

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
 Data File : VY011246.D
 Acq On : 02 Nov 2022 01:54
 Operator : KP/MD
 Sample : N5337-03
 Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-02-11.5-12.0

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\82Y110122S.M
 Title : SW846 8260

Signal : TIC: VY011246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.179	1362	1371	1379	rBV	23465	41235	1.03%	0.123%
2	11.288	1547	1553	1562	rVB8	20632	58181	1.45%	0.173%
3	11.489	1580	1586	1591	rBV	27268	47444	1.18%	0.141%
4	11.739	1621	1627	1631	rBV4	21824	50974	1.27%	0.151%
5	11.928	1654	1658	1663	rVB3	29069	43346	1.08%	0.129%
6	12.001	1663	1670	1676	rBV4	138600	313396	7.82%	0.931%
7	12.117	1685	1689	1693	rVB	216413	293680	7.33%	0.873%
8	12.197	1693	1702	1705	rBV2	142303	307804	7.68%	0.914%
9	12.233	1705	1708	1713	rVB3	170858	250425	6.25%	0.744%
10	12.312	1713	1721	1725	rBV8	47671	146402	3.65%	0.435%
11	12.379	1725	1732	1734	rBV6	108346	240316	6.00%	0.714%
12	12.410	1734	1737	1742	rVB2	155469	209216	5.22%	0.622%
13	12.459	1742	1745	1752	rVB5	67976	154137	3.85%	0.458%
14	12.520	1752	1755	1758	rBV2	98187	126169	3.15%	0.375%
15	12.568	1758	1763	1767	rBV5	77361	139884	3.49%	0.416%
16	12.642	1770	1775	1782	rVB4	305247	651791	16.27%	1.936%
17	12.727	1782	1789	1794	rBV6	179974	498666	12.45%	1.482%
18	12.806	1795	1802	1806	rBV5	302893	800653	19.98%	2.379%
19	12.910	1816	1819	1821	rBV	50318	67496	1.68%	0.201%
20	12.946	1821	1825	1829	rVV4	318109	455075	11.36%	1.352%
21	13.001	1829	1834	1836	rBV2	346691	590564	14.74%	1.755%
22	13.038	1836	1840	1846	rVV	1446735	2135898	53.31%	6.346%
23	13.099	1847	1850	1853	rVB2	150064	178830	4.46%	0.531%
24	13.166	1857	1861	1865	rBV	407100	637362	15.91%	1.894%
25	13.215	1866	1869	1872	rBV2	264463	379556	9.47%	1.128%
26	13.288	1877	1881	1882	rVV2	417708	573722	14.32%	1.705%
27	13.312	1883	1885	1889	rVV2	583234	900438	22.48%	2.675%
28	13.355	1889	1892	1896	rVV3	735668	1239200	30.93%	3.682%
29	13.391	1896	1898	1903	rVB3	399053	550621	13.74%	1.636%
30	13.562	1922	1926	1929	rBV3	248305	415204	10.36%	1.234%
31	13.672	1941	1944	1945	rBV	146568	161137	4.02%	0.479%
32	13.745	1950	1956	1960	rVV3	1223148	2220469	55.42%	6.597%
33	13.788	1960	1963	1968	rVV4	310178	504842	12.60%	1.500%
34	13.849	1970	1973	1979	rVV6	305445	639709	15.97%	1.901%
35	13.910	1979	1983	1989	rVV4	446703	911760	22.76%	2.709%
36	14.007	1996	1999	2004	rVB	556721	847124	21.14%	2.517%

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37	14.068	2005	2009	2014	rBV6	402257	699769	17.47%	2.079%
38	14.141	2015	2021	2026	rBV5	471223	919262	22.95%	2.731%
39	14.190	2026	2029	2032	rBV3	245584	371213	9.27%	1.103%
40	14.257	2032	2040	2054	rVB9	1232253	4006343	100.00%	11.903%
41	14.373	2055	2059	2062	rBV3	353741	618925	15.45%	1.839%
42	14.416	2062	2066	2070	rVB3	691000	971334	24.24%	2.886%
43	14.611	2096	2098	2102	rBV5	132870	164801	4.11%	0.490%
44	14.678	2105	2109	2113	rVV2	356941	599749	14.97%	1.782%
45	14.727	2113	2117	2124	rVB2	1212817	1970518	49.18%	5.854%
46	14.800	2124	2129	2133	rBV6	176252	342353	8.55%	1.017%
47	14.842	2134	2136	2138	rBV2	107479	125137	3.12%	0.372%
48	14.940	2148	2152	2156	rVB2	543547	829857	20.71%	2.465%
49	15.001	2156	2162	2164	rBV3	175139	372740	9.30%	1.107%
50	15.050	2165	2170	2177	rVB2	424124	853012	21.29%	2.534%
51	15.208	2191	2196	2201	rBV2	430605	666670	16.64%	1.981%
52	15.275	2202	2207	2212	rBV7	127145	242351	6.05%	0.720%
53	15.336	2213	2217	2223	rBV8	159621	345231	8.62%	1.026%
54	15.519	2242	2247	2254	rVV2	210330	450545	11.25%	1.339%
55	15.598	2256	2260	2265	rVB4	191469	339522	8.47%	1.009%
56	15.684	2267	2274	2284	rVB5	150877	439441	10.97%	1.306%
57	15.879	2301	2306	2311	rVB3	87129	174616	4.36%	0.519%
58	16.019	2326	2329	2334	rVB4	75089	130074	3.25%	0.386%
59	16.153	2347	2351	2354	rBV4	33686	48759	1.22%	0.145%
60	16.470	2398	2403	2418	rVB7	62488	193923	4.84%	0.576%

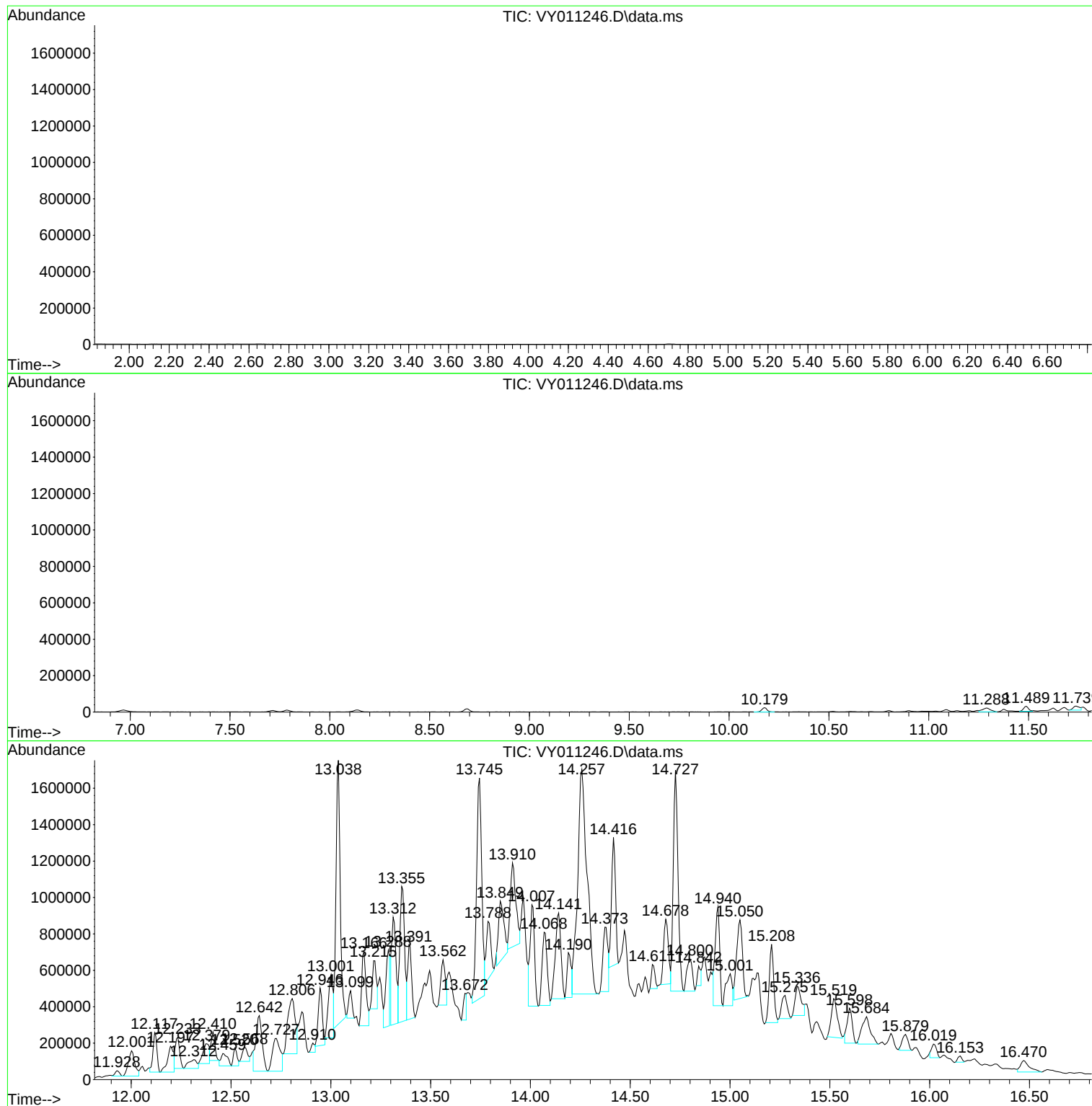
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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SB-02-11.5-12.0

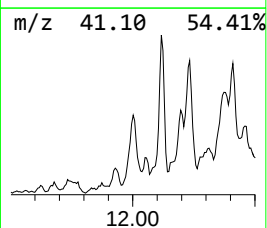
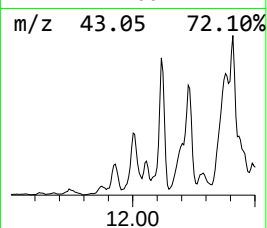
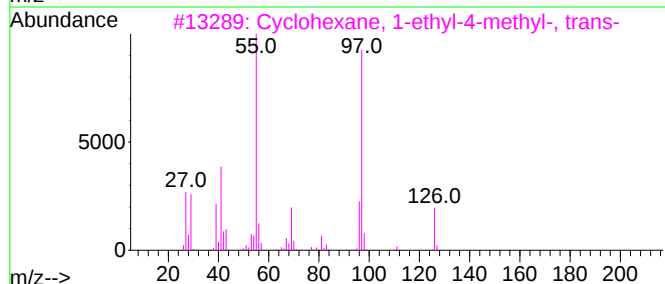
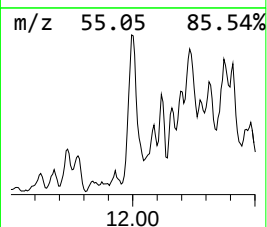
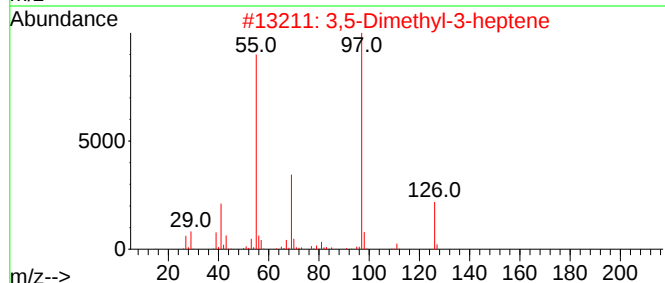
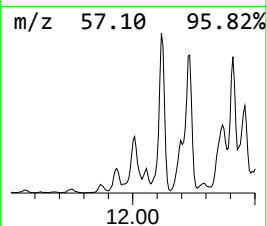
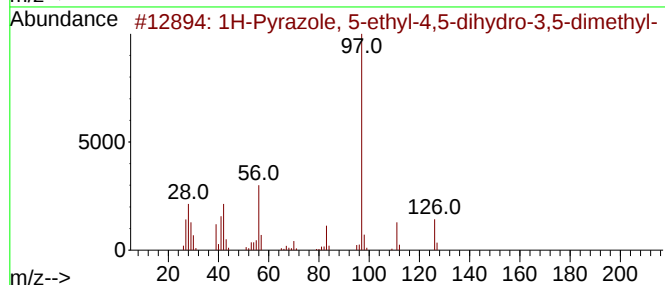
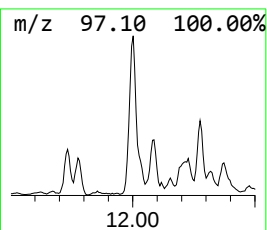
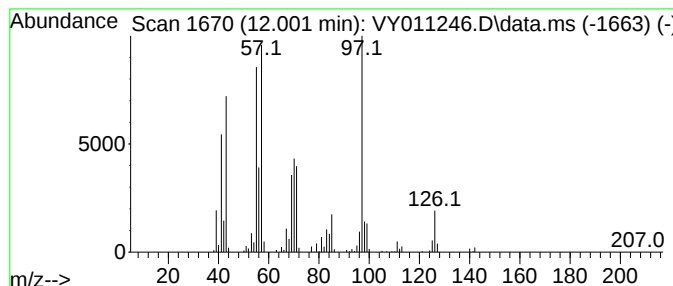
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.002 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.002	330.28 ug/l	313396	Chlorobenzene-d5	11.489

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	46
2		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	38
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	38
4		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	38
5		1-Heptene, 3-methyl-	112	C8H16	004810-09-7	35



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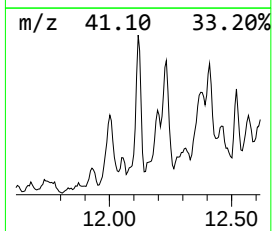
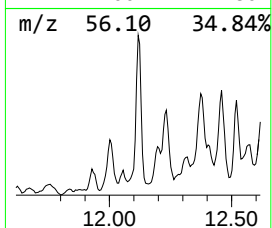
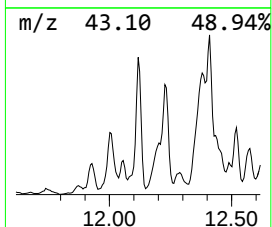
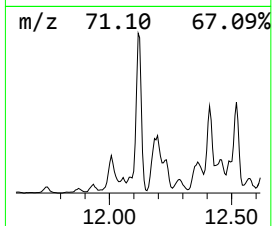
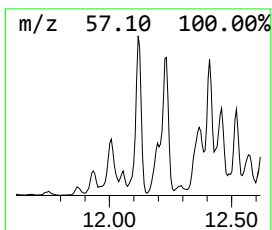
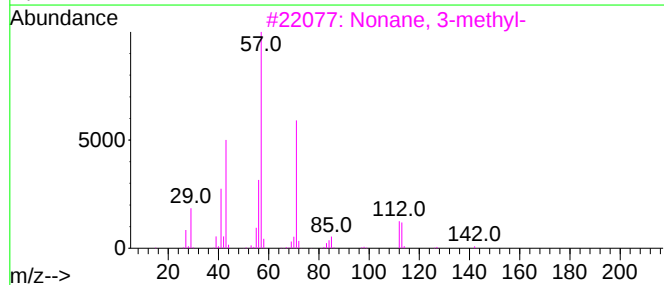
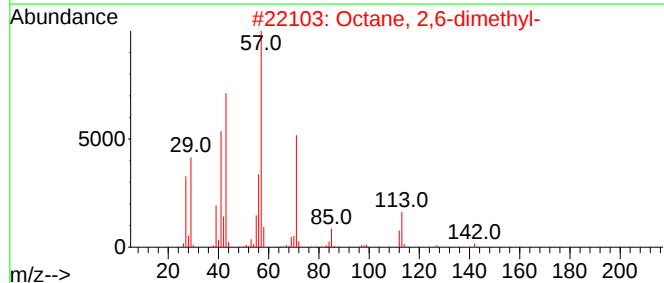
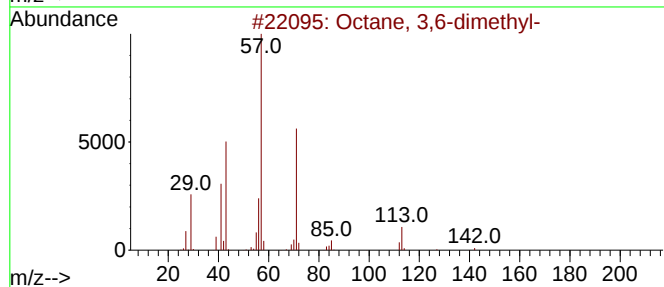
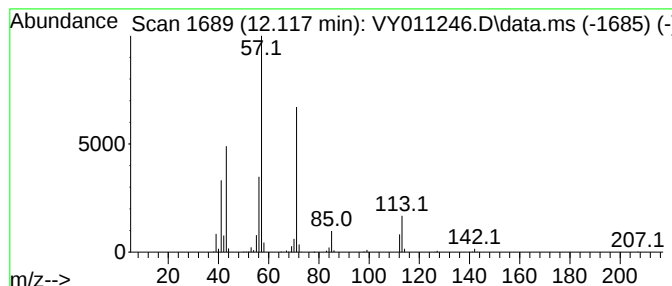
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 3,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.117	309.50 ug/l	293680	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	90
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	59
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	53



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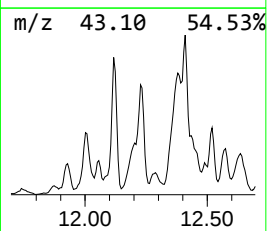
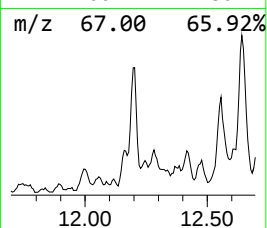
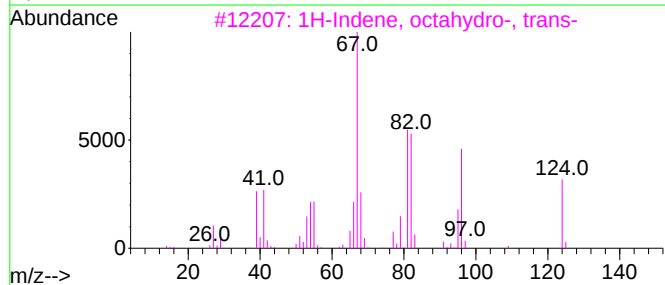
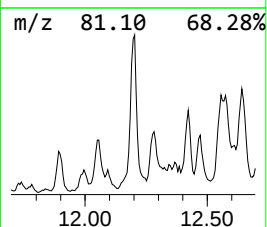
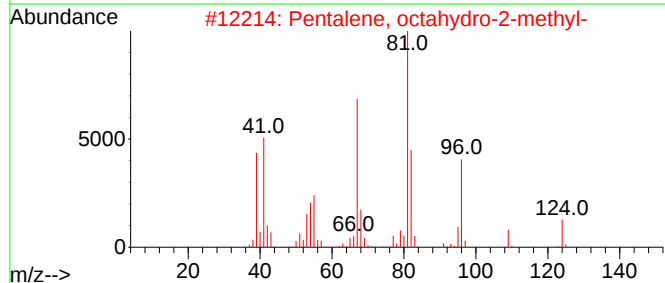
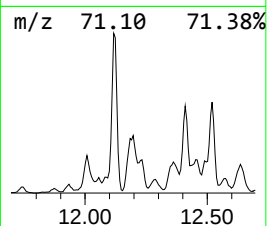
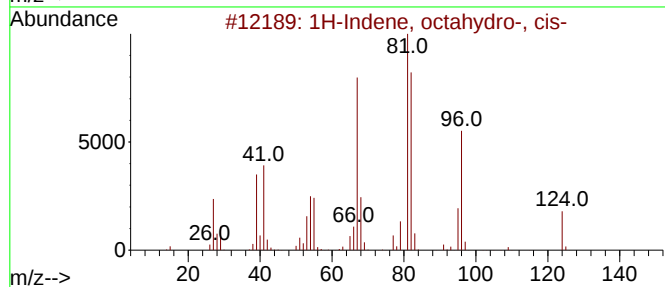
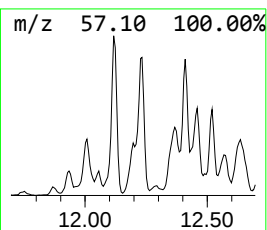
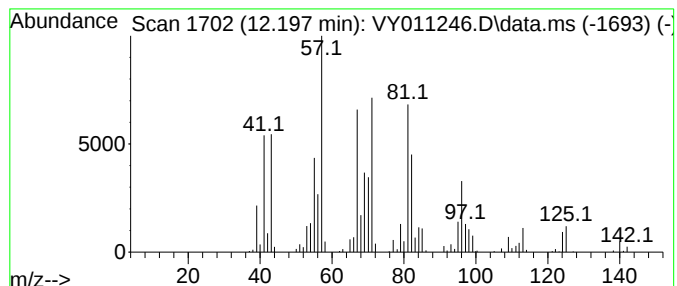
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Indene, octahydro-, cis- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.197	324.39 ug/l	307804	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	90
2			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	70
3			1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
4			Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	49
5			Butanoic acid, 3-hexenyl ester, ...	170	C10H18O2	016491-36-4	47



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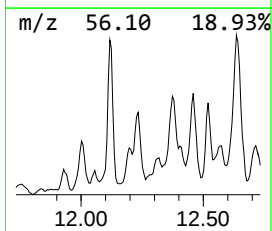
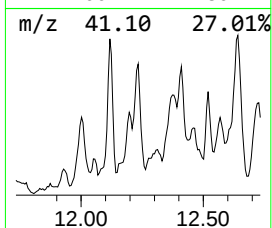
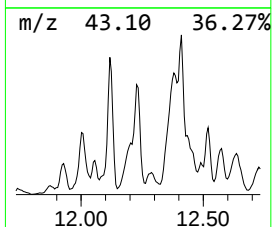
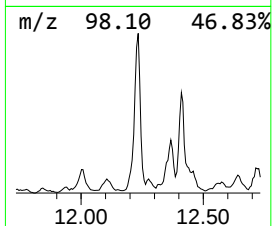
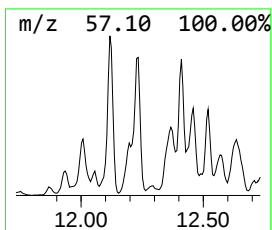
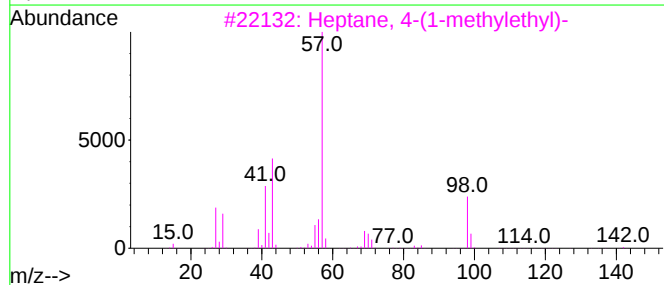
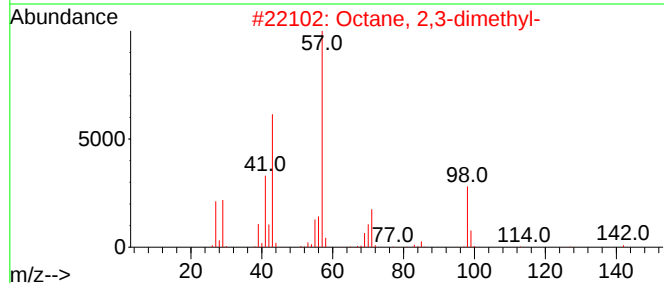
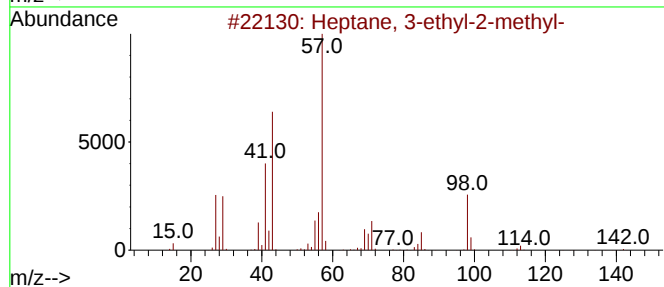
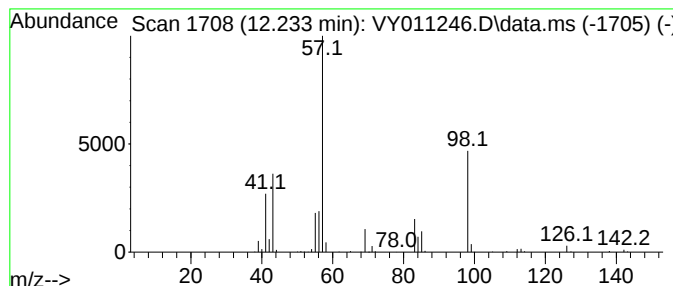
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Quant Title : SW846 8260

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Peak Number 4 Heptane, 3-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	263.92 ug/l	250425	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	80
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
3			Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	59
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	42
5			4-Octylcyclohexanone	210	C14H26O	1000428-94-1	38



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ClientSampleId :
SB-02-11.5-12.0

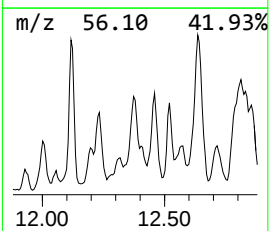
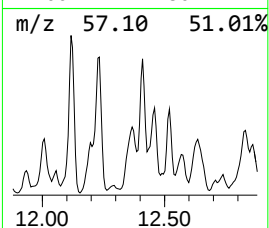
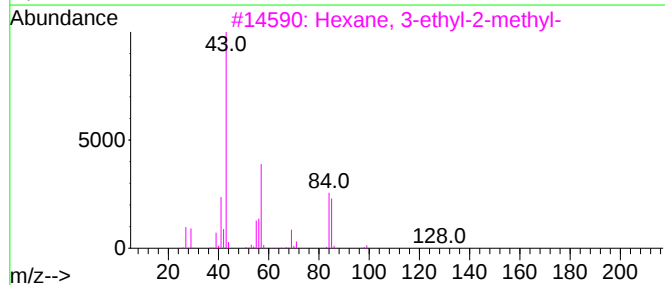
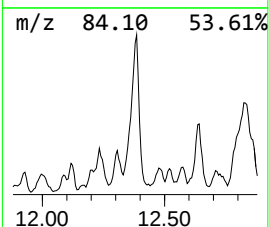
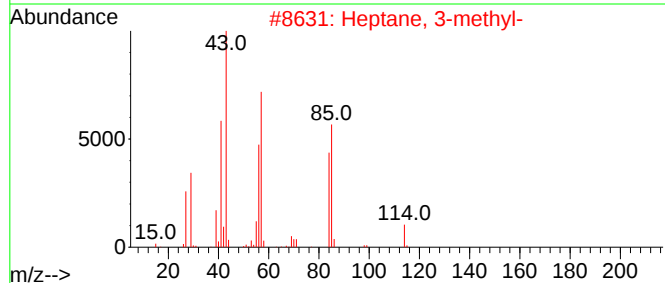
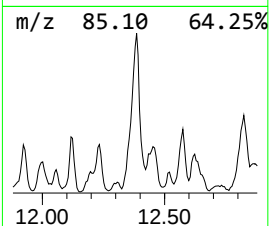
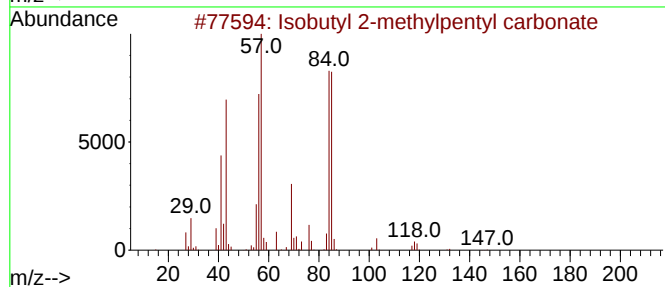
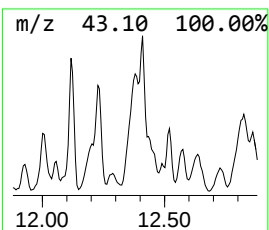
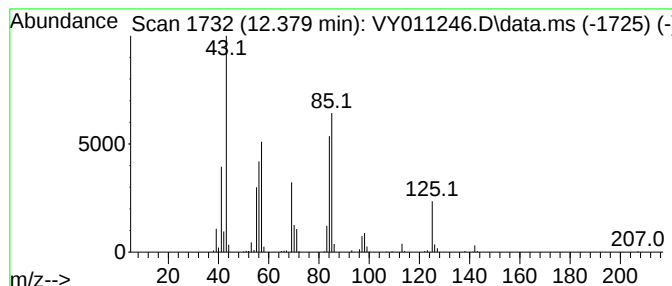
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Quant Title : SW846 8260

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

Peak Number 5 Isobutyl 2-methylpentyl car... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	253.26 ug/l	240316	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl 2-methylpentyl carbonate	202	C11H22O3	1000372-75-2	59
2			Heptane, 3-methyl-	114	C8H18	000589-81-1	47
3			Hexane, 3-ethyl-2-methyl-	128	C9H20	016789-46-1	43
4			Nonane, 5-methyl-	142	C10H22	015869-85-9	38
5			Valeric acid, 2-tetradecyl ester	298	C19H38O2	055193-14-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

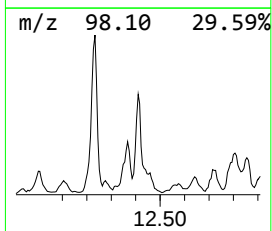
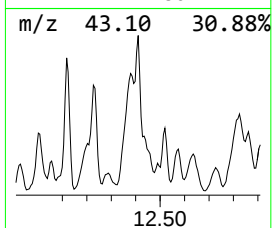
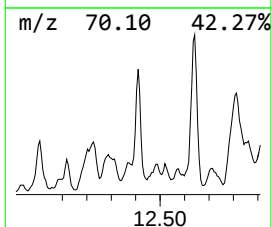
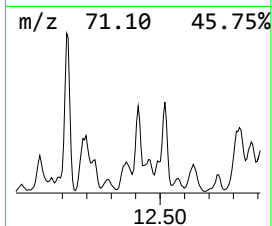
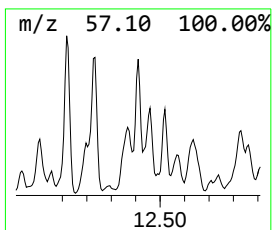
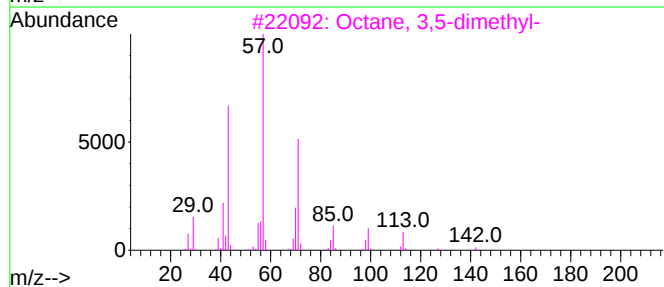
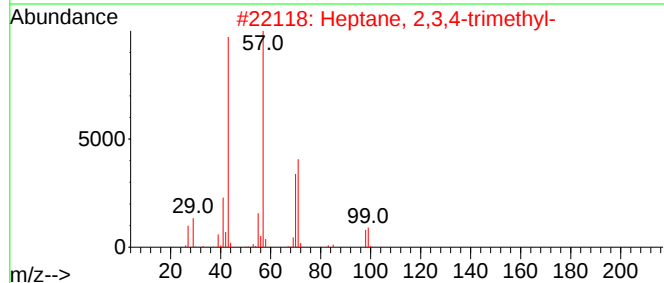
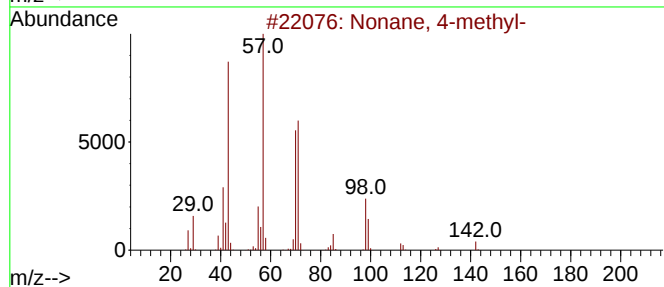
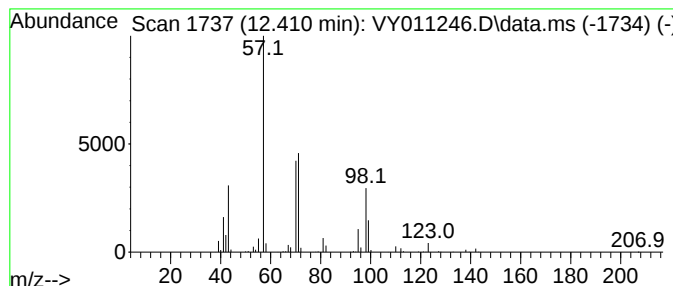
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Quant Title : SW846 8260

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

Peak Number 6 Nonane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	220.49 ug/l	209216	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2			Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	59
3			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	47
4			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	46
5			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

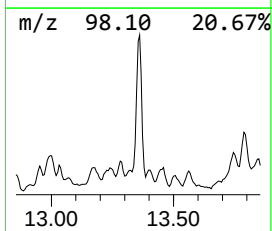
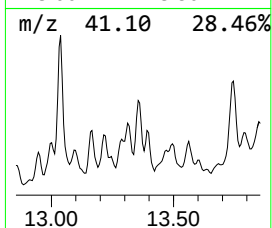
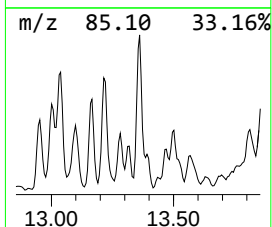
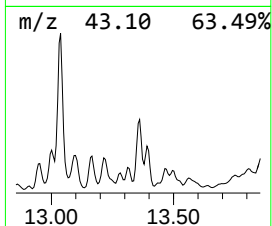
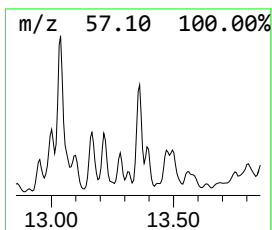
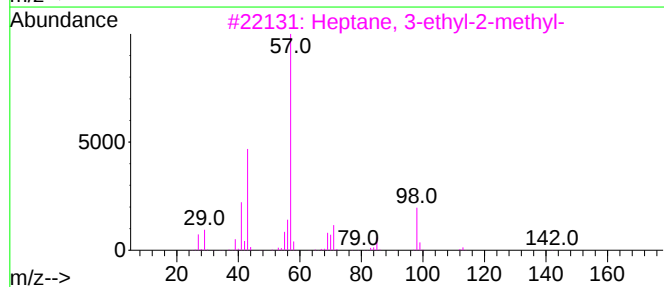
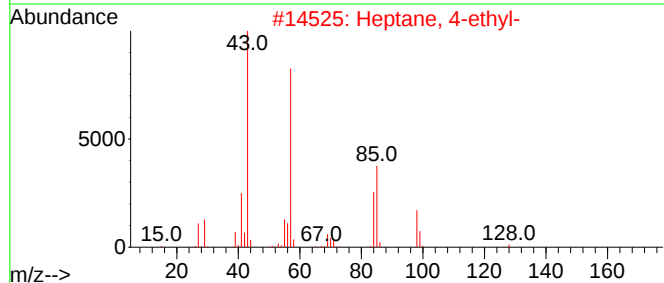
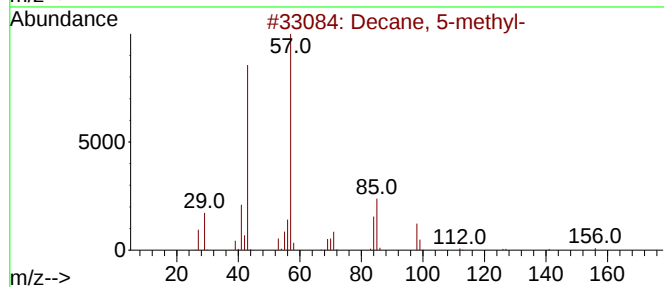
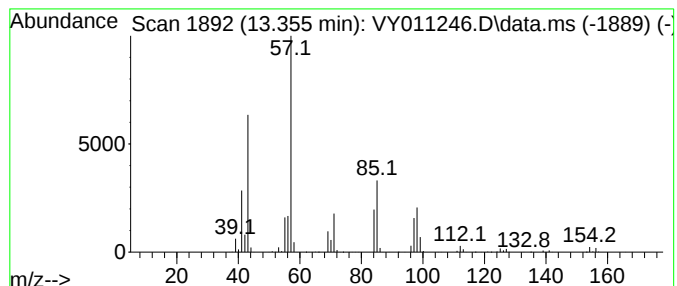
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Quant Title : SW846 8260

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

Peak Number 7 Decane, 5-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.355	112.53 ug/l	1239200	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 5-methyl-	156	C11H24	013151-35-4	87
2			Heptane, 4-ethyl-	128	C9H20	002216-32-2	53
3			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	50
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	47
5			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

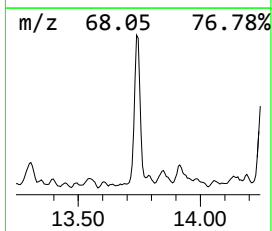
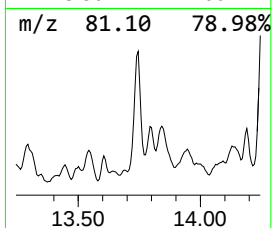
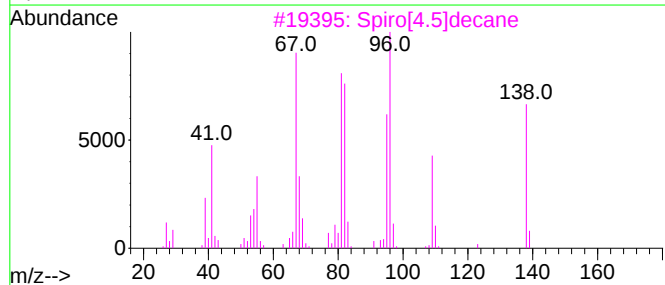
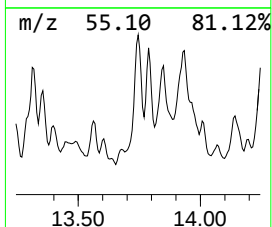
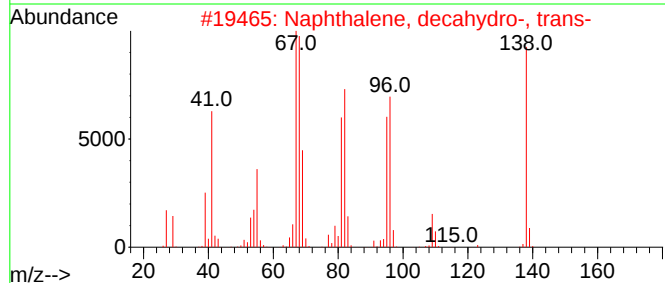
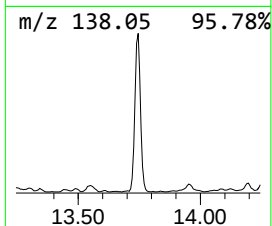
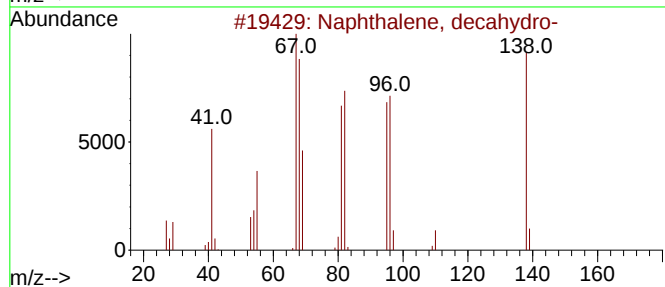
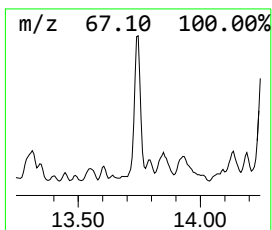
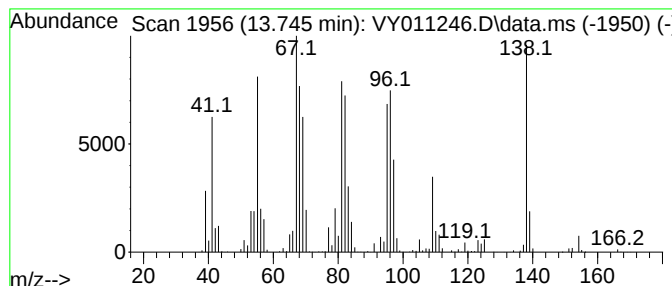
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, decahydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	201.63 ug/l	2220470	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	94
3			Spiro[4.5]decane	138	C10H18	000176-63-6	93
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	81
5			Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

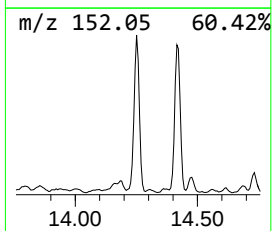
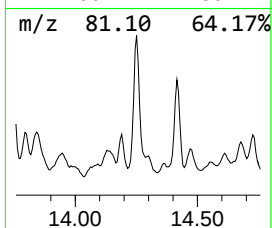
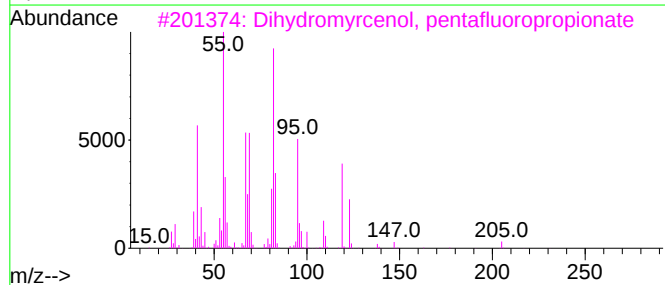
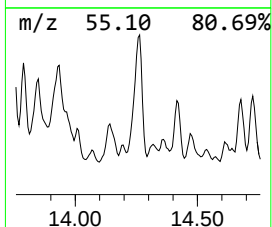
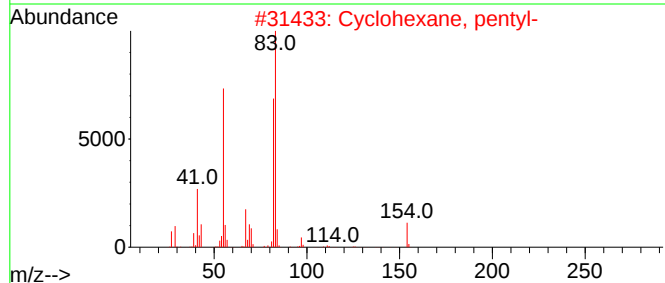
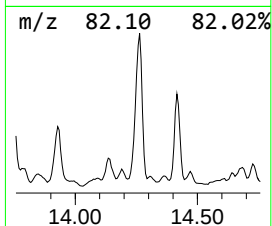
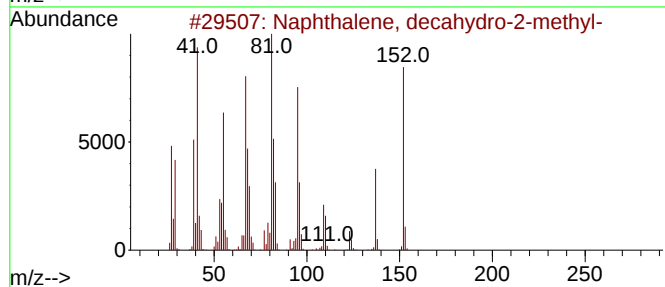
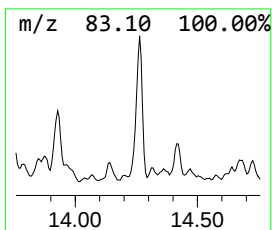
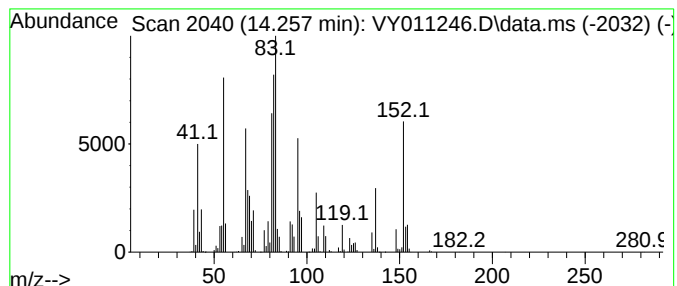
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Quant Title : SW846 8260

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

Peak Number 9 unknown14.257 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	363.80 ug/l	4006340	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	46
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	45
3			Dihydromyrcenol, pentafluoroprop...	302	C13H19F5O2	1000463-72-1	43
4			(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	43
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

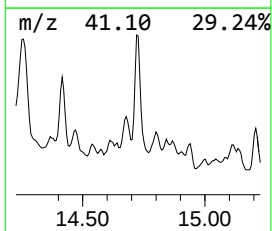
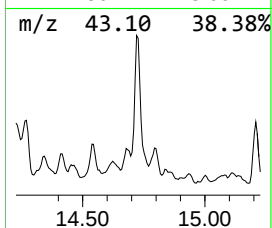
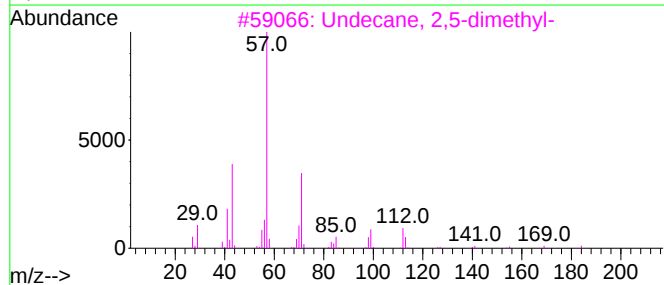
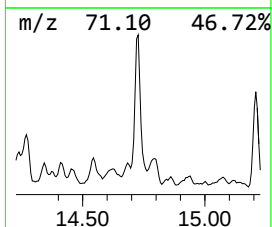
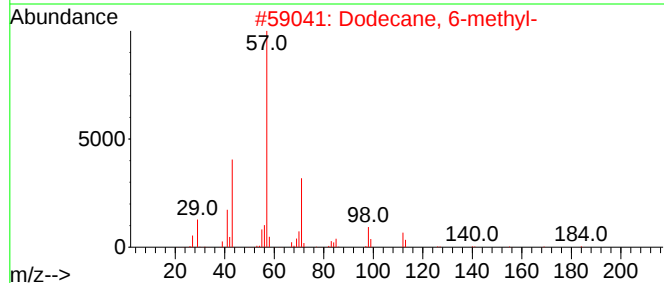
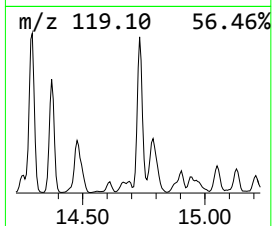
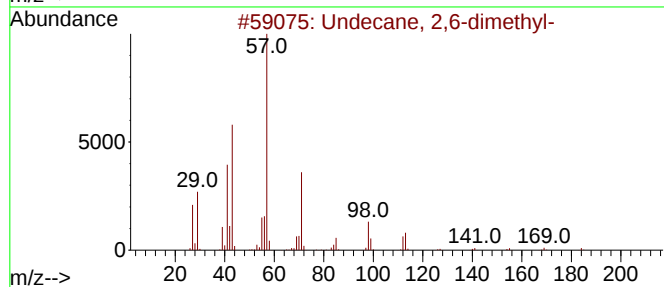
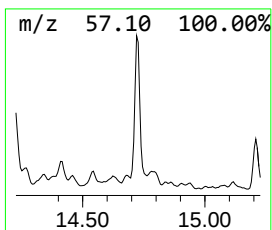
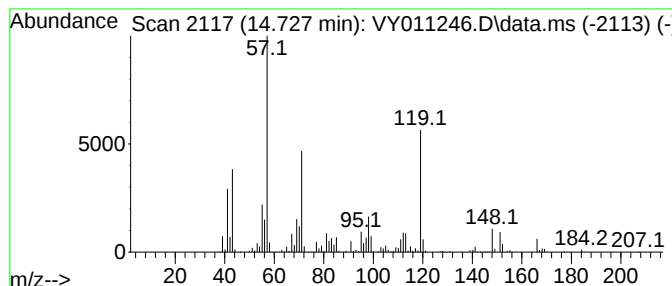
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Quant Title : SW846 8260

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

Peak Number 10 Undecane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	178.94 ug/l	1970520	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	42
3			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	38
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	38
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
Data File : VY011246.D
Acq On : 02 Nov 2022 01:54
Operator : KP/MD
Sample : N5337-03
Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02-11.5-12.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.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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1H-Indene, octa...	12.197	324.4	ug/l	307804	3	11.489	47444	50.0
Heptane, 3-ethy...	12.233	263.9	ug/l	250425	3	11.489	47444	50.0
Isobutyl 2-meth...	12.380	253.3	ug/l	240316	3	11.489	47444	50.0
Nonane, 4-methyl-	12.410	220.5	ug/l	209216	3	11.489	47444	50.0
Decane, 5-methyl-	13.355	112.5	ug/l	1239200	4	13.422	550621	50.0
Naphthalene, de...	13.745	201.6	ug/l	2220470	4	13.422	550621	50.0
unknown14.257	14.257	363.8	ug/l	4006340	4	13.422	550621	50.0
Undecane, 2,6-d...	14.727	178.9	ug/l	1970520	4	13.422	550621	50.0