

Supporting Information (S1)

1. Characteristic RDM patterns
2. Frequently observed unique RDM patterns

RDM pattern with a single atomic region is represented as follows.

R1-R2:D1-D2:M1-M2

RDM pattern with multiple atomic regions is represented as follows.

R1-R2:D1-D2:M1-M2_R1-R2:D1-D2:M1-M2

or R1 R2:D1-D2:M1-M2_R1-R2:D1-D2:M1-M2_R1-R2:D1-D2:M1-M2

1. Characteristic RDM patterns

1-1. Carbohydrate metabolism

C1a-C1b:*-C1c:C5a-C5a

C1b-C1a:C6a-*:C5a-C5a

C1b-C1y:*-C1y:C5a+O1a-C1z+O1a_C5a-C1z:*-O2x:C1b+C1b+O5a-C1b+C1y+O1a

C1b-C2a:C6a-*:C5a-C2c_O5a-O2b:*-P1b:C5a-C2c

C1c-C1c:*-*:C1c+C5a+O1a-C1c+C5a+O1a

C1c-C5a:*-*:C1b+C1c+O1a-C1b+C1c+O5a

C1y-C5x:*-*:C1y+C1y+O1a-C1y+C1y+O5x

C2a-C1b:*-C6a:C2c-C5a_O2b-O5a:P1b-*:C2c-C5a

C5a-C1c:*-*:C1b+C1c+O5a-C1b+C1c+O1a

C5a-C1d:*-C1b:C1b+C6a+O5a-C1b+C6a+O1a

C5x-C1y:*-*:C1y+C1y+O5x-C1y+C1y+O1a

N1a-N1b:*-C5a:C1y-C1y

O1a-O2a:*-C1y:C1y-C1y

O1a-O2b:*-P1b:C1b-C1b_O2b-O1a:P1b-*:C1y-C1y

O2a-O1a:C1y-*:C1b-C1b

O2b-O1a:P1b-*:C1b-C1b_O1a-O2b:*-P1b:C1y-C1y

O7a-O6a:P1b-*:C7a-C6a

1-2. Lipid metabolism

C1a-C1b:*-O1a:C5a-C5a

C1b-C2b:*-*:C1b+C1b-C1b+C2b_C1b-C2b:*-*:C1b+C5a-C2b+C5a

C1c-C5a:*-*:C1b+C1b+O1a-C1b+C1b+O5a

C5a-C1c:*-*:C1b+C1b+O5a-C1b+C1b+O1a

C5x-C1y:*-*:C1x+C1x+O5x-C1x+C1x+O1a

O1a-O7a:*-C7a:C1c-C1c

O2b-O1c:C1b-*:P1b-P1b

O2c-O2b:P1b-C1b:P1b-P1b

O7a-O1a:C7a-*:C1c-C1c

1-3. Amino acid metabolism

C1b-C1a:C5a-*:C5a-C5a_S2a-S2a:C5a-C5a:C1b-C1b

C1b-C4a:*-*:C1b+O1a-C1b+O4a

C1b-C4a:N1a-O4a:C1b-C1b

C1c-C1b:C6a-*:C1b+N1a-C1b+N1a

C1c-C1c:*-*:C1b+C6a+N1a-C1b+C6a+N1a

C1c-C2b:N1a-*:C1b+C6a-C2b+C6a

C1c-C5a:N1a-O5a:C1b+C6a-C1b+C6a

C1c-C5a:N1a+*-*+O5a:C1b+C6a-C1b+C6a

C4a-C1b:*-*:C1b+O4a-C1b+O1a

C4a-C1b:O4a-N1a:C1b-C1b

C4a-C6a:*-O6a:C1b+O4a-C1b+O6a

C4a-C6a:*-O6a:C1c+O4a-C1c+O6a

C5a-C1c:*-*:C1b+C6a+O5a-C1b+C6a+O1a

C5a-C1c:*+O5a-N1a+*:C1b+C6a-C1b+C6a

C5a-C1c:O5a-N1a:C1b+C6a-C1b+C6a

C5a-C1c:O5a-N1a:C1c+C6a-C1c+C6a

C5a-C6a:N1a-O6a:C1b+O5a-C1b+O6a

C5a-C6a:N1b-O6a:C1b+O5a-C1b+O6a

C6a-C4a:O6a-*:C1b+O6a-C1b+O4a
C8x-C8y:*-O1a:C8x+C8x-C8x+C8x
C8x-C8y:*-O1a:C8x+C8y-C8x+C8y
N1a-N1b:*-C5a:C1b-C1b
N1a-N1b:*-C5a:C1c-C1c
N1a-N1b:*-P1b:C2c-C2c
N1b-N1a:C2c-*:C1b-C1b
N1b-N1a:C5a-*:C1b-C1b
N1b-N1a:C5a-*:C1c-C1c
O1a-O2a:*-C1a:C8y-C8y
O6a-O7a:*-C1y:C6a-C7a
O6a-O7a:*-P1b:C6a-C7a
S1a-S2a:*-C1a:C1b-C1b
S1a-S3a:*-S3a:C1b-C1b
S2a-S1a:C1b-*:C1b-C1b
S3a-S1a:S3a-*:C1b-C1b

1-4. Xenobiotics biodegradation metabolism

C1a-C1b:*-O1a:C8y-C8y
C1b-C1a:C1c-*:C5a-C5a
C1b-C4a:*-*:C8y+O1a-C8y+O4a
C1c-C4a:C1b-*:C1a+O1a-C1a+O4a
C1y-C8y:*-*:C1y+C2x+O1a-C8y+C8x+O1a_C1y-C8y:*-*:C2y+C1y+O1a-C8y+C8y+O1a
C2b-C1c:*-O1a:C2a+C2b-C1a+C1b
C2b-C2a:C5a-*:C2b-C2b
C4a-C6a:*-O6a:C8y+O4a-C8y+O6a
C6a-C5a:O6a-S2a:C8y+O6a-C8y+O5a
C8x-C4a:*+C8y-O4a+*:C8x-C2b_C8y-C6a:*+C8x-O6a+*:C8y+O1a-C2c+O6a

2. Frequently observed category-unique RDM patterns

2-1. Carbohydrate metabolism

C1a-C1b:*-C1d:C5a-C6a_C5a-C6a:S2a-O6a:C1a+O5a-C1b+O6a

C1b-C1c:*-O1a:C1c+C5a-C1c+C1c

C1b-C1y:*-O2x:C1c+O1a-C1y+O1a_O1a-O2x:* C1y:C1c-C1y

C1b-C1y:*-O2x:C1z+O1a-C1y+O1a_C1z-C1y:O2x-*:C1y+C1b+O1a-C1y+C1y+O1a_O2x-O2x:*+C1z-C1y+*:C1y+O1a-C1y+O1a

C1b-C6a:*-O6a:C1y+O1a-C1y+O6a

C1c-C1b:O1a-*:C1c+C1c-C1c+C5a

C1c-C1z:*-O2x:C1b+C1c+O1a-C1b+C1y+O1a_O1a-O2x:* C1z:C1b-C1x

C1c-C4a:C1b-*:C1c+O1a-C1c+O4a

C1c-C5a:*-*:C1a+C6a+O1a-C1a+C6a+O5a

C1y-C1b:C1y-*:C1z+O1a-C5a+O1a_C1z-C5a:O2x-*:C1b+C1y+O1a-C1b+C1b+O5a

C1y-C1b:O2x-*:C1y+O1a-C1c+O1a_O2x-O1a:C1y-*:C1y-C1c

C1y-C1b:O2x-*:C1y+O1a-C1z+O1a_C1y-C1z:*-O2x:C1y+C1y+O1a-C1y+C1b+O1a_O2x-O2x:C1y+*-*+C1z:C1y+O1a-C1y+O1a

C1y-C1y:*-*:C1y+C1y+N1b-C1y+C1y+N1b

C1y-C1y:*-*:C1y+C1y+O1a-C1y+C1y+O1a

C1y-C1y:*-*:C1y+O1a+O2x-C1y+O1a+O2x

C1y-C7x:*-*:C1y+O1a+O2x-C1y+O7x+O7x

C1z-C1c:O2x-*:C1b+C1y+O1a-C1b+C1c+O1a_O2x-O1a:C1z-*:C1x-C1b

C4a-C1c:*-C1b:C1c+O4a-C1c+O1a

C4a-C6a:*-O6a:C1a+O4a-C1a+O6a

C5a-C6a:S2a-O6a:C1a+O5a-C1a+O6a

C6a-C4a:O6a-*:C1a+O6a-C1a+O4a

C7x-C1y:*-*:C1y+O7x+O7x-C1y+O1a+O2x

O1a-O2b:*-P1b:C1b-C1b_O1a-O2b:*-P1b:C1b-C1b

O1c-O2c:*-P1b:P1b-P1b_O1c-O2c:*-P1b:P1b-P1b

O2a-O1a:C1b-*:C1y-C1y

O2a-O1a:C1y-*:C1z-C1z

2-2. Lipid metabolism

C1b-C1b:C6a+*-*+C5a:C5a-C5a

C1c-C2b:O1a-*:C1b+C1b-C1b+C2b

C1y-C1c:O2x+*-*+O1a:C1y+C1b-C1c+C1b_O2x-O1a:C1y-*:C1y-C1c

C1y-C5x:*-*:C1x+C1x+O1a-C1x+C2x+O5x

C2b-C1b:*-*:C1b+C2b-C1b+C1b_C2b-C1b:*-*:C2b+C5a-C1b+C5a

C2b-C1c:*-O1a:C1b+C2b-C1b+C1b

C2b-C1y:*-O2x:C1b+C2b-C1b+C1y_C2b-C1y:*-O2x:C2b+C1b-C1y+C1b

C2x-C1x:*-*:C2y+C5x-C1y+C5x_C2y-C1y:*-*:C1x+C1z+C2x-C1x+C1z+C1x

C5x-C1y:*-*:C1x+C1z+O5x-C1x+C1z+O1a

2-3. Amino acid metabolism

C1b-C4a:N1a-O4a:C6a-C6a

C1c-C5a:C6a-O5a:C1b+N1a-C1b+N1a

C1x-C2x:*-*:C1x+N1x-C1x+N2x_N1x-N2x:*-*:C1x+C1y-C2x+C1y

C2c-C2c:N1b-N1b:N1a+N2a-N1a+N2a

C7a-C4a:O7a-*:C1b+O7a-C1b+O4a

N1a-N1b:*-C1c:C1b-C1b

N1a-N1b:*-C2c:C1b-C1b

N1b-N1a:P1b-*:C2c-C2c

S0-S2a:C1b-*:C1a+C1b-C1a+C1b

S1a-S2a:*-C1b:C1b-C1b

2-4. Xenobiotics biodegradation metabolism

C1y-C1y:O2x+*-*+S2a:C2x+C1y-C2x+C1y_O2x-O1a:C1y-*:C1y-C1y

C2b-C1a:C2b-*:C5a-C5a

C6a-C4a:O6a-*:C8y+O6a-C8y+O4a

C8x-C1y:*-O1a:C8x+C8x-C1y+C2x_C8x-C1y:*-O1a:C8x+C8y-C1y+C2y

C8x-C1y:*-O1a:C8x+C8y-C2x+C1z_C8y-C1z:*-O1a:C6a+C8x+C8x-C6a+C1y+C2x

C8y-C8x:X-*:C8y+C8x-C8y+C8x