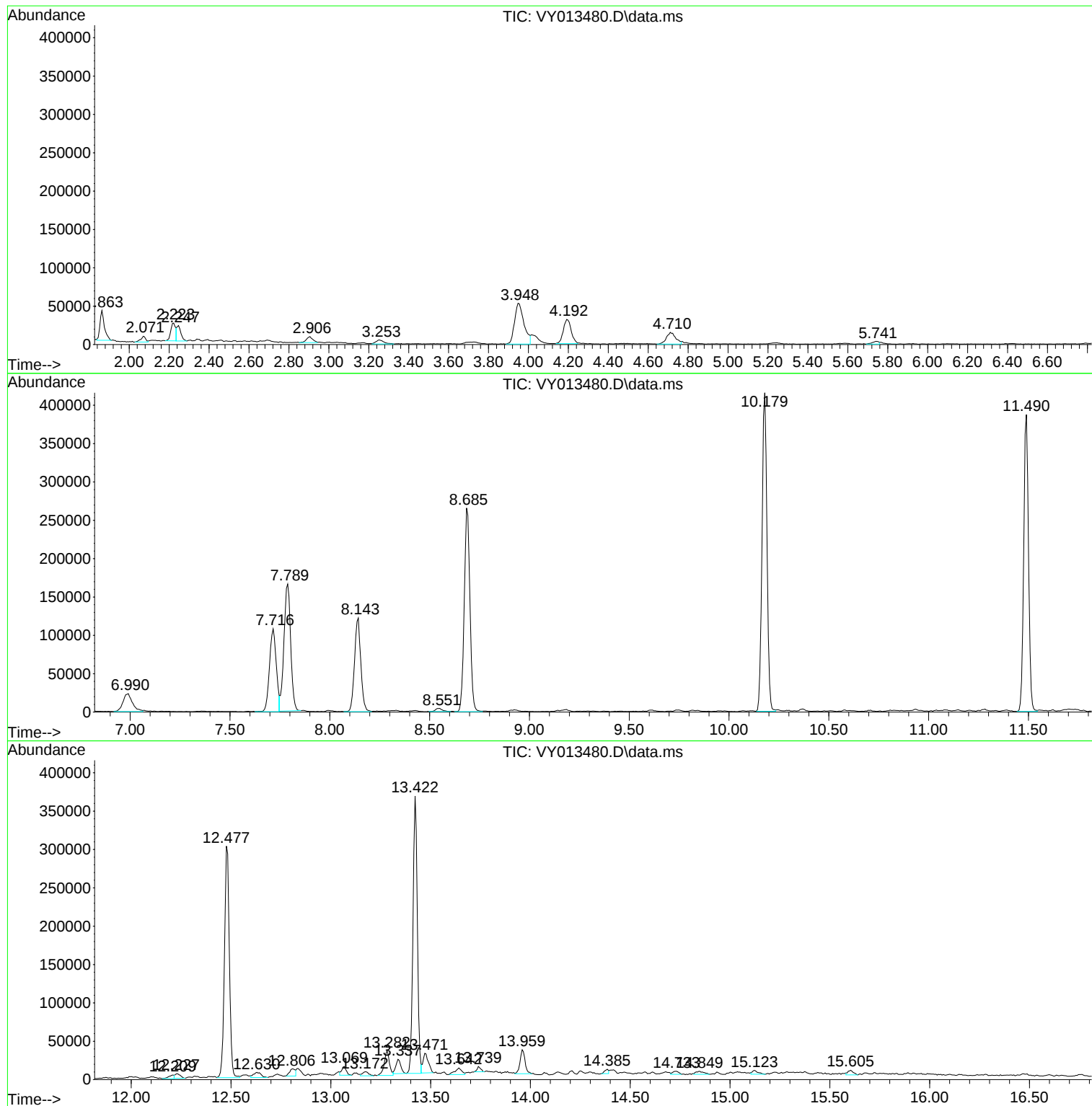
Sum of corrected areas: 4781375

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

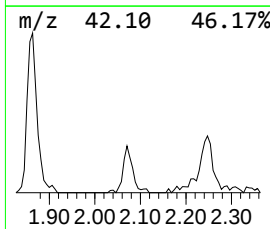
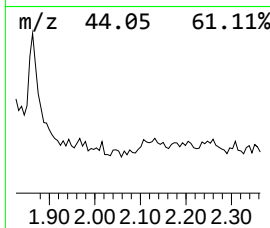
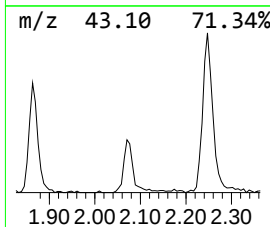
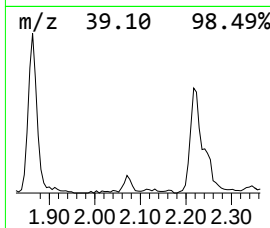
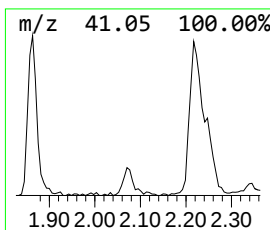
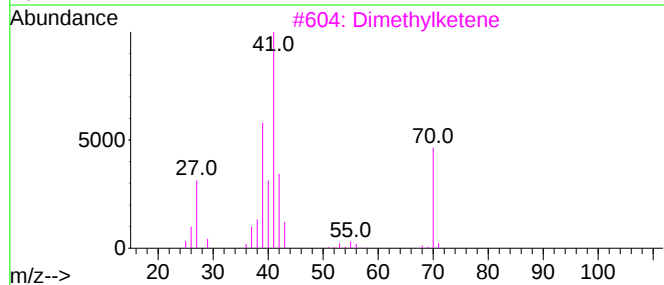
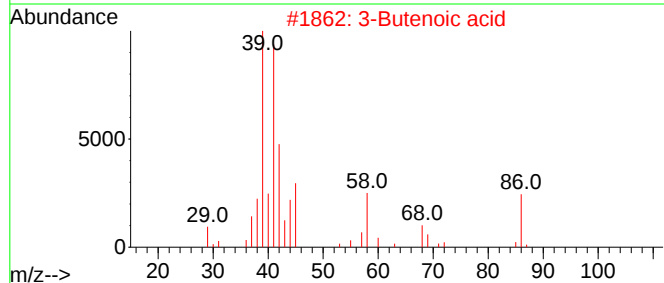
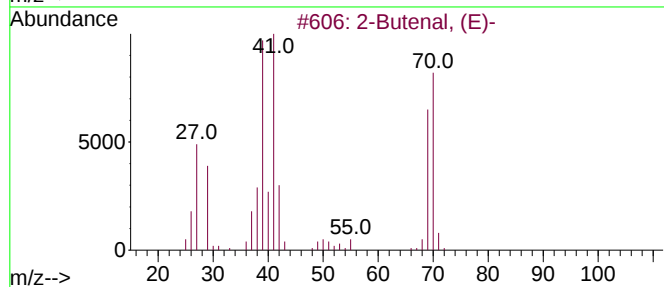
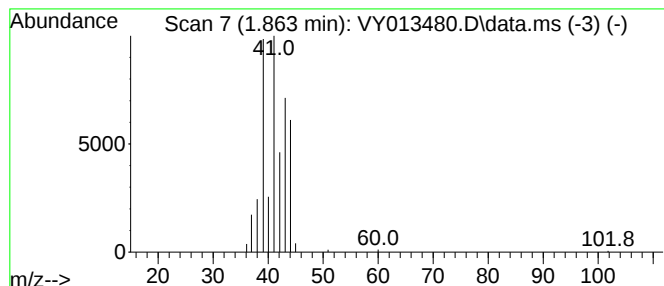
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 1 2-Butenal, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.863	7.70 ug/l	59427	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-			70	C4H6O	000123-73-9	72
2	3-Butenoic acid			86	C4H6O2	000625-38-7	64
3	Dimethylketene			70	C4H6O	000598-26-5	40
4	Cyclopropanecarboxamide			85	C4H7NO	006228-73-5	40
5	2-Butenal			70	C4H6O	004170-30-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

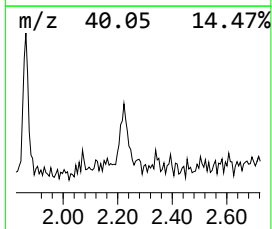
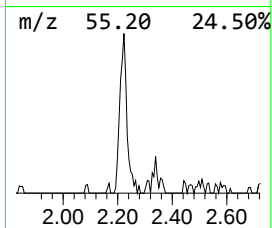
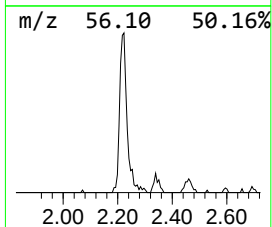
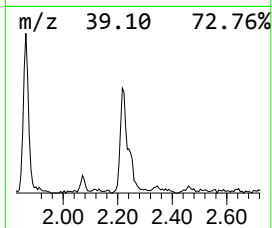
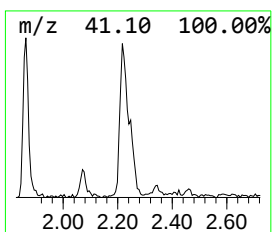
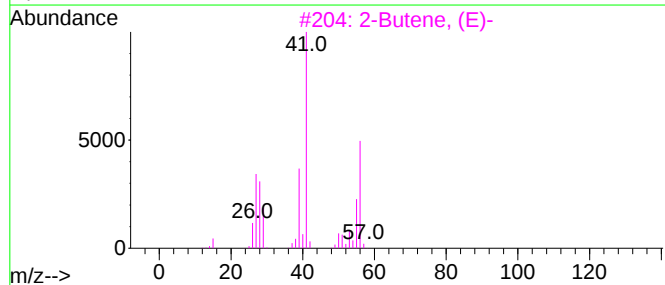
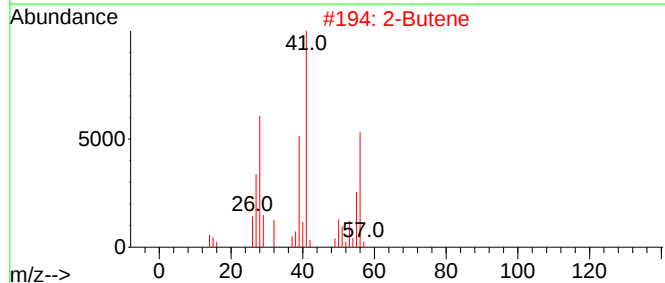
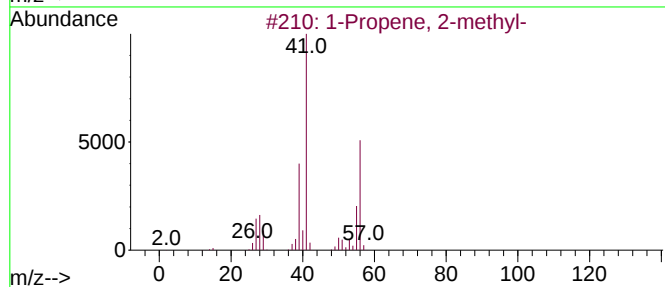
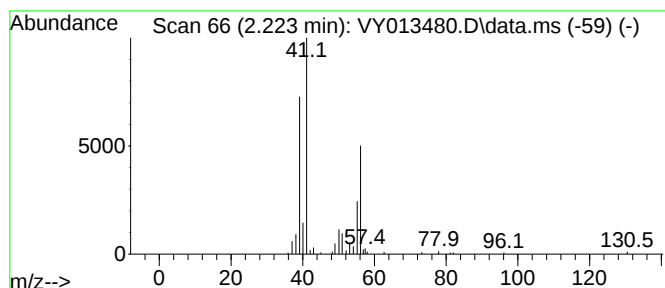
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.223	5.27 ug/l	40695	Pentafluorobenzene	7.789

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propene, 2-methyl-	56	C4H8	000115-11-7	72
2		2-Butene	56	C4H8	000107-01-7	50
3		2-Butene, (E)-	56	C4H8	000624-64-6	38
4		2-Butene, (Z)-	56	C4H8	000590-18-1	38
5		1-Butene	56	C4H8	000106-98-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

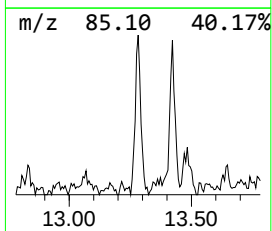
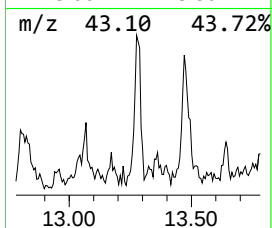
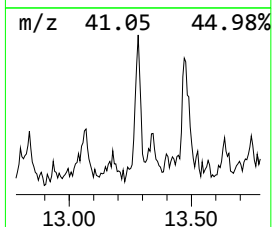
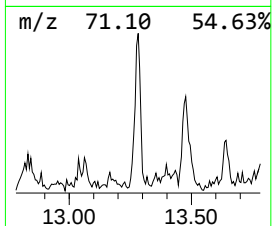
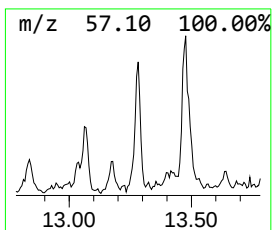
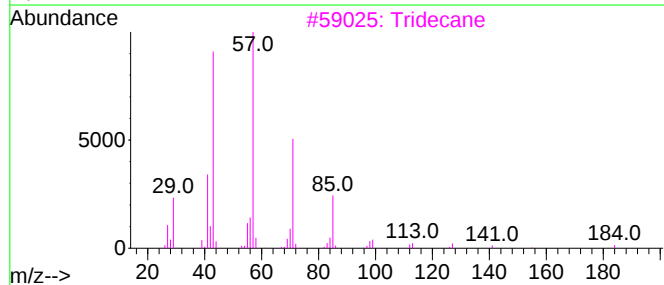
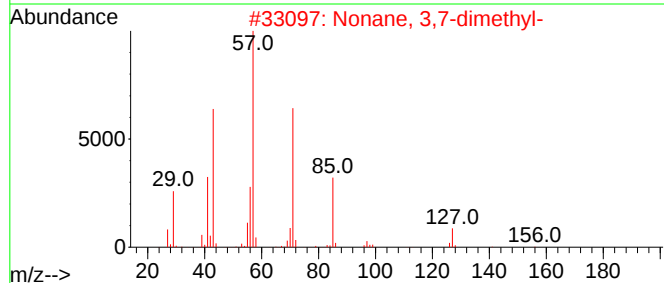
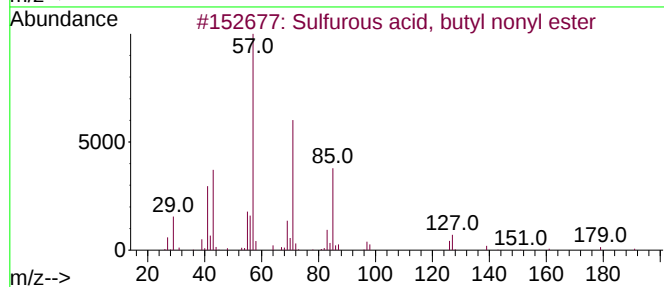
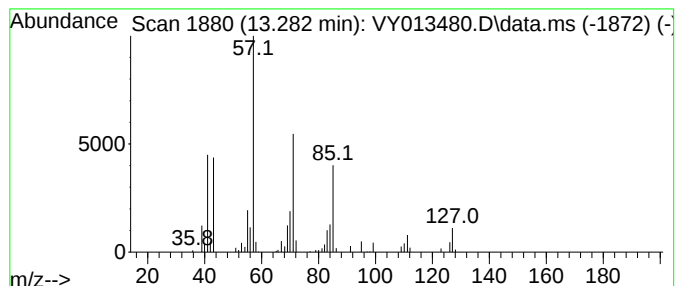
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 4 Sulfurous acid, butyl nonyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	5.33 ug/l	58959	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
3			Tridecane	184	C13H28	000629-50-5	59
4			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
Data File : VY013480.D
Acq On : 26 Apr 2023 17:50
Operator : KP/MD
Sample : 02448-01
Misc : 3.86g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20230283-23-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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-Butenal, (E)-	1.863	7.7	ug/l	59427	1	7.789	385751	50.0
1-Propene, 2-me...	2.223	5.3	ug/l	40695	1	7.789	385751	50.0
Sulfurous acid,...	13.282	5.3	ug/l	58959	4	13.422	553086	50.0