

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
 Data File : VY011972.D
 Acq On : 22 Dec 2022 14:14
 Operator : KP/MD
 Sample : N6160-03
 Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VOC-7-3051

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\82Y122022S.M
 Title : SW846 8260

Signal : TIC: VY011972.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	25	rVB2	13820	33119	4.80%	0.584%
2	3.942	337	348	359	rBV2	6246	16890	2.45%	0.298%
3	4.198	380	390	401	rBV	13299	37094	5.38%	0.654%
4	4.716	461	475	487	rBV	5854	18418	2.67%	0.325%
5	5.753	635	645	654	rVB3	3974	12332	1.79%	0.218%
6	7.350	900	907	916	rVB5	2987	8152	1.18%	0.144%
7	7.716	957	967	973	rBV2	99011	236337	34.26%	4.168%
8	7.789	973	979	990	rVB	185716	419314	60.78%	7.396%
9	8.143	1028	1037	1050	rBV	93811	201152	29.16%	3.548%
10	8.691	1118	1127	1142	rBV	260959	521357	75.57%	9.196%
11	10.179	1363	1371	1379	rBV	403692	689893	100.00%	12.168%
12	11.087	1513	1520	1525	rBV8	4092	8529	1.24%	0.150%
13	11.294	1548	1554	1564	rBV9	3217	8155	1.18%	0.144%
14	11.489	1579	1586	1598	rVB	319417	523618	75.90%	9.235%
15	11.685	1613	1618	1622	rBV6	4914	10706	1.55%	0.189%
16	11.843	1638	1644	1647	rBV6	4695	8108	1.18%	0.143%
17	11.995	1664	1669	1676	rBV8	5472	14419	2.09%	0.254%
18	12.093	1681	1685	1692	rVB7	4411	9876	1.43%	0.174%
19	12.203	1697	1703	1713	rBV8	12541	33112	4.80%	0.584%
20	12.319	1713	1722	1727	rBV9	7936	24422	3.54%	0.431%
21	12.392	1729	1734	1737	rVV5	6216	9491	1.38%	0.167%
22	12.483	1743	1749	1755	rBV	219182	344334	49.91%	6.073%
23	12.562	1755	1762	1767	rBV10	6814	19096	2.77%	0.337%
24	12.642	1772	1775	1780	rVB6	7960	12533	1.82%	0.221%
25	12.733	1783	1790	1794	rBV6	15213	38570	5.59%	0.680%
26	12.794	1796	1800	1805	rBV4	11899	24380	3.53%	0.430%
27	12.916	1815	1820	1822	rBV4	9369	16715	2.42%	0.295%
28	12.947	1822	1825	1829	rVV4	15654	23491	3.41%	0.414%
29	13.068	1838	1845	1851	rVB9	11712	27007	3.91%	0.476%
30	13.136	1851	1856	1858	rBV6	14088	24436	3.54%	0.431%
31	13.166	1858	1861	1868	rVB6	13617	28799	4.17%	0.508%
32	13.257	1871	1876	1879	rBV6	10042	21369	3.10%	0.377%
33	13.294	1879	1882	1888	rVV4	15812	35242	5.11%	0.622%
34	13.349	1888	1891	1896	rVV5	14675	26317	3.81%	0.464%
35	13.422	1897	1903	1911	rVB	230485	394319	57.16%	6.955%
36	13.495	1912	1915	1918	rBV4	9369	13400	1.94%	0.236%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	13.568	1923	1927	1931	rVB3	18536	29285	4.24%	0.517%
38	13.611	1931	1934	1937	rBV3	11588	16424	2.38%	0.290%
39	13.690	1942	1947	1950	rBV6	23124	47248	6.85%	0.833%
40	13.806	1962	1966	1970	rBV7	18285	38040	5.51%	0.671%
41	14.141	2018	2021	2027	rVB7	35016	65804	9.54%	1.161%
42	14.196	2027	2030	2035	rBV4	20172	33014	4.79%	0.582%
43	14.257	2035	2040	2043	rBV2	74172	127321	18.46%	2.246%
44	14.367	2055	2058	2062	rBV4	22857	45339	6.57%	0.800%
45	14.422	2064	2067	2070	rVV4	39584	60314	8.74%	1.064%
46	14.550	2083	2088	2091	rBV2	69551	126177	18.29%	2.225%
47	14.617	2096	2099	2104	rVV5	51515	85349	12.37%	1.505%
48	14.733	2115	2118	2124	rVB5	56609	88630	12.85%	1.563%
49	14.849	2134	2137	2140	rBV4	55673	83433	12.09%	1.472%
50	15.123	2178	2182	2189	rVB4	139639	253277	36.71%	4.467%
51	15.446	2230	2235	2242	rBV4	121988	307991	44.64%	5.432%
52	15.605	2257	2261	2268	rVB2	207585	367517	53.27%	6.482%

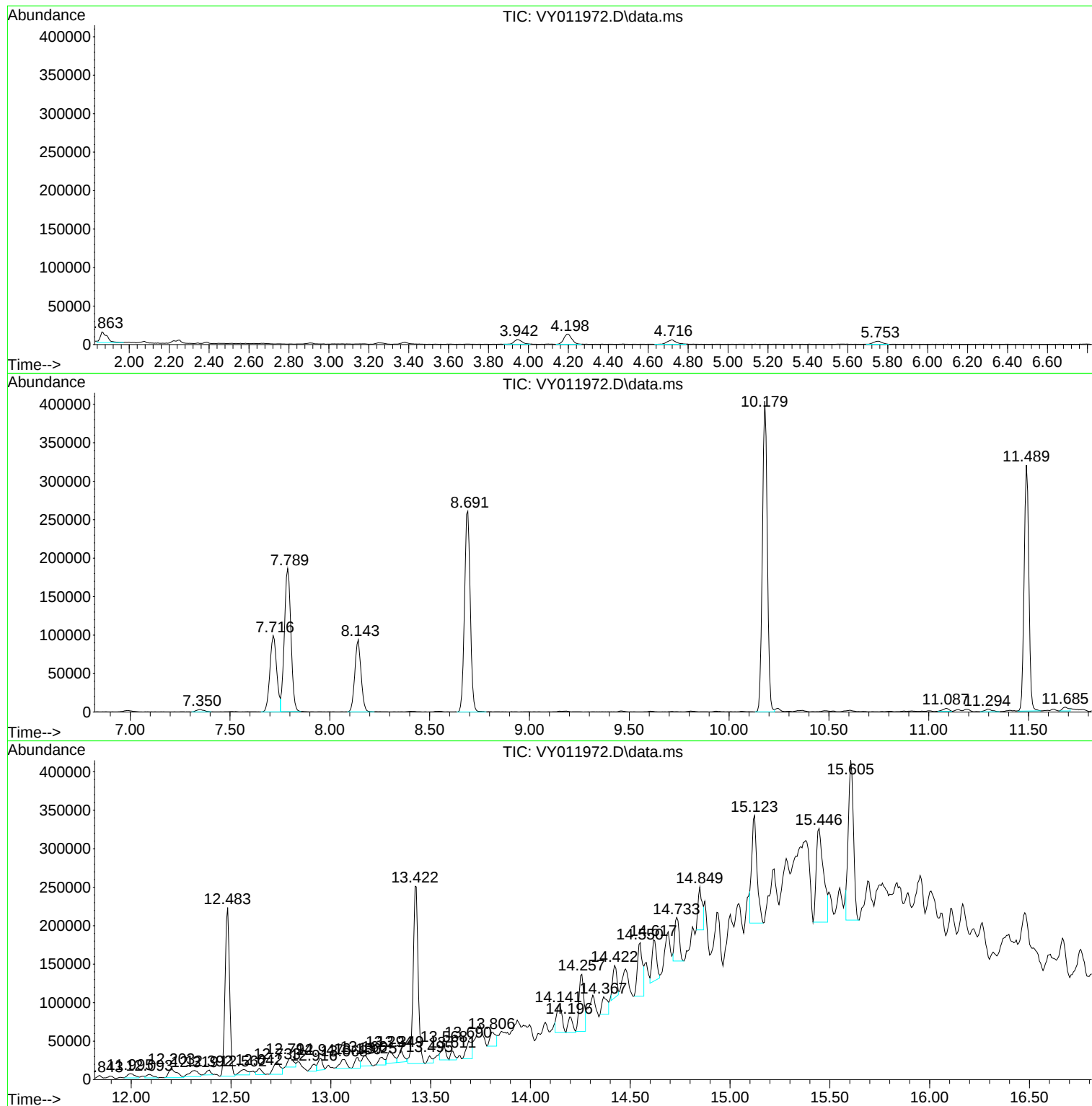
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ClientSampleId :
VOC-7-3051

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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



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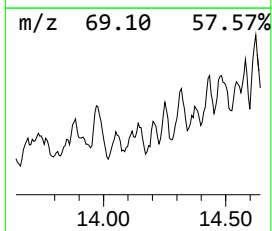
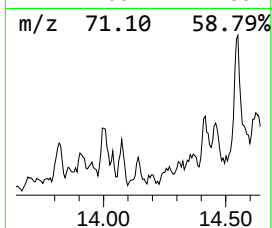
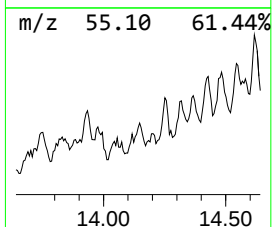
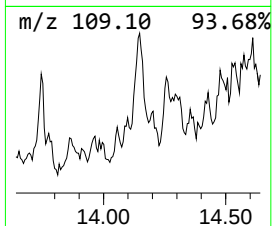
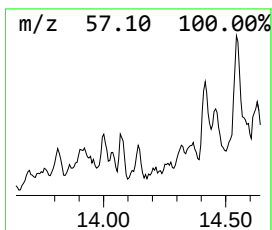
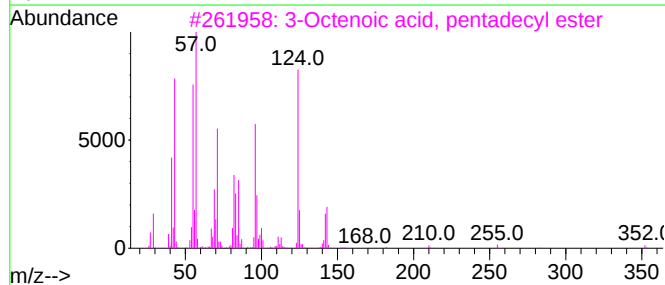
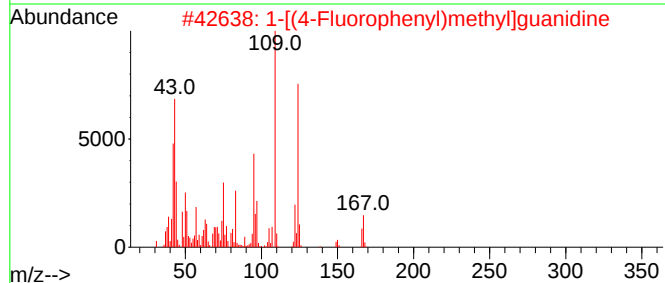
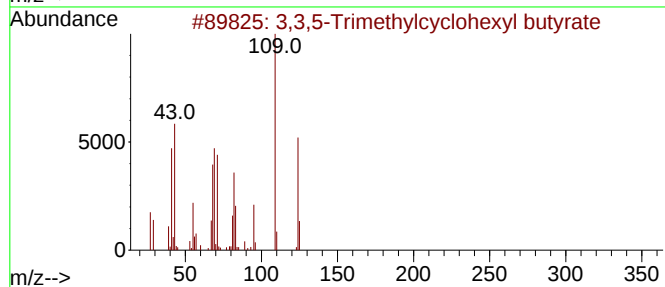
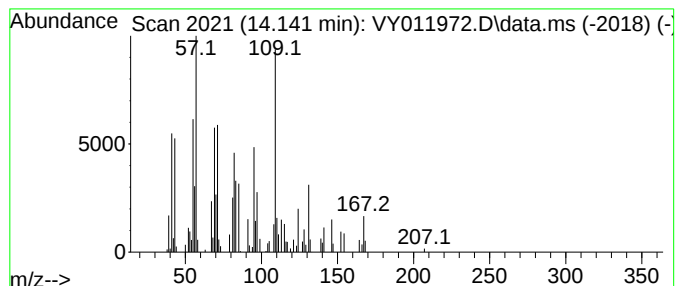
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 1 3,3,5-Trimethylcyclohexyl b... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.141	8.34 ug/l	65804	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3,5-Trimethylcyclohexyl butyrate	212	C13H24O2	1000430-81-6	50
2			1-[(4-Fluorophenyl)methyl]guanidine	167	C8H10FN3	000459-33-6	43
3			3-Octenoic acid, pentadecyl ester	352	C23H44O2	1000406-13-4	27
4			2-Cyclopenten-1-one, 3,5,5-trime...	124	C8H12O	024156-95-4	22
5			1,2,4,4-Tetramethylcyclopentene	124	C9H16	065378-76-9	22



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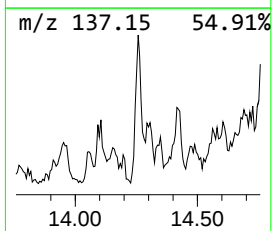
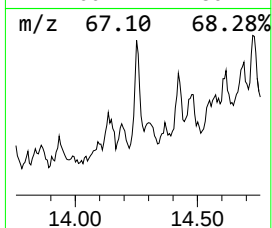
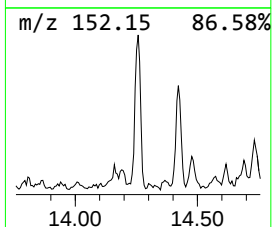
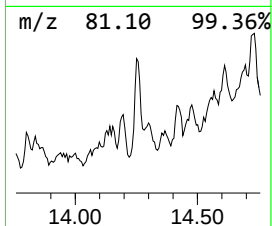
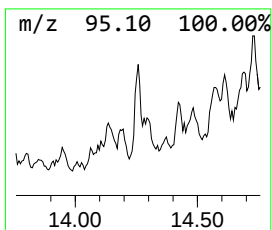
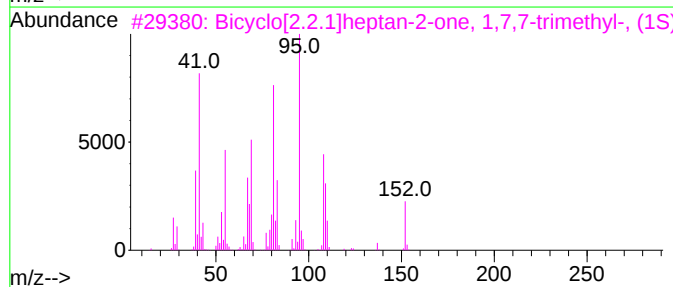
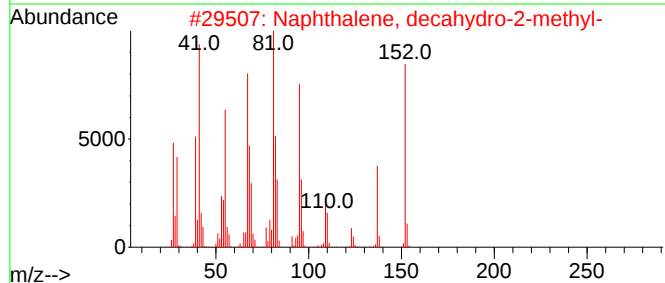
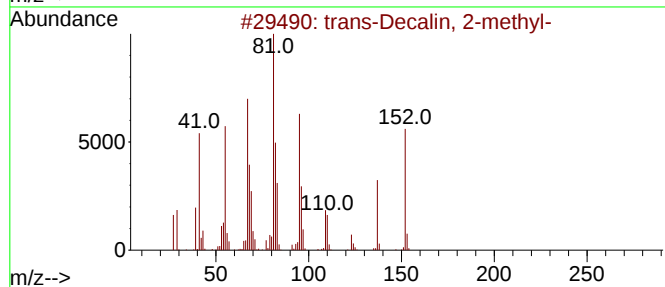
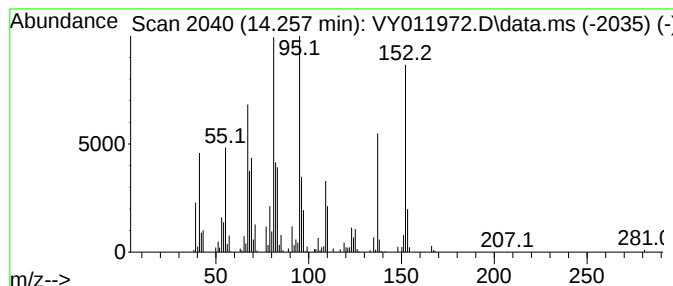
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 2 trans-Decalin, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	16.14 ug/l	127321	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	94
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	68
4			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	55
5			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	55



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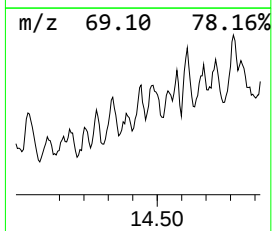
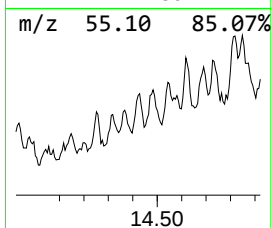
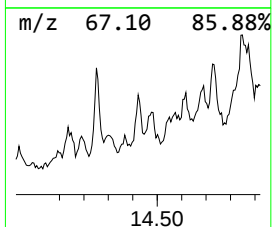
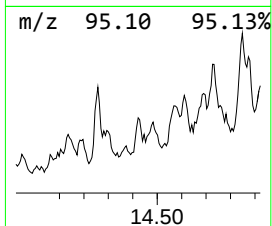
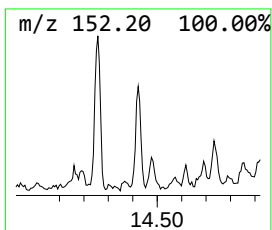
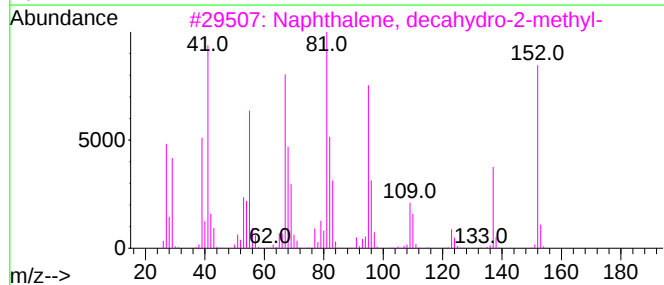
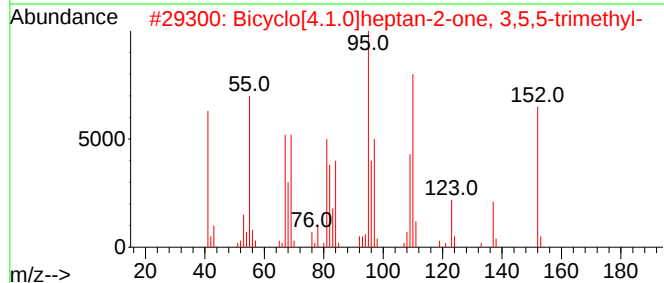
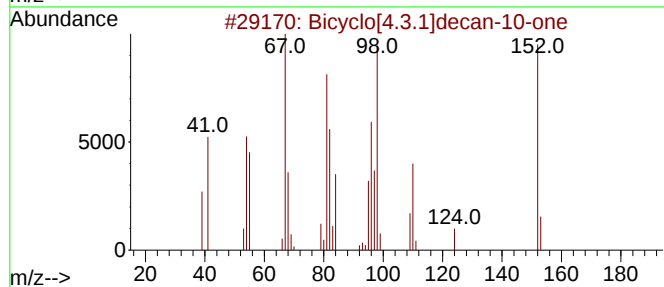
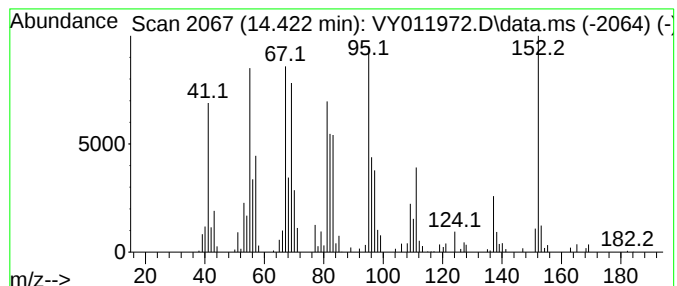
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 3 Bicyclo[4.3.1]decan-10-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	7.65 ug/l	60314	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.3.1]decan-10-one	152	C10H16O	020440-21-5	64
2			Bicyclo[4.1.0]heptan-2-one, 3,5,...	152	C10H16O	029750-24-1	58
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	53
4			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	45
5			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	43



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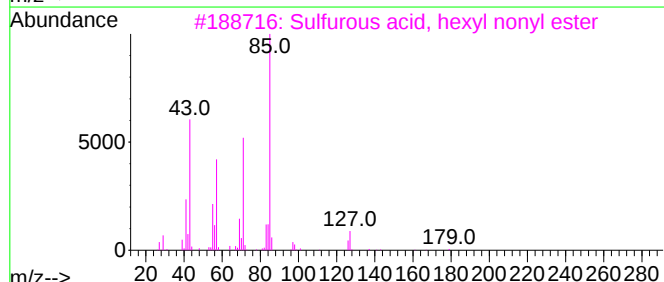
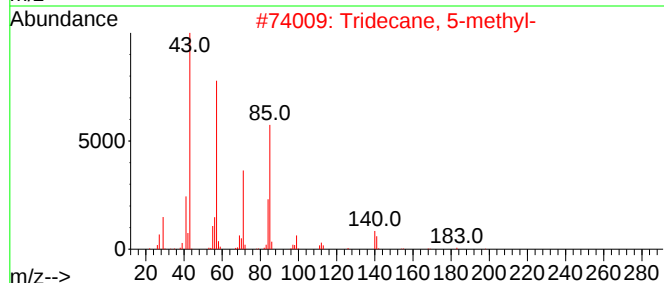
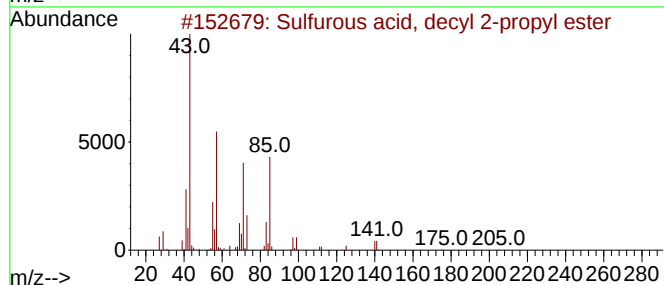
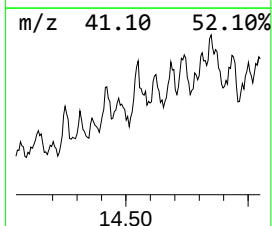
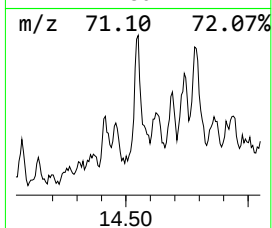
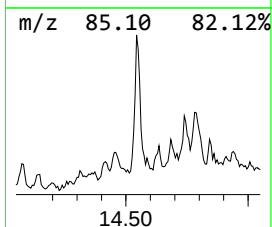
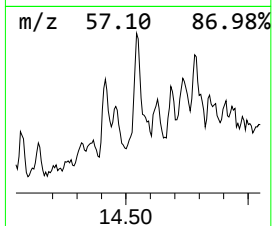
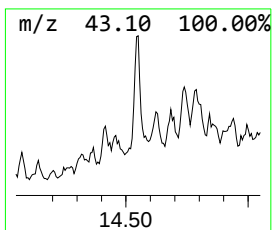
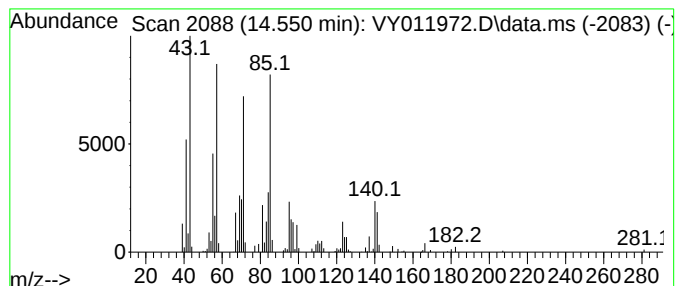
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sulfurous acid, decyl 2-pro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	16.00 ug/l	126177	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	50
2			Tridecane, 5-methyl-	198	C14H30	025117-31-1	47
3			Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	43
4			Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	43
5			Sulfurous acid, dodecyl hexyl ester	334	C18H38O3S	1000309-13-4	38



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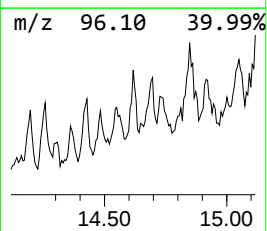
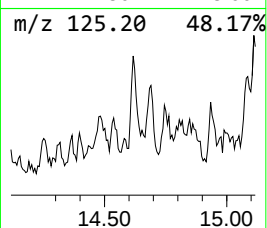
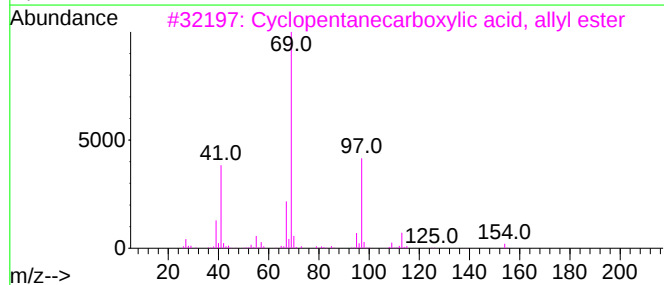
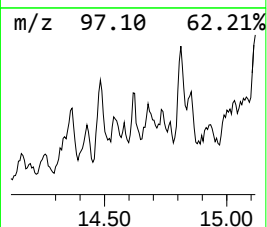
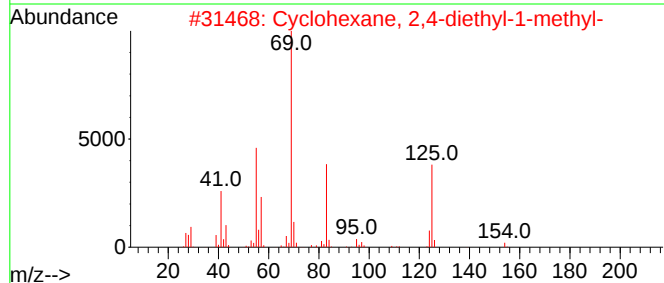
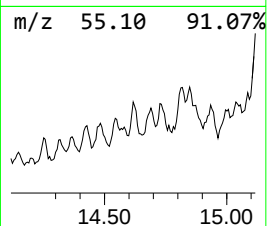
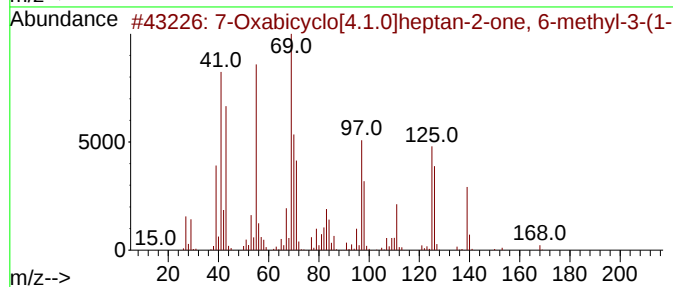
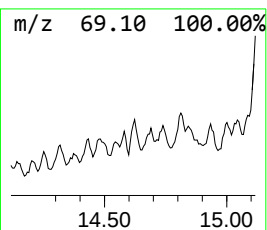
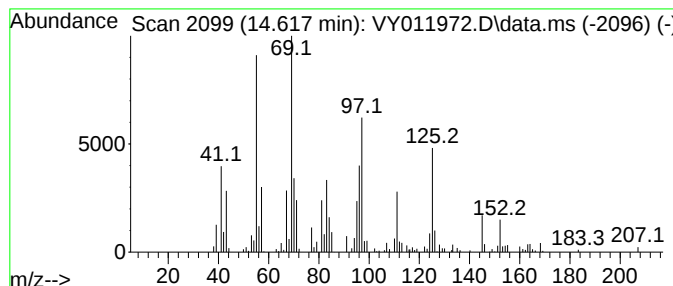
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Quant Title : SW846 8260

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

Peak Number 5 7-Oxabicyclo[4.1.0]heptan-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.617	10.82 ug/l	85349	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[4.1.0]heptan-2-one,...	168	C10H16O2	005286-38-4	52
2			Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	38
3			Cyclopentanecarboxylic acid, all...	154	C9H14O2	178905-33-4	35
4			Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	35
5			Tetradecanenitrile	209	C14H27N	000629-63-0	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

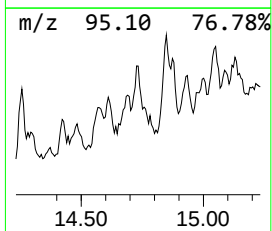
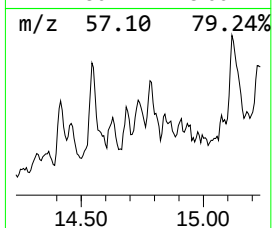
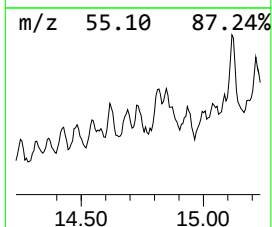
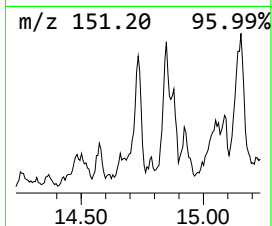
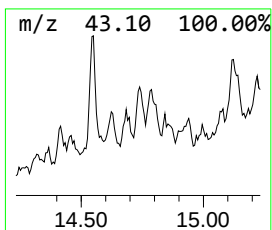
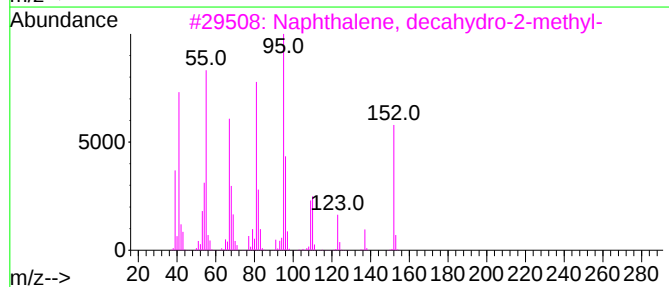
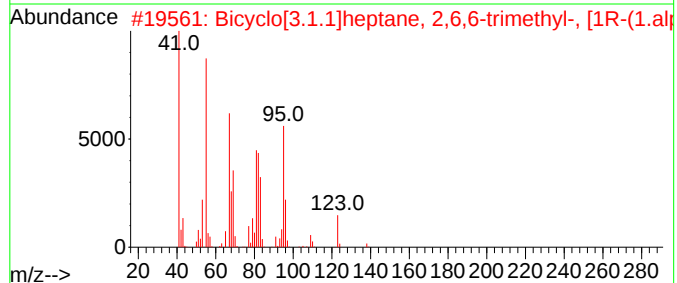
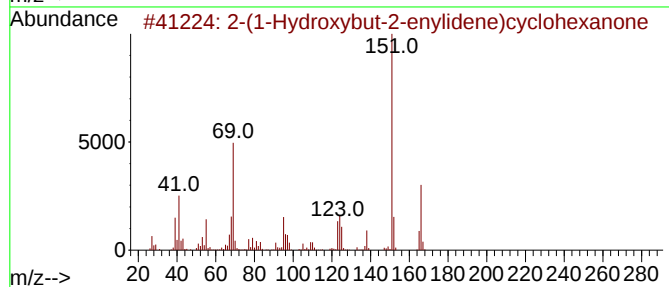
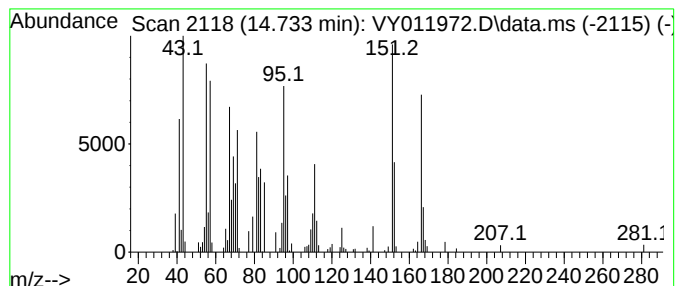
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Quant Title : SW846 8260

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

Peak Number 6 2-(1-Hydroxybut-2-enylidene... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	11.24 ug/l	88630	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Hydroxybut-2-enylidene)cycl...	166	C10H14O2	1000186-18-9	53		
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	38		
3	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	22		
4	Apocynin	166	C9H10O3	000498-02-2	18		
5	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	18		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

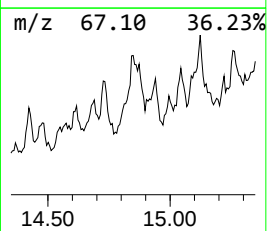
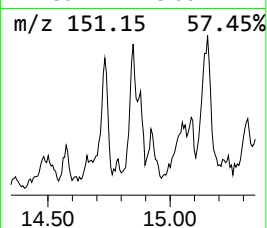
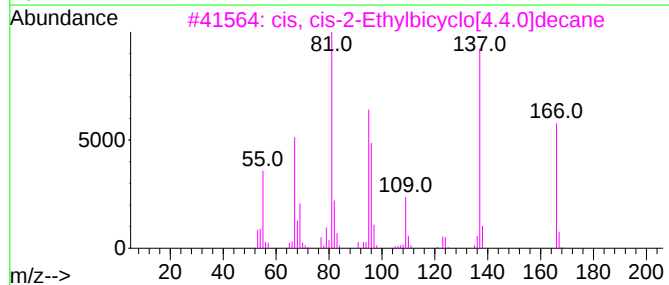
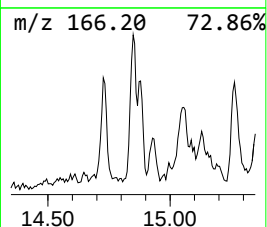
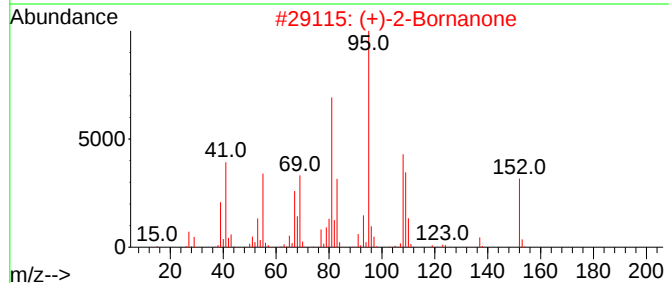
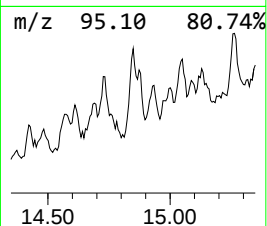
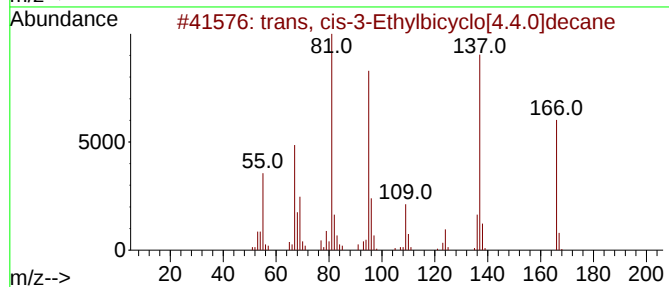
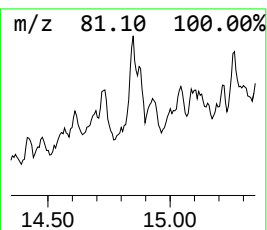
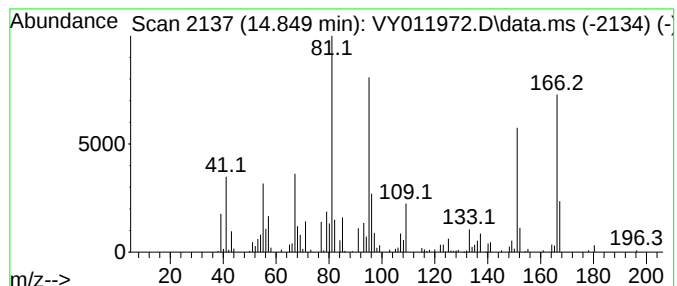
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Quant Title : SW846 8260

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

Peak Number 7 trans, cis-3-Ethylbicyclo[4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.849	10.58 ug/l	83433	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	76
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	49
3			cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	38
4			Cyclopropane, 1-(1-methylethyl)-...	152	C11H20	056259-17-7	30
5			Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

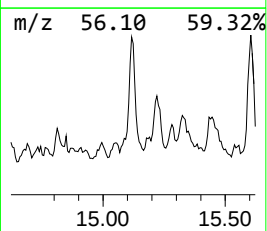
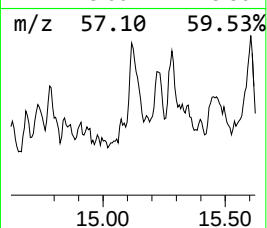
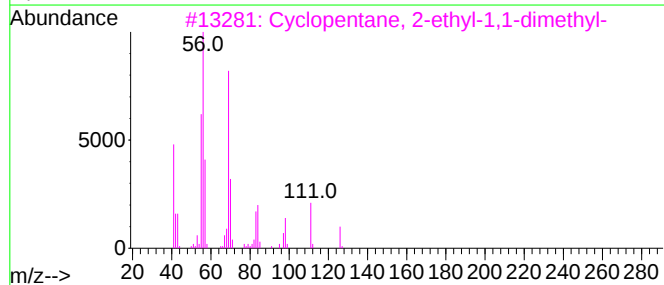
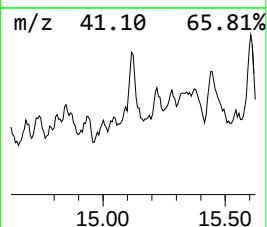
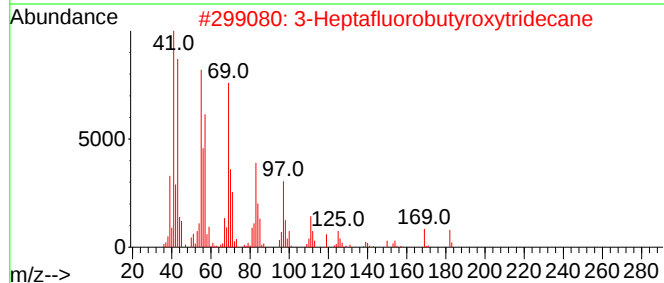
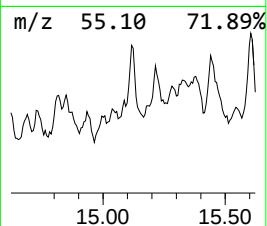
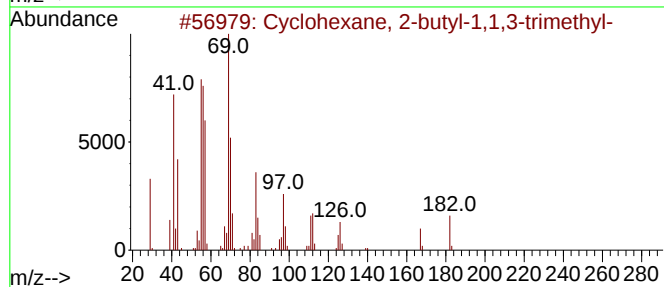
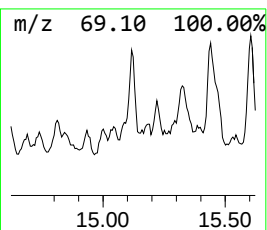
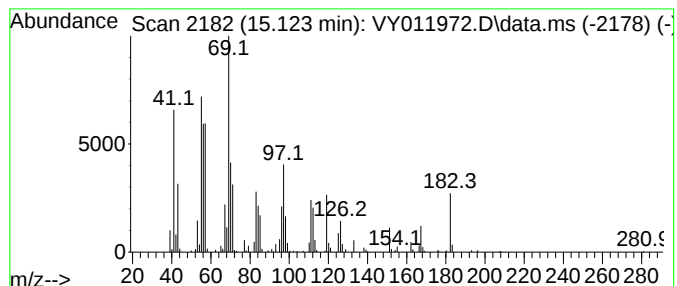
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 2-butyl-1,1,3-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	32.12 ug/l	253277	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	76
2			3-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-5	64
3			Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	58
4			Cyclopentane, butyl-	126	C9H18	002040-95-1	53
5			2-Decanol, trifluoroacetate	254	C12H21F3O2	1010352-32-8	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

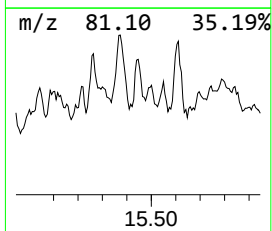
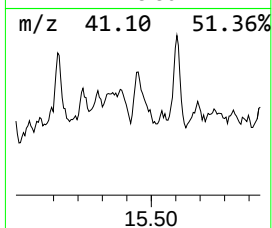
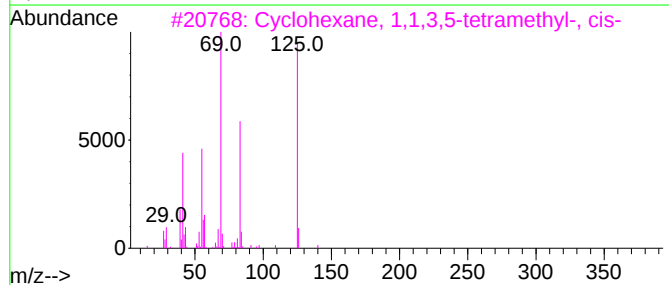
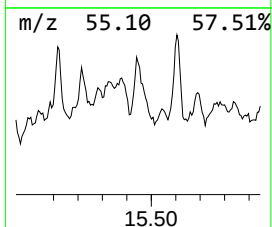
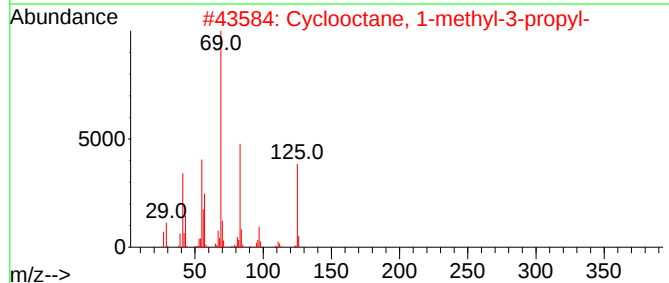
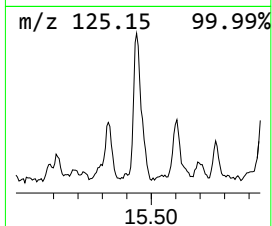
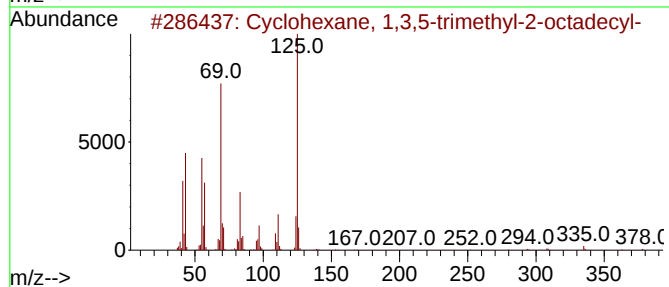
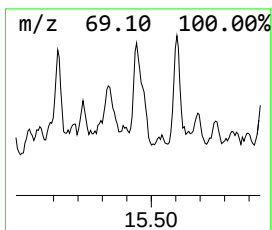
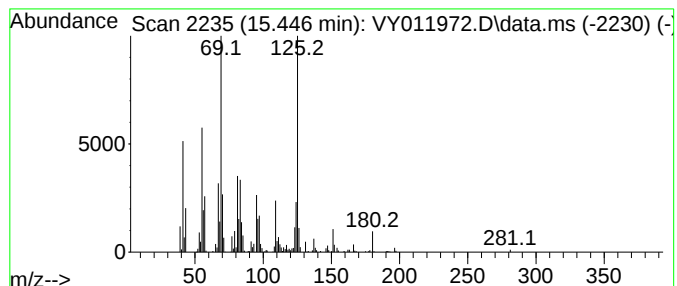
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1,3,5-trimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.446	39.05 ug/l	307991	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-trimethyl-2-o...	378	C27H54	055282-34-3	59
2			Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	52
3			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	47
4			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	47
5			1,7-Nonadiene, 4,8-dimethyl-	152	C11H20	062108-28-5	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

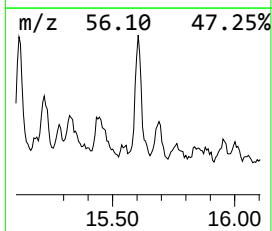
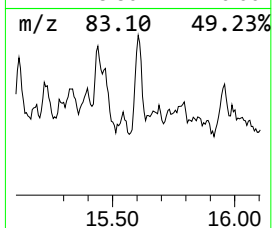
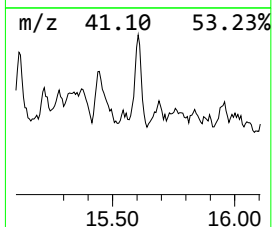
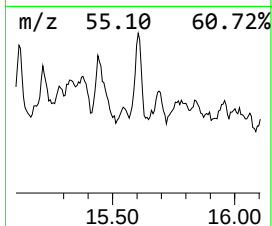
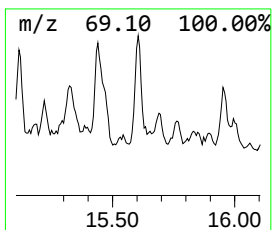
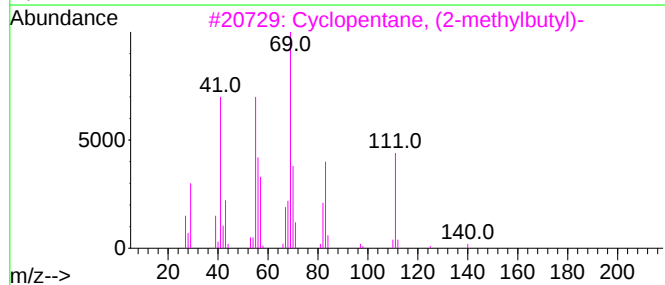
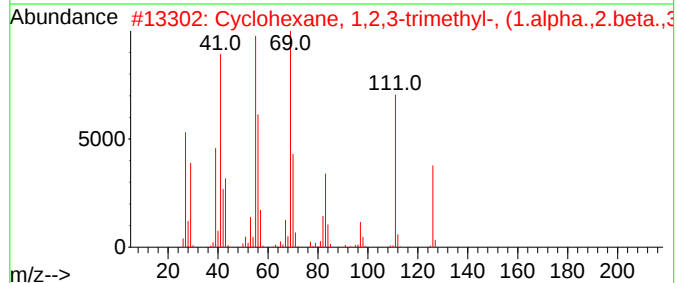
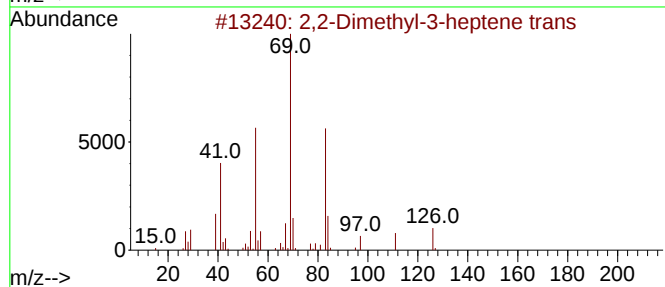
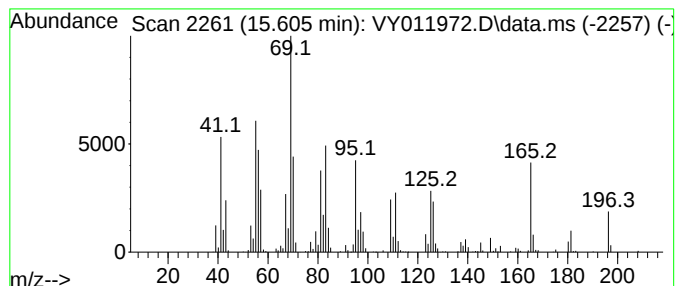
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.605 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.605	46.60 ug/l	367517	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	43
2			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	41
3			Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	38
4			2-Hexanone, 3-cyclohexylidene-4-...	208	C14H24O	1000150-19-2	38
5			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY122222\
Data File : VY011972.D
Acq On : 22 Dec 2022 14:14
Operator : KP/MD
Sample : N6160-03
Misc : 4.41g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VOC-7-3051

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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trans-Decalin, ...	14.257	16.1	ug/l	127321	4	13.428	394319	50.0
Bicyclo[4.3.1]d...	14.422	7.7	ug/l	60314	4	13.428	394319	50.0
Sulfurous acid,...	14.550	16.0	ug/l	126177	4	13.428	394319	50.0
7-Oxabicyclo[4....	14.617	10.8	ug/l	85349	4	13.428	394319	50.0
2-(1-Hydroxybut...	14.733	11.2	ug/l	88630	4	13.428	394319	50.0
trans, cis-3-Et...	14.849	10.6	ug/l	83433	4	13.428	394319	50.0
Cyclohexane, 2-...	15.123	32.1	ug/l	253277	4	13.428	394319	50.0
Cyclohexane, 1,...	15.446	39.0	ug/l	307991	4	13.428	394319	50.0
unknown15.605	15.605	46.6	ug/l	367517	4	13.428	394319	50.0