Table S1: Weights for PRs branch with TNFα and LTs with CCL_2

PRs branch (w_{PR_i})	**Weight ($\boldsymbol{w_{PR_i}}$)** TNFα	LTs branch	**Weight ($\boldsymbol{w_{LT_i}}$)** CCL_2
w_{PGE_2}	0.25	w_{LTB_4}	0.45
$w_{PGF_{2\alpha}}$	0.27	w_{epiLTB_4}	0.32
w_{PGD_2}	0.22	w_{12LTB_4}	0.23
w_{TxB_2}	0.26		

1 Materials and Methods

The rate balance equations for all the metabolites of PRs and LTs branches are:

$$\frac{d[5-HETE]}{dt} = k_{5-HETE}[AA]e_{5-HETE}(1 + k_{ATP}[ATP]) - g_{5-HETE}[5 - HETE] \quad (1)$$

$$\frac{d[15-HETE]}{dt} = k_{15-HETE}[AA]e_{15-HETE}(1 + k_{ATP}[ATP]) - g_{15-HETE}[15 - HETE] \quad (2)$$

1.1 PRs branch

$$\frac{d[PGH_2]}{dt} = e_{PGH_2}k_{PGH_2}[AA](1 + k_{ATP}[ATP]) - g_{PGH_2}[PGH_2] - v_{PGD_2}e_{PGD_2}k_{PGD_2}[PGH_2] - v_{PGE_2}e_{PGE_2}k_{PGE_2}[PGH_2] - v_{PGF_{2\alpha}}e_{PGF_{2\alpha}}k_{PGF_{2\alpha}}[PGH_2] - v_{TXB_2}e_{TXB_2}k_{TXB_2}[PGH_2] \quad (3)$$

$$\frac{d[PGD_2]}{dt} = v_{PGD_2}e_{PGD_2}k_{PGD_2}[PGH_2] - g_{PGD_2}[PGD_2] - k_{dPGD_2}[PGD_2] - k_{PGJ_2}[PGD_2] \quad (4)$$

$$\frac{d[PGE_2]}{dt} = v_{PGE_2}e_{PGE_2}k_{PGE_2}[PGH_2] - g_{PGE_2}[PGE_2] \quad (5)$$

$$\frac{d[PGF_{2\alpha}]}{dt} = v_{PGF_{2\alpha}}e_{PGF_{2\alpha}}k_{PGF_{2\alpha}}[PGH_2] - g_{PGF_{2\alpha}}[PGF_{2\alpha}] \quad (6)$$

$$\frac{d[TxB_2]}{dt} = v_{TxB_2}e_{TxB_2}k_{TxB_2}[PGH_2] - g_{TxB_2}[TxB_2] \quad (7)$$

$$\frac{d[PGJ_2]}{dt} = k_{PGJ_2}[PGD_2] - g_{PGJ_2}[PGJ_2] - k_{dPGJ_2}[PGJ_2] \quad (8)$$

$$\frac{d[dPGJ_2]}{dt} = k_{dPGJ_2}[PGJ_2] - g_{dPGJ_2}[dPGJ_2] \quad (9)$$

$$\frac{d[dPGD_2]}{dt} = k_{dPGD_2}[PGD_2] - g_{dPGD_2}[dPGD_2] \quad (10)$$

For PRs branch, there are control variables u_{PR_i} associated with each PR_i. As an example, enzyme balance for dimensionless e_{PGD_2}, ε_{PGD_2} is Eq. (11). Similarly, for LTs branch, there are control variables u_{LT_i} corresponding to each LT_i.

$$\frac{d\varepsilon_{PGD_2}}{dt} = \beta\left(\alpha' + \frac{k'_{e_{PGD_2}}[PGH_2]u_{PGD_2}}{K_{e_{PGD_2}} + [PGH_2]}\right) - \beta\varepsilon_{PGD_2} \quad (11)$$

The control variables for enzyme synthesis u_{PR_i} are defined as

$$u_{PR_i} = \frac{\rho_{PR_i}}{\sum_{j=1}^{4}\rho_{PR_j}} \text{ for } PR_j = \{PGD_2, PGE_2, PGF_{2\alpha}, TxB_2\} \quad (12)$$

The cybernetic variable for enzyme activity v_{PR_i} is defined as

$$v_{PR_i} = \frac{\rho_{PR_i}}{\max_{j=1,2,3,4}(\rho_{PR_j})}; \ PR_j = \{PGD_2, PGE_2, PGF_{2\alpha}, TxB_2\} \quad (13)$$

1.2 LTs branch

$$\frac{d[LTA_4]}{dt} = e_{LTA_4} k_{LTA_4}[AA](1 + k_{ATP}[ATP]) - g_{LTA_4}[LTA_4] - \sum_{i=1}^{3} v_{LT_i} e_{LT_i} k_{LT_i}[LTA_4], \quad \text{for } LT_i = \{LTB_4, \ 12LTB_4, \ 6tLTB_4\} \quad (14)$$

The cybernetic control variable for a LT, LT_i, is v_{LT_i}. e_{LT_i} is the relevant enzyme level and g_{LTA_4} is the degradation rate of LTA_4. k_{LT_i} is the rate constant of the product LT_i. Eq. (15) is the detailed version of Eq. (14).

$$\frac{d[LTA_4]}{dt} = e_{LTA_4} k_{LTA_4}[AA](1 + k_{ATP}[ATP]) - g_{LTA_4}[LTA_4] - v_{LTB_4} e_{LTB_4} k_{LTB_4}[LTA_4] - v_{12LTB_4} e_{12LTB_4} k_{12LTB_4}[LTA_4] - v_{6tLTB_4} e_{6tLTB_4} k_{6tLTB_4}[LTA_4] \quad (15)$$

The kinetic equation for an LT, LT_i is Eq. (16) . There are no further conversions of LTs, making the downstream fluxes zero (Fig. 1).

$$\frac{d[LT_i]}{dt} = v_{LT_i} e_{LT_i} k_{LT_i}[LTA_4] - g_{LT_i}[LT_i] \quad \text{for } LT_i = \{LTB_4, 6tLTB_4, 12LTB_4\} \quad (16)$$

$$\frac{d[LTB_4]}{dt} = v_{LTB_4} e_{LTB_4} k_{LTB_4}[LTA_4] - g_{LTB_4}[LTB_4] \quad (17)$$

$$\frac{d[6tLTB_4]}{dt} = v_{6tLTB_4} e_{6tLTB_4} k_{6tLTB_4}[LTA_4] - g_{6tLTB_4}[6tLTB_4] \quad (18)$$

$$\frac{d[12LTB_4]}{dt} = v_{12LTB_4} e_{12LTB_4} k_{12LTB_4}[LTA_4] - g_{12LTB_4}[12LTB_4] \quad (19)$$

The control variables for enzyme synthesis u_{LT_i} are defined as

$$u_{LT_i} = \frac{\rho_{LT_i}}{\sum_{j=1}^{3} \rho_{LT_j}} \text{ for } LT_j = \{LTB_4, 6tLTB_4, 12LTB_4\} \quad (20)$$

The cybernetic variable for enzyme activity v_{PR_i} is defined as

$$v_{LT_i} = \frac{\rho_{LT_i}}{\max_{j=1,2,3}(\rho_{LT_j})}; \ LT_j = \{LTB_4, 6tLTB_4, 12LTB_4\} \quad (21)$$

2 RSTE

The AA network is a well-characterized network where the causality between any two metabolites is known. For instance, AA (cause) leads to downstream production of metabolites PGD_2, PGE_2, $PGF_{2\alpha}$,TxB_2 (effect). To determine the hyperparameters, we run simulations for $m =$

$\{1, 2, 3, \ldots, 10\}$, $q = \{0.1, 0.25, 0.4, \ldots, 3\}$, and $\tau = \{1, 2, 3, \ldots, 50\}$, and predict the causality for any two metabolites. We choose the m, τ and q combination for which the RSTE model best captures causality for the AA network. The RSTE model developed using the optimized hyperparameters is representative of the AA network causality. We predict causality between AA and the cytokine TNFα as well as AA and the chemokine CCL_2 using the same hyperparameters.

Table S2: RSTE values for AA network and AA, TNFα (and CCL_2) combination

Connections ($m = 3,\ q = 0.85,\ \tau = 13$)	**RSTE**
AA_PGD_2 − PGD_2_AA	0.00162
AA_PGF_{2a} − PGF_{2a}_AA	-0.01007
AA_TxB_2 − TxB_2_AA	0.0156
AA_15ddPGD$_2$ −15ddPGD$_2$_AA	0.0301
AA_PGJ_2 − PGJ_2_AA	0.0224
AA_15ddPGJ$_2$ −15ddPGJ$_2$_AA	0.028
AA_ketPGD$_2$ − ketPGD$_2$_AA	0.037
AA_LTB_4 − LTB_4_AA	0.031
AA_epiL − epiL_AA	0.09
AA_transL − transL_AA	0.014
AA_HETE5 − HETE5_AA	-0.025
AA_HETE15 − HETE15_AA	-0.005
PGD$_2$_15ddPGD$_2$ −15ddPGD$_2$_PGD$_2$	0.0014
PGD$_2$_PGJ_2 − PGJ_2_PGD$_2$	0.025
PGD$_2$_15ddPGJ$_2$ −15ddPGJ$_2$_PGD$_2$	0.033
PGD$_2$_ketPGD$_2$ − ketPGD$_2$_PGD$_2$	0.008
PGJ$_2$_15ddPGJ$_2$ −15ddPGJ$_2$_PGJ$_2$	-0.015
AA_TNFα − TNFα_AA	0.0002
AA_CCL_2 − CCL_2_AA	0.0004

Table S3 Calculated kinetic parameters for the COX pathway. The columns represent parameters calculated for the cybernetic model. The parameters are estimated using the simulation strategy discussed in the paper.

Parameter	Values	Parameter	Values	Parameter	Values	Parameter	Values
k_{PGE_2}	0.0062	$k'_{e_{PGE_2}}$	0.8778	$LTA4_{K_0}$	0.0005	$k_{eHETE15}$	0.6863
$k_{PGF_{2\alpha}}$	0.0018	$k'_{e_{PGF_{2\alpha}}}$	0.3786	$e_{LTB4_{K_0}}$	0.5566	$K_{m_{LK}}$	0.0135
k_{TxB_2}	0.0103	$k'_{e_{TxB_2}}$	0.4835	$e_{epiL_{K_0}}$	0.7405	β	0.8909
k_{dPGD_2}	0.0520	$e_{PGH2_{K_0}}$	0.8286	$e_{transL_{K_0}}$	0.7306		
k_{PGJ_2}	0.0207	$e_{PGD2_{K_0}}$	0.1651	$e_{LTA_{4_{K_0}}}$	0.7975		
k_{dPGJ_2}	0.0388	$e_{PGE2_{K_0}}$	0.1622	$e_{HETE15_{K_0}}$	0.6656		
g_{PGH_2}	0.4186	$e_{PGF2\alpha_{K_0}}$	0.7993	k'_{eLTB_4}	0.4317		
g_{PGD_2}	0.0045	$e_{TxB2_{K_0}}$	0.5614	k'_{eepiL}	0.2715		
g_{PGE_2}	1.32E-06	k_{LTB_4}	4.9256	$k'_{etransL}$	0.3207		
$g_{PGF_{2\alpha}}$	7.11E-07	k_{epiL}	4.4478	k'_{eLTA_4}	0.5733		
g_{TxB_2}	7.12E-07	k_{transL}	4.4778	$LTA4_0$	0.0010		
g_{dPGD_2}	7.07E-07	k_{LTA_4}	0.0002	$LTA4_{K_0}$	0.0005		
g_{PGJ_2}	7.10E-07	k_{HETE5}	0.0005	$e_{LTB4_{K_0}}$	0.5566		
g_{dPGJ_2}	0.1032	k_{HETE15}	0.0001	$e_{epiL_{K_0}}$	0.7405		
$PGH2_0$	0.0074	g_{LTB_4}	0.8706	$e_{transL_{K_0}}$	0.7306		
$PGH2_{K_0}$	0.9999	g_{epiL}	0.4394	$e_{LTA4_{K_0}}$	0.7975		
k_{ATP}	4.9991	g_{transL}	0.7316	$e_{HETE15_{K_0}}$	0.6656		
K_{mAA}	48.0240	g_{LTA_4}	0.3299				

3 Development of Mutual information formulation for time series

In what follows, we briefly describe our approach for formulating mutual information for bivariate time series.

Note that Shannon's mutual information $I(X;Y)$, Eq. (10) can be written in terms of expectation as follows

$$I(X;Y) = \mathbb{E}_p[\lambda(x_i,y_j)] \quad ; \quad \lambda(x_i,y_j) = \log p(x_i,y_j) - \log p(x_i) - \log p(y_j) \qquad (22)$$

where $\mathbb{E}_p[.]$ denotes the expectation operator. $I(X;Y)$ is the expectation of the difference between the log likelihood of two variables $\log p(x_i,y_j)$ and single variable $\log p(x_i)$, $\log p(y_j)$ with respect to the joint probability distribution $p(x_i,y_j)$. Galka et al. [1] redefined $\lambda(x_i,y_j)$ in Eq. (22) by pairing the time points as

$$\lambda(\vec{X}_t,\vec{Y}_t) = \log\left(p_{xy}\left((x_1,y_1),(x_2,y_2),\dots,(x_N,y_{N_t})\right)\right) - \log p_x(x_1,x_2,\dots,x_{N_t}) - \log p_y(y_1,\dots,y_{N_t})$$

(23)

The short-hand notation for Eq. 23 is $\lambda(\vec{X}_t, \vec{Y}_t) = L(\vec{X}_t, \vec{Y}_t) - L(\vec{X}_t) - L(\vec{Y}_t)$ where $L(.)$ denotes the log-likelihood operation. Eq. 23 involves estimating high-dimensional joint probability densities; evaluating them is computationally expensive due to the intra and inter-temporal correlations. To overcome this obstacle, Galka et al. [1] suggest formulating them in terms of probability densities of the corresponding innovation series [1]. The authors recommend describing the temporal correlations by a time series prediction model. This model makes future time predictions using past time points, ensuring that the system follows causality. Conventionally, the vector autoregressive (VAR) model for a two-dimension time series ($z_t^{(1)}$) and ($z_t^{(2)}$) is used to capture the data's inter and intra-temporal correlations based on causality [2]. The VAR model has a hyperparameter p that denotes the temporal dependency to the past time points. More precisely, this model entails the target variable ($z_t^{(1)}$) which equals to a weighted linear combination of its p past values and p past values of the other time series, an error term series (e_t) and a constant μ, as shown in Eq. 24 and Eq. 25.

$$z_t^{(1)} = \sum_{k=1}^{p} \alpha_k^{(1)} z_{t-k}^{(1)} + \sum_{i=1}^{p} \beta_k^{(1)} z_{t-k}^{(2)} + e_t + \mu^{(1)}; \qquad z_t^{(1)} - \hat{z}_t^{(1)} = e_t \tag{24}$$

$$z_t^{(2)} = \sum_{k=1}^{p} \alpha_k^{(2)} z_{t-k}^{(1)} + \sum_{i=1}^{p} \beta_k^{(2)} z_{t-k}^{(2)} + f_t + \mu^{(2)}; \qquad z_t^{(2)} - \hat{z}_t^{(2)} = f_t \tag{25}$$

VAR makes one-step ahead prediction, $\widehat{z_t}^{(1)}$ of the target variable ($z_t^{(1)}$). The innovation of the prediction ($\widehat{z_t}^{(1)}$) at an instant, e_t is the difference between the observed $z_t^{(1)}$ and predicted value $\widehat{z_t}^{(1)}$. The innovations conceptually represent the error between the model predictions and the observed values. We use the VAR model to determine the innovation series for $\vec{X}_t$ and $\vec{Y}_t$ using Eq. 24 and 25, respectively. Our method uses VAR only unlike Galka's technique which employs both AR and VAR [1]. We use VAR only because (1) mutual dependence estimations tend to improve by applying VAR filters and (2) the two series are generated according to a joint probability distribution, indicating that $\vec{X}_t$ and $\vec{Y}_t$ are correlated. Moreover, this approach is better consistent with the standard definition of MI. We mathematically derived that the joint probability density of $\vec{X}_t$ is the same as the joint probability density of the corresponding innovation series e_t. This is true for the $\vec{Y}_t$ series and the paired ($\vec{X}_t$, $\vec{Y}_t$) series.

$$p_X(x_1, x_2, x_3, \dots, x_{N_t}) = p_e(e_1, e_2, \dots, e_{N_t}); p_Y(y_1, y_2, y_3, \dots, y_{N_t}) = p_f(f_1, f_2, \dots, f_{N_t}) \tag{26}$$

$$p_{XY}\left((x_1 y_1), (x_2, y_2), (x_3, y_3), \dots, (x_{N_t}, y_{N_t})\right) = p_{ef}\left((e_1 f_1), (e_2, f_2), \dots, (e_{N_t}, f_{N_t})\right) \tag{27}$$

A befitting time series forecasting method yields a white noise innovation data set. If the time points are from an independent and identically distributed (i.i.d) sequence, the joint probability of the innovation time series deciphers as the product of marginal probability densities per Eq. (28). This is true for joint probability distribution of time series Y_t per Eq. (28).

$$p_e(e_1, e_2, \dots, e_t) = p_e(e_1) p_e(e_2) \dots p_e(e_t); \quad p_f(f_1, f_2, \dots, f_t) = p_f(f_1) p_f(f_2) \dots p_f(f_t) \tag{28}$$

$$p_{ef}\big((e_1, f_1), .., (e_t, f_t)\big) = p_{ef}(e_1, f_1)\, p_{ef}(e_2, f_2) .., p_{ef}(e_t, f_t) \tag{29}$$

We write Eq. 29 as mentioned because $\{(e_1, f_1), .., (e_t, f_t)\}$ are independent of each other. Thus, Eq. 23 takes the form

$$\lambda(\vec{X}_t, \vec{Y}_t) = \sum_{i=1}^{N_t} \log\left(\frac{p_{ef}(e_i,f_i)}{p_e(e_i)p_f(f_i)}\right) \quad (30)$$

$$IT(\vec{X}_t; \vec{Y}_t) = \int_{-\infty}^{\infty} \sum_{i=1}^{N_t} \log\left(\frac{p_{ef}(e_i,f_i)}{p_e(e_i)p_f(f_i)}\right) p(e_1,f_1)p(e_2,f_2)\ldots p(e_{N_t},f_{N_t}) de_1..de_{N_t} df_1..df_{N_t} \quad (31)$$

To derive MI formulation for continuous variables, we take the average of Eq. 30 with respect to the joint probability distribution and integrate as per Eq. 31. We know that $\int_{-\infty}^{\infty} p(e_i,f_i)de_i df_i = 1$, hence MI formulation for bivariate temporally correlated time series, $IT(\vec{X}_t; \vec{Y}_t)$, is

$$IT(\vec{X}_t; \vec{Y}_t) = N_t \iint_{-\infty}^{\infty} p_{ef}(e_i,f_i) \log\left(\frac{p_{ef}(e_i,f_i)}{p_e(e_i)p_f(f_i)}\right) de_i df_i \quad (32)$$

For Eq. 32 derivation, we employ the fact that the integral for all time points will be the same as they all belong to identical probability distributions.

Galka et al. developed the "innovation approach to compute mutual information" for temporally correlated time series [1]. The authors originally considered time series with Gaussian distribution as the innovation series. However, the innovation series can also follow nonparametric distributions. We build upon Galka et al.'s innovation approach and propose an estimation method for $IT(\vec{X}_t; \vec{Y}_t)$, valid for parametric and nonparametric distributions of the innovation series. Our method uses VAR only for innovation series determination unlike Galka's technique which employs both AR and VAR [1]. We use VAR only because (1) mutual dependence estimations tend to improve by applying VAR filters and (2) the two series are generated according to a joint probability distribution, indicating that $\vec{X}_t$ and $\vec{Y}_t$ are correlated. Moreover, this approach is consistent with the standard definition of MI.

Eq. 33 denotes the $IT(\vec{X}_t; \vec{Y}_t)$ formulation in terms of joint entropy, $HT(\vec{X}_t, \vec{Y}_t)$, defined in Eq. 34, and entropies for X_t, $HT(\vec{X}_t)$ and $\vec{Y}_t$, $HT(Y_t)$, detailed in Eq. 35. Eq. 32 indicates that $IT(\vec{X}_t; \vec{Y}_t)$ quantifies the shared interaction between the bivariate time series similar to Shannon's MI representation.

$$IT(\vec{X}_t; \vec{Y}_t) = HT(\vec{X}_t) + HT(\vec{Y}_t) - HT(\vec{X}_t, \vec{Y}_t) \quad (33)$$

$$HT(\vec{X}_t, \vec{Y}_t) = -N_t \iint_{-\infty}^{\infty} p_{ef}(e_i,f_i) \log p_{ef}(e_i,f_i)\, de_i df_i \quad (34)$$

$$HT(\vec{X}_t) = -N_t \int_{-\infty}^{\infty} p_e(e_i) \log p_e(e_i)\, de_i; \quad HT(\vec{Y}_t) = -N_t \int_{-\infty}^{\infty} p_f(f_i) \log p_f(f_i)\, df_i \quad (35)$$

Remark: Note that $IT(\vec{X}_t; \vec{Y}_t)$, Eq. 32 observes the following properties:

(a) $IT(\vec{X}_t; \vec{Y}_t) \geq 0$. It is always non-negative.

(b) $IT(\vec{X}_t; \vec{Y}_t) = 0$ if and only if the time series are independent of each other.

(c) $IT(\vec{X}_t; \vec{Y}_t) = IT(\vec{Y}_t; \vec{X}_t)$ implies that $IT(\vec{X}_t; \vec{Y}_t)$ is symmetric.

$IT(\vec{X}_t; \vec{Y}_t) \leq \min(HT(\vec{X}_t), HT(\vec{Y}_t))$, following the similar arguments based on Jensen's inequality application to Shanon's MI formulation $I(X;Y)$. It is important to note that the properties (a)-(d) of $IT(\vec{X}_t; \vec{Y}_t)$ retains the standard characteristics of Shannon's MI formulation $I(X;Y)$.

4 F-test calculation

$$F = \frac{\left(\sum_{j=1}^{nt}\left(Y_j^{trt}-\bar{X}_j^{trt}\right)^2+\sum_{j=1}^{nt}\left(Y_j^{ctrl}-\bar{X}_j^{ctrl}\right)^2\right)\Big/_{(ne\times nt)}}{\left(\sum_{j=1}^{nt}\sum_{i=1}^{nr}\left(X_{ij}^{trt}-\bar{X}_j^{trt}\right)^2+\sum_{j=1}^{nt}\sum_{i=1}^{nr}\left(X_{ij}^{ctrl}-\bar{X}_j^{ctrl}\right)^2\right)\Big/_{(ne\times nt\times(nr-1))}} \quad (36)$$

where X_j, $\bar{X}_j$, and Y_j denote the experimental data, mean experimental data, and simulated (fitted) data at time point j, respectively. nr is the number of replicates (nr = 3, indexed as i), nt is the number of time points (nt = 7, indexed as j). ne is the number of experimental conditions used, and trt and ctrl are treatment and control groups, respectively. The degrees of freedom for determining the F distribution are $df_1 = (ne \times nt)$ and $df_2 = (ne \times nt \times (nr - 1))$.

Table S4. Model Accuracy for the formulated cybernetic goal. Goodness of fit, *F*-test, for simulated/optimized (control, adenosine triphosphate (ATP) stimulated, and Kdo2-Lipid A (KLA) primed data) and predicted (Kdo2-Lipid A (KLA) primed and ATP stimulated) cases. *F* values smaller than $F_{0.05}(21, 42) = 0.51$ indicate that the fit-error is statistically smaller than the experimental error; whereas, the *F* values smaller than $F_{0.95}(21, 42) = 1.81$ indicate statistically equal variance in simulated (fitted) and experimental data.

Metabolite	Model Fit to Data	Model Prediction to KLA+ATP Data
PGD_2	0.4462	0.6549
PGE_2	0.6382	0.827
$PGF_{2\alpha}$	0.2873	0.4174
TXB_2	0.4209	0.3783
$dPGD_2$	0.4869	1.8715
PGJ_2	0.4453	0.6674
$dPGJ_2$	0.4534	1.0044
LTB_4	0.233	0.2499
12-epi-LTB_4	0.2473	0.291
6-trans-epi-LTB_4	0.2321	0.2508
5-HETE	0.289	0.5084
15-HETE	0.2833	0.3755

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