



Faculty of Information and Communication Technology

**THREE-DIMENSIONAL EXACT LEGENDRE MOMENT
INVARIANTS FOR AMPHETAMINE-TYPE STIMULANTS
MOLECULAR STRUCTURE REPRESENTATION**

Satrya Fajri Pratama

Doctor of Philosophy

2017

**THREE-DIMENSIONAL EXACT LEGENDRE MOMENT INVARIANTS
FOR AMPHETAMINE-TYPE STIMULANTS
MOLECULAR STRUCTURE REPRESENTATION**

SATRYA FAJRI PRATAMA

**A thesis submitted
in fulfillment of the requirements for the degree of Doctor of Philosophy**

Faculty of Information and Communication Technology

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2017

DECLARATION

I declare that this thesis entitled “Three-Dimensional Exact Legendre Moment Invariants for Amphetamine-Type Stimulants Molecular Structure Representation” is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

Signature :

Name : Satrya Fajri Pratama

Date :

APPROVAL

I hereby declare that I have read this thesis and in my opinion this thesis is sufficient in terms of scope and quality for the award of Doctor of Philosophy.

Signature :

Supervisor Name : Assoc. Prof. Dr. Azah Kamilah Muda

Date :

DEDICATION

For the glory of Islam, and to my family.

ABSTRACT

The abuse of amphetamine-type stimulants (ATS) drugs has become a global, harrowing social problem. The technical limitations of the current test kits to detect new brand of ATS drugs present a challenge to national law enforcement authorities and scientific staff of forensic laboratories. Meanwhile, new molecular imaging devices which allowed mankind to characterize the physical three-dimensional (3D) molecular structure have been recently introduced, and it can be used to remedy the limitations of existing drug test kits. Thus, a new type of 3D molecular structure representation technique, or molecular descriptors, should be developed to cater the 3D molecular structure acquired physically using these molecular imaging devices. One of the image processing methods to represent a 3D image is 3D moments and moment invariants. However, there are problems exhibited by the existing 3D moments and moment invariants. Therefore, it is necessary to propose a new 3D moment invariants which is free from these problems. This study compares various 3D moments and identified 3D Legendre moments as the best moments to construct 3D moment invariants, namely 3D exact Legendre moment invariants (3D ELMI), which is used to represent the 3D molecular structure of ATS drugs. Since the 3D molecular structure of ATS drugs dataset obtained using molecular imaging devices are currently unavailable, this study acquired the 3D molecular structure of ATS drugs data from United Nations Office of Drug and Crime (UNODC) and pihkal.info database instead. The proposed technique was compared to the existing 3D moment invariants and molecular descriptors techniques in terms of processing time, memory consumption, single instance invariance, intra- and inter-class variance, and classification accuracy. The comparative study conducted found that 3D ELMI performs better than the existing 3D moment invariants, such as 3D geometric moment invariants (3D GMI), 3D Gaussian–Hermite moment invariants (3D GHMI), and 3D Zernike descriptors (3D ZD). The satisfactory performance of 3D ELMI is attributed to numerous factors, such as the quality of the 3D Legendre, exact computation of the 3D Legendre, and the novelty of the proposed invariants techniques. The proposed technique was also compared to existing 3D molecular descriptors, for example weighted holistic invariants molecular (WHIM), geometry, topology, and atom weights assembly (GETAWAY), radial distribution function (RDF), and 3D molecule representation of structure based on electron diffraction (3D-MoRSE) descriptors. Despite 3D ELMI is capable to overcome the limitations of existing 3D molecular descriptors which depends on 3D molecular structure model instead of physical molecular structure obtained from molecular imaging devices, the test reveals 3D ELMI is not as good as these techniques, primarily due to the substantial number of features produced by the proposed technique. Nevertheless, the promising applicability and the unique approach of the proposed technique to represent the 3D molecular structure of ATS drugs has been demonstrated and worth to receive further exploration in the future works.

ABSTRAK

Penyalahgunaan dadah perangsang jenis amfetamin (ATS) telah menjadi masalah sosial antarabangsa yang menakutkan. Batasan teknikal kit ujian semasa untuk mengesan jenama baru dadah ATS memberi cabaran kepada pihak penguat kuasa undang-undang dan kakitangan saintifik makmal forensik. Sementara itu, peranti pengimejan molekul yang membenarkan umat manusia untuk melihat struktur molekul tiga dimensi (3D) baru saja diperkenalkan, dan ianya dapat digunakan untuk mengatasi batasan kit ujian semasa. Oleh itu, teknik perwakilan struktur molekul 3D, atau deskriptor molekul 3D, berjenis baru yang dapat mewakili bentuk molekul 3D yang dikesan melalui peranti pengimejan molekul perlu dibangunkan. Salah satu kaedah pemprosesan imej untuk mewakili imej 3D ialah momen dan momen kekal 3D. Walau bagaimanapun, terdapat pelbagai masalah yang ditunjukkan oleh teknik momen dan momen kekal 3D sedia ada. Oleh itu, ianya penting untuk mencadangkan momen kekal 3D baru yang bebas dari masalah-masalah teknik sedia ada. Kajian ini membandingkan pelbagai teknik momen 3D dan berjaya mengenalpasti momen Legendre 3D sebagai teknik terbaik untuk dijadikan asas untuk membangunkan momen kekal 3D baru bernama momen kekal Legendre tepat 3D (3D ELMI), yang dapat digunakan untuk mewakili struktur molekul 3D dadah ATS. Disebabkan struktur molekul 3D dadah yang diperolehi dengan menggunakan peranti pengimejan molekul belum lagi tersedia, kajian ini mendapatkan struktur molekul 3D dadah ATS dari pangkalan data Pejabat Dadah dan Jenayah Pertubuhan Bangsa-bangsa Bersatu (UNODC) dan pihkal.info sebagai gantinya. Teknik yang dicadangkan dibandingkan dengan teknik momen kekal dan deskriptor molekul 3D sedia ada dari segi masa pemrosesan, penggunaan memori, kekekalan sebuah sampel, variasi dalam dan antar kelas, serta ketepatan pengelasan. Perbandingan yang dijalankan mendapati 3D ELMI berprestasi lebih baik berbanding momen kekal 3D sedia ada, seperti momen kekal geometrik 3D (3D GMI), momen kekal Gaussian–Hermite 3D (3D GHMI), dan deskriptor Zernike 3D (3D ZD). Hasil 3D ELMI yang memuaskan disebabkan oleh banyak faktor, antaranya kualiti asal Legendre 3D, pengiraan tepat Legendre 3D, dan juga kebaharuan teknik pengekalan yang dicadangkan. Teknik yang dicadangkan juga dibandingkan dengan deskriptor molekul 3D sedia ada, seperti deskriptor molekul holistik kekal berwajaran (WHIM), perhimpunan geometri, topologi, dan berat atom (GETAWAY), fungsi distribusi radial (RDF), dan perwakilan struktur molekul 3D berdasarkan pembelahan elektron (3D-MORSE). Walaupun 3D ELMI mampu mengatasi batasan deskriptor molekul 3D sedia ada yang bergantung kepada model struktur molekul 3D, ujian yang dijalankan mendedahkan bahawa 3D ELMI tidak sebaik deskriptor molekul 3D sedia ada, terutamanya disebabkan bilangan ciri-ciri yang banyak dari teknik yang dicadangkan. Walau bagaimanapun, kebolegunaan yang cerah dan pendekatan yang khas daripada teknik yang dicadangkan untuk mewakili struktur molekul 3D dadah ATS telah pun ditunjukkan dan berbaloi untuk diteroka secara lebih lanjut dalam kerja-kerja masa depan.

ACKNOWLEDGEMENTS

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

In the name of Allah, the Most Gracious and the Most Merciful, for without Him, I would never be where I am today. Not to forget, greetings and eulogy to our beloved, The Great Prophet Muhammad SAW, for without him, we'll still be living the age of darkness.

I am deeply indebted to lecturers of UTeM, especially those in FTMK, and to my supervisors: Assoc. Prof. Drs. Azah Kamilah Muda and Choo Yun Huoy for all their helps, supports, interests, valuable hints and patience, and to Prof. Dr. Ajith Abraham for his insightful wisdom and expertise. I'd also express gratitude to Prof. Ing. Dr. Jan Flusser and colleagues in UTIA, Czech Republic, Stephen Chapman and peers in Isomer Design Ltd., Canada, for assisting me in conducting this study. I'd also like to thank ICGEB, Italy, and UTeM for providing me financial support for my study, via CRP – ICGEB Research Grant (CRP/MYS13-03) and UTeM Postgraduate Fellowship (Zamalah) Scheme, respectively.

I am truly and forever obliged to Lustiana Pratiwi, for without her endearing support and loving company I wouldn't make this far, and with whom I have the greatest blessing from Him and the joy of my life, Mus'ab Khyrissiddiq Pratama. Especially, I would like to forever give my deepest and most special thanks to my parents, Dahrina and Fitrizal Raini, whose patient love and life-long teaching enabled me to complete this work and have pushed me to go this far. I'd also like to thank my parents-in-law, Sugianto and Lustiawati, for making me part of their family.

TABLE OF CONTENTS

	PAGE
DECLARATION	
APPROVAL	
DEDICATION	
ABSTRACT	i
ABSTRAK	ii
ACKNOWLEDGEMENTS	iii
TABLE OF CONTENTS	iv
LIST OF TABLES	vii
LIST OF FIGURES	xi
LIST OF ABBREVIATIONS	xxiv
LIST OF SYMBOLS	xxvii
LIST OF APPENDICES	xxix
LIST OF PUBLICATIONS	xxx
CHAPTER	
1 INTRODUCTION	1
1.1 Overview	1
1.2 Research Background	2
1.3 Problem Statements	6
1.4 Research Questions	8
1.5 Objectives	9
1.6 Hypothesis Statement	10
1.7 Scope	10
1.8 Research Significance	11
1.9 Thesis Organization	13
1.10 Summary	14
2 LITERATURE REVIEW	16
2.1 Introduction	16
2.2 Amphetamine-Type Stimulants (ATS)	16
2.3 ATS Drugs Identification and Analysis	23
2.4 Molecular Descriptors	34
2.4.1 Weighted Holistic Invariant Molecular Descriptors	38
2.4.2 Geometry, Topology, and Atom Weights Assembly Descriptors	41
2.4.3 Radial Distribution Function Descriptors	48
2.4.4 3D Molecule Representation of Structure Based on Electron Diffraction Descriptors	49
2.4.5 3D Zernike Descriptors	51
2.4.6 Review of 3D Molecular Descriptors	53
2.5 Moments and Moment Invariants Shape Descriptors	54
2.5.1 Geometric Moments and Moment Invariants	64
2.5.2 Complex Moments and Moment Invariants	70
2.5.3 Legendre Moments and Moment Invariants	74
2.5.4 Gegenbauer Moments and Moment Invariants	79
2.5.5 Gaussian–Hermite Moments and Moment Invariants	84

2.5.6	Discrete Chebyshev Moments and Moment Invariants	89
2.5.7	Weighted Krawtchouk Moments and Moment Invariants	97
2.5.8	Hahn Moments and Moment Invariants	101
2.5.9	Zernike Moments and Moment Invariants	107
2.5.10	Orthogonal Fourier–Mellin Moments and Moment Invariants	117
2.5.11	Chebyshev–Fourier Moments and Moment Invariants	121
2.5.12	Assessment of the Moments and Moment Invariants	124
2.6	Summary	126
3	RESEARCH METHODOLOGY	130
3.1	Introduction	130
3.2	Problem Situation and Solution Concept	131
3.2.1	Problem Situation	131
3.2.2	Solution Concept	133
3.3	Research Design	135
3.3.1	Investigation Phase	136
3.3.2	Implementation Phase	138
3.3.2.1	Research Development Process	138
3.3.2.2	Performance Measurement Process	139
3.4	Detailed Research Development Process	151
3.4.1	Dataset Preparation	151
3.4.2	Feature Extraction	166
3.4.3	Classification	172
3.5	Development Tools and Environmental Setup	178
3.6	Summary	178
4	A COMPARATIVE STUDY ON THE PERFORMANCES OF 3D MOMENTS TECHNIQUES	179
4.1	Introduction	179
4.2	Modification of Existing 2D to 3D Orthogonal Moments	180
4.2.1	3D Hahn Moments	180
4.2.2	3D Orthogonal Fourier–Mellin Moments	181
4.2.3	3D Chebyshev–Fourier Moments	181
4.3	Standardization of Moments	182
4.4	Results and Discussion	188
4.5	Summary	214
5	3D EXACT LEGENDRE MOMENT INVARIANTS	215
5.1	Introduction	215
5.2	Technique Formulations	215
5.2.1	3D Exact Legendre Moments	216
5.2.2	3D Exact Geometric Moment Invariants	221
5.2.3	3D Exact Legendre Moment Invariants	227
5.3	Performance Measurements	231
5.3.1	Comparison with 3D Approximated Legendre Moments	233
5.3.2	Comparison of Two Versions of 3D Exact Legendre Moment Invariants	241

5.3.3	Comparison with Existing 3D Moment Invariants	246
5.3.4	Comparison with Existing 3D Molecular Descriptors	266
5.4	Summary	293
6	CONCLUSION	295
6.1	Introduction	295
6.2	Research Summary	295
6.3	Research Findings	298
6.3.1	3D Exact Legendre Moments and Moment Invariants	298
6.3.2	3D Exact Geometric Moments and Moment Invariants	301
6.3.3	3D Hahn Moments	302
6.3.4	3D Orthogonal Fourier–Mellin Moments	302
6.3.5	3D Chebyshev–Fourier Moments	303
6.3.6	2D Molecular Structure to 3D Binary Voxel Converter	303
6.3.7	3D Moments and Moment Invariants Calculator and Viewer	305
6.3.8	Complex Number Representation	307
6.3.9	Database of ATS Drugs Molecular Structure in Various Format	307
6.4	Research Contributions	309
6.5	Research Limitations	311
6.6	Recommendations for Future Works	312
6.6.1	Feature Selection	312
6.6.2	Generation of Moment Invariants from Higher Order Moments	313
6.6.3	Validation of 3D Exact Geometric Moment Invariants	313
6.6.4	Exploration on the Other 3D Moments	314
6.6.5	Application of Exact Computation and Proposed Invariants to Other 3D Moments	315
6.6.6	Classification Technique for the 3D Moment Invariants for 3D Molecular Structure Representation	315
6.7	Summary	316
	REFERENCES	317
	APPENDICES	358

LIST OF TABLES

TABLE	TITLE	PAGE
2.1	WHIM descriptors	39
2.2	GETAWAY descriptors based on matrix operators and information indices	44
2.3	GETAWAY descriptors based on autocorrelation functions	46
3.1	Summary of the investigation phase	137
3.2	Sample of first 5 extracted features of ecstasy using existing molecular descriptors	172
3.3	Summary of classifiers parameters	174
3.4	Overview of frequently used molecular similarity coefficients	176
4.1	Polar Cantor, polar Szudzik, polar bit-interleaved, and Cartesian bit-interleaved pairing functions values of zeroth-order moments for each 3D moments of ecstasy	187
4.2	Average of processing time, memory consumption, and intra-class variance ratio of 3D moments	189
4.3	Average of classification accuracies of 3D moments represented using polar Cantor pairing function	191
4.4	Average of classification accuracies of 3D moments represented using polar Szudzik pairing function	192
4.5	Average of classification accuracies of 3D moments represented using polar bit-interleaved pairing function	192
4.6	Average of classification accuracies of 3D moments represented using	193

	Cartesian bit-interleaved pairing function	
4.7	Sum of ranks of 3D moments	197
4.8	Tests of normality for random forests classification accuracy of 3D moments	199
4.9	Tests of normality for RIPPER classification accuracy of 3D moments	200
4.10	Ranks for random forests classification accuracy	204
4.11	Kruskal–Wallis H test results for random forests classification accuracy	205
4.12	Post-hoc test results using multiple Mann–Whitney U tests for random forests classification accuracy of 3D Legendre moments	205
4.13	Ranks for RIPPER classification accuracy of polar Cantor and polar bit-interleaved	207
4.14	Kruskal–Wallis H test results for RIPPER classification accuracy of polar Cantor and polar bit-interleaved	207
4.15	Post-hoc test results using multiple Mann–Whitney U tests for RIPPER classification accuracy of polar Cantor and polar bit-interleaved for 3D Legendre moments	208
4.16	Test of homogeneity of variances results for RIPPER classification accuracy of polar Szudzik and Cartesian bit-interleaved	209
4.17	ANOVA results for RIPPER classification accuracy of polar Szudzik and Cartesian bit-interleaved	209
4.18	Robust tests of equality of means results for RIPPER classification accuracy of polar Szudzik and Cartesian bit-interleaved	209
4.19	Post-hoc test results using Tukey HSD and Games–Howell tests for RIPPER classification accuracy of polar Szudzik and Cartesian bit-interleaved for 3D Legendre moments	210
5.1	Average of processing time, memory consumption, and intra-class variance ratio of 3D approximated and exact Legendre moments	234

5.2	Average of classification accuracies of 3D approximated and exact Legendre moments represented using proposed pairing functions	234
5.3	Tests of normality for random forests classification accuracy of 3D approximated and exact Legendre moments	238
5.4	Tests of normality for RIPPER classification accuracy of 3D approximated and exact Legendre moments	238
5.5	Levene's equality of variances tests of 3D approximated and exact Legendre moments	239
5.6	Independent samples <i>t</i> -test for equality of means for 3D approximated and exact Legendre moments	240
5.7	Average of processing time, memory consumption, and single instance invariance ratio of 3D exact Legendre moment invariants	242
5.8	Average of classification accuracies of 3D exact Legendre moment invariants	243
5.9	Percentage of single instance invariance of 3D moment invariants	248
5.10	Percentage of intra- and inter-class variance of 3D moment invariants	248
5.11	Average of classification accuracies of 3D moment invariants	249
5.12	Difference of two scenarios classification accuracies of 3D moment invariants	256
5.13	Tests of normality for classification accuracy of 3D moment invariants	258
5.14	Ranks for classification accuracy of 3D moment invariants	261
5.15	Kruskal–Wallis <i>H</i> test results for classification accuracy of 3D moment invariants	262
5.16	Post-hoc test results using multiple Mann–Whitney <i>U</i> tests for classification accuracy of 3D ELMI against existing 3D moment invariants	263
5.17	Percentage of single instance invariance of 3D molecular descriptors	267
5.18	Percentage of intra- and inter-class variance of 3D molecular descriptors	267

5.19	Average of classification accuracies of 3D molecular descriptors	268
5.20	Difference of two scenarios classification accuracies of 3D molecular descriptors	278
5.21	Tests of normality for classification accuracy of 3D molecular descriptors	280
5.22	Ranks for classification accuracy of 3D molecular descriptors	283
5.23	Kruskal–Wallis H test results for classification accuracy of 3D molecular descriptors	285
5.24	Post-hoc test results using multiple Mann–Whitney U tests for classification accuracy of 3D ELMI against existing 3D molecular descriptors	286
A.1	Sample of drugs molecular information	358

LIST OF FIGURES

FIGURE	TITLE	PAGE
1.1	Thesis organization	14
2.1	2D molecular structure of β -phenethylamine (United Nations Office of Drugs and Crime, 2006b)	17
2.2	Basic 2D molecular structure of ATS	19
2.3	Sub-groups of ATS per substitution patterns: (a) no substitution, (b) methylenedioxy-substitution, and (c) other substitution patterns	20
2.4	Samples of ATS drug molecular structure: (a) amphetamine, (b) methamphetamine, (c) 2C-B, (d) MDMA, and (e) fenethylamine	21
2.5	Categories of drug identification and analysis methods (Spectra Analysis, 2009)	26
2.6	2D molecular structure of (a) <i>d</i> -methamphetamine and (b) <i>l</i> -methamphetamine	29
2.7	3D molecular structure of (a) <i>d</i> -methamphetamine and (b) <i>l</i> -methamphetamine	30
2.8	2D molecular structure of structurally similar ATS, (a) 2C-B and (b) 2C-C	30
2.9	Comparison of STM images, nc-AFM images, and 3D molecular structures model (de Oteyza <i>et al.</i> , 2013)	33
2.10	Taxonomy of moments	61
2.11	Orthogonal moments	62

2.12	Summary of the flow and coverage of the literature review	129
3.1	Research design	136
3.2	Summary of performance measurement phase	150
3.3	Summary of the	151
3.4	MarvinSketch used to draw 2D molecular structure	153
3.5	MarvinSketch used for 3D conversion	154
3.6	Jmol used for verifying conversion process and converting to VRML file	155
3.7	Rotation transformation results of one molecular structure	156
3.8	binvox used to convert VRML to BINVOX format	158
3.9	Output of the voxelization process visualized using viewvox	158
3.10	Voxelization results of the same molecular structure from training dataset (blue) and testing datasets (red)	159
3.11	Open Babel used to convert MDL SDF to (a) MOP and (b) PDB format	161
3.12	MOPAC2016 used to convert MOP to OUT format	163
3.13	Summary of dataset preparation phase	165
3.14	E-Dragon software to calculate molecular descriptors (a) by uploading SDF format and (b) view the result	167
3.15	3dmorse used to calculate 3D-MoRSE descriptors from OUT format	169
3.16	3D-SURFER used to calculate 3D Zernike descriptors (a) by uploading PDB format and (b) view the result	170
3.17	Summary of feature extraction phase	172
3.18	Procedures taken during the classification phase during (a) preliminary and (b) benchmark studies	177
4.1	Average of processing time of 3D moments (nanoseconds/voxel)	189
4.2	Average of memory consumption of 3D moments (bytes/voxel)	190
4.3	Average of intra- and inter-class variance ratio of 3D moments	191

4.4	Average of classification accuracies of 3D moments represented using polar Cantor pairing function	193
4.5	Average of classification accuracies of 3D moments represented using polar Szudzik pairing function	194
4.6	Average of classification accuracies of 3D moments represented using polar bit-interleaved pairing function	195
4.7	Average of classification accuracies of 3D moments represented using Cartesian bit-interleaved pairing function	196
5.1	The proposed translation invariant is applied to three different original images and produces same image projection	223
5.2	Average of classification accuracies of 3D approximated and exact Legendre moments represented using polar Cantor pairing function	235
5.3	Average of classification accuracies of 3D approximated and exact Legendre moments represented using polar Szudzik pairing function	235
5.4	Average of classification accuracies of 3D approximated and exact Legendre moments represented using polar bit-interleaved pairing function	236
5.5	Average of classification accuracies of 3D approximated and exact Legendre moments represented using Cartesian bit-interleaved pairing function	236
5.6	Average of classification accuracies of 3D exact Legendre moment invariants for classification of known drugs molecular structure	244
5.7	Average of classification accuracies of 3D exact Legendre moment invariants for classification of unknown drugs molecular structure	245
5.8	Percentage of single instance invariance of 3D moment invariants	248
5.9	Percentage of intra- and inter-class variance of 3D moment invariants	248
5.10	Average of random forests classification accuracies of 3D moment invariants	250
5.11	Average of naïve Bayes classification accuracies of 3D moment invariants	250

5.12	Average of SVM classification accuracies of 3D moment invariants	251
5.13	Average of C4.5 classification accuracies of 3D moment invariants	251
5.14	Average of RIPPER classification accuracies of 3D moment invariants	251
5.15	Average of <i>k</i> -NN–Tanimoto coefficient classification accuracies of 3D moment invariants	252
5.16	Average of <i>k</i> -NN–Hodgkin coefficient classification accuracies of 3D moment invariants	252
5.17	Average of <i>k</i> -NN–Cosine coefficient classification accuracies of 3D moment invariants	253
5.18	Average of <i>k</i> -NN–Pearson coefficient classification accuracies of 3D moment invariants	253
5.19	Average of <i>k</i> -NN–Euclidian distance classification accuracies of 3D moment invariants	254
5.20	Average of <i>k</i> -NN–Hamming distance classification accuracies of 3D moment invariants	254
5.21	Average of <i>k</i> -NN–Soergel distance classification accuracies of 3D moment invariants	255
5.22	Percentage of single instance invariance of 3D molecular descriptors	267
5.23	Percentage of intra- and inter-class variance of 3D molecular descriptors	268
5.24	Average of random forests classification accuracies of 3D molecular descriptors	270
5.25	Average of naïve Bayes classification accuracies of 3D molecular descriptors	271
5.26	Average of SVM classification accuracies of 3D molecular descriptors	271
5.27	Average of C4.5 classification accuracies of 3D molecular descriptors	272
5.28	Average of RIPPER classification accuracies of 3D molecular descriptors	272
5.29	Average of <i>k</i> -NN–Tanimoto coefficient classification accuracies of 3D	273

	molecular descriptors	
5.30	Average of k -NN–Hodgkin coefficient classification accuracies of 3D molecular descriptors	273
5.31	Average of k -NN–Cosine coefficient classification accuracies of 3D molecular descriptors	274
5.32	Average of k -NN–Pearson coefficient classification accuracies of 3D molecular descriptors	274
5.33	Average of k -NN–Euclidian distance classification accuracies of 3D molecular descriptors	275
5.34	Average of k -NN–Hamming distance classification accuracies of 3D molecular descriptors	275
5.35	Average of k -NN–Soergel distance classification accuracies of 3D molecular descriptors	276
5.42	3D molecular structure ecstasy with (a) original atom coordinates and (b) randomized atom coordinates	292
6.1	Proposed software to convert 2D molecular structure to 3D binary voxel grid	304
6.2	Proposed software to calculate the 3D moments and moment invariants by (a) setting the parameters and (b) executing the calculation	306
6.3	Proposed software to view the 3D moments and moment invariants results	307
B.1	Normal Q-Q plot of random forests classification accuracy for 3D geometric moments	362
B.2	Normal Q-Q plot of random forests classification accuracy for 3D complex moments	363
B.3	Normal Q-Q plot of random forests classification accuracy for 3D Legendre moments	363
B.4	Normal Q-Q plot of random forests classification accuracy for 3D	364

	Gegenbauer moments	
B.5	Normal Q-Q plot of random forests classification accuracy for 3D Gaussian– Hermite moments	364
B.6	Normal Q-Q plot of random forests classification accuracy for 3D discrete Chebyshev moments	365
B.7	Normal Q-Q plot of random forests classification accuracy for 3D weighted Krawtchouk moments	365
B.8	Normal Q-Q plot of random forests classification accuracy for 3D Hahn moments	366
B.9	Normal Q-Q plot of random forests classification accuracy for 3D Zernike moments	366
B.10	Normal Q-Q plot of random forests classification accuracy for 3D orthogonal Fourier–Mellin moments	367
B.11	Normal Q-Q plot of random forests classification accuracy for 3D Chebyshev–Fourier moments	367
B.12	Normal Q-Q plot of RIPPER classification accuracy for 3D geometric moments	368
B.13	Normal Q-Q plot of RIPPER classification accuracy for 3D complex moments	368
B.14	Normal Q-Q plot of RIPPER classification accuracy for 3D Legendre moments	369
B.15	Normal Q-Q plot of RIPPER classification accuracy for 3D Gegenbauer moments	369
B.16	Normal Q-Q plot of RIPPER classification accuracy for 3D Gaussian– Hermite moments	370
B.17	Normal Q-Q plot of RIPPER classification accuracy for 3D discrete	370

	Chebyshev moments	
B.18	Normal Q-Q plot of RIPPER classification accuracy for 3D weighted Krawtchouk moments	371
B.19	Normal Q-Q plot of RIPPER classification accuracy for 3D Hahn moments	371
B.20	Normal Q-Q plot of RIPPER classification accuracy for 3D Zernike moments	372
B.21	Normal Q-Q plot of RIPPER classification accuracy for 3D orthogonal Fourier–Mellin moments	372
B.22	Normal Q-Q plot of RIPPER classification accuracy for 3D Chebyshev–Fourier moments	373
C.1	Average of processing time of 3D approximated and exact Legendre moments (nanoseconds/voxel)	374
C.2	Average of memory consumption of 3D approximated and exact Legendre moments (bytes/voxel)	374
C.3	Average of intra- and inter-class variance ratio of 3D approximated and exact Legendre moments	375
C.4	Processing time of 3D exact Legendre moment invariants (nanoseconds/voxel)	375
C.5	Memory consumption of 3D exact Legendre moment invariants (bytes/voxel)	375
C.6	Percentage of single instance invariance of 3D exact Legendre moment invariants	376
D.1	Normal Q-Q plot of random forests classification accuracy for 3D exact Legendre moments	377
D.2	Normal Q-Q plot of RIPPER classification accuracy for 3D exact Legendre moments	378
D.3	Normal Q-Q plot of random forests classification accuracy of 3D moments invariants for classification of known drugs molecular structure	379

D.4	Normal Q-Q plot of random forests classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	379
D.5	Normal Q-Q plot of naïve Bayes classification accuracy of 3D moments invariants for classification of known drugs molecular structure	380
D.6	Normal Q-Q plot of naïve Bayes classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	380
D.7	Normal Q-Q plot of SVM classification accuracy of 3D moments invariants for classification of known drugs molecular structure	381
D.8	Normal Q-Q plot of SVM classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	381
D.9	Normal Q-Q plot of C4.5 classification accuracy of 3D moments invariants for classification of known drugs molecular structure	382
D.10	Normal Q-Q plot of C4.5 classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	382
D.11	Normal Q-Q plot of RIPPER classification accuracy of 3D moments invariants for classification of known drugs molecular structure	383
D.12	Normal Q-Q plot of RIPPER classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	383
D.13	Normal Q-Q plot of <i>k</i> -NN–Tanimoto coefficient classification accuracy of 3D moments invariants for classification of known drugs molecular structure	384
D.14	Normal Q-Q plot of <i>k</i> -NN–Tanimoto coefficient classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	384
D.15	Normal Q-Q plot of <i>k</i> -NN–Cosine coefficient classification accuracy of 3D moments invariants for classification of known drugs molecular structure	385
D.16	Normal Q-Q plot of <i>k</i> -NN–Cosine coefficient classification accuracy of 3D moments invariants for classification of unknown drugs molecular structure	385