

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042122\
 Data File : VY008448.D
 Acq On : 21 Apr 2022 18:12
 Operator : KP/MD
 Sample : N2511-04
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 1529

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\82Y042122S.M
 Title : SW846 8260

Signal : TIC: VY008448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.058	34	39	46	rBV2	6527	11879	1.74%	0.261%
2	2.223	60	66	77	rVB2	11058	23116	3.39%	0.508%
3	2.345	80	86	89	rBV	10527	18172	2.66%	0.399%
4	2.387	89	93	100	rVV	37935	63808	9.35%	1.402%
5	2.461	100	105	112	rVB	13290	22155	3.24%	0.487%
6	2.906	169	178	187	rBV2	11644	26472	3.88%	0.582%
7	3.253	228	235	245	rVB3	4334	10704	1.57%	0.235%
8	3.826	320	329	339	rVV	12194	30504	4.47%	0.670%
9	3.948	339	349	370	rVB	70247	196581	28.79%	4.319%
10	4.198	381	390	404	rBV2	4600	14962	2.19%	0.329%
11	4.564	441	450	461	rVB8	3096	11563	1.69%	0.254%
12	4.716	463	475	483	rBV4	7474	29123	4.27%	0.640%
13	4.887	495	503	512	rVB2	7962	25677	3.76%	0.564%
14	5.576	607	616	630	rBV5	4044	13572	1.99%	0.298%
15	5.747	630	644	661	rBV	216364	682783	100.00%	15.002%
16	5.905	663	670	681	rVB5	4338	13155	1.93%	0.289%
17	6.698	786	800	810	rBV2	36184	114583	16.78%	2.518%
18	6.795	811	816	822	rVB6	2941	7005	1.03%	0.154%
19	6.874	824	829	838	rVB3	3897	9788	1.43%	0.215%
20	6.984	838	847	859	rBV2	32473	94393	13.82%	2.074%
21	7.338	896	905	914	rVB5	2186	7503	1.10%	0.165%
22	7.716	958	967	973	rBV	71971	171719	25.15%	3.773%
23	7.789	973	979	988	rVV2	115268	268341	39.30%	5.896%
24	7.868	988	992	1000	rVB3	5282	12556	1.84%	0.276%
25	8.142	1022	1037	1049	rVV3	73883	195700	28.66%	4.300%
26	8.325	1058	1067	1073	rVV3	5970	17429	2.55%	0.383%
27	8.392	1073	1078	1089	rVB2	16850	37450	5.48%	0.823%
28	8.551	1094	1104	1113	rBV2	26811	59845	8.76%	1.315%
29	8.691	1119	1127	1135	rBV	179349	348853	51.09%	7.665%
30	8.770	1135	1140	1147	rVB2	11441	22050	3.23%	0.484%
31	9.136	1192	1200	1205	rBV	27235	49137	7.20%	1.080%
32	9.185	1206	1208	1213	rVV3	4569	6961	1.02%	0.153%
33	9.258	1213	1220	1234	rVB2	45992	95800	14.03%	2.105%
34	9.526	1255	1264	1272	rVV4	5145	13508	1.98%	0.297%
35	9.612	1272	1278	1289	rVB2	11058	22719	3.33%	0.499%
36	9.752	1294	1301	1308	rVB3	4339	10414	1.53%	0.229%

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37	10.069	1348	1353	1357	rBV2	4894	9333	1.37%	0.205%
38	10.112	1357	1360	1364	rVV4	7241	12233	1.79%	0.269%
39	10.179	1364	1371	1378	rVV	264275	462893	67.80%	10.171%
40	10.246	1378	1382	1385	rVV	4719	8112	1.19%	0.178%
41	10.282	1385	1388	1395	rVB4	4404	7874	1.15%	0.173%
42	10.368	1395	1402	1409	rBV4	4929	10758	1.58%	0.236%
43	10.441	1409	1414	1416	rBV2	4249	6930	1.01%	0.152%
44	10.484	1416	1421	1428	rVB4	13199	32485	4.76%	0.714%
45	10.581	1428	1437	1442	rBV2	8076	15745	2.31%	0.346%
46	10.721	1456	1460	1466	rVB5	3896	7256	1.06%	0.159%
47	10.831	1469	1478	1482	rBV3	13330	26859	3.93%	0.590%
48	10.935	1489	1495	1506	rVB2	61246	103010	15.09%	2.263%
49	11.148	1524	1530	1536	rBV4	4355	9473	1.39%	0.208%
50	11.319	1554	1558	1563	rVB3	6353	10846	1.59%	0.238%
51	11.386	1563	1569	1576	rVB4	5429	11420	1.67%	0.251%
52	11.489	1579	1586	1593	rBV	230862	375223	54.95%	8.244%
53	11.709	1616	1622	1624	rBV4	5365	9932	1.45%	0.218%
54	11.739	1624	1627	1633	rVB4	8224	14578	2.14%	0.320%
55	11.806	1633	1638	1643	rBV3	4920	8241	1.21%	0.181%
56	12.105	1682	1687	1695	rVB3	7633	12957	1.90%	0.285%
57	12.209	1698	1704	1715	rBV3	16276	29684	4.35%	0.652%
58	12.386	1728	1733	1740	rVV3	7253	14426	2.11%	0.317%
59	12.483	1742	1749	1761	rVB2	170065	274973	40.27%	6.042%
60	12.739	1783	1791	1795	rBV4	7085	14102	2.07%	0.310%
61	12.806	1795	1802	1812	rVB6	14319	36884	5.40%	0.810%
62	13.276	1870	1879	1883	rBV7	8693	16813	2.46%	0.369%
63	13.428	1897	1904	1910	rVB	151075	237732	34.82%	5.223%
64	13.965	1986	1992	1997	rVB2	5908	10509	1.54%	0.231%

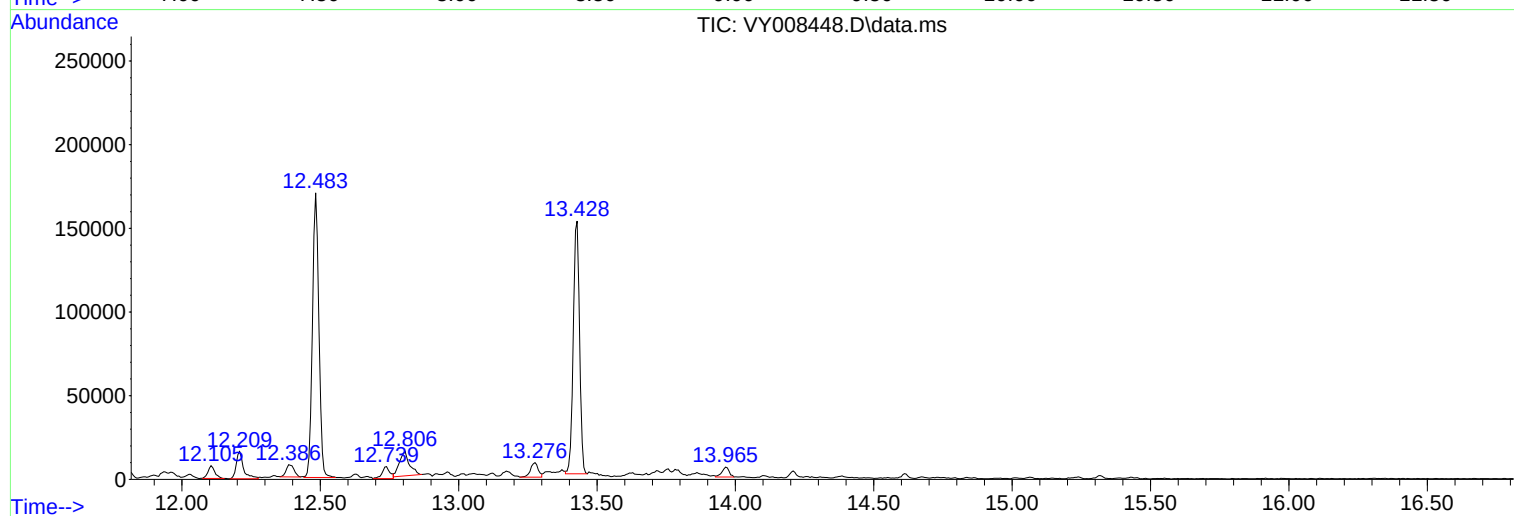
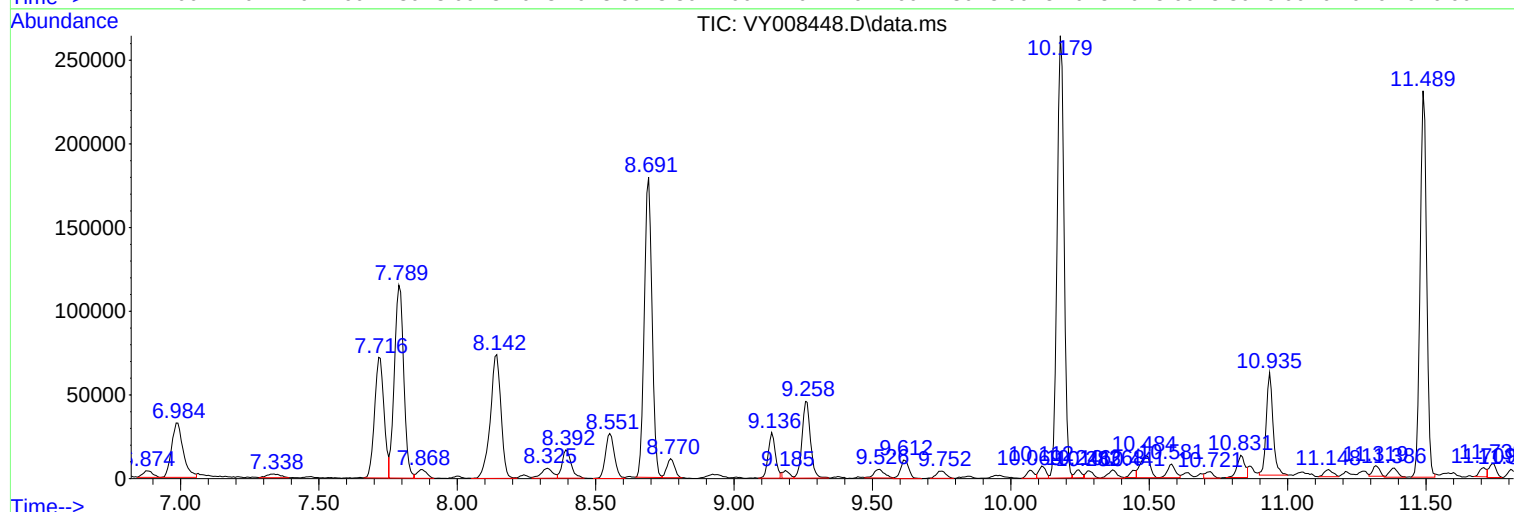
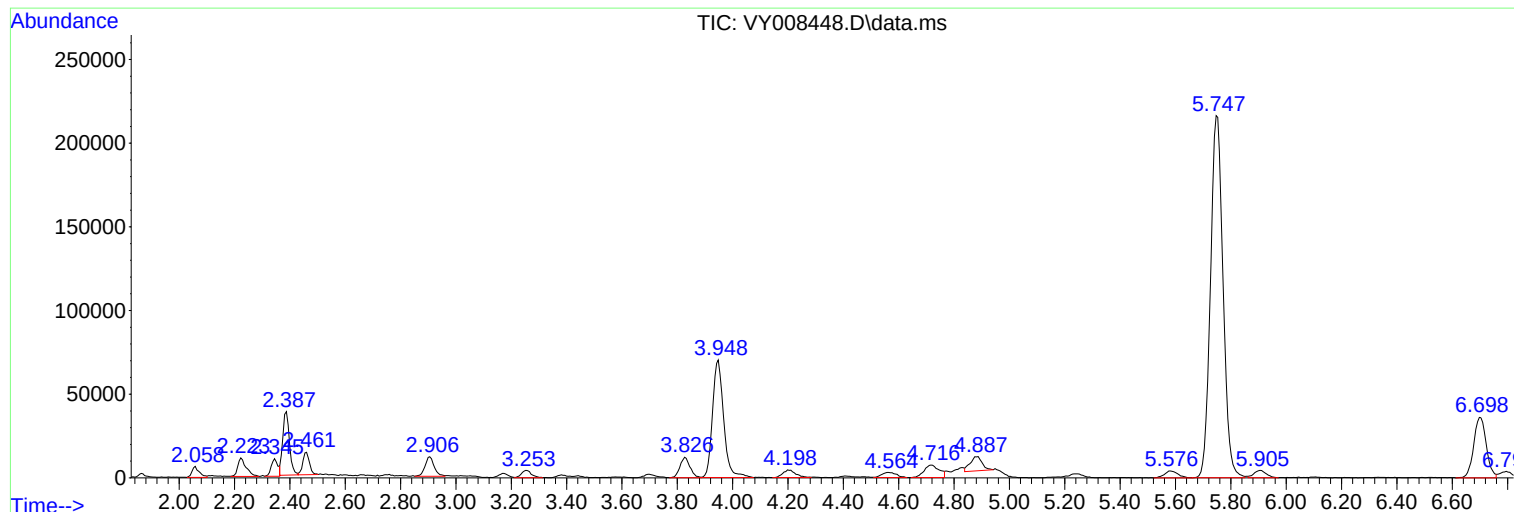
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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



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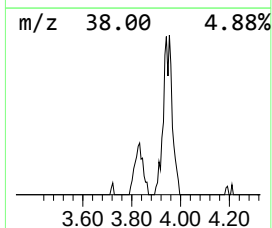
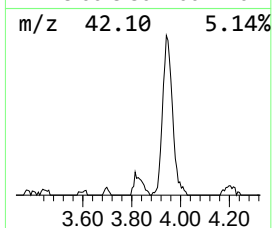
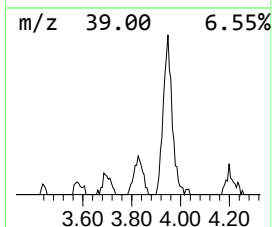
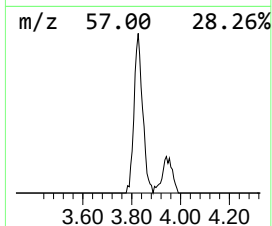
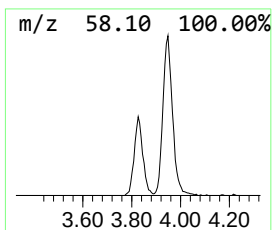
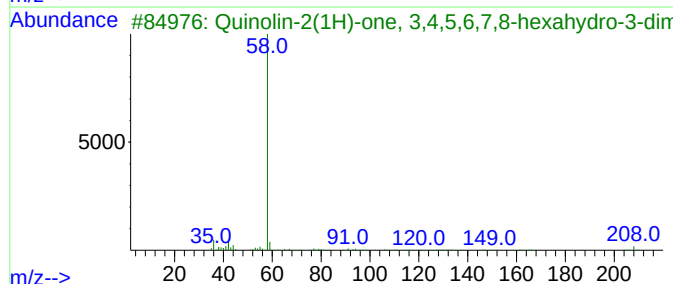
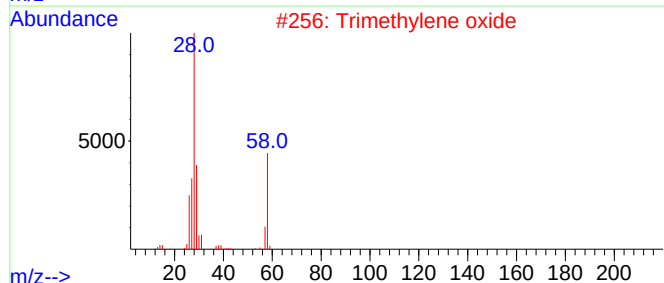
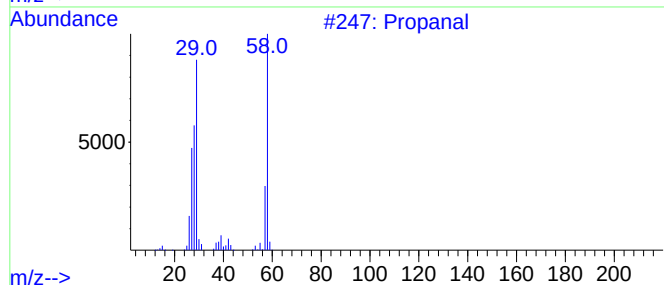
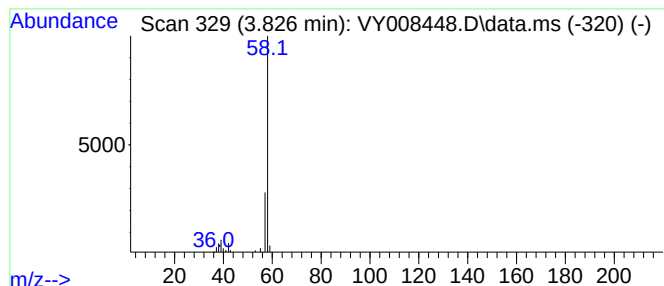
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.826	5.68 ug/l	30504	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	64
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			Benzedrex	155	C10H21N	000101-40-6	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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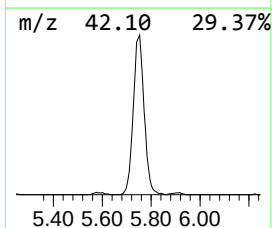
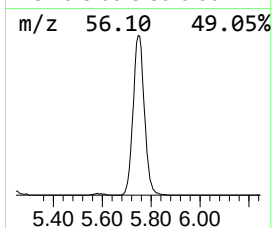
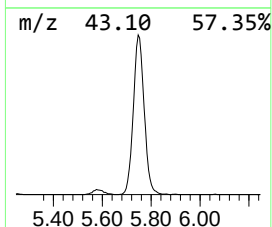
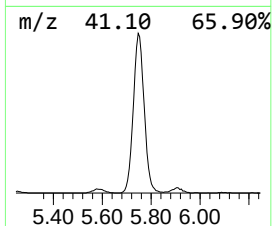
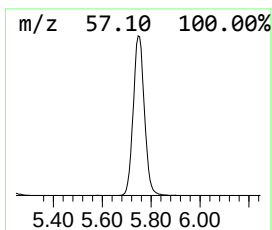
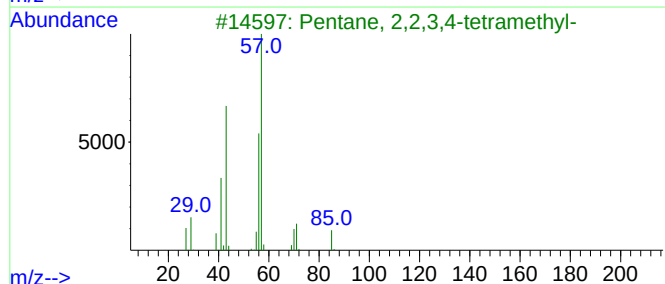
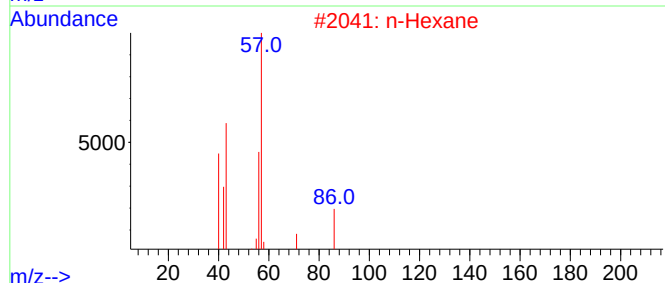
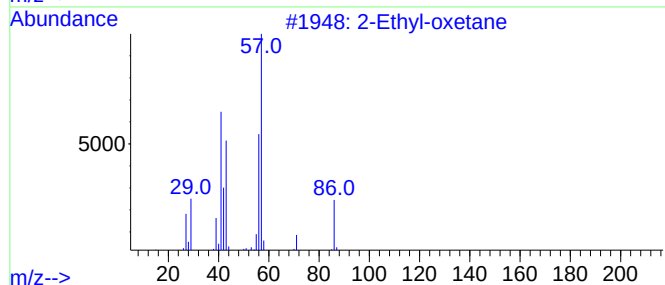
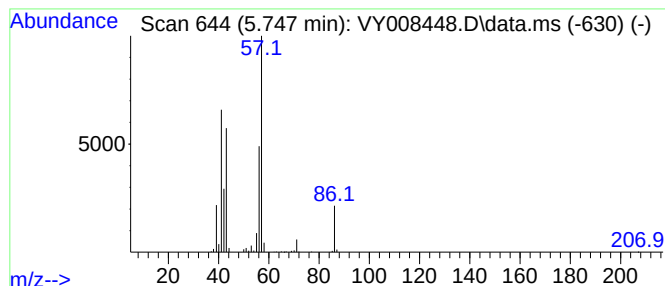
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 4 2-Ethyl-oxetane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.747	127.22 ug/l	682783	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	86
2			n-Hexane	86	C6H14	000110-54-3	86
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4			Morpholine	87	C4H9NO	000110-91-8	38
5			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	38



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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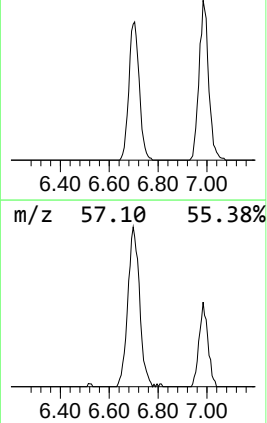
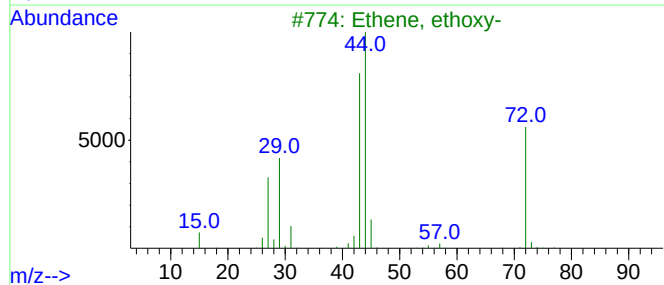
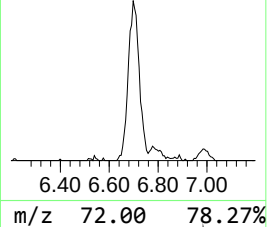
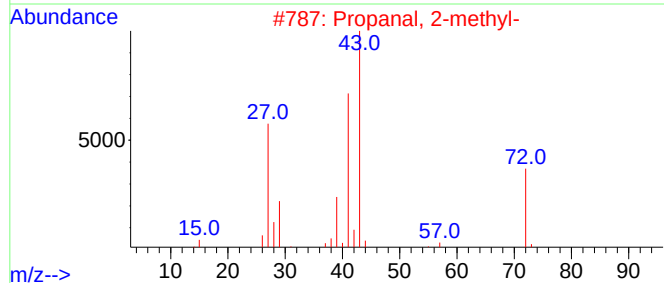
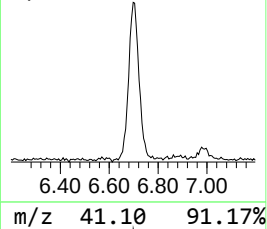
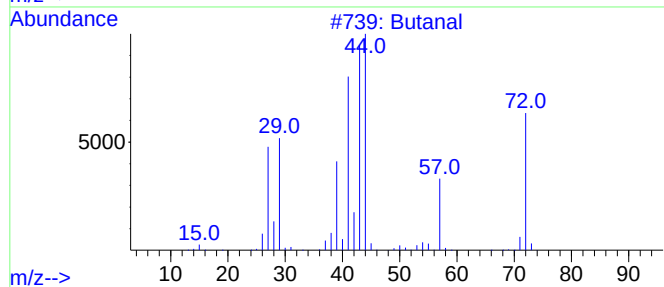
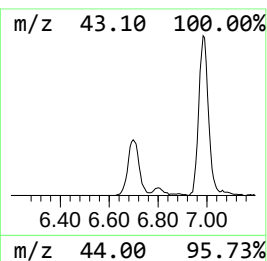
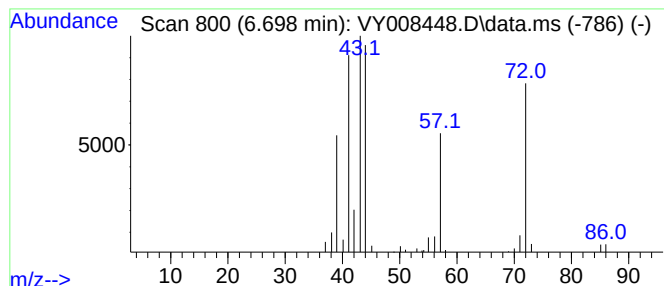
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.698	21.35 ug/l	114583	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	37



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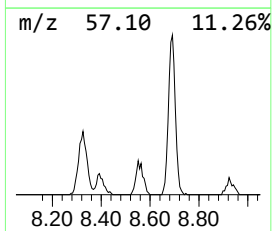
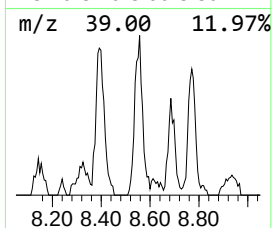
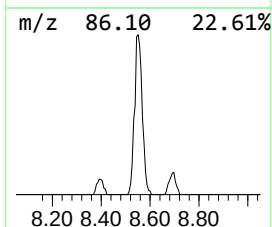
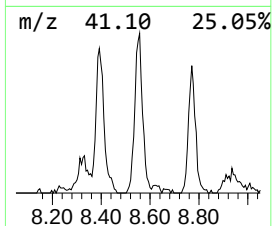
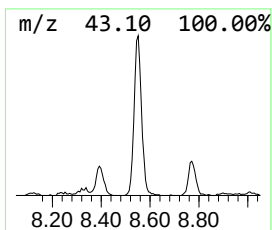
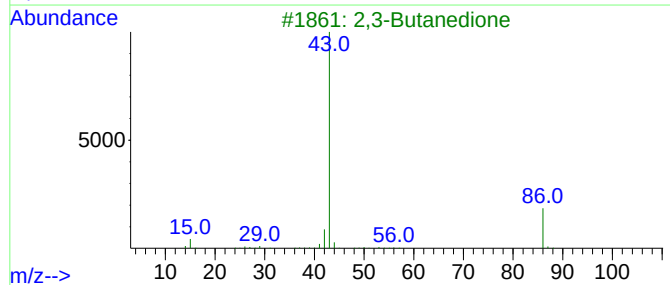
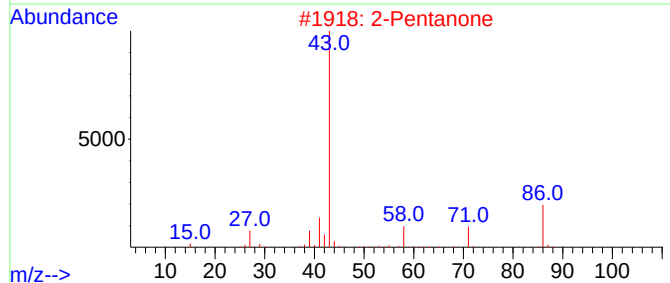
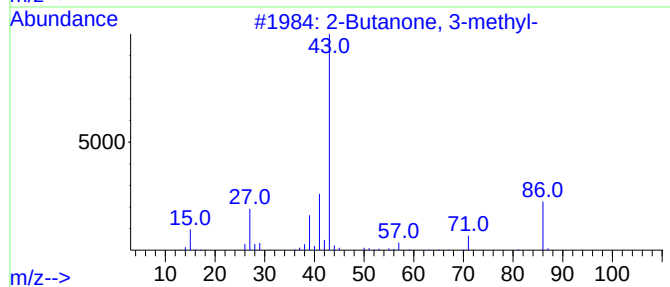
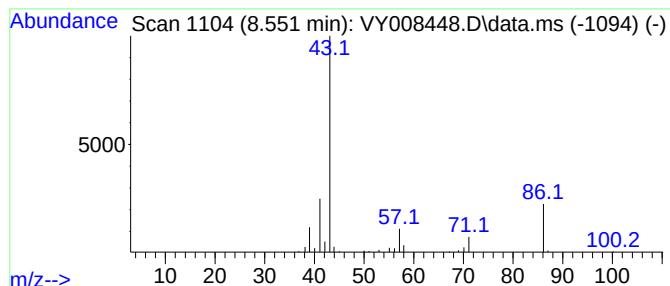
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 6 2-Butanone, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	8.58 ug/l	59845	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	58
2	2-Pentanone			86	C5H10O	000107-87-9	53
3	2,3-Butanedione			86	C4H6O2	000431-03-8	37
4	1-Propen-2-ol, formate			86	C4H6O2	032978-00-0	33
5	Pentanal, 2-methyl-			100	C6H12O	000123-15-9	23



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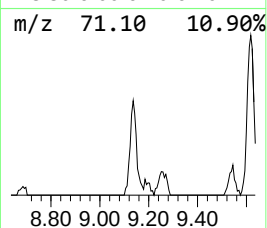
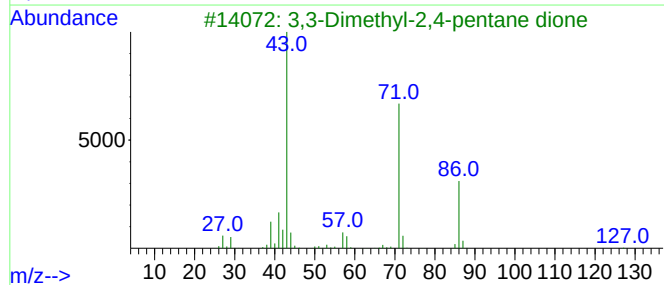
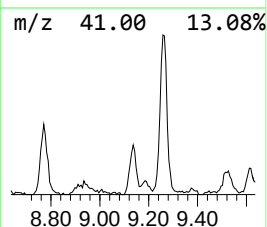
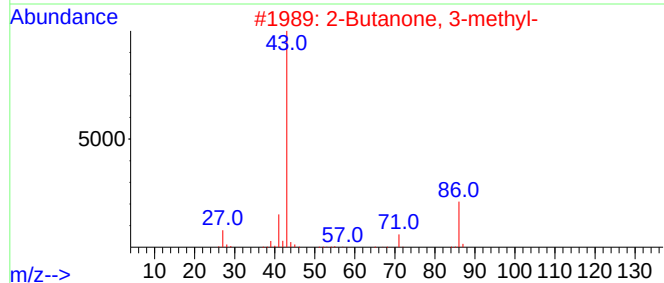
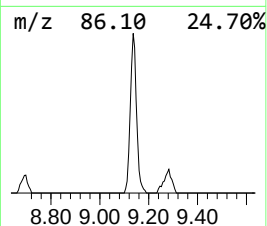
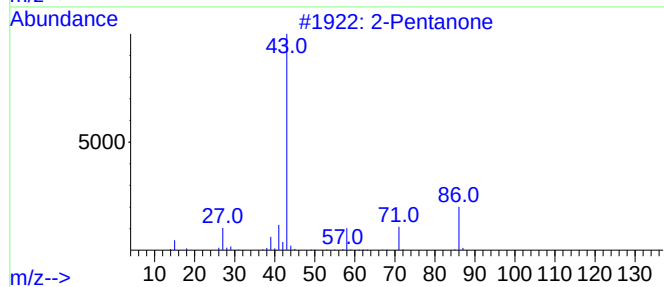
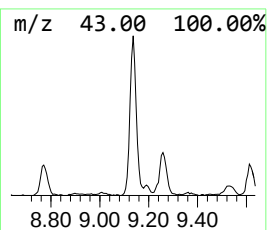
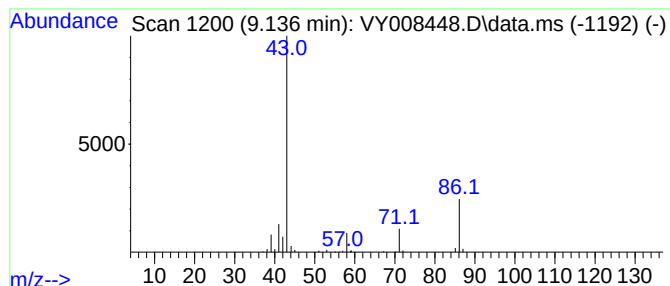
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Quant Title : SW846 8260

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

Peak Number 7 2-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.136	7.04 ug/l	49137	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	86
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
4			2-Propanone, methylhydrazone	86	C4H10N2	005771-02-8	17
5			Butane	58	C4H10	000106-97-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042122\
Data File : VY008448.D
Acq On : 21 Apr 2022 18:12
Operator : KP/MD
Sample : N2511-04
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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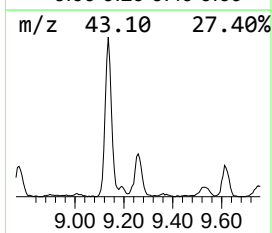
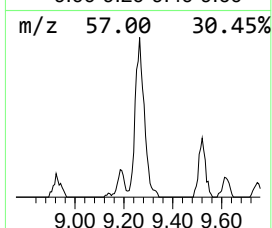
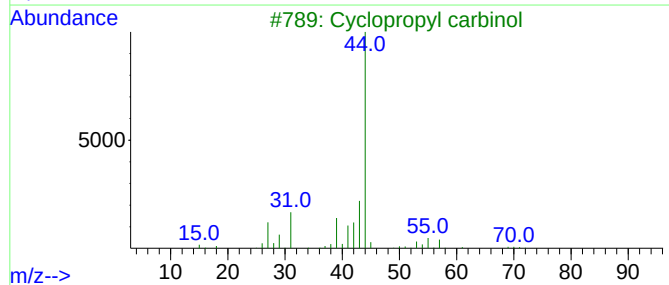
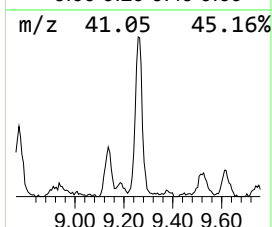
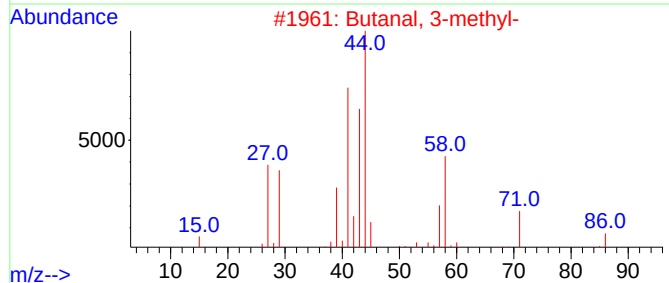
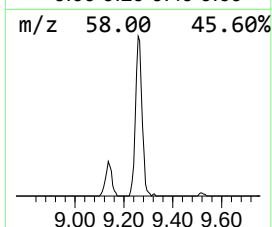
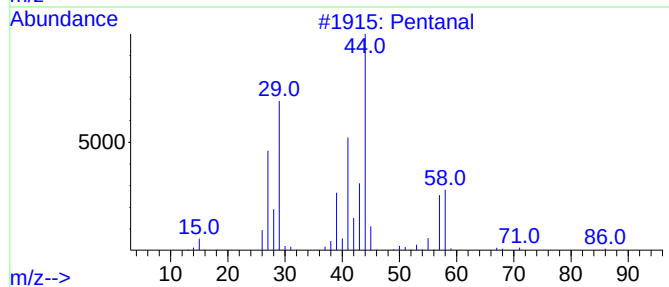
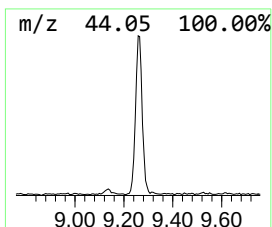
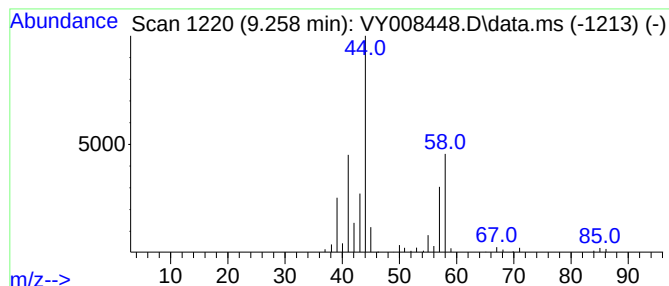
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Quant Title : SW846 8260

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

Peak Number 8 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.258	13.73 ug/l	95800	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	90
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	78
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
4			(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	9
5			Alanylglycine, TMS	218	C8H18N2O3Si	1000475-96-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042122\
Data File : VY008448.D
Acq On : 21 Apr 2022 18:12
Operator : KP/MD
Sample : N2511-04
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1529

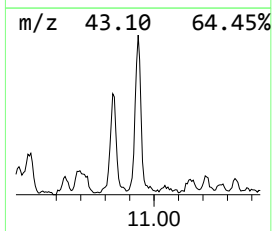
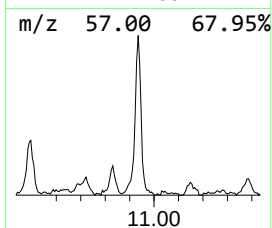
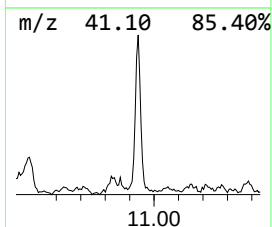
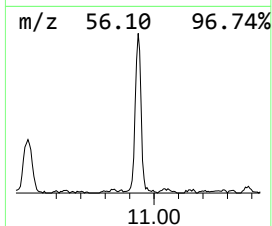
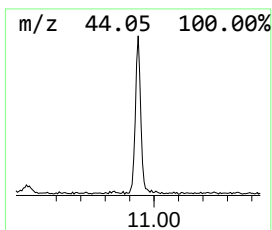
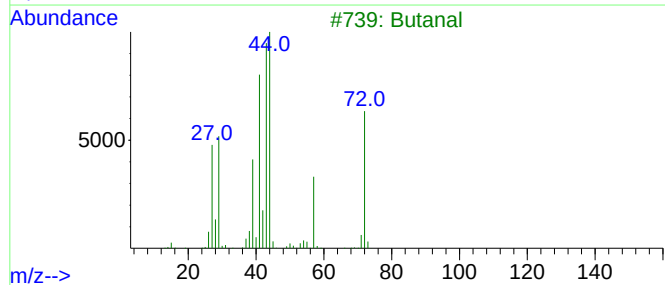
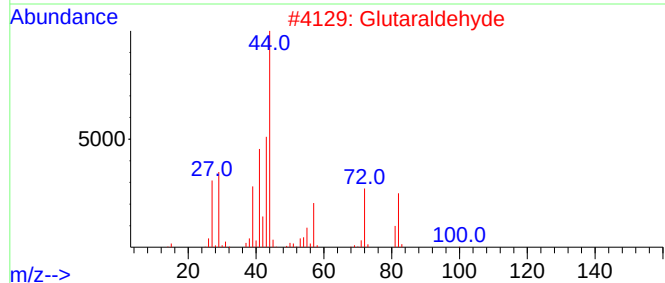
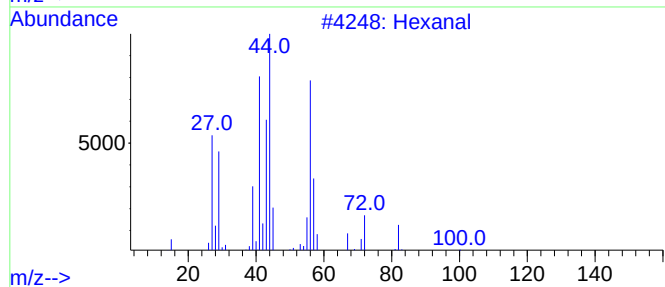
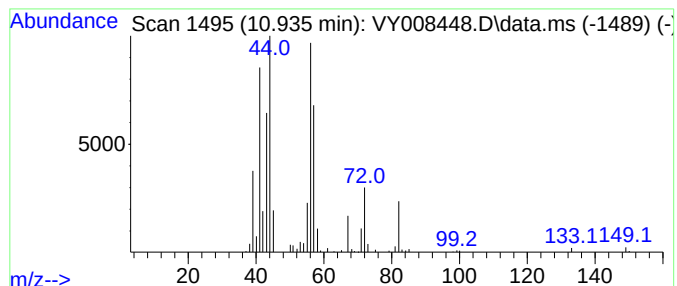
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Quant Title : SW846 8260

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

Peak Number 9 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	13.73 ug/l	103010	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	91
2			Glutaraldehyde	100	C5H8O2	000111-30-8	32
3			Butanal	72	C4H8O	000123-72-8	30
4			Pentanal, 3-methyl-	100	C6H12O	015877-57-3	25
5			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042122\
Data File : VY008448.D
Acq On : 21 Apr 2022 18:12
Operator : KP/MD
Sample : N2511-04
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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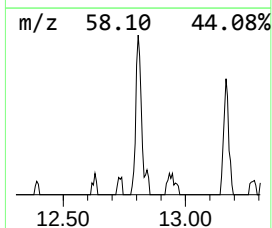
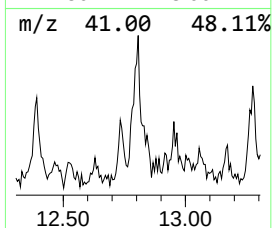
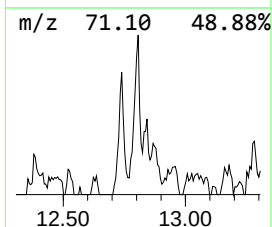
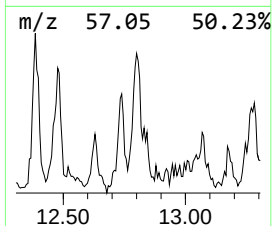
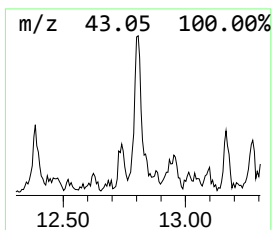
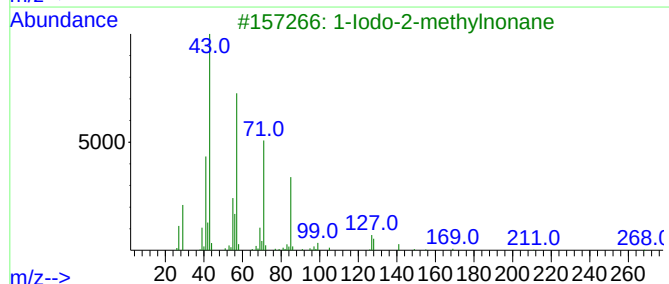
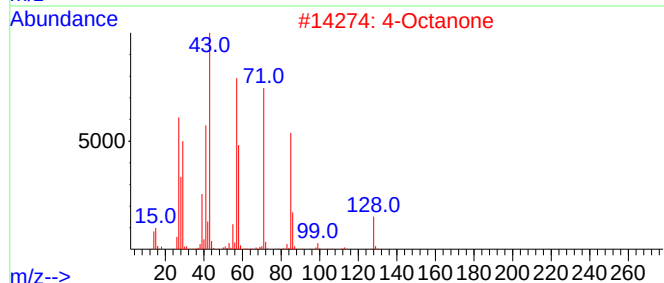
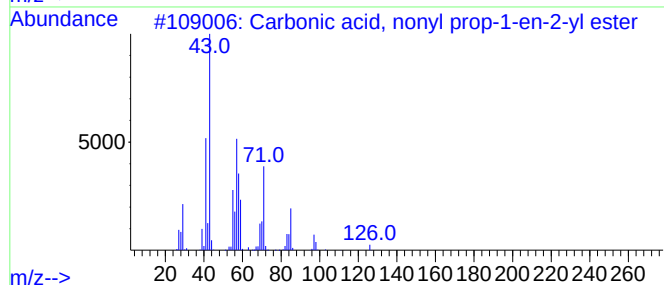
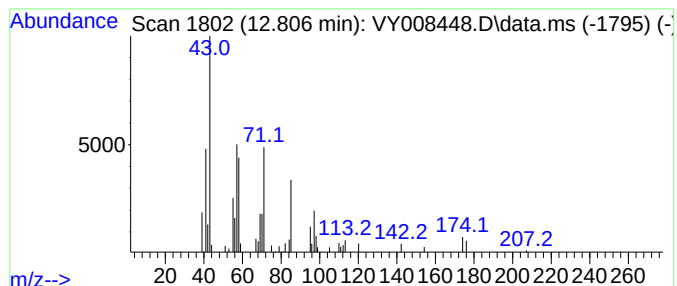
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Quant Title : SW846 8260

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

Peak Number 10 Carbonic acid, nonyl prop-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	7.76 ug/l	36884	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	53
2			4-Octanone	128	C8H16O	000589-63-9	50
3			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	27
4			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	27
5			Dodecane	170	C12H26	000112-40-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042122\
Data File : VY008448.D
Acq On : 21 Apr 2022 18:12
Operator : KP/MD
Sample : N2511-04
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1529

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.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
Propanal	3.826	5.7	ug/l	30504	1	7.789	268341	50.0
2-Ethyl-oxetane	5.747	127.2	ug/l	682783	1	7.789	268341	50.0
Butanal	6.698	21.4	ug/l	114583	1	7.789	268341	50.0
2-Butanone, 3-m...	8.551	8.6	ug/l	59845	2	8.691	348853	50.0
2-Pentanone	9.136	7.0	ug/l	49137	2	8.691	348853	50.0
Pentanal	9.258	13.7	ug/l	95800	2	8.691	348853	50.0
Hexanal	10.935	13.7	ug/l	103010	3	11.489	375223	50.0
Carbonic acid, ...	12.806	7.8	ug/l	36884	4	13.428	237732	50.0