Supplementary Information. Matlab code of the mathematical model.

The Ratio of Acetate-to-Glucose Oxidation in Astrocytes from a Single ^{13}C NMR Spectrum of Cerebral Cortex

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Abbreviations:

aKG, alpha-ketoglutarate; CAC, citric acid cycle; GLN, glutamine; NMR, nuclear magnetic resonance

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----------------------------------------
File name: Metabolic.m
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global N data
% input the raw data (normalized or not) as:
% rawdata=[E4s E4d34 E4d45 E4q Q4s Q4d34 Q4d45 Q4q];
% for example:
rawdata = [0.106170;0.780196;0.040584;0.073050;0.127703;0.362109;0.182212;0.327976]
M=8;
Mh=M/2; Earea=0; Qarea=0;
% Normalizing the raw data
for k=1:Mh
kp=k+Mh;
Earea=Earea+rawdata(k);
Qarea=Qarea+rawdata(kp);
end;
for k=1:Mh
kp=k+Mh;
data(k)=rawdata(k)/Earea;
data(kp)=rawdata(kp)/Qarea;
end;
% calculation of the parameter a-h
N=5;
% starting values for a, b, f, g, h.
xs=[0.1 0.1 0.1 0.1 0.2];
for i=1:N
lub(i)=0.0001;
ubo(i)=0.99999999;
end;
ubo(4)=20;
ubo(5)=20;
fun=@DataDifference;
options=optimset('Jacobian','off');
[x,resnorm]=lsqnonlin(fun,xs,lub,ubo,options);
abp=x(1)+x(2);
cp=x(1)/abp-x(1);
dp=x(2)/abp-x(2);
ep=1-x(3);
% pr = computed values of a,b,c,d,e,f,g,h
pr=[x(1) x(2) cp dp ep x(3) x(4) x(5)]'
%dat=calculated data based on found a-h
dat(1) = (dp + x(4)*x(3))/(1+x(4));
dat(2) = (cp + x(4)*ep)/(1 + x(4));
dat(3) = x(2)/(1 + x(4));
dat(4) = x(1)/(1 + x(4));
```

```
dat(5) = (dp + x(5)*x(3))/(1 + x(5));
dat(6) = (cp + x(5)*ep)/(1 + x(5));
dat(7) = x(2)/(1 + x(5));
dat(8) = x(1)/(1 + x(5));
datadif=dat'-data';
for n=1:M
pdiff(n)=datadif(n)*100/data(n);
end;
%datacompare= actual data,data generated from a-h, difference, % diff
datacompare=[data' dat' datadif pdiff']
%type pr to see the found parameters
%type datacompare to see computed data using the found parameters.
```

File name: DataDifference.m

```
function [F] = nmrfit(pp)
global N data
p=abs(pp);
fact=1;
a=p(1);
b=p(2);
f=p(3);
g=p(4);
h=p(5);
c=(a/(a+b)-a);
d=(b/(a+b)-b);
e=(1-f);
g2=1+g;
h2=1+h;
F(1) = fact*[data(1)-(d + g*f)/g2];
F(2) = fact*[data(2)-(c + g*e)/g2];
F(3) = fact*[data(3)- b/g2];
F(4) = fact*[data(4)- a/g2];
F(5) = fact*[data(5)- (d + h*f)/h2];
F(6) = fact*[data(6)- (c + h*e)/h2];
F(7) = fact*[data(7)- b/h2];
F(8) = fact*[data(8)- a/h2];
if (a+b>1-.0001)
F(9)=100000;
else;
F(9)=0;
end;
```