

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041322\
 Data File : VY008312.D
 Acq On : 13 Apr 2022 15:03
 Operator : KP/MD
 Sample : N2349-13
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 DEL-7

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\82Y040822S.M
 Title : SW846 8260

Signal : TIC: VY008312.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.900	169	177	186	rBV4	2896	7473	1.33%	0.198%
2	3.948	340	349	363	rBV	11144	29848	5.32%	0.792%
3	4.716	465	475	490	rBV3	10943	40597	7.24%	1.077%
4	5.753	632	645	655	rVB4	5653	17729	3.16%	0.470%
5	6.984	839	847	856	rBV	7549	19212	3.42%	0.510%
6	7.716	956	967	973	rBV	66175	158201	28.20%	4.198%
7	7.789	973	979	989	rVB	134939	299580	53.40%	7.950%
8	8.142	1028	1037	1053	rVB	71832	164108	29.25%	4.355%
9	8.545	1096	1103	1114	rVB2	8288	18130	3.23%	0.481%
10	8.691	1118	1127	1137	rBV	204391	398466	71.03%	10.574%
11	9.136	1193	1200	1215	rVV	23743	52003	9.27%	1.380%
12	9.276	1215	1223	1233	rVB3	3298	8313	1.48%	0.221%
13	9.819	1305	1312	1321	rVB5	2287	6534	1.16%	0.173%
14	10.069	1347	1353	1363	rBV	11902	21617	3.85%	0.574%
15	10.179	1363	1371	1378	rBV	331683	560973	100.00%	14.886%
16	10.276	1384	1387	1394	rVB3	6404	12092	2.16%	0.321%
17	10.368	1394	1402	1409	rVB3	5482	10023	1.79%	0.266%
18	10.721	1454	1460	1467	rVB2	6851	12149	2.17%	0.322%
19	10.831	1467	1478	1487	rBV	25395	46002	8.20%	1.221%
20	10.929	1489	1494	1499	rVV5	3664	5790	1.03%	0.154%
21	11.203	1533	1539	1545	rBV3	3582	6929	1.24%	0.184%
22	11.386	1564	1569	1577	rVB6	3645	7806	1.39%	0.207%
23	11.489	1578	1586	1595	rBV	288705	463719	82.66%	12.306%
24	11.599	1595	1604	1610	rVV3	9500	20087	3.58%	0.533%
25	11.739	1616	1627	1632	rVB3	10002	23897	4.26%	0.634%
26	12.026	1668	1674	1679	rVB2	9180	14419	2.57%	0.383%
27	12.105	1679	1687	1696	rVB	44642	71435	12.73%	1.896%
28	12.209	1696	1704	1706	rBV5	3305	7254	1.29%	0.192%
29	12.239	1706	1709	1718	rVB6	4100	8558	1.53%	0.227%
30	12.416	1732	1738	1743	rBV5	4312	8819	1.57%	0.234%
31	12.483	1743	1749	1763	rVV	214905	337540	60.17%	8.957%
32	12.629	1765	1773	1778	rVV5	6735	15027	2.68%	0.399%
33	12.684	1778	1782	1788	rVB5	3344	6242	1.11%	0.166%
34	12.764	1788	1795	1797	rBV4	5967	10073	1.80%	0.267%
35	12.806	1797	1802	1809	rVV	94957	142033	25.32%	3.769%
36	12.934	1817	1823	1831	rBV2	7112	19376	3.45%	0.514%

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37	13.038	1837	1840	1845	rBV4	5105	9710	1.73%	0.258%
38	13.166	1855	1861	1866	rVB	29159	45117	8.04%	1.197%
39	13.276	1873	1879	1886	rBV	3911	10621	1.89%	0.282%
40	13.428	1897	1904	1910	rBV	250094	379794	67.70%	10.079%
41	13.526	1915	1920	1926	rBV	48008	82278	14.67%	2.183%
42	13.660	1938	1942	1948	rBV7	3928	7174	1.28%	0.190%
43	13.757	1951	1958	1969	rBV4	20109	52251	9.31%	1.387%
44	13.849	1969	1973	1979	rBV	20934	34031	6.07%	0.903%
45	14.105	2010	2015	2023	rBV	19614	31292	5.58%	0.830%
46	14.507	2076	2081	2090	rVB2	15469	25864	4.61%	0.686%
47	14.623	2095	2100	2105	rVV3	9461	16668	2.97%	0.442%
48	14.958	2148	2155	2164	rBV2	9887	21491	3.83%	0.570%

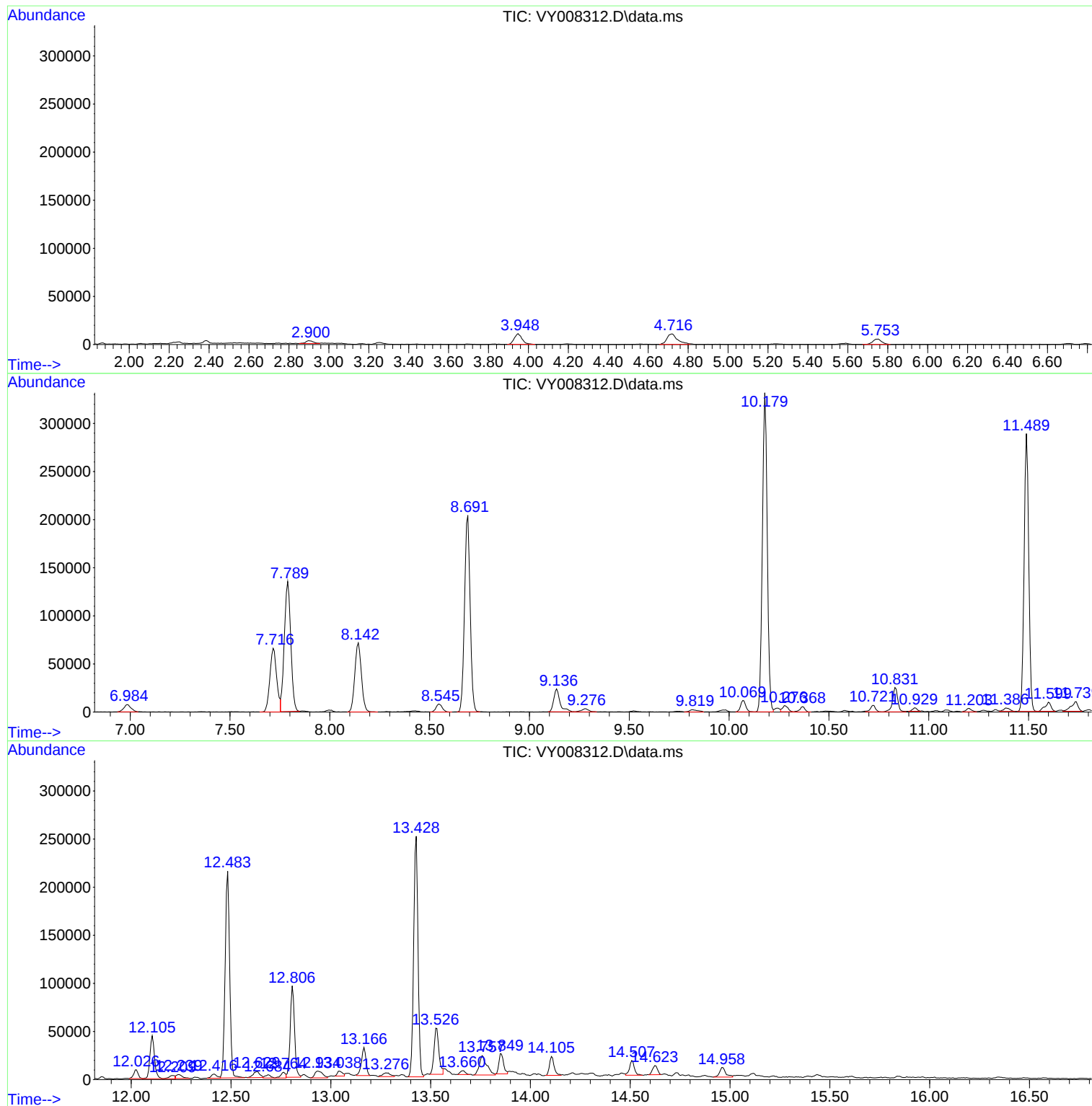
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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



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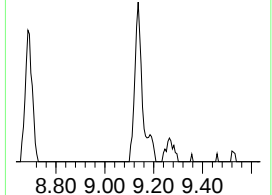
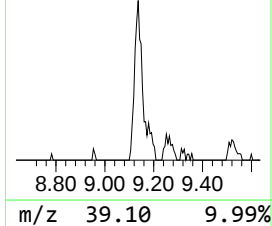
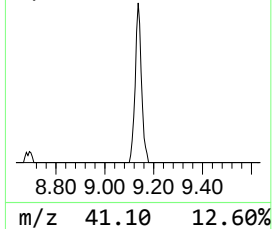
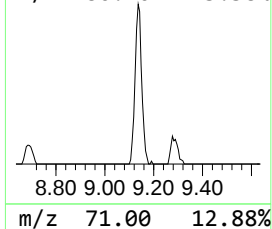
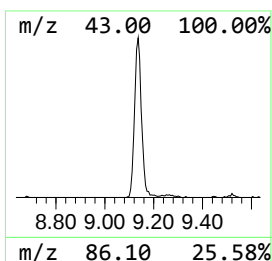
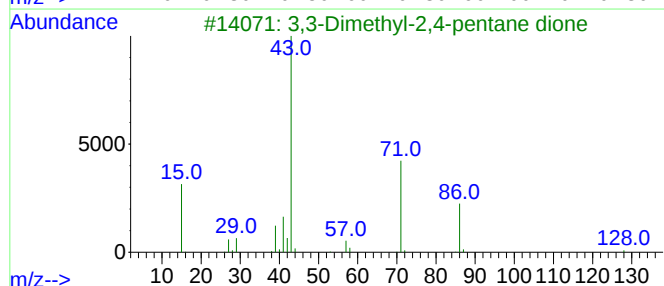
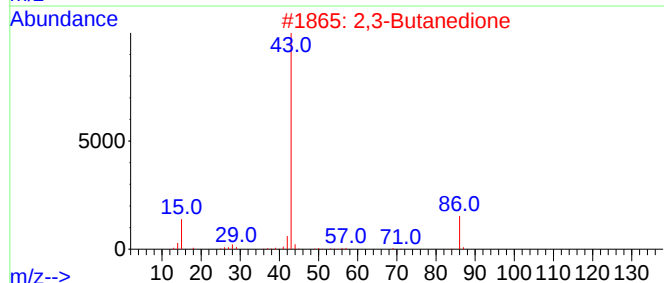
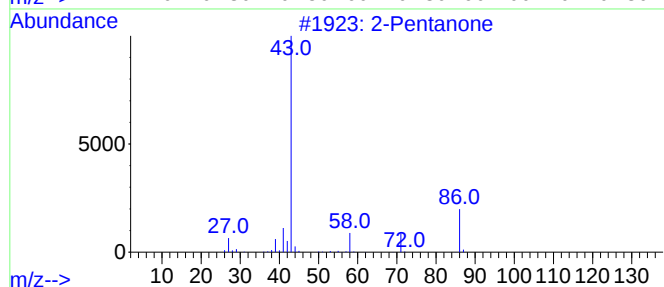
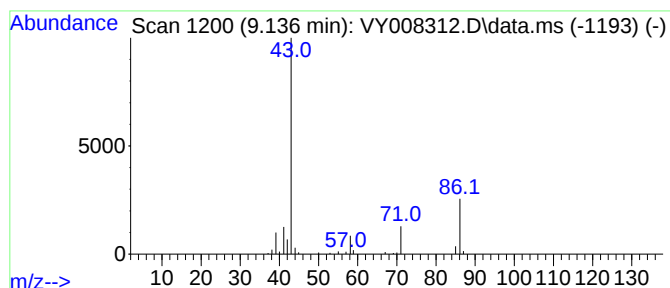
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.136	6.53 ug/l	52003	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	80
2			2,3-Butanedione	86	C4H6O2	000431-03-8	50
3			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	33
4			Butane	58	C4H10	000106-97-8	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



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Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DEL-7

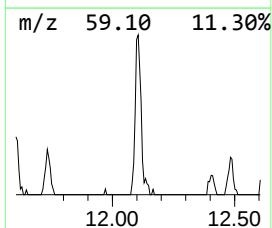
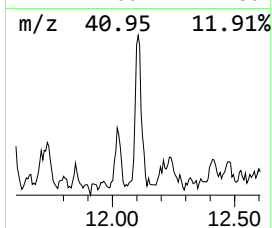
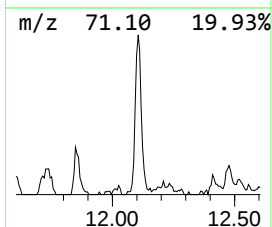
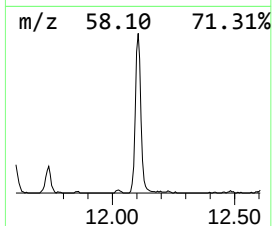
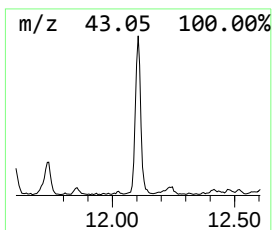
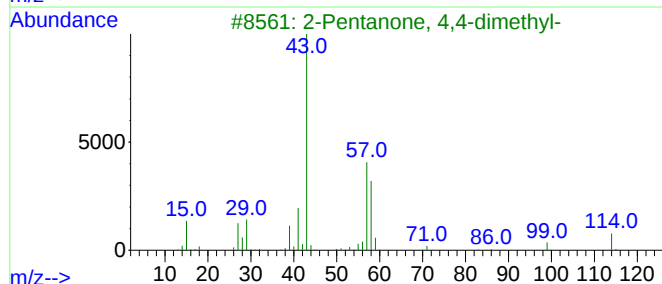
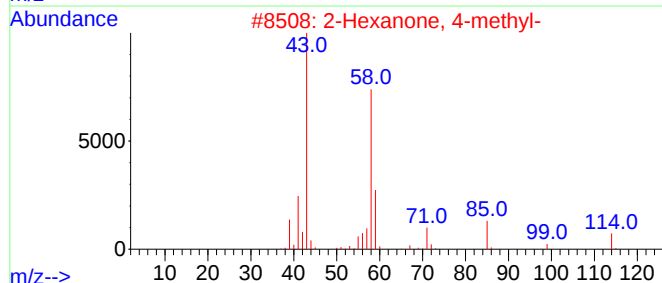
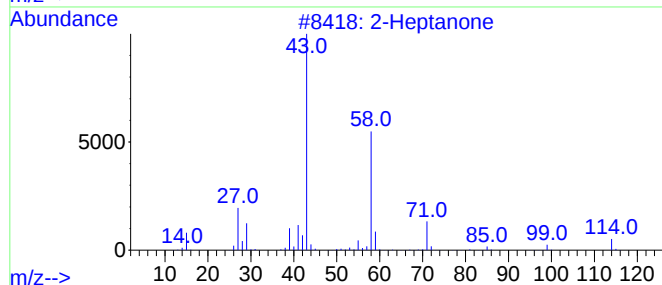
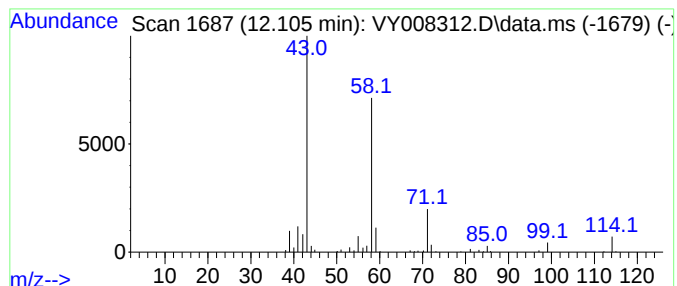
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	7.70 ug/l	71435	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	58
3			2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	47
4			3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	025910-96-7	40
5			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	38



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Misc : 5.02g/5.0mL/MSVOA_Y/soil
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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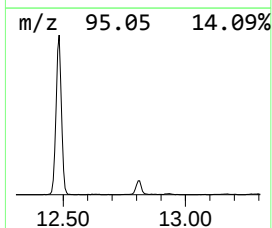
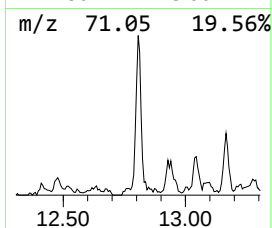
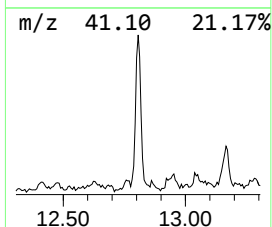
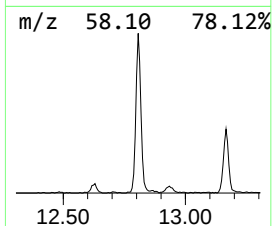
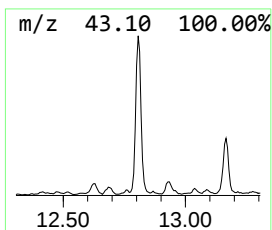
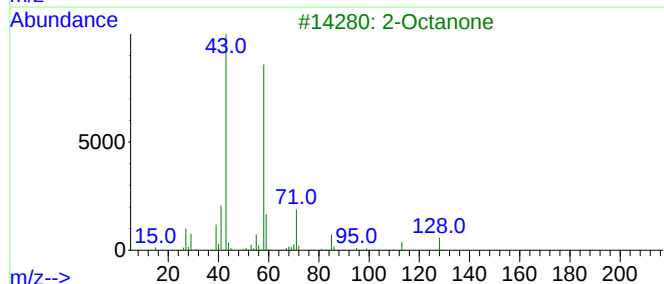
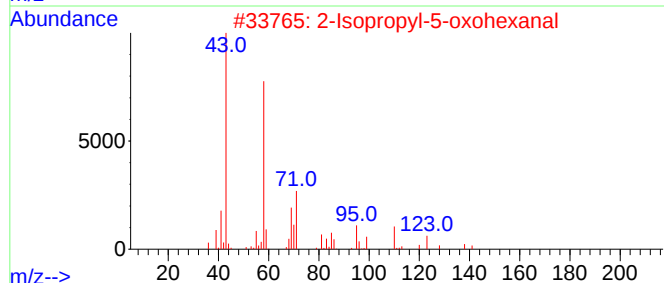
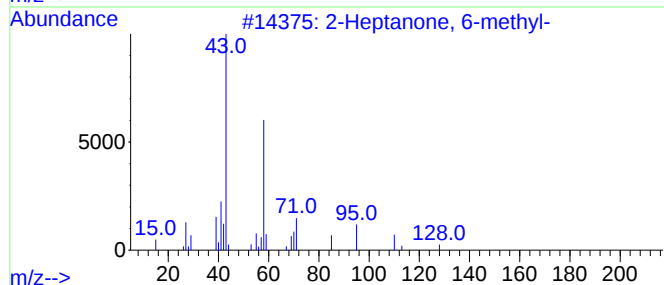
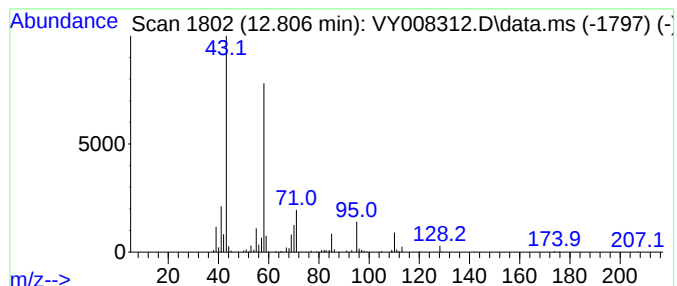
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Heptanone, 6-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	18.70 ug/l	142033	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2			2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	74
3			2-Octanone	128	C8H16O	000111-13-7	64
4			2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	42
5			1-Methyl-1-ethoxycyclobutane	114	C7H14O	059416-06-7	38



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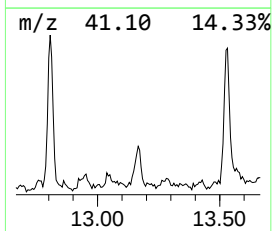
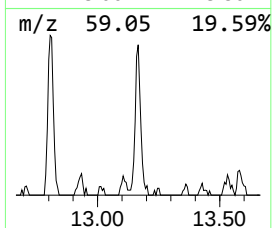
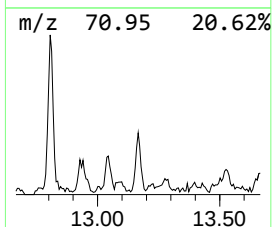
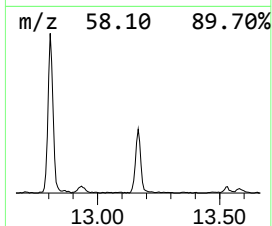
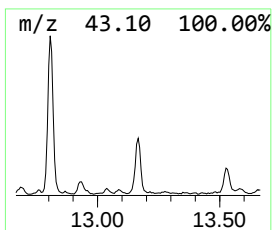
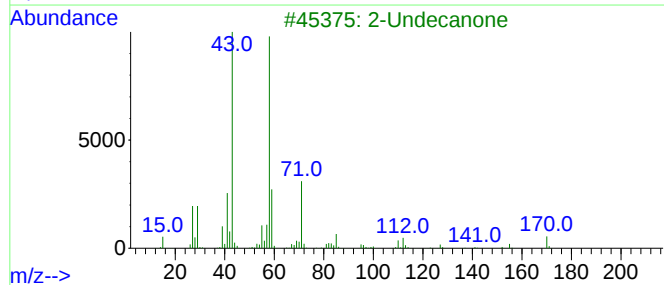
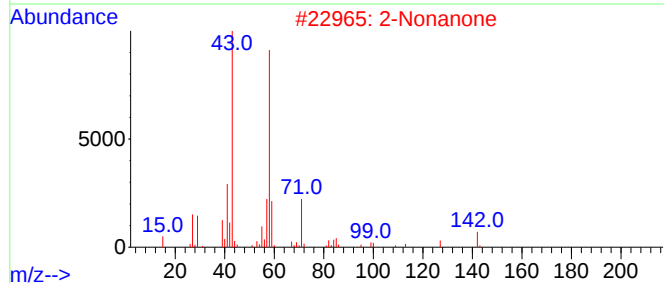
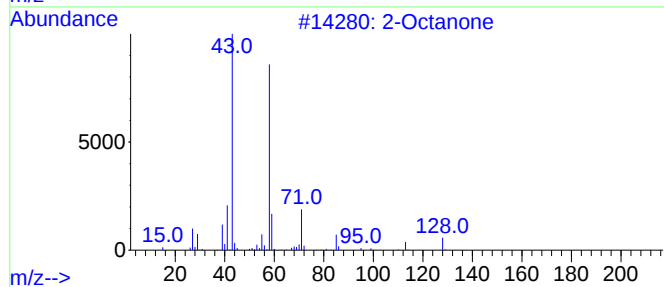
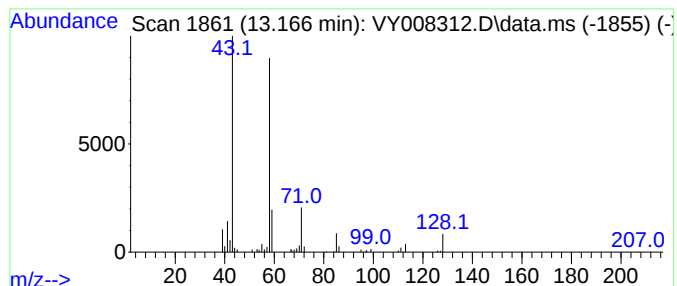
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Octanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.166	5.94 ug/l	45117	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	91
2			2-Nonanone	142	C9H18O	000821-55-6	78
3			2-Undecanone	170	C11H22O	000112-12-9	64
4			Butanimidamide	86	C4H10N2	000107-90-4	59
5			5-Nonanone, 2,8-dimethyl-	170	C11H22O	002050-99-9	56



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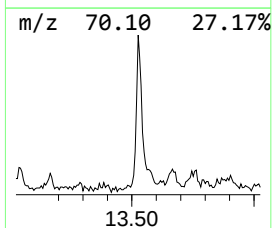
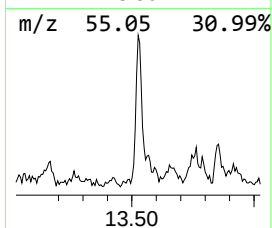
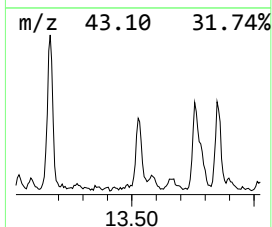
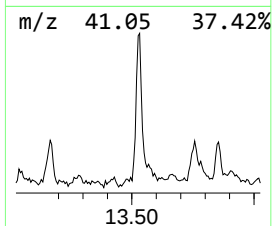
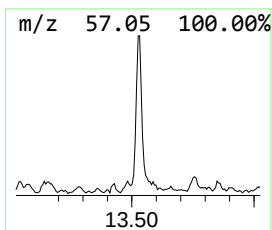
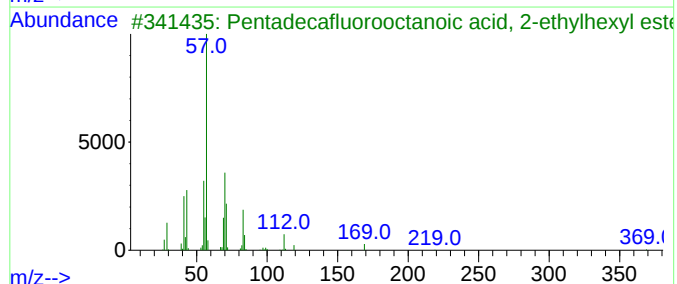
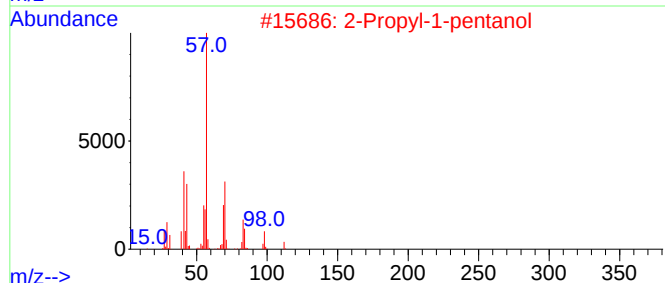
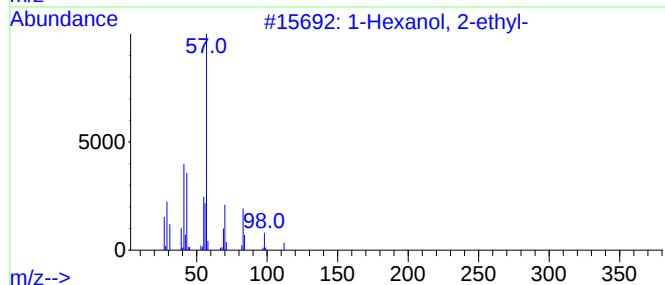
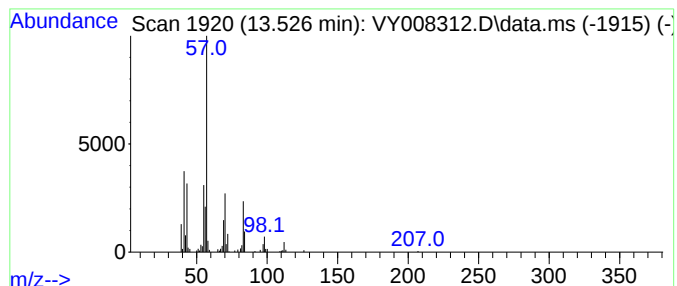
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	10.83 ug/l	82278	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
3	Pentadecafluorooctanoic acid, 2-...			526	C16H17F15O2	1000406-80-9	53
4	Butyl tetradecyl ether			270	C18H38O	1000406-40-4	50
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041322\
Data File : VY008312.D
Acq On : 13 Apr 2022 15:03
Operator : KP/MD
Sample : N2349-13
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DEL-7

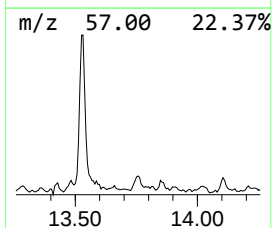
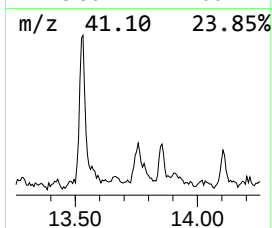
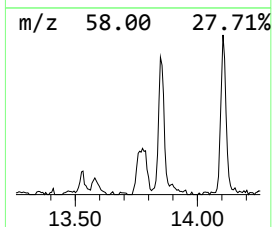
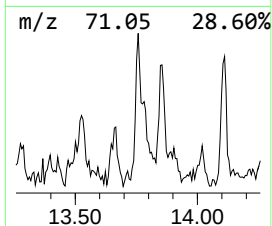
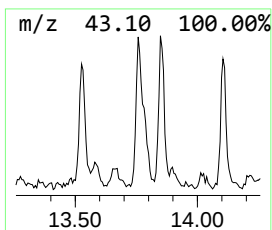
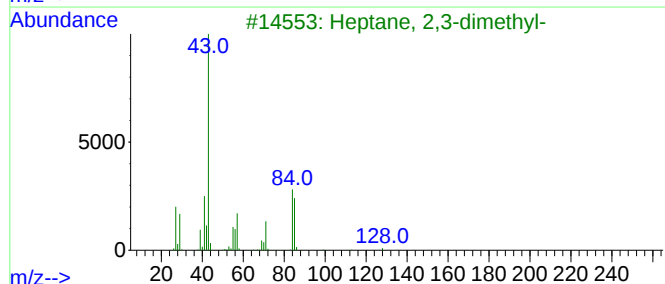
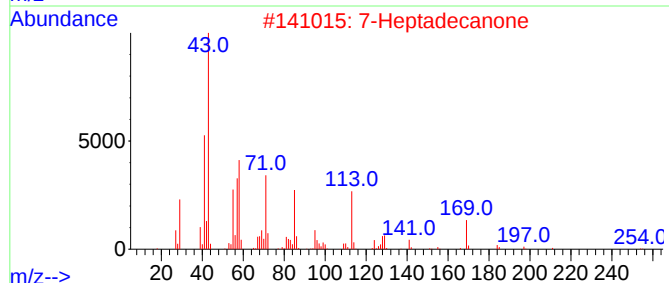
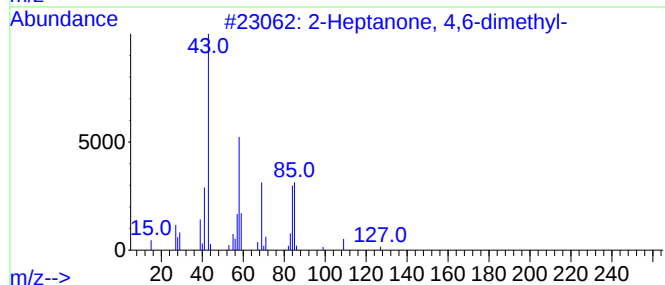
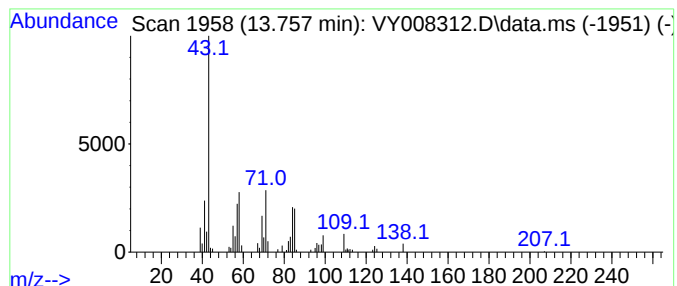
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.757 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	6.88 ug/l	52251	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	47
2		7-Heptadecanone	254	C17H34O	006064-42-2	38
3		Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	35
4		Octane, 4-methyl-	128	C9H20	002216-34-4	35
5		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041322\
Data File : VY008312.D
Acq On : 13 Apr 2022 15:03
Operator : KP/MD
Sample : N2349-13
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DEL-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.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
2-Pentanone	9.136	6.5	ug/l	52003	2	8.691	398466	50.0
2-Heptanone	12.105	7.7	ug/l	71435	3	11.489	463719	50.0
2-Heptanone, 6-...	12.806	18.7	ug/l	142033	4	13.428	379794	50.0
2-Octanone	13.166	5.9	ug/l	45117	4	13.428	379794	50.0
1-Hexanol, 2-et...	13.526	10.8	ug/l	82278	4	13.428	379794	50.0
unknown13.757	13.757	6.9	ug/l	52251	4	13.428	379794	50.0