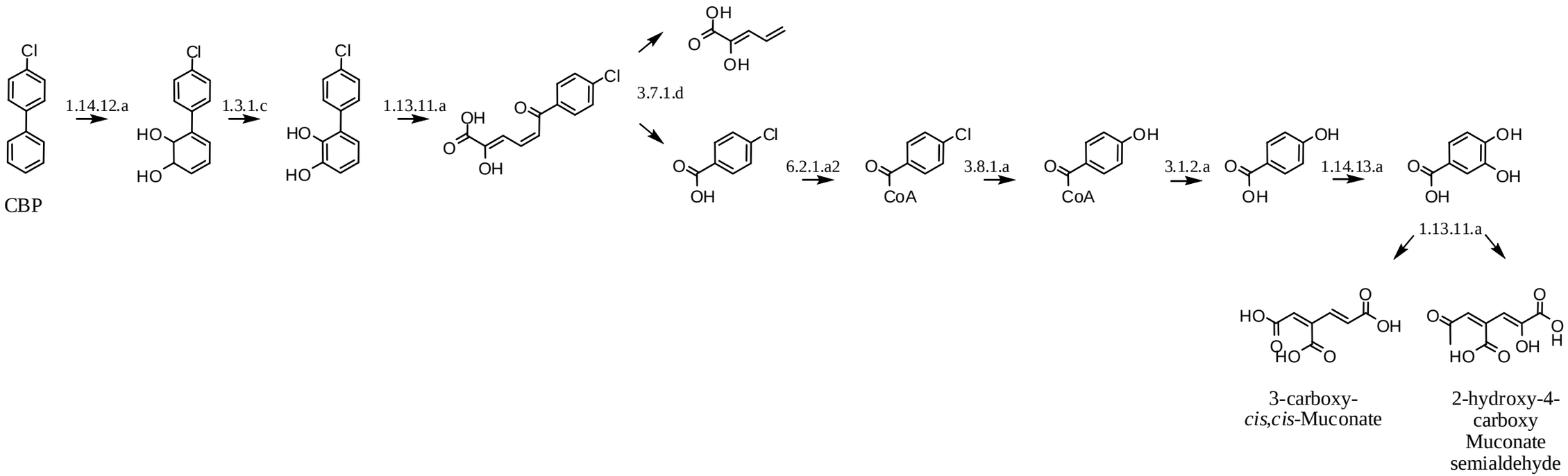
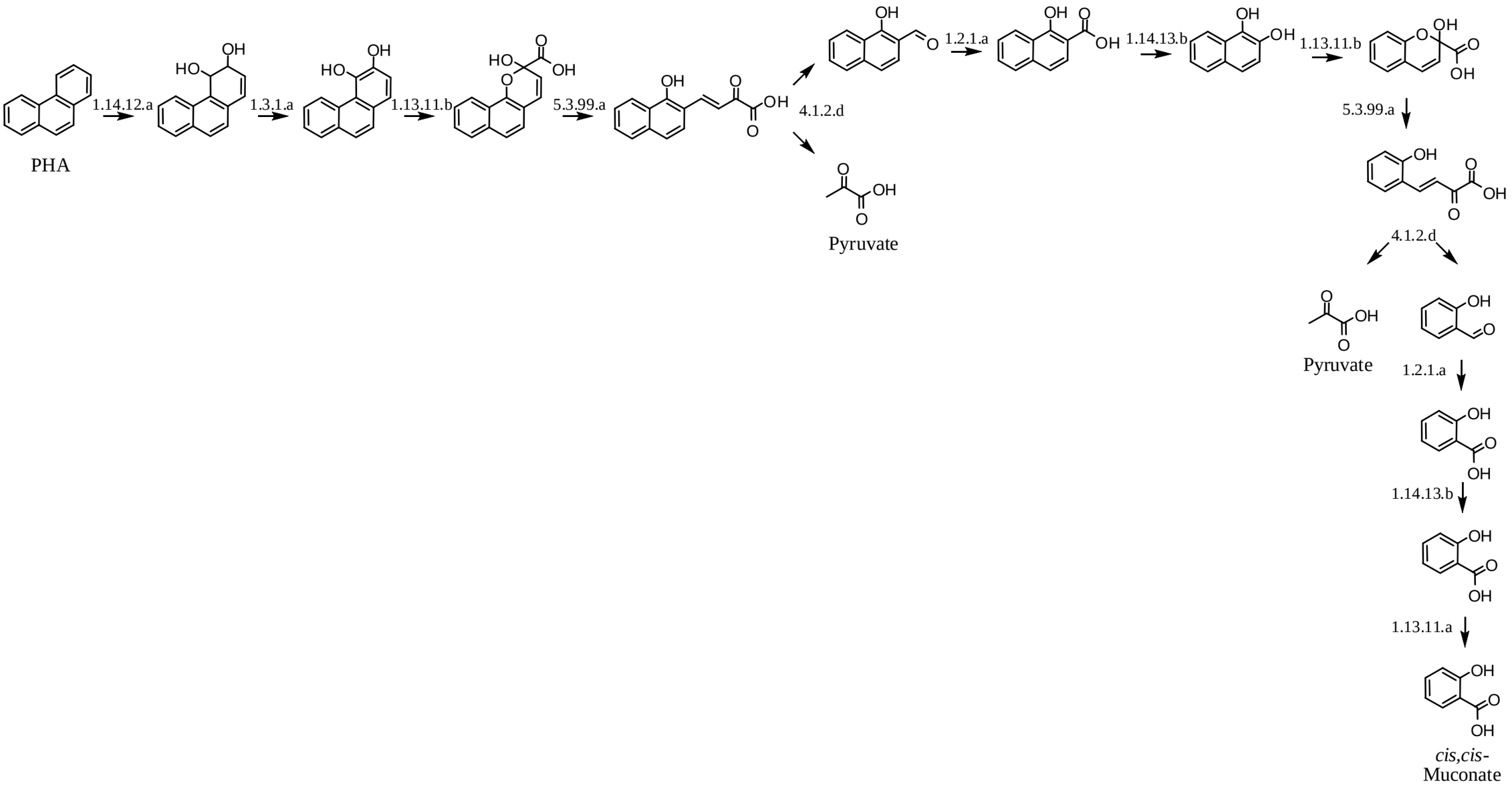
Supplementary Figure 1. Known biodegradation pathway of four xenobiotic compounds. A, 4-chlorobiphenyl (CBP); B, phenanthrene (PHE); C, γ-hexachlorocyclohexane (GHCH); D, 1,2,4-trichlorobenzene (1,2,4-TCB).

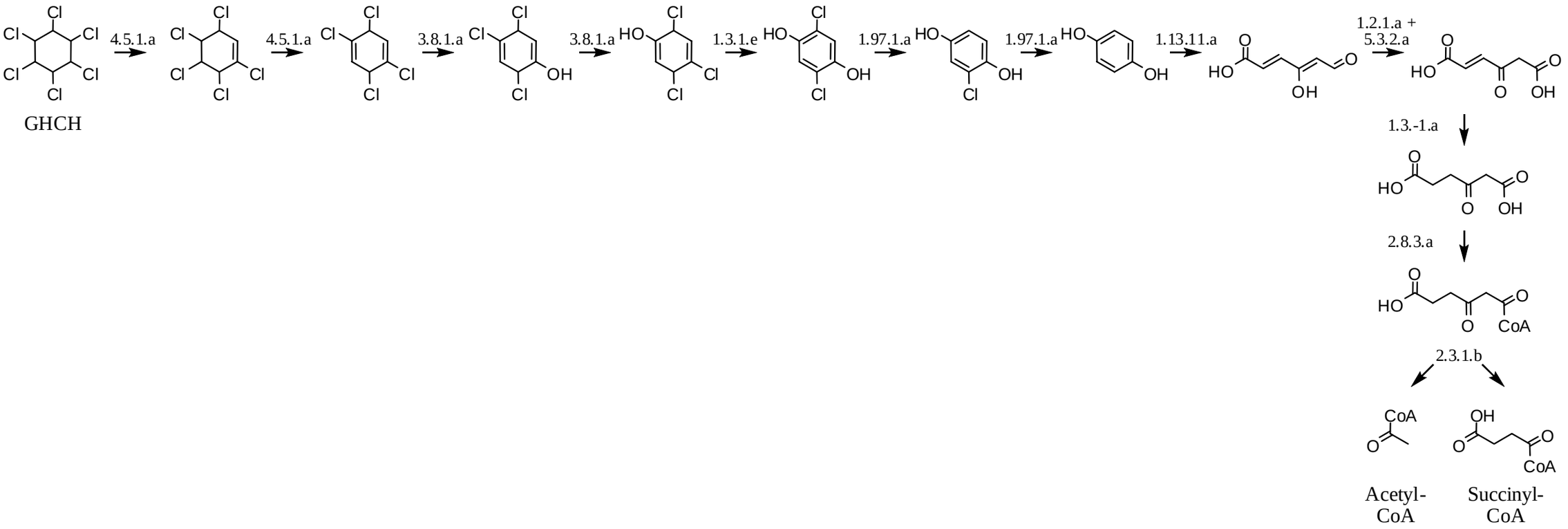
A



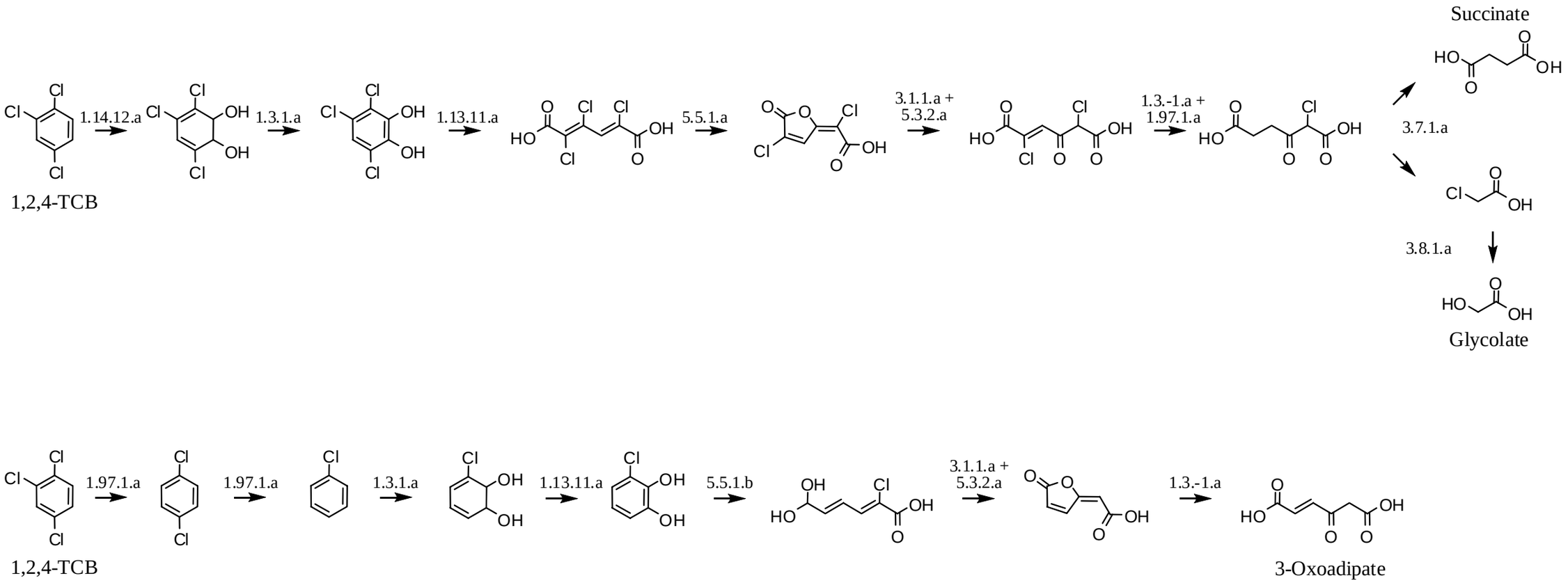
B


PHA
1.14.12.a
1.3.1.a
1.13.11.b
5.3.99.a
4.1.2.d
Pyruvate
1.2.1.a
1.14.13.b
1.13.11.b
5.3.99.a
4.1.2.d
Pyruvate
1.2.1.a
1.14.13.b
1.13.11.a
cis,cis-
Muconate

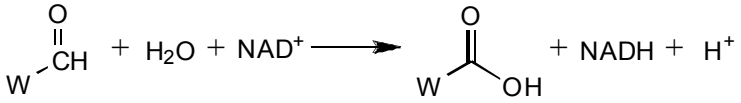
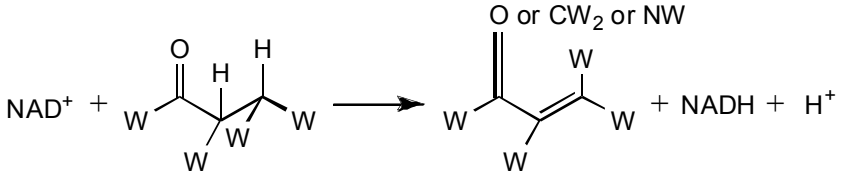
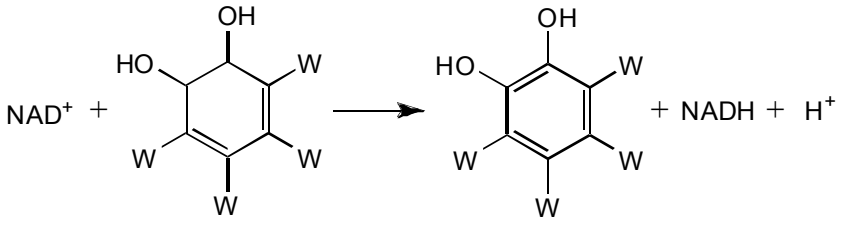
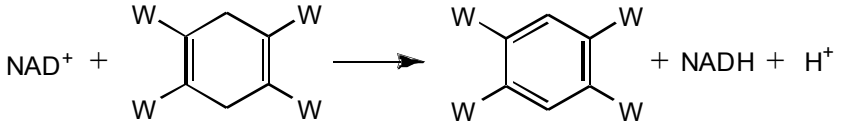
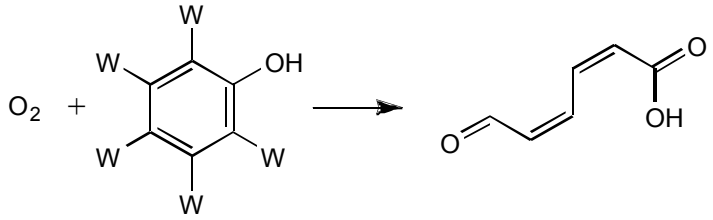
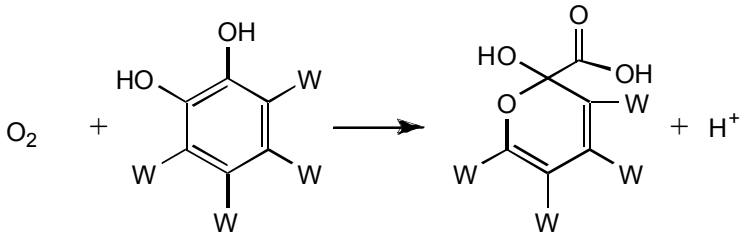
C


GHCH
4.5.1.a
4.5.1.a
3.8.1.a
3.8.1.a
1.3.1.e
1.97.1.a
1.97.1.a
1.13.11.a
1.2.1.a +
5.3.2.a
1.3.-1.a
2.8.3.a
2.3.1.b
Acetyl-
CoA
Succinyl-
CoA

D

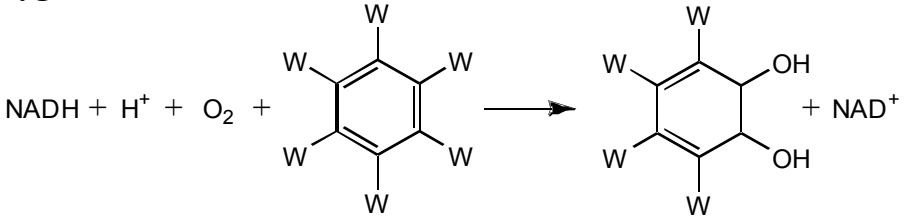

1,2,4-TCB
1.14.12.a
1.3.1.a
1.13.11.a
5.5.1.a
3.1.1.a +
5.3.2.a
1.3.-1.a +
1.97.1.a
Succinate
3.7.1.a
3.8.1.a
Glycolate
1,2,4-TCB
1.97.1.a
1.97.1.a
1.3.1.a
1.13.11.a
5.5.1.b
3.1.1.a +
5.3.2.a
1.3.-1.a
3-Oxoadipate

Supplementary Table I. Description of reaction operators.

Operator	Operator action
1.2.1: Oxidoreductases acting on the aldehyde or oxo group of donors	
1.2.1.a	 W must be carbon or hydrogen.
1.3.1: Oxidoreductases acting on the CH-CH group of donors	
1.3.1.a	 All W's can be any type of atom.
1.3.-1.a	Exact reverse of 1.3.1.a
1.3.1.c	 All W's can be any type of atom.
1.3.1.e	 W must be OH, Br, Cl, F, or I.
1.13.11: Acting on single donors with O_2 as oxidant and incorporation of two atoms of oxygen	
1.13.11.a	 W can be any type of atom.
1.13.11.b	 All W's can be any type of atom.

1.14.12: Dioxygenases with NADH or NADPH as one donor

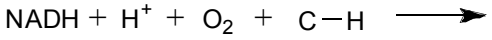
1.14.12.a



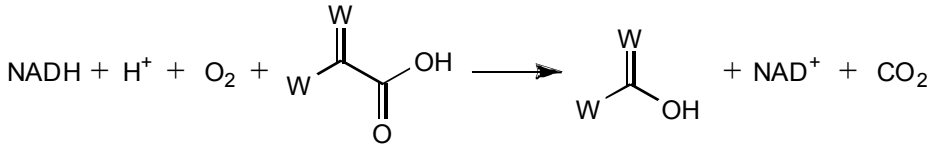
All W's can be any type of atom.

1.14.12: Monoxygenases with NADH or NADPH as one donor

1.14.13.a



1.14.13.b



All W's can be any type of atom.

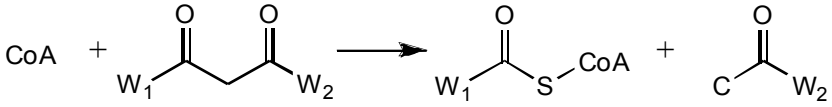
1.97.1: Oxidoreductases

1.97.1.a

W_1 = C, H, or halogen; W_2 = halogen

2.3.1: Transferring groups other than amino-acyl groups

2.3.1.b



W_1 must be carbon; W_2 = C or S.

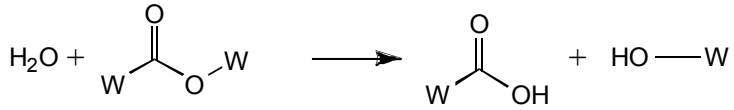
2.8.3: CoA-transferases

2.8.3.a

W must be carbon.

3.1.1: Carboxylic ester hydrolases

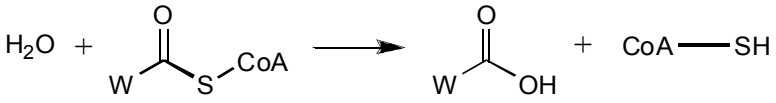
3.1.1.a



W must be carbon.

3.1.2: Thiolester hydrolases

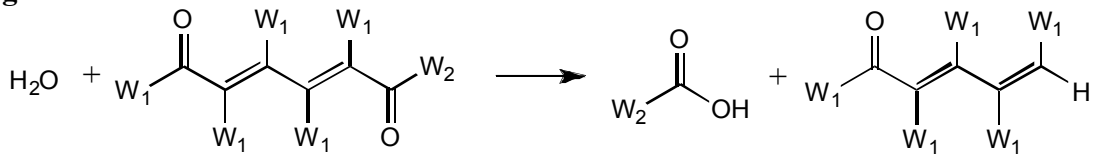
3.1.2.a



W can be any type of atom.

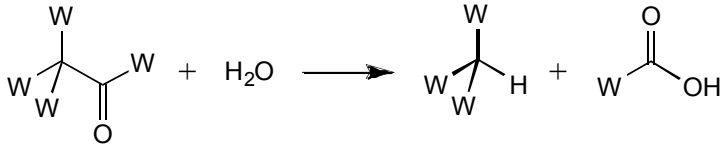
3.7.1: Acting on carbon-carbon bonds in ketonic substances

3.7.1.d



W_1 can be anything. W_2 cannot be oxygen.

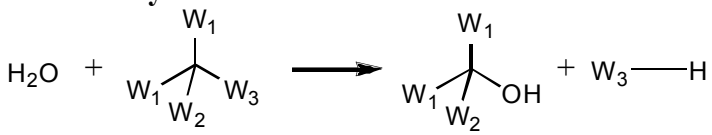
3.7.1.e



W must be carbon or nitrogen

3.8.1: Carbon-halide hydrolases

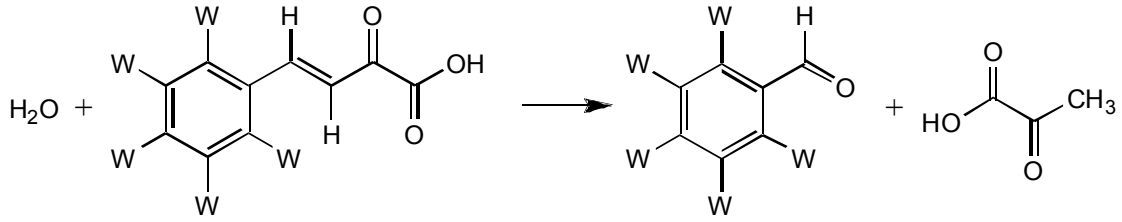
3.8.1.a



W_1 must be carbon. W_2 = C, H, or N. W_3 = halogen.

4.2.1: Carbon-oxygen hydrolyases

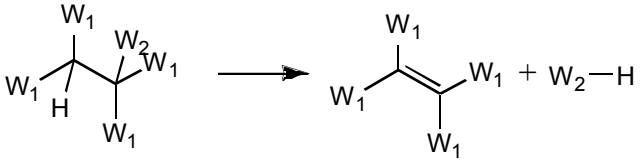
4.2.1.j



All W's can be any type of atom.

4.5.1: Carbon-halide lyases

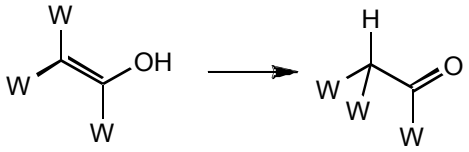
4.5.1.a



W_1 = C or halogen. W_2 must be a halogen.

5.3.2: Interconverting keto- and enol- groups

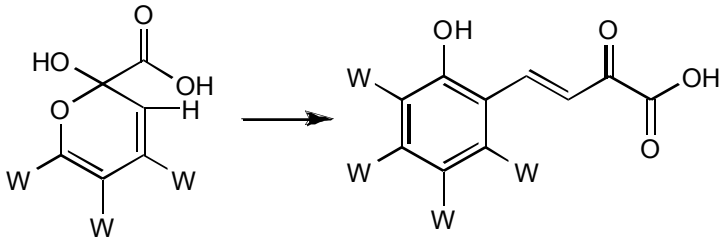
5.3.2.a



W can be anything, but the double bond must not be in an aromatic ring. This operator is spontaneous.

5.3.99: Intramolecular oxidoreductases

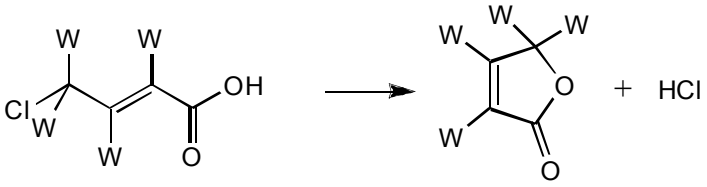
5.3.99.a



W can be any type of atom.

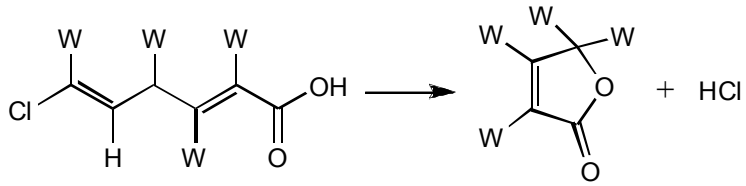
5.5.1: Intramolecular lyases

5.5.1.a



W can be any type of atom.

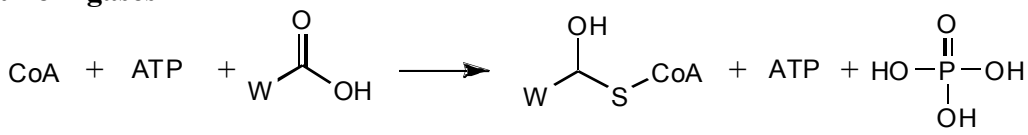
5.5.1.b



W can be any type of atom.

6.2.1: Acid-thiol ligases

6.2.1.a



W can be any type of atom.