

Concatenated
Features

Input
Features

x_1

\vdots

x_n

Molecule
Embedding

x_1

\vdots

x_8

x_1

\vdots

x_8

Isotopologue
Embedding

Hidden Layers (256 \rightarrow 128)

a_1

a_2

a_3

a_4

\vdots

a_{256}

a_1

a_2

a_3

\vdots

a_{128}

Isotopologue-Specific
Corrections

b_1

\vdots

b_{64}

\vdots

($n = 12$)

b_1

\vdots

b_{64}

y_1

y_n