

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
 Data File : VY013781.D
 Acq On : 17 May 2023 17:13
 Operator : KP/MD
 Sample : 02812-01
 Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WG-0516-B5-0-2

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\82Y051723S.M
 Title : SW846 8260

Signal : TIC: VY013781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	3	8	24	rVB	178731	248097	3.45%	0.828%
2	2.247	61	70	84	rBV	229880	391291	5.44%	1.306%
3	4.722	465	476	496	rBV3	25870	87306	1.21%	0.291%
4	7.722	957	968	974	rBV2	130146	317230	4.41%	1.059%
5	7.789	974	979	991	rVB	207042	472029	6.57%	1.575%
6	8.143	1027	1037	1048	rBV	134109	304367	4.23%	1.016%
7	8.691	1118	1127	1139	rBV	333607	658045	9.15%	2.196%
8	10.179	1363	1371	1386	rBV	619619	1085663	15.10%	3.623%
9	10.368	1394	1402	1412	rVB	91546	168490	2.34%	0.562%
10	10.520	1422	1427	1433	rVB	44761	78746	1.10%	0.263%
11	10.618	1433	1443	1448	rBV3	47630	93221	1.30%	0.311%
12	10.801	1463	1473	1479	rBV	59048	100548	1.40%	0.336%
13	10.904	1479	1490	1496	rBV3	33407	79952	1.11%	0.267%
14	10.971	1496	1501	1505	rVV	79841	142596	1.98%	0.476%
15	11.038	1508	1512	1516	rVV	89034	148771	2.07%	0.496%
16	11.087	1516	1520	1526	rVV	135147	246606	3.43%	0.823%
17	11.203	1533	1539	1543	rBV3	71118	131878	1.83%	0.440%
18	11.288	1543	1553	1563	rVB4	279838	753019	10.47%	2.513%
19	11.380	1563	1568	1573	rBV	222464	342771	4.77%	1.144%
20	11.490	1580	1586	1596	rVB	513521	850352	11.83%	2.838%
21	11.593	1596	1603	1607	rBV	721942	1194717	16.62%	3.987%
22	11.703	1612	1621	1630	rVV2	3328426	7189273	100.00%	23.991%
23	11.776	1630	1633	1639	rVB3	142616	241213	3.36%	0.805%
24	12.026	1662	1674	1682	rBV	1231829	2521777	35.08%	8.415%
25	12.124	1686	1690	1693	rVV	188604	245392	3.41%	0.819%
26	12.203	1699	1703	1705	rVV2	140501	225960	3.14%	0.754%
27	12.245	1705	1710	1719	rVV4	259711	608349	8.46%	2.030%
28	12.331	1719	1724	1728	rVV3	123680	248556	3.46%	0.829%
29	12.380	1728	1732	1734	rVV4	73016	134323	1.87%	0.448%
30	12.410	1734	1737	1740	rVV	155271	249599	3.47%	0.833%
31	12.483	1744	1749	1753	rVV	401674	604173	8.40%	2.016%
32	12.526	1753	1756	1760	rVB3	99280	133182	1.85%	0.444%
33	12.642	1771	1775	1782	rVB3	159343	297376	4.14%	0.992%
34	12.727	1782	1789	1793	rBV3	123781	276575	3.85%	0.923%
35	12.800	1793	1801	1807	rVV3	1218306	2259282	31.43%	7.539%
36	12.861	1807	1811	1815	rVV2	200556	351494	4.89%	1.173%

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37	12.947	1815	1825	1829	rVV5	149034	395633	5.50%	1.320%
38	13.008	1829	1835	1836	rVV2	143478	294977	4.10%	0.984%
39	13.038	1836	1840	1847	rVV	381560	713138	9.92%	2.380%
40	13.123	1847	1854	1857	rVV5	94309	274510	3.82%	0.916%
41	13.166	1857	1861	1867	rVV6	111410	335679	4.67%	1.120%
42	13.221	1867	1870	1872	rVV2	105755	175745	2.44%	0.586%
43	13.245	1872	1874	1878	rVV3	118981	179436	2.50%	0.599%
44	13.318	1878	1886	1890	rVV4	335276	848717	11.81%	2.832%
45	13.361	1890	1893	1896	rVV2	191641	310369	4.32%	1.036%
46	13.422	1896	1903	1912	rVV2	622713	1266605	17.62%	4.227%
47	13.501	1912	1916	1919	rVV3	129316	212087	2.95%	0.708%
48	13.562	1920	1926	1930	rVV6	80418	200477	2.79%	0.669%
49	13.611	1930	1934	1941	rVB7	38163	76558	1.06%	0.255%
50	13.751	1951	1957	1961	rBV	588863	897311	12.48%	2.994%
51	13.788	1961	1963	1968	rVB3	64277	86623	1.20%	0.289%
52	13.849	1968	1973	1980	rBV7	42573	87207	1.21%	0.291%
53	14.251	2033	2039	2046	rVB8	60514	129635	1.80%	0.433%

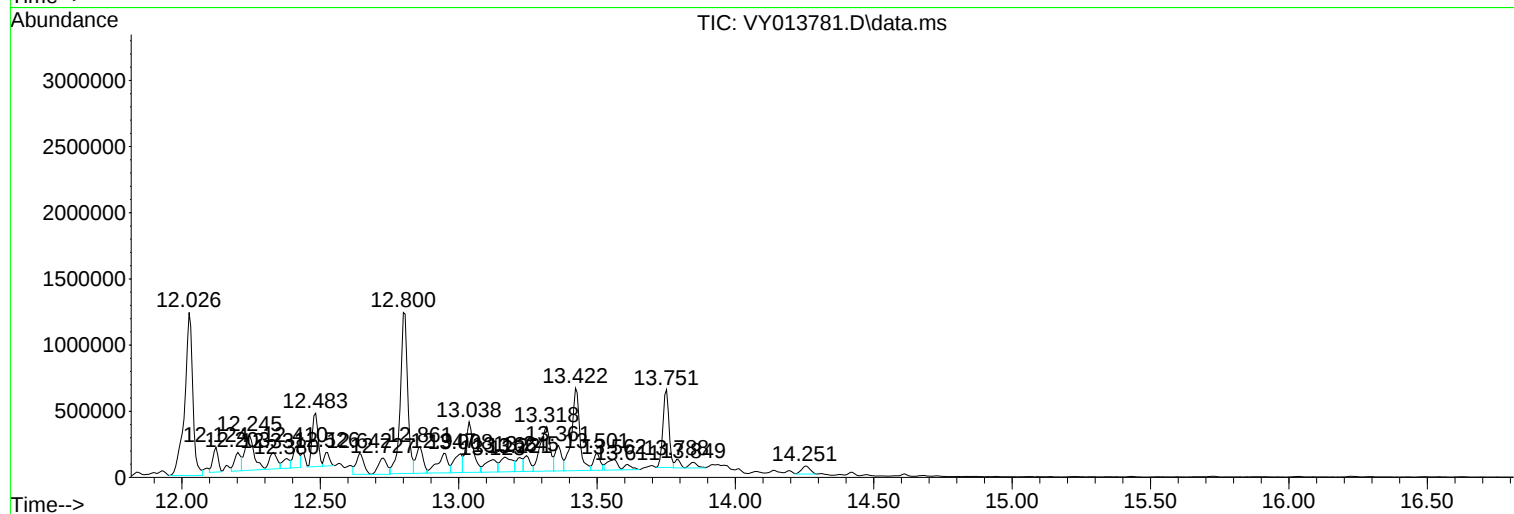
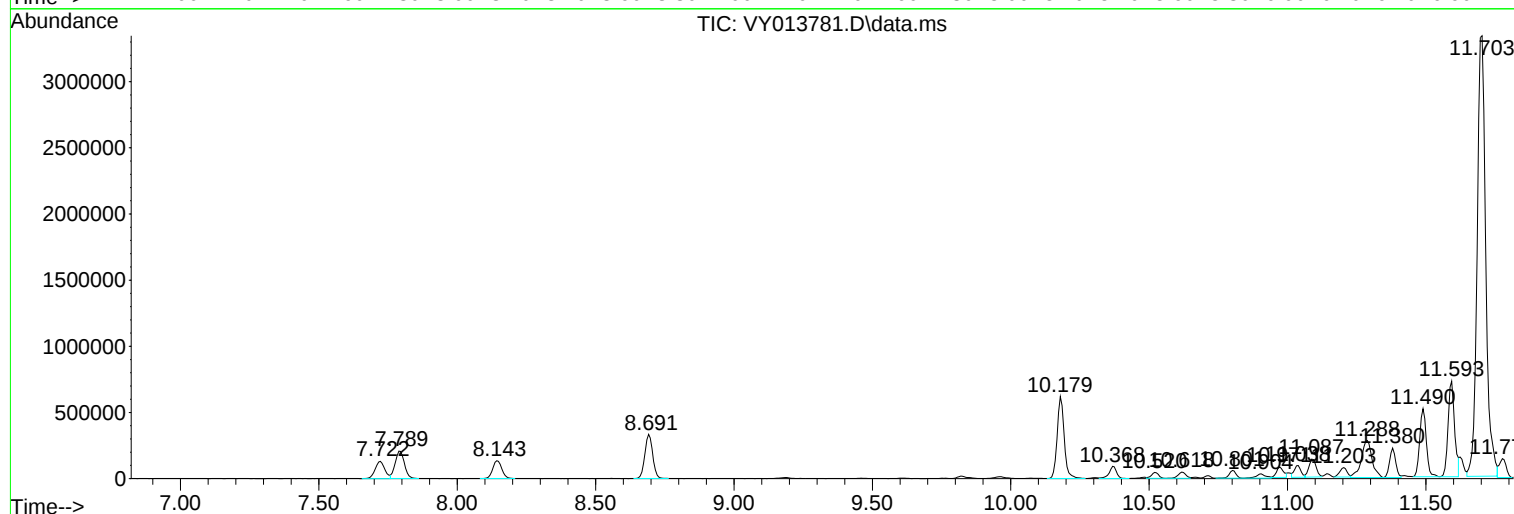
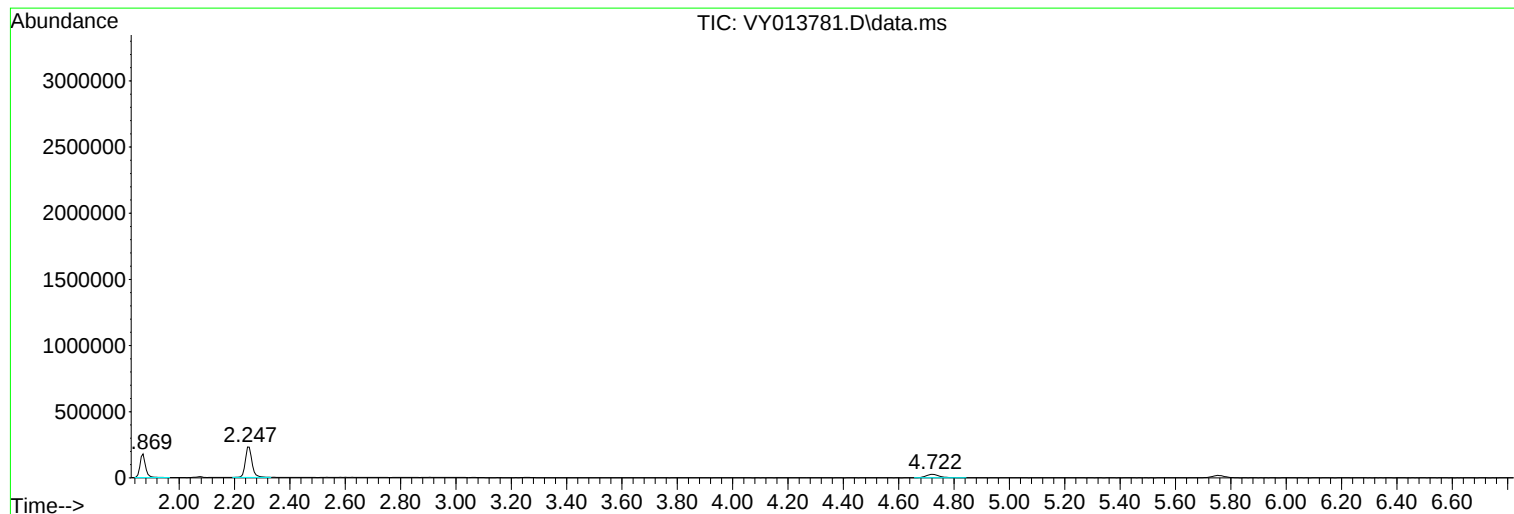
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
WG-0516-B5-0-2

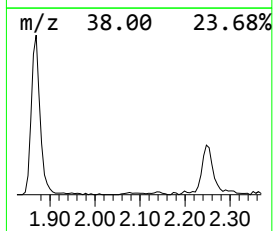
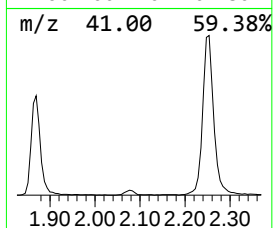
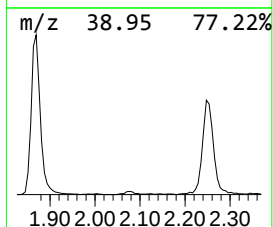
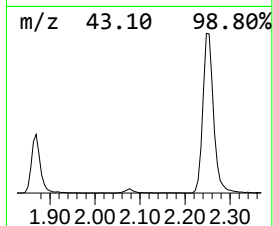
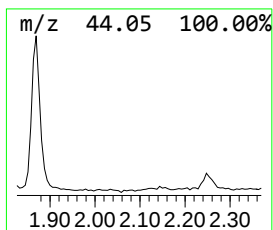
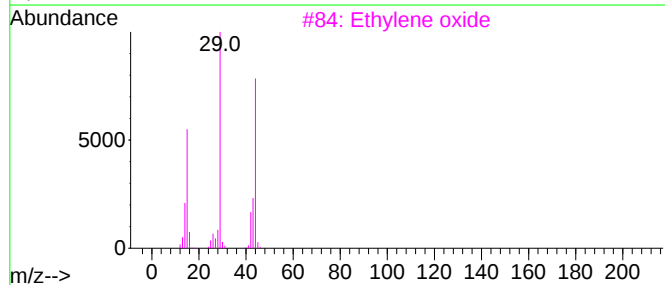
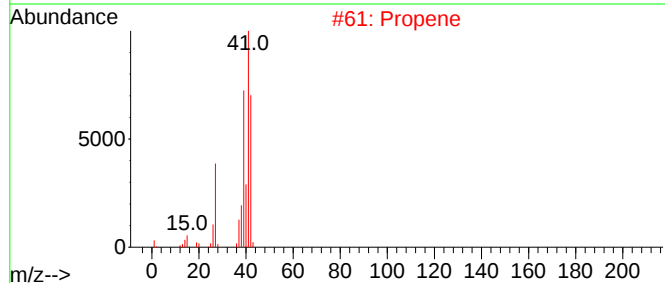
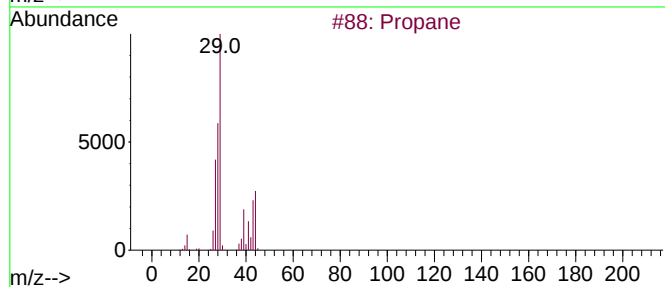
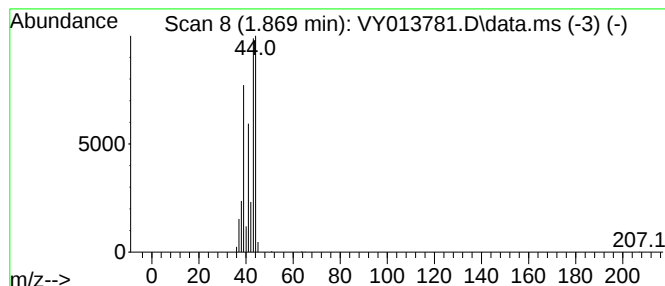
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051723S.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.869	26.28 ug/l	248097	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	90
2	Propene			42	C3H6	000115-07-1	9
3	Ethylene oxide			44	C2H4O	000075-21-8	5
4	Acetaldehyde			44	C2H4O	000075-07-0	5
5	Chloro(prop-2-yn-1-yloxy)methanone			118	C4H3ClO2	035718-08-2	4



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WG-0516-B5-0-2

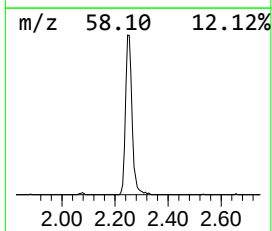
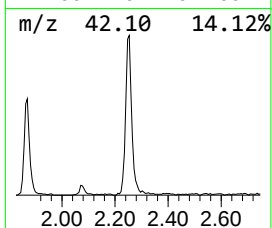
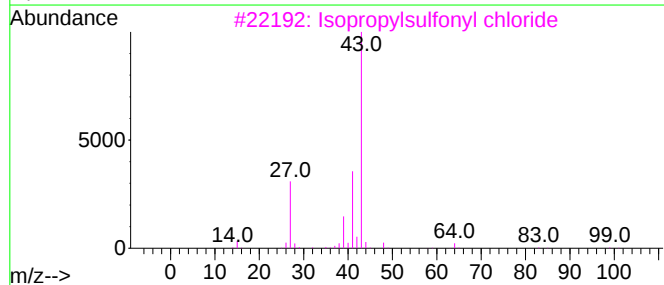
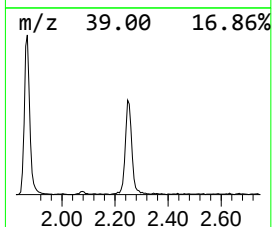
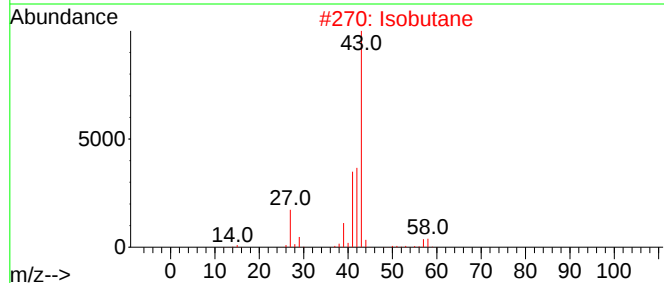
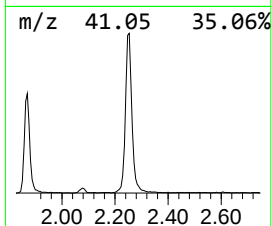
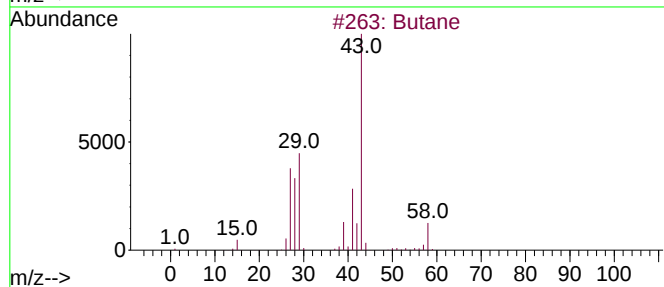
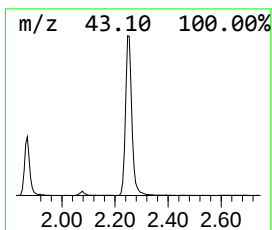
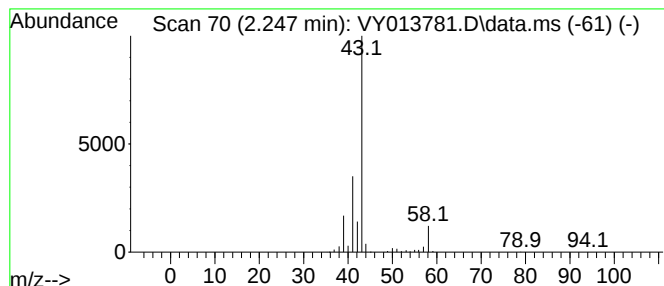
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051723S.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.247	41.45 ug/l	391291	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isobutane	58	C4H10	000075-28-5	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
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Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

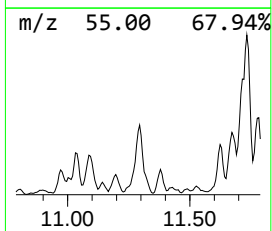
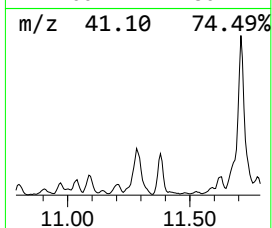
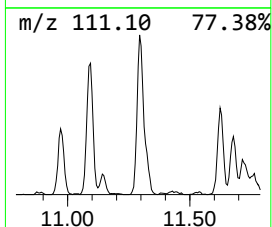
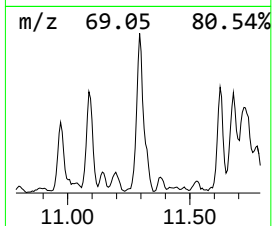
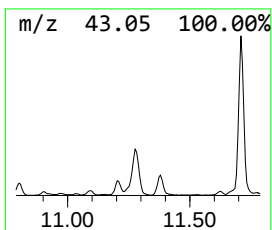
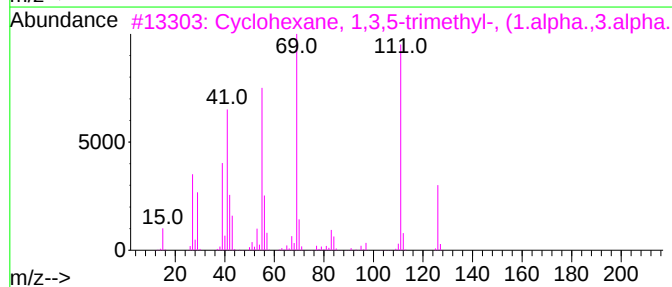
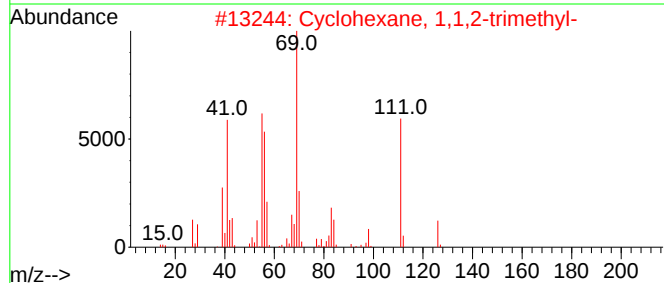
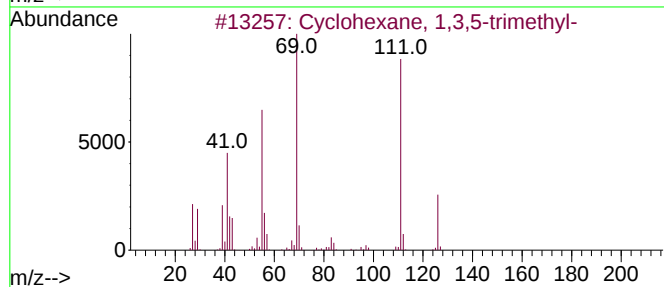
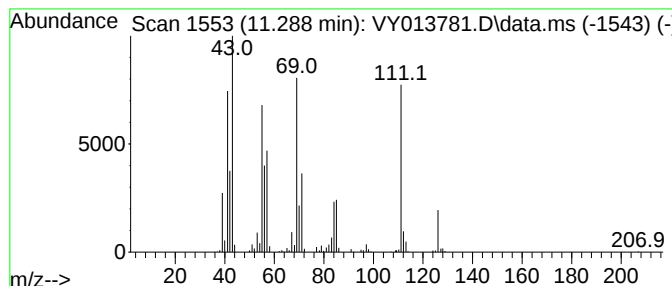
Instrument :
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.288	44.28 ug/l	753019	Chlorobenzene-d5	11.490	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
2	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	64
3	Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	58
4	Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-27-3	52
5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	49



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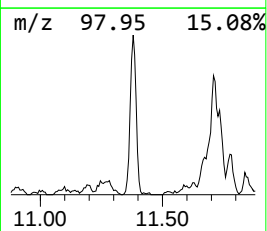
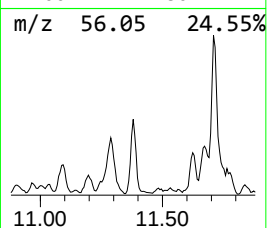
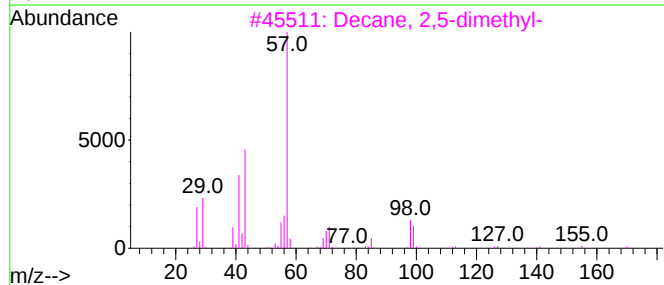
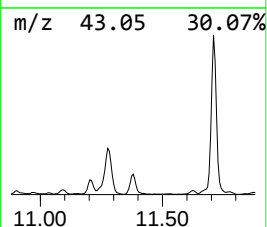
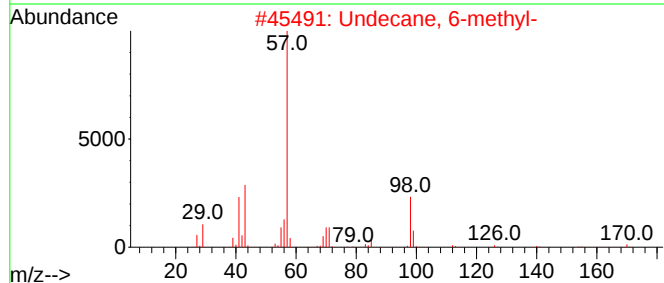
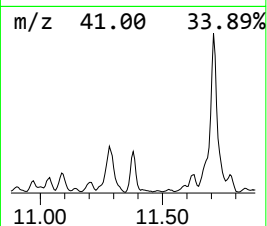
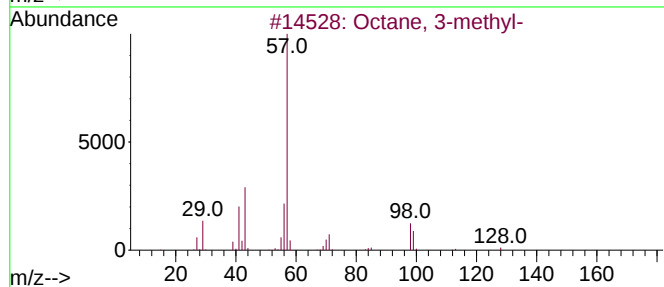
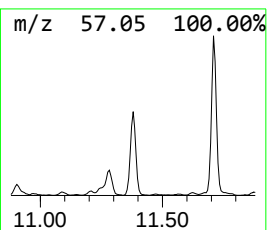
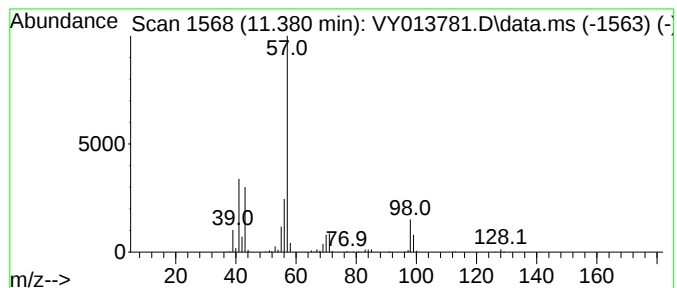
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051723S.M
Quant Title : SW846 8260

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

Peak Number 4 Octane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	20.15 ug/l	342771	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	87
2			Undecane, 6-methyl-	170	C12H26	017302-33-9	59
3			Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	59
4			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	53
5			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50



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WG-0516-B5-0-2

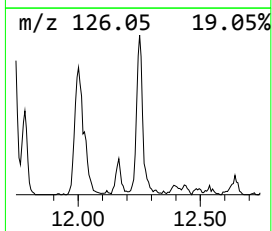
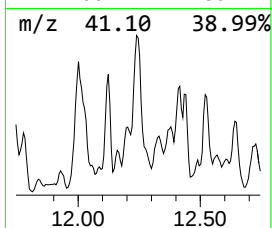
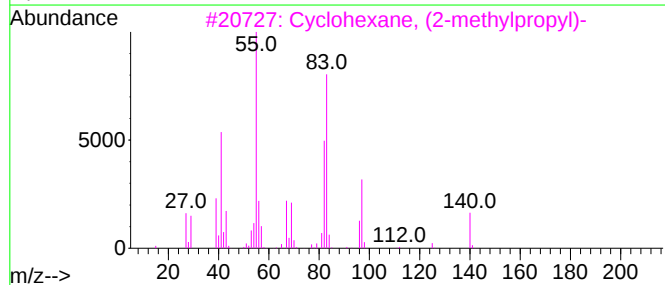
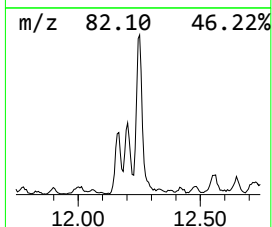
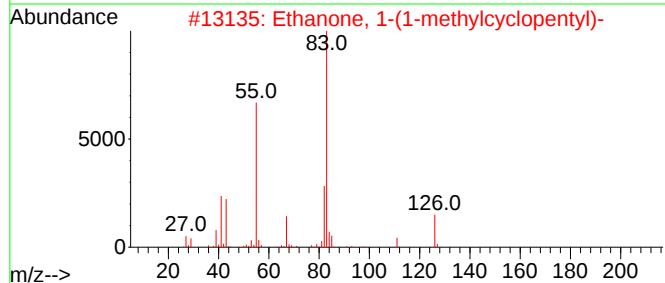
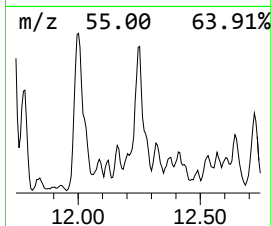
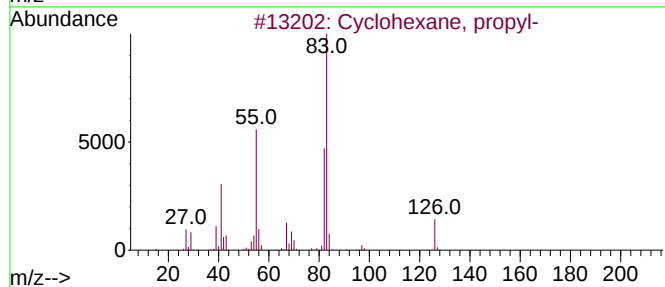
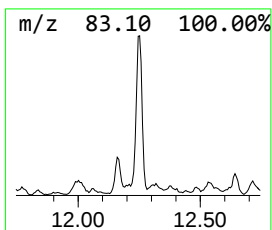
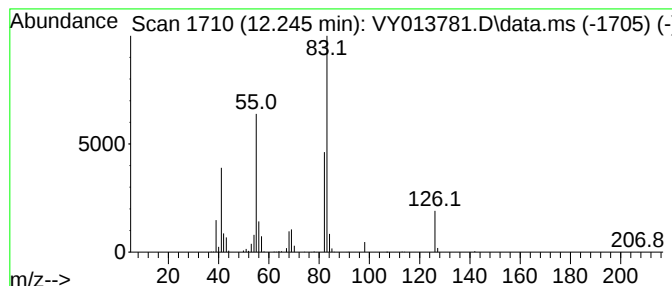
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.246	35.77 ug/l	608349	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59
3			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	59
4			3,3-Dimethylhex-5-en-2-one	126	C8H14O	1000424-30-3	53
5			Lomustine	233	C9H16ClN3O2	013010-47-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

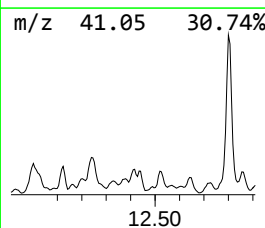
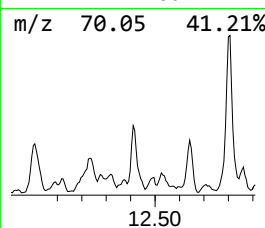
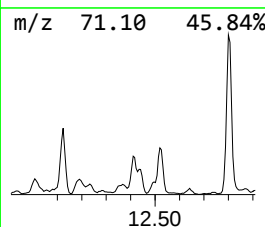
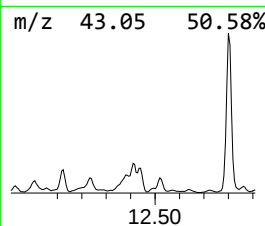
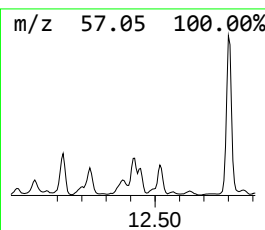
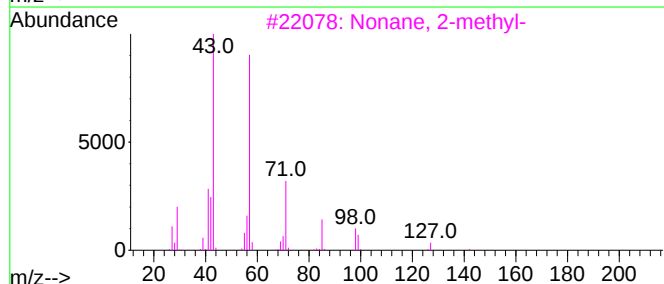
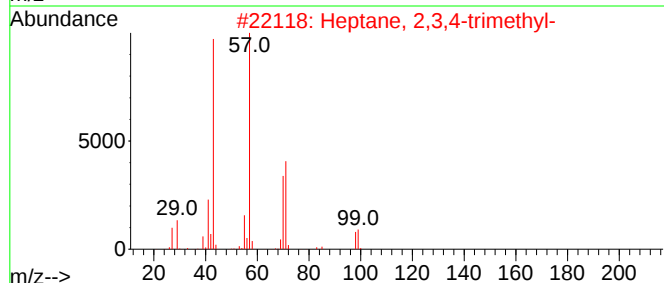
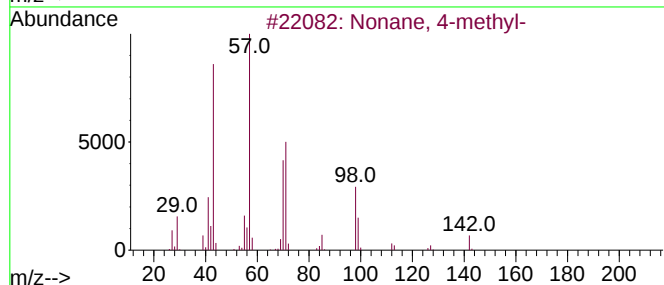
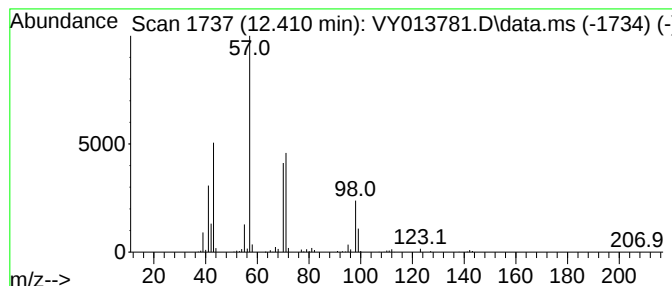
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Quant Title : SW846 8260

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

Peak Number 6 Nonane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	14.68 ug/l	249599	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-	142	C10H22	017301-94-9	78
2			Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
3			Nonane, 2-methyl-	142	C10H22	000871-83-0	47
4			Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	42
5			Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

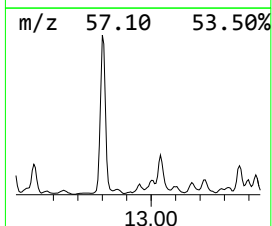
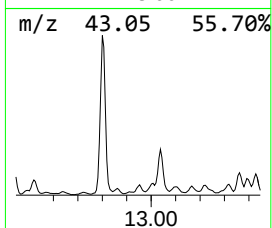
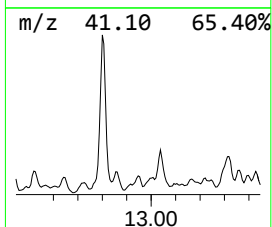
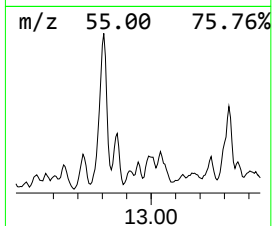
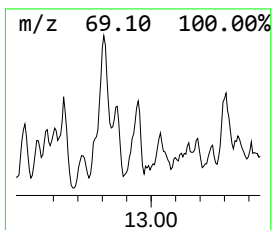
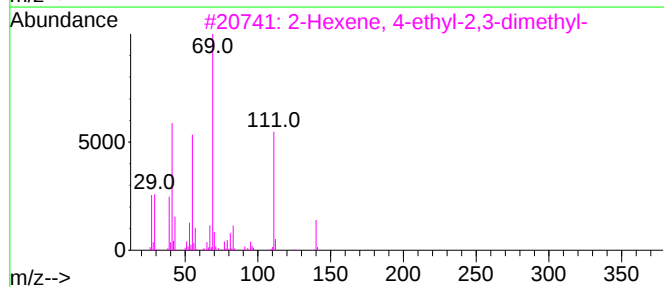
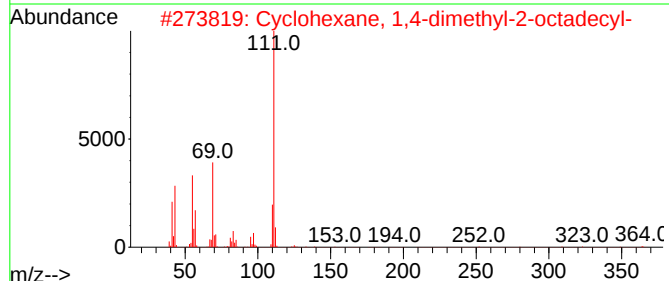
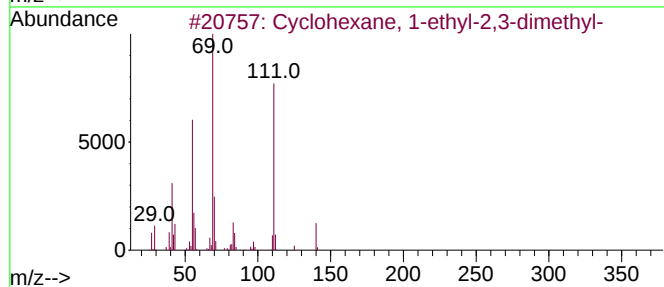
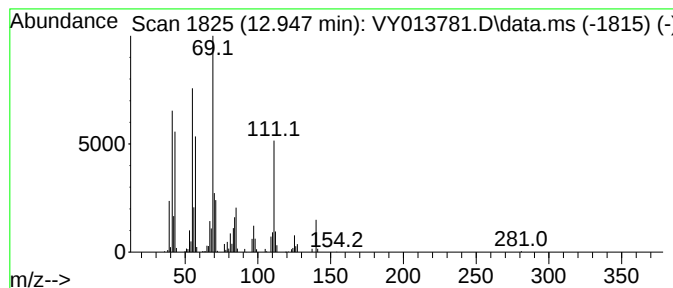
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1-ethyl-2,3-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.947	15.62 ug/l	395633	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2,3-dimethyl-	140	C10H20	007058-05-1	68
2			Cyclohexane, 1,4-dimethyl-2-octa...	364	C26H52	055282-02-5	64
3			2-Hexene, 4-ethyl-2,3-dimethyl-	140	C10H20	1000149-19-7	49
4			Cyclopropane, 1,1-dimethyl-2-pen...	140	C10H20	062167-97-9	49
5			3-Nonene, 2-methyl-	140	C10H20	053966-53-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

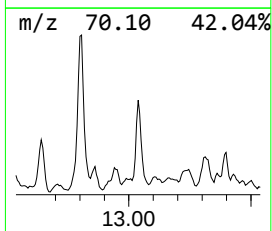
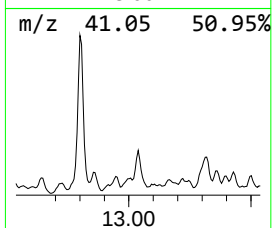
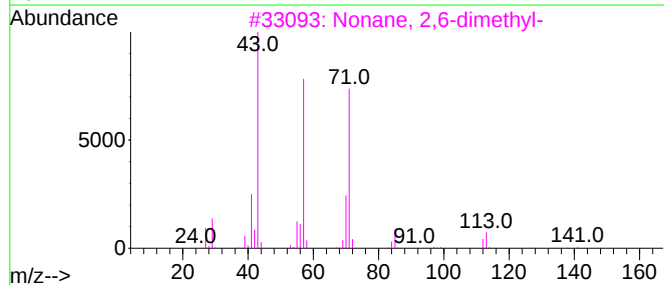
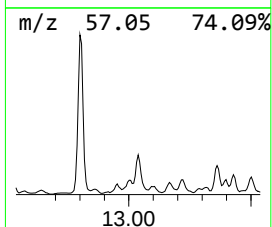
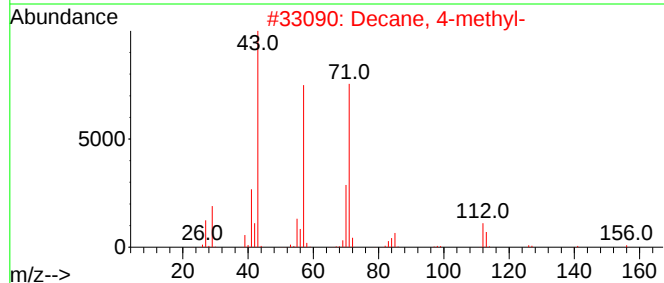
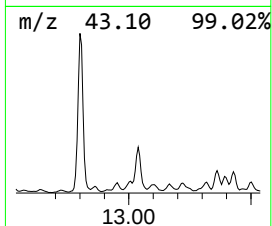
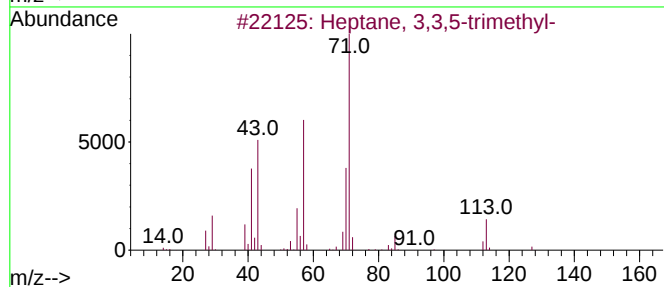
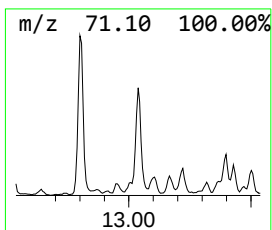
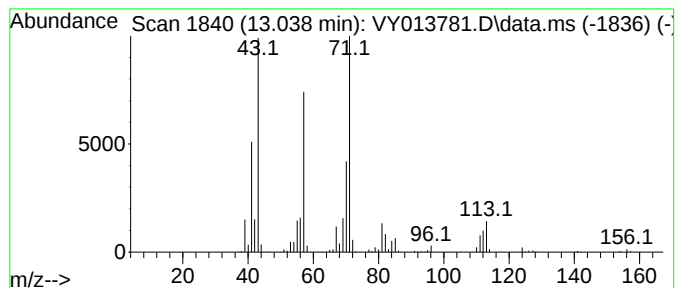
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Quant Title : SW846 8260

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

Peak Number 8 Heptane, 3,3,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.038	28.15 ug/l	713138	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	78
2			Decane, 4-methyl-	156	C11H24	002847-72-5	74
3			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	72
4			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
5			4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

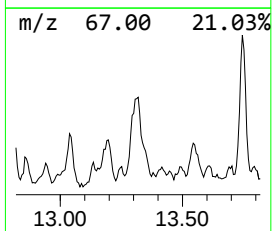
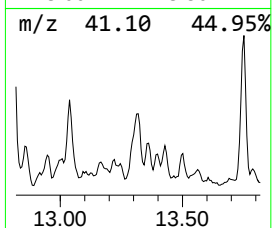
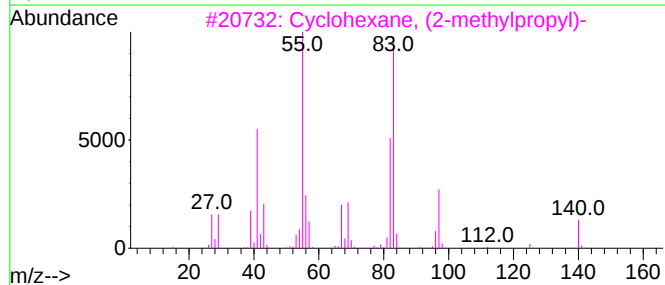
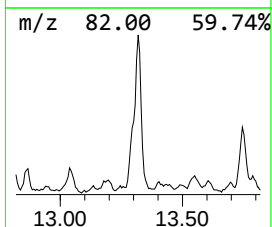
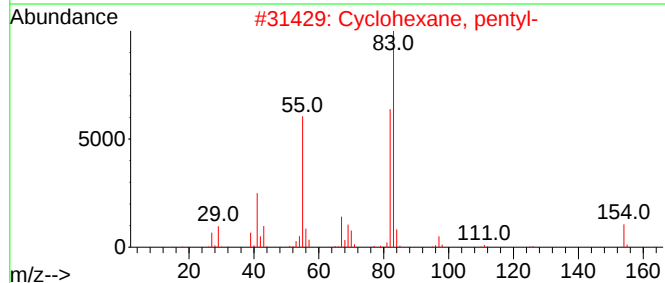
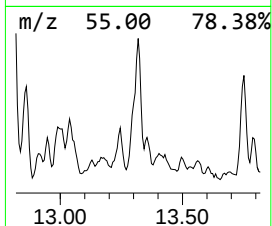
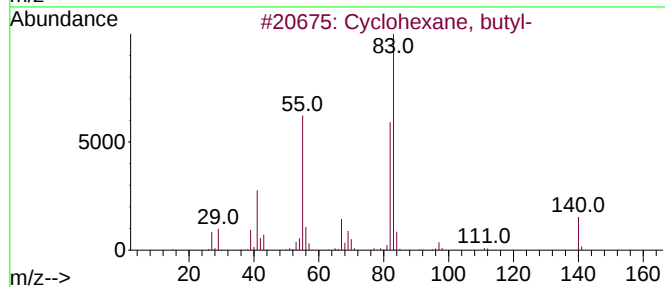
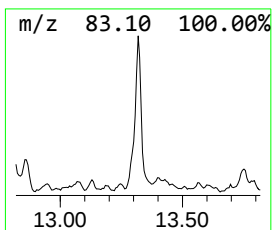
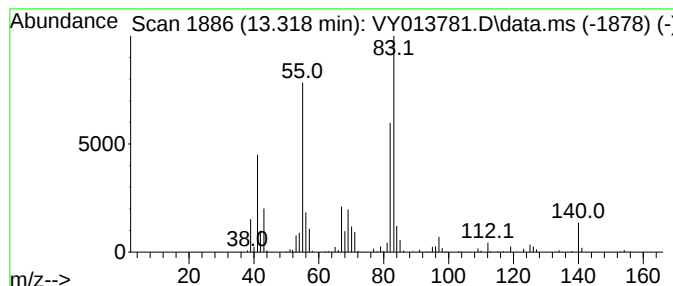
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.318	33.50 ug/l	848717	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	90
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	87
3			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	80
4			Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
5			Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

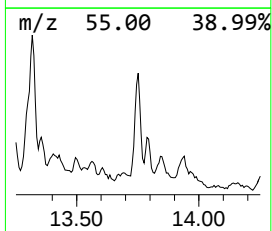
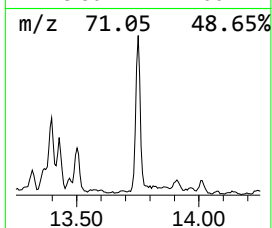
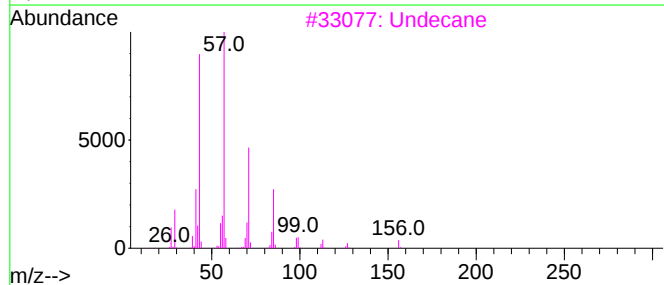
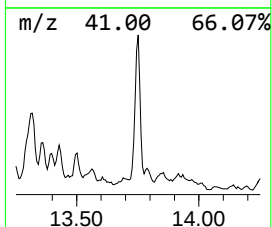
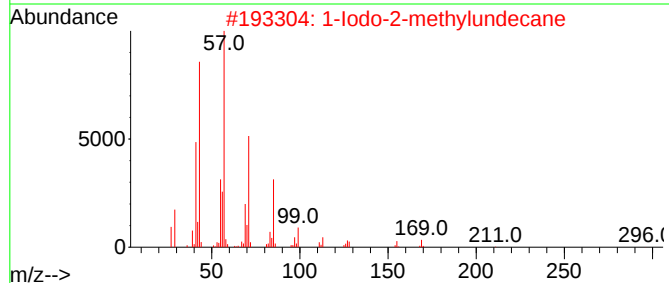
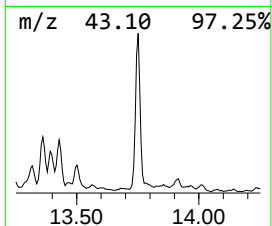
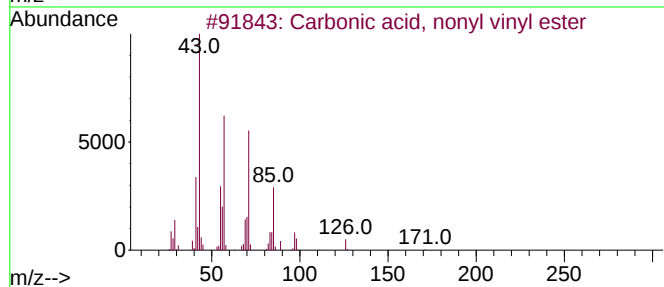
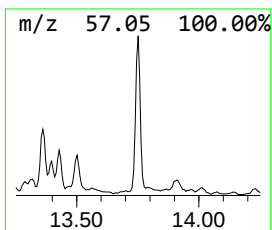
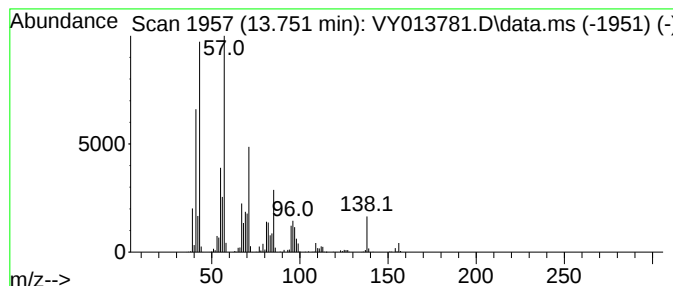
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Quant Title : SW846 8260

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

Peak Number 10 unknown13.751 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	35.42 ug/l	897311	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	49
2			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	47
3			Undecane	156	C11H24	001120-21-4	46
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	46
5			Tridecane	184	C13H28	000629-50-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051723\
Data File : VY013781.D
Acq On : 17 May 2023 17:13
Operator : KP/MD
Sample : 02812-01
Misc : 6.39g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WG-0516-B5-0-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051723S.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
Propane	1.869	26.3	ug/l	248097	1	7.795	472029	50.0
Butane	2.247	41.5	ug/l	391291	1	7.795	472029	50.0
Cyclohexane, 1,...	11.288	44.3	ug/l	753019	3	11.490	850352	50.0
Octane, 3-methyl-	11.380	20.1	ug/l	342771	3	11.490	850352	50.0
Cyclohexane, pr...	12.246	35.8	ug/l	608349	3	11.490	850352	50.0
Nonane, 4-methyl-	12.410	14.7	ug/l	249599	3	11.490	850352	50.0
Cyclohexane, 1-...	12.947	15.6	ug/l	395633	4	13.422	1266610	50.0
Heptane, 3,3,5-...	13.038	28.1	ug/l	713138	4	13.422	1266610	50.0
Cyclohexane, bu...	13.318	33.5	ug/l	848717	4	13.422	1266610	50.0
unknown13.751	13.751	35.4	ug/l	897311	4	13.422	1266610	50.0