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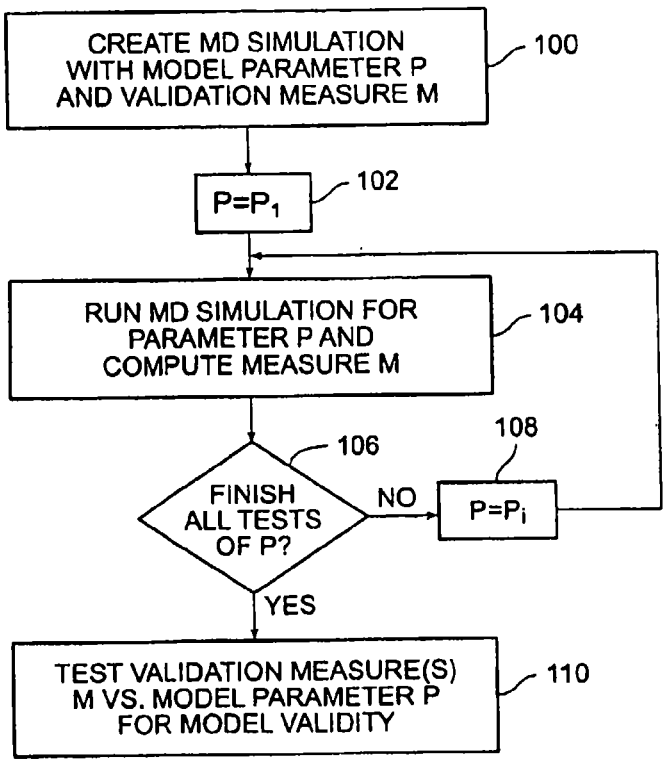
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(54) Title: METHOD FOR SELF-VALIDATION OF MOLECULAR MODELING



(57) Abstract: A method for validating a computer model of a molecular system (100), comprising selecting a model parameter of the molecular system (102); selecting a validation measure of the molecular system (102); simulating the molecular system by modeling with the selected model parameter (104); determining a value of the validation measure of said molecular system from the simulating step; and testing whether the value of the validation measure is in a predetermined range to validate the computer modeling (110).



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