Faculty of Information and Communication Technology

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

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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 dataPejabat 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, penggunakan 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, kebolehgunaan 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.

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