

Contents

1	Introduction	1
2	Fundamentals of Infrared and Raman Spectroscopy, SERS, and Theoretical Simulations	9
2.1	Vibrations of Molecules	9
2.2	Infrared Spectroscopy	12
2.2.1	Basics.....	12
2.2.2	FT-Infrared Measurements	15
2.3	Raman Spectroscopy	16
2.3.1	Basics.....	16
2.3.2	FT-Raman Measurements	18
2.4	Surface-Enhanced Raman Spectroscopy	18
2.4.1	Basics	18
2.4.2	Mechanisms of Surface Enhancement	19
2.4.3	SERS-Active Substrates	21
2.4.4	SERS Measurements.....	24
2.5	Theoretical Simulations.....	25
2.5.1	Molecular Mechanics and Electronic Structure Methods	25
2.5.2	The Simulation Model	26
2.5.3	DFT Methods.....	27
2.5.4	The Basis Set	28
2.5.5	Computational Details	29
3	Tranquilizers and Sedatives	37
3.1	Phenothiazine Derivatives.....	37
3.1.1	Vibrational Analysis	38
3.1.2	Adsorption on the Silver Surface.....	46
3.1.3	Conclusions.....	55

3.2	Anthranil	56
3.2.1	Vibrational Analysis	57
3.2.2	Adsorption on the Silver Surface	59
3.2.3	Conclusions.....	66
4	Anti-Inflammatory Drugs.....	69
4.1	Diclofenac Sodium.....	69
4.1.1	Vibrational Analysis	71
4.1.2	Adsorption on the Silver Surface	77
4.1.3	Conclusions.....	82
4.2	Diclofenac Sodium – β -Cyclodextrin Complex	83
4.2.1	Vibrational Analysis	83
4.2.2	Adsorption on the Silver Surface	90
4.2.3	Conclusions.....	93
5	Molecules with Antibacterial Properties	97
5.1	Potassium Benzylpenicillin	97
5.1.1	Vibrational Analysis	98
5.1.2	Adsorption on the Silver Surface	104
5.1.3	Conclusions.....	109
5.2	Trihydrate Amoxicillin.....	110
5.2.1	Vibrational Analysis	111
5.2.2	Adsorption on the Silver Surface	115
5.2.3	Conclusions.....	118
5.3	Rivanol.....	118
5.3.1	Vibrational Analysis	119
5.3.2	Adsorption on the Silver Surface	121
5.3.3	Conclusions.....	122
6	Vitamins	125
6.1	Vitamin B1	125
6.1.1	Vibrational Analysis	126
6.1.2	Adsorption on the Gold Surface	133
6.1.3	Conclusions.....	136
6.2	Vitamin PP	137
6.2.1	Adsorption on the Silver Surface	137
6.2.2	Conclusions.....	141
7	Other Molecules with Pharmacological Activity	143
7.1	2-Formylfuran Derivatives	143
7.1.1	2-Formylfuran.....	143
7.1.2	5-(4-Fluor-phenyl)-2-formylfuran and 5-(4-Brom-phenyl)-2-formylfuran	152

7.2	Quinoline Derivatives	163
7.2.1	Isoquinoline	163
7.2.2	Lepidine	169
7.3	9-Phenylacridine	176
7.3.1	Vibrational Analysis	176
7.3.2	Adsorption on the Silver Surface	179
7.3.3	Conclusions.....	182
8	New Developments in SERS-Active Substrates	187
9	Summary	207
	Index	211