**What is claimed is:**

1. A method of predicting *in vivo* pharmacokinetics and pharmacodynamics of a mixture with multiple components, comprising the steps of:

    a) determining the rate of metabolism of individual and interacting components in the mixture in gastrointestinal tract and liver;

    b) determining distribution of the components in blood or plasma;

    c) determining the rate of the components' renal elimination; and

    d) determining the potency of an individual component and synergism or inhibition among the components,

wherein the above determinations comprise mathematical models that will predict the pharmacokinetics and pharmacodynamics properties of the mixture *in vivo*.

2. The method of claim 1, further comprising the steps of determining parameters for active metabolites of the components according to steps (a) through (d), wherein outputs of the mathematical models will predict the pharmacokinetics and pharmacodynamics properties of the mixture and their metabolites *in vivo*.

3. The method of any one of claims 1-2, wherein the pharmacokinetics and pharmacodynamics properties comprise concentration-time profiles and response-time profiles for the components and their metabolites.

4. The method of any one of claims 1-3, wherein the mathematical models are capable of solving multiple unknowns which are linearly independent or interacting with each other.

5. The method of any one of claims 1-4, wherein the mathematical models comprises

$r \approx \bar{r} + \sum_i w_i(d_i - \bar{d}_i) + \sum_i w_i'(d_i - \bar{d}_i)^2 + \sum_{i,j} w_{i,j}(d_i - \bar{d}_i)(d_j - \bar{d}_j)$, wherein r is linearized response, $\bar{r}$ is the average linearized response; $w_i$ is weight of the $i$ component (relates to potency), $d_i$ is the dose of component $i$ and $\overline{d_i}$ and $\overline{d_j}$ are average dose of the $i^{th}$ and $j^{th}$ component, $w_{i,j}$ is the weight of the interacting pair.

6. The method of any one of claims 1-5, wherein the mathematical models comprises

$A = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \beta_{i,j} x_i x_j$, wherein $\alpha_0$ and $\alpha_i$ are baseline activity and activity coefficient of component $i$ respectively, $x_i$ and $x_j$ are components $i$ and j respectively, $\beta_{i,j}$ is the activity coefficient of the interacting pair, $x_i$ and $x_j$, wherein said equation is able to predict an optimized composition of the mixture to achieve maximum possible potency.

7. The method of any one of claims 1-6, wherein the rate of metabolism comprises rate of degradation and rate of absorption.

8. The method of any one of claims 1-7, wherein the determination of the rate of metabolism in gastrointestinal tract comprises assays using artificial gastric or intestinal juice, intestinal flora, intestinal microsomes, or permeability studies using cultured cells or intestinal tissues.

9. The method of any one of claims 1-8, wherein the determination of the rate of metabolism in liver comprises assays using freshly harvested hepatocytes, cryopreserved hepatocytes, hepatic microsomes, hepatic cytosol or S-9 fractions.

10. The method of any one of claims 1-9, wherein the determination of distribution in blood or plasma comprises determining binding to plasma protein, binding to blood protein, pKa, log P, log D, and volume of distribution of a component.

11. The method of any one of claims 1-10, wherein the determination of renal elimination is based on the components' chemical structure.

12. The method of any one of claims 1-11, wherein the determination of potency comprises receptor binding assay, enzymatic assay, biochemical response assay, and assays with isolated tissues or organs.

13. A composition comprising multiple components as identified by any one of the method of claims 1-12, wherein the components have desirable *in vivo* pharmacokinetics and pharmacodynamics properties as determined by any one of the method of claims 1-12.

14. The composition of claim 13, comprising Red clover (*Trifolium pratense*).

15. The composition of claim 14, wherein the Red clover comprises formononetin, biochanin A and their glycosides in amounts determined by any one of the method of claims 1-12.

**What is claimed is:**

1. A method for preparing optimized drug formulations through the prediction of *in vivo* pharmacokinetics and pharmacodynamics of a mixture with multiple components, wherein the identities of or interactions among the components are not known a priori, said method comprises the steps of:
   a) determining the rate of metabolism of individual and interacting components in the mixture in the gastrointestinal tract and liver using *in vitro* assays;
   b) determining distribution of said components in blood or plasma using *in vitro* assays or *in silico* methods;
   c) determining the rate of renal elimination of said components using *in vitro* assays or *in silico* methods;
   d) determining the potency of an individual component and synergism or inhibition among the components using *in vitro* assays;
   e) inputting the results from (a) to (d) into mathematical models *in silico* to obtain concentration time profiles and response time profiles for the components, and the time course for the composite mixture's response; and
   f) using the results from (e) to prepare a composition comprising specified components, wherein the components have desirable *in vivo* pharmacokinetic and pharmacodynamic properties.

2. The method of claim 1, wherein the concentration time profiles or response time profiles predict the pharmacokinetics and pharmacodynamics properties of the components and their active metabolites *in vivo*.

3. The method of any one of claims 1-2, wherein the mathematical models solve multiple unknowns which are linearly independent or interacting with each other.

4. The method of any one of claims 1-3, wherein the mathematical models comprise $r \approx \bar{r} + \sum_i w_i(d_i - \bar{d}_i) + \sum_i w_i'(d_i - \bar{d}_i)^2 + \sum_{i,j} w_{i,j}(d_i - \bar{d}_i)(d_j - \bar{d}_j)$, wherein r is linearized response, $\bar{r}$ is the average linearized response; $w_i$ is weight of the $i$ component (relates to

potency), $d_i$ is the dose of component $i$ and $\overline{d_i}$ and $\overline{d_j}$ are average dose of the $i^{th}$ and $j^{th}$ component, $w_{i,j}$ is the weight of the interacting pair.

5. The method of any one of claims 1-4, wherein the mathematical models comprise $A = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \beta_{i,j} x_i x_j$, wherein $\alpha_0$ and $\alpha_i$ are baseline activity and activity coefficient of component $i$ respectively, $x_i$ and $x_j$ are components $i$ and j respectively, $\beta_{i,j}$ is the activity coefficient of the interacting pair, $x_i$ and $x_j$, wherein said equation is able to predict an optimized composition of the components to achieve maximum possible potency.

6. The method of any one of claims 1-5, wherein the rate of metabolism comprises rate of degradation and rate of absorption.

7. The method of any one of claims 1-6, wherein determining the rate of metabolism in gastrointestinal tract comprises assays using artificial gastric or intestinal juice, intestinal flora, or intestinal microsomes, or permeability studies using cultured cells or intestinal tissues.

8. The method of any one of claims 1-7, wherein determining the rate of metabolism in liver comprises assays using freshly harvested hepatocytes, cryopreserved hepatocytes, hepatic microsomes, hepatic cytosol or S-9 fractions.

9. The method of any one of claims 1-8, wherein determination of distribution in blood or plasma comprises determining binding to plasma protein, binding to blood protein, pKa, log P, log D, or volume of distribution of a component.

10. The method of any one of claims 1-9, wherein determining the rate of renal elimination is calculated on the basis of known properties originating from the components' chemical structure.

11. The method of any one of claims 1-10, wherein determination of potency comprises receptor binding assay, enzymatic assay, biochemical response assay, or assays with isolated tissues or organs.

12. A composition comprising multiple components as identified by any one of the method of claims 1-11, wherein the components have desirable *in vivo* pharmacokinetics and pharmacodynamics properties as determined by any one of the method of claims 1-11.

13. The composition of claim 12, comprising components of Red clover (an herb of the scientific name *Trifolium pratense*).

14. The composition of claim 13, wherein the Red clover comprises formononetin, biochanin A and their glycosides in amounts determined by any one of the method of claims 1-11.