

การศึกษาทางเภสัชควอนตัมของสารประกอบกลุ่มคล้ายคลอโรควินและกลุ่มคล้ายเมโฟลควิน



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QUANTUM PHARMACOLOGICAL STUDIES ON CHLOROQUINE AND MEFLOQUINE ANALOGS

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สภา พลมัน : การศึกษาทางเภสัชควอนตัมของสารประกอบกลุ่มคล้ายคลอโรควินและกลุ่มคล้ายเมโฟลควิน (QUANTUM PHARMACOLOGICAL STUDIES ON CHLOROQUINE AND MEFLOQUINE ANALOGS) อ.ที่ปรึกษา : รศ.ดร.ศิริรัตน์ กักผล, อ.ที่ปรึกษาร่วม ศ.ดร.บี เอ็ม โรเด, 226 หน้า

ได้ทำการประเมินแบบจำลองเชิงเส้นสำหรับความสัมพันธ์ระหว่าง โครงสร้างอิเล็กทรอนิกส์ และฤทธิ์ในการต้านเชื้อมาลาเรีย ของสารประกอบกลุ่มคล้ายคลอโรควินและกลุ่มคล้ายเมโฟลควิน ที่ได้จากการคำนวณแบบซีเอนดีโอ (CNDO/2) โมเลกุลาร์ออร์บิทัล ได้คำนวณสารประกอบกลุ่มคล้ายคลอโรควินโดยวิธีแอบอินนิซิโอด้วย เพื่อเปรียบเทียบผลจากวิธีซีเอนดีโอ จากสมการพิตติงเชิงเส้นที่ได้พบว่าวิธีแอบอินนิซิโอไม่ได้ปรับปรุงให้แบบจำลองให้ดีขึ้น อย่างไรก็ตามค่าพารามิเตอร์ที่สำคัญของทั้งสองวิธีให้ผลที่คล้ายคลึงกัน การศึกษาในแนวทางเดียวกันนี้ ได้กระทำกับสารในกลุ่มคล้ายเมโฟลควินโดยวิธีใช้ประจุมูลฐานจากวิธีซีเอนดีโอ จากขนาดของค่าพารามิเตอร์ของสมการได้นำมาทำนายศูนย์กลางความไวของยาในกลุ่มทั้งสอง การศึกษานี้ทำให้ทราบว่าผลการคำนวณโดยวิธีเคมีเอ็มไพริคัลแบบซีเอนดีโอ เป็นวิธีที่สามารถช่วยในการออกแบบยาตัวใหม่และทำให้ทราบถึงศูนย์กลางความไวของยาด้วย

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ลายมือชื่อนิสิต
ลายมือชื่ออาจารย์ที่ปรึกษา APD



SUPA POLMAN : QUANTUM PHARMACOLOGICAL STUDIES ON CHLOROQUINE AND
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Linear models for the relationships between electronic structure and antimalarial activity of chloroquine and mefloquine analogs have been evaluated, based on CNDO/2 molecular orbital calculations. Ab initio method has also been calculated for chloroquine series. According to the linear fitting equations, the models are not improved by the ab initio approach compared to CNDO/2 data. However, the relative important of parameters from both calculations is well comparable. A similar approach has been made for the CNDO/2 net charges of mefloquine analogs. The active center of both drugs have been predicted according to the parameter size of the fitting equations. This study have suggested that semiempirical CNDO/2 calculations seem to be good enough for searching of electronic structure - activity relationships and can be a useful tool in designing potential new drugs and revealing a drug's active center.

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CONTENTS



Pages

ABSTRACT IN THAI	IV
ABSTRACT IN ENGLISH	V
ACKNOWLEDGEMENT	VI
LIST OF FIGURES	XI
LIST OF TABLES	XIII

CHAPTER

I INTRODUCTION

1.1 Historical Outline of Antimalarial Drug	3
1.2 General Chemical Structure of Antimalarials ..	9
1.3 Quantitative Structure-Activity Relationships in Quantum Pharmacological Studies	12

II MOLECULAR ORBITAL THEORY IN QUANTUM PHARMACOLOGICAL STUDIES

2.1 Quantum Mechanical Principles	17
2.1.1 The Schroedinger Wave Equation	18
2.1.2 The Born-Oppenheimer Approximation	21
2.1.3 The Antisymmetry of Pauli Exclusion Principle	23
2.1.4 Molecular Orbital and Linear Combination of Atomic Orbital (LCAO) Approximation..	26
2.2 Self-Consistent Field Molecular Orbital Theory.	30
2.2.1 Hartree Fock Equation	32
2.2.2 The Roothaan Equation	34
2.2.3 The Charge Density and Population Analysis	36

2.2.4	The Central Field Approximation and the Self-Consistent Field Procedure	38
2.2.5	The Form of the Basis sets	39
2.3	Approximate Molecular Orbital Theories	40
2.3.1	The Nature of Semiempirical Theory	41
2.3.2	Invariant Levels of Approximation	42
2.3.3	Approximate with Complete Neglect of Differential Overlap (CNDO)	45
2.3.3.1	The Neglect of Overlap (NO) ..	45
2.3.3.2	The Zero-Differential Overlap (ZDO) Approximation	45
2.3.3.3	The Core Hamiltonian Approximation	46
2.3.4	The CNDO parametrization	49
2.3.4.1	The local Core Matrix Element.	49
2.3.4.2	The electron-Core Potential Integrals	50
2.3.4.3	The Bonding Parameters, B_{AB} ..	50
2.3.5	The CNDO Basis Set	51
2.3.6	The SCF Procedure for CNDO	52

III CALCULATIONS

3.1	The model	53
3.2	Methodical Steps	57
3.2.1	Calculation of the Coordinates of Atoms in Chloroquine and Mefloquine Drugs ...	59

	Pages
3.2.2 Calculation of the Electron Distribution of Chloroquine and Mefloquine Drugs ...	75
IV FITTING OF ELECTRON DISTRIBUTION TO THE ACTIVITY OF DRUGS BY LINEAR MODELS	97
4.1 Fitting of the Linear Equations of Chloroquine by CNDO/2 Method	98
4.2 Fitting of the Linear Equations of Chloroquine by Ab initio Method	105
4.3 Fitting of the Linear Equations of Mefloquine by CNDO/2 Method	113
V DISCUSSION AND CONCLUSION	
5.1 Chloroquine Analog Antimalarial Drugs	120
5.1.1 Electron Distribution in Quinoline ring	120
5.1.2 Electron Distribution - Activity Relationships of Chloroquine Antimalarial Drugs According to CNDO/2 Method	122
5.1.3 Comparison of Electron Distribution - Activity of Chloroquine Antimalarial Drugs According to CNDO/2 and Ab initio Calculations	125
5.1.4 Prediction of Active Center	127
5.2 Mefloquine Analog Antimalarial Drugs	131
5.2.1 Electron Distribution in Mefloquine Drug	
5.2.2 Electron Distribution-Activity Relationships of Mefloquine Antimalarial Drugs According to CNDO/2 Calculation ..	133

	Pages
5.2.3 Prediction of Active Center	136
CONCLUSION	138
REFERENCES	139
APPENDIX I	147
APPENDIX II	189
APPENDIX III	223
VITA	226

List of Figure

Figure	Pages
1.1 Malaria Situation in the World, 1985	4
1.2 Quinine	6
1.3 Chloroquine	7
1.4 Mefloquine	8
1.5 Quinoline ring	10
1.6 Acridine	11
1.7 Phenantrene	11
1.8 Biguanide	11
1.9 Sulfone	12
1.10 Sulfonamide	12
3.1 Molecular backbone of chloroquine	53
3.2 Molecular backbone of mefloquine	53
3.3 Structure of chloroquine with atomic numbering	60
3.4 Structure of mefloquine with atomic numbering	60
5.1 Net charges at various atoms in quinoline ring, and amino nitrogen, N2 of chloroquine	121
5.2a The plot of calculated versus observed antimalarial activity ($\ln A$) for model 12	124
5.2b The plot of $\ln A$ versus $\ln A_{cal}$ for model 12	124
5.3 Predicted active center of chloroquine drug	127
5.4 Net charges at various atoms in quinoline ring, C13, O and N2 of mefloquine	132
5.5a The plot of calculated versus observed antimalarial activity ($\ln A$) for model 26	135
5.5b The plot of $\ln A$ versus $\ln A_{cal}$ for model 26	135

Figure	Pages
5.6 Predicted active center of chloroquine drug	136
5.7a The two possibilities of an active site of mefloquine The hydrogen bond acceptor via N1 and hydrogen bond donor via N2	137
5.7b The two possibilities of an active site of mefloquine The hydrogen bond acceptor via N1 and hydrogen bond donor via O-H.....	137

List of Table

Table	Pages
3.1a	Chemical structure and antimalarial activity of nuclear substituents of chloroquine drugs 54
3.1b	Chemical structure and antimalarial activity of different amino side chain of chloroquine drugs 55
3.1c	Chemical structure and antimalarial activity of nuclear substituents of mefloquine drugs 56
3.2a	The geometry parameters of chloroquine drugs 61
3.2b	The geometry parameters of mefloquine drugs 62
3.3	The cartesian coordinates (\AA) of atoms in quinoline ring of chloroquine drugs 63
3.4	The cartesian coordinates (\AA) of nuclear substituents in quinoline ring of chloroquine drugs 64
3.5	The cartesian coordinates (\AA) of additional nuclear substituents in quinoline ring of chloroquine drugs 65
3.6a	The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ1-CQ13 66
3.6b	The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ14 and CQ15 67
3.6c	The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ16-CQ17 68
3.6d	The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ18-CQ19 69
3.6e	The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ20-CQ21 70

Table	Pages
3.6f The cartesian coordinates (\AA) of atoms in amino side chain of chloroquine drugs, CQ22	71
3.7 The cartesian coordinates (\AA) of mefloquine, MF1	72
3.8a The cartesian coordinates (\AA) of nuclear substituent in quinoline ring of mefloquine drugs	73
3.8b The cartesian coordinates (\AA) of nuclear substituent in quinoline ring of mefloquine drugs	74
3.9a Atomic charges of atoms in chloroquine drugs, CQ1 and CQ2	76
3.9b Atomic charges of atoms in chloroquine drugs, CQ3 and CQ4	77
3.9c Atomic charges of atoms in chloroquine drugs, CQ5 and CQ6	78
3.9d Atomic charges of atoms in chloroquine drugs, CQ7 and CQ8	79
3.9e Atomic charges of atoms in chloroquine drugs, CQ9 and CQ10	80
3.9f Atomic charges of atoms in chloroquine drugs, CQ11 and CQ12	81
3.9g Atomic charges of atoms in chloroquine drugs, CQ14 and CQ15	82
3.9h Atomic charges of atoms in chloroquine drugs, CQ15 and CQ16	83
3.9i Atomic charges of atoms in chloroquine drugs, CQ17 and CQ18	84

Table	Pages
3.9j Atomic charges of atoms in chloroquine drugs, CQ19 and CQ20	85
3.9k Atomic charges of atoms in chloroquine drugs, CQ21 and CQ22	86
3.10a Atomic charges of atoms in mefloquine drugs, MF1, MF2 and MF3	88
3.10b Atomic charges of atoms in mefloquine drugs, MF3, MF4 and MF4	89
3.10c Atomic charges of atoms in mefloquine drugs, MF7, MF8 and MF9	90
3.10d Atomic charges of atoms in mefloquine drugs, MF10, MF11 and MF12	91
3.10e Atomic charges of atoms in mefloquine drugs, MF13, MF14 and MF15	92
3.10f Atomic charges of atoms in mefloquine drugs, MF16, MF17 and MF18	93
3.10g Atomic charges of atoms in mefloquine drugs, MF19, MF20 and MF21	94
3.11 Dipole moments and the total energies of chloroquine compounds	95
3.12 Dipole moments and the total energies of mefloquine compounds	96
4.1 The net charges for CNDO/2 calculation of atoms in chloroquine drugs as use for linear model fitting	101

Table	Pages
4.2a	Parametes for linear model and fitting characteristics of the equation including all CNDO/2 net charges of all atoms in quinoline ring and N2 of chloroquine drugs (no. of compounds = 22) 101
4.2b	Parametes for linear model and fitting characteristics of the equation including all CNDO/2 net charges of atoms N1, C2, C3, C4 and N2 of chloroquine drugs (no. of compounds = 22) 102
4.2c	Parametes for linear model and fitting characteristics of the equation including all CNDO/2 net charges of atoms N1, C4, C9, C10 and N2 of chloroquine drugs (no. of compounds = 22) 103
4.2d	Parametes for linear model and fitting characteristics of the equation including all CNDO/2 net charges of atoms N1, C2, C3, C4, C9, C10 and N2 of chloroquine drugs (no. of compounds = 22) 104
4.3	The net charges for ab initio calculation of atoms in chloroquine drugs as use in linear model fitting 106
4.4a	Parameters for linear model and fitting characteristics of the equation including CNDO/2 net carges of atoms N1, C2, C3, C4 and N2 of chloroquine drugs (no. of compounds = 17) 108
4.4b	Parameters for linear modil and fitting characteristics of the equation including CNDO/2 net carges of atoms N1, C4, C9, C10 and N2 of chloroquine drugs (no. of compounds = 17) 109

Table	Pages
4.4c Parameters for linear model and fitting characteristics of the equation including CNDO/2 net charges of atoms N1, C2, C3, C4, C9, C10 and N2 of chloroquine drugs (no. of compounds = 17)	110
4.5a Parameters for linear model and fitting characteristics of the equation including ab initio net charges of atoms N1, C2, C3, C4 and N2 of chloroquine drugs (no. of compounds = 17)	111
4.5b Parameters for linear model and fitting characteristics of the equation including ab initio net charges of atoms N1, C4, C9, C10 and N2 of chloroquine drugs (no. of compounds = 17)	112
4.5c Parameters for linear model and fitting characteristics of the equation including ab initio net charges of atoms N1, C2, C3, C4 and N2 of chloroquine drugs (no. of compounds = 17)	113
4.6 The net charge for CNDO/2 calculation of atoms in mefloquine drugs as use in linear model fitting	114
4.7a Parameters for linear model and fitting characteristics of the equation including all CNDO/2 net charges of all atoms in quinoline ring and N2 of mefloquine drugs (no. of compounds = 21)	115
4.7b Parameters for linear model and fitting characteristics of the equation including all CNDO/2 net charges of N1, C2, C3, C4, C13, O and N2 of mefloquine drugs (no. of compounds = 21)	116

Table	Pages
4.7c Parameters for linear model and fitting characteristics of the equation including all CNDO/2 net charges of N1, C4, C9, C10, C13, O and N2 of mefloquine drugs (no. of compounds = 21)	117
4.7d Parameters for linear model and fitting characteristics of the equation including all CNDO/2 net charges of N1, C2, C3, C4, C9, C10, C13, O and N2 of mefloquine drugs (no. of compounds = 21)	118
4.7e Parameters for linear model and fitting characteristics of the equation including all CNDO/2 net charges of C13, C26, O and N2 of mefloquine drugs (no. of compounds = 21)	119
5.1 Effect of the number and position of ring nitrogens on antimalarial activity	129
5.2 Effect on antimalarial activity of increasing the size of the heterocyclic ring	130