

Yufeng Jane Tseng



Professor

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CURRENT POSITIONS:

- 2015 – **Director**, Drug Research Center, National Taiwan University
- 2014 – **Professor**, Graduate Institute of Biomedical Electronics, and
Bioinformatics, Department of Computer Science and Information
Engineering, School of Pharmacy, National Taiwan University, Taiwan
- 2009 – **Principle Investigator**, Metabolomics Core Laboratory, Genomic Center,
National Taiwan University

PROFESSIONAL EXPERIENCES:

- 2010 – 2015 **Group Leader**, Molecular modeling unit, Drug Research Center,
National Taiwan University
- 2008 – 2014 **Associate Professor**, Graduate Institute of Biomedical
Electronics, and Bioinformatics, Department of Computer Science
and Information Engineering, School of Pharmacy, National
Taiwan University, Taiwan
- 2006 – 2008 **Assistant Professor**, Institute of Biomedical Electronics, and
Bioinformatics, Department of Computer Science and
Information Engineering (joint position), School of Pharmacy
(joint position since 2007), National Taiwan University, Taipei,
Taiwan
- 2004 – 2006 **Research Fellow**, National Center of Biotechnology Information,
National Institute of Health, Bethesda, MD, USA
- 1998 – 2006 **Principal Molecular Modeling Software Developer**, The
Chem21 Group, Inc., Lake Forest, USA

HONORS AND AWARDS

- 2015 Drug Repurposing Innovation Award, TWi Pharmaceutical Foundation,
Taiwan
- 2015 IBM Faculty Award, USA
- 2013 NTU EECS Outstanding Research Contribution Award, Taiwan
- 2013 American Chemical Society Chemluminary award, USA

- 2012 American Chemical Society Innovation Award, USA
- 2005- 2006 Intramural Training Award, National Center of Biotechnology Information, National Institute of Health, Bethesda, MD, USA
- 2001 Charles Bell Award for Computational Chemistry, University of Illinois at Chicago, Chicago, IL, USA

SELECTED PROFESSIONAL SERVICES

Guest-Editor-in-Chief, Special Issue, The Journal of Combinatorial Chemistry and High Throughput Screening, 2013

Editorial Advisor, The Journal of Molecular Graphics and Modelling (~2013)

Editorial Advisor, The Journal of Combinatorial Chemistry and High Throughput Screening (~ 2013)

Grant Viewer, National Science of Council (Integrated interdisciplinary program) 2007, 2008, 2009, 2010, (Biomedical Informatics), 2009, 2010, 2011,2012,2013 Taiwan

Ad hoc Grant Reviewer, Agency for Science, Technology and Research (A*STAR), Singapore, 2010

Programming Board, Division of Computers in Chemistry, American Chemical Society National Meetings, since 2010

Reviewer, Scientific Reports, PLOS One, Journal of Toxicological Sciences, Journal of Molecular Modeling, Journal of Chemical Information and Modeling, Journal of Chemical Information and Computer Science, Journal of the Biomedical Sciences, Journal of the Formosan Medical Association, Journal of the Taiwan Institute of Chemical Engineers, Journal of Biomedical Engineering: Applications, Basis and Communications

Registered Pharmacist, Taiwan, since 1997

EDUCATION:

2002 - Ph.D., Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL

1997 – B.S., Pharmacy, National Taiwan University, Taiwan

SELECTED PEER-REVIEWED PUBLICATIONS (IN CHRONOLOGICAL ORDER SINCE 2003)

Journal paper:

1. Chiu, H. H., Tsai, S. J., Tseng, Y. J., Wu, M. S., Liao, W. C., Huang, C. S., & Kuo, C. H. (2015). An efficient and robust fatty acid profiling method for plasma metabolomic studies by gas chromatography–mass spectrometry. *Clinica*

Chimica Acta, In press. (IF = 2.824, Ranking=7/31, 22% Category: Medical Laboratory Technology)

2. Tzeng, T. H., Kuo, C. Y., Wang, S. Y., Huang, P. K., Kuo, P. H., Huang, Y. M., Tseng, Y. J.*, Tian, W. C., Lee, S. C., & Lu, S. S., (2015). A portable micro gas chromatography system for volatile compounds detection with 15ppb of sensitivity, *IEEE Journal of Solid-State Circuits*, *accepted*. (IF=3.009, Ranking = 23/249, 9%, Category: Engineering, Electrical & Electronic)
3. Chen, G. Y., Liao, H. W., Tsai, I.L., Tseng, Y. J., & Kuo, C. H., (2015). Using the matrix-induced ion suppression method for concentration normalization in cellular metabolomics studies. *Analytical chemistry*, 87(19), 9731-9739. (IF=5.636, Ranking = 4/74, 5%, Category: Chemistry, Analytical)
4. Lin, M. I., Su, B. H., Lee, C. H., Wang, S. T., Wu, W. C., Dangate, P., Wang, S. Y., Huang, W. I., Cheng, T. J., Lin, O. A., Cheng, Y. S., Tseng, Y. J.*, & Sun, C. M. (2015). Synthesis and inhibitory effects of novel pyrimido-pyrrolo-quinoxalinedione analogues targeting nucleoproteins of influenza A virus H1N1. *European journal of medicinal chemistry*, 102, 477-486 (IF =3.447, Ranking = 11/59, 18%, Category: Chemistry, Medicinal)
5. Lai, Y. S., Chen, W. C., Kuo, T. C., Ho, C. T., Kuo, C. H., Tseng, Y. J., ... & Sheen, L. Y. (2015). Mass spectrometry-based serum metabolomics of a C57BL/6J mouse model of high-fat diet induced nonalcoholic fatty liver disease development. *Journal of Agricultural and Food Chemistry*, 63(35), 7873-7884. (IF = 2.912, Ranking=2/56, 3%, Category: Agriculture, Multidisciplinary)
6. Esposito, E. X., Hopfinger, A. J., Shao, C. Y., Su, B. H., Chen, S. Z., & Tseng, Y. J. (2015). Exploring possible mechanisms of action for the nanotoxicity and protein binding of decorated nanotubes: Interpretation of physicochemical properties from optimal QSAR models. *Toxicology and applied pharmacology*, 288(1), 52-62. (IF =3.705, Ranking = 13/88, 14%, Category: Toxicology)
7. Su, B. H., Tu, Y. S., Lin, C, Shao, C. Y., Lin, O. A., & Tseng, Y. J.* (2015). Rule-based Prediction Models of Cytochrome P450 Inhibition. *Journal of chemical information and modeling*, 55(7), 1426-1434. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
8. Chen H. H., Tseng, Y. J., Wang, S. Y., Tsai, Y. S., Chang, C. S., Kuo, T. C., Yao, W. J., Shieh, C. C., Wu, C. H., & Kuo, P. H. (2015). The metabolome profiling and pathway analysis in metabolic healthy and abnormal. *International Journal of Obesity*, 39(8), 1241-1248. (IF =5.004, Ranking = 8/77, 10%, Category: Nutrition & Dietetics)

9. Su, B. H., Tu, Y. S., Lin, O. A., Harn, Y. C., Shen, M. Y., & Tseng, Y. J.* (2015). Rule-based Classification Models of Molecular Autofluorescence. *Journal of chemical information and modeling*, 55(2), 434-445. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
10. Wang, S. Y., Kuo, C. H., & Tseng, Y. J.* (2015). An Ion Trace Detection Algorithm to Extract Pure Ion Chromatograms to Improve Untargeted Peak Detection Quality for Liquid Chromatography/Time-of-Flight Mass Spectrometry-based Metabolomics Data. *Analytical chemistry*, 87(5), 3048-3055 (IF=5.636, Ranking = 4/74, 5%, Category: Chemistry, Analytical)
11. Chen, G. Y., Liao, H. W., Tseng, Y. J., Tsai, I. L., & Kuo, C. H. (2015). A matrix-induced ion suppression method to normalize concentration in urinary metabolomics studies using flow injection analysis electrospray ionization mass spectrometry. *Analytica Chimica Acta*, 864, 21-29 (IF= 4.513, Ranking = 5/74, 6%, Category: Chemistry, Analytical)
12. Shao, C. Y., Su, B. H., Tu, Y. S., Lin, C., Lin, O. A., & Tseng, Y. J.* (2015). CypRules: A rule-based P450 inhibition prediction server. *Bioinformatics*, 31(11), 1869-1871. (IF = 4.981, Ranking = 3/57, 5%, Category: Mathematical & Computational Biology)
13. Hung, C. S., Li, H. Y., Kuo, C. H., Lin, M. S., Kuo, T. C., Tsai, S. J., Liu, P. H., Lin, C. H., Yang, C.Y., Chuang, L.M., Chen, M.F., Tseng, Y.J.*, & Kao, H. L. (2015). Fasting But Not Changes of Plasma Metabolome During Oral Glucose Tolerance Tests Improve the Diagnosis of Severe Coronary Arterial Stenosis. *Clinical endocrinology*. (IF = 3.457, Ranking=48/128, 37% Category: Endocrinology & Metabolism)
14. Chen, G. Y., Chiu, H. H., Lin, S. W., Tseng, Y. J., Tsai, S. J., & Kuo, C. H. (2015). Development and application of a comparative fatty acid analysis method to investigate voriconazole-induced hepatotoxicity. *Clinica Chimica Acta*, 438, 126-134. (IF = 2.764, Ranking=7/31, 22% Category: Medical Laboratory Technology)
15. Lin, S. W., Kang, W. Y., Lin, D. T., Lee, J. C., Wu, F. L. L., Chen, C. L., & Tseng, Y. J.* (2014). Comparison of warfarin therapy clinical outcomes following implementation of an automated mobile phone-based critical laboratory value text alert system. *BMC medical genomics*, 7(Suppl 1), S13. (IF = 2.873, Ranking=69/167, 41% Category: Genetics & Heredity)
16. Su, B. H., Huang, Y. S., Chang, C. Y., Tu, Y. S., & Tseng, Y. J.* (2013). Template-Based de Novo Design for Type II Kinase Inhibitors and Its Extended

Application to Acetylcholinesterase Inhibitors. *Molecules*, 18(11), 13487-13509. (IF = 2.416, Ranking=22/58, 37%, Category: Chemistry, Organic)

17. Tsai, I. L., Weng, T. I., Tseng, Y. J., Tan, H. K. L., Sun, H. J., & Kuo, C. H. (2013). Screening and Confirmation of 62 Drugs of Abuse and Metabolites in Urine by Ultra-High-Performance Liquid Chromatography–Quadrupole Time-of-Flight Mass Spectrometry. *Journal of analytical toxicology*, 37(9), 642-651. (IF = 2.858, Ranking=18/74, 24% Category: Chemistry, Analytical)
18. Liu, C. T., Raghu, R., Lin, S. H., Wang, S. Y., Kuo, C. H., Tseng, Y. J., & Sheen, L. Y. (2013). Metabolomics of ginger essential oil against alcoholic fatty liver in mice. *Journal of agricultural and food chemistry*, 61(46), 11231-11240. (IF = 2.912, Ranking=2/56, 3%, Category: Agriculture, Multidisciplinary)
19. Kuo, T. C., Tian, T. F., & Tseng, Y. J.* (2013). 3Omics: a web-based systems biology tool for analysis, integration and visualization of human transcriptomic, proteomic and metabolomic data. *BMC systems biology*, 7(1), 64. (IF = 2.435, Ranking= 13/57, 22%, Category: Mathematical & Computational Biology)
20. Tsai, I. L., Kuo, T. C., Ho, T. J., Harn, Y. C., Wang, S. Y., Fu, W. M., ... & Tseng, Y. J.* (2013). Metabolomic dynamic analysis of hypoxia in MDA-MB-231 and the comparison with inferred metabolites from transcriptomics data. *Cancers*, 5(2), 491-510.
21. Huang, C. C., McDermott, M. M., Liu, K., Kuo, C. H., Wang, S. Y., Tao, H., & Tseng, Y. J.* (2013). Plasma metabolomic profiles predict near-term death among individuals with lower extremity peripheral arterial disease. *Journal of vascular surgery*, 58(4), 989-996. (IF = 3.021, Ranking= 33/198, 16%, Category: Surgery)
22. Tseng, Y. J.*, Martin, E., Bologa, C. G., & Shelat, A. A. (2013). Cheminformatics aspects of high throughput screening: from robots to models: symposium summary. *Journal of computer-aided molecular design*, 27(5), 443-453. (IF =2.99, Ranking = 12/102, 11%, Category: Computer Science, Interdisciplinary Applications)
23. Tseng, Y. J., Kuo, C. T., Wang, S. Y., Liao, H. W., Chen, G. Y., Ku, Y. L., Shao, W.C., & Kuo, C. H. (2013). Metabolomic characterization of rhubarb species by capillary electrophoresis and ultra - high - pressure liquid chromatography. *Electrophoresis*, 34(19), 2918-2927. (IF = 3.028, Ranking= 14/74, 18%, Category: Chemistry, Analytical)
24. Chang, C. Y., Hsu, M. T., Esposito, E. X., & Tseng, Y. J.* (2013). Oversampling to overcome overfitting: exploring the relationship between data set composition,

molecular descriptors, and predictive modeling methods. *Journal of chemical information and modeling*, 53(4), 958-971. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)

25. Ho, T. J., Kuo, C. H., Wang, S. Y., Chen, G. Y., & Tseng, Y. J.* (2013). True ion pick (TIPick): a denoising and peak picking algorithm to extract ion signals from liquid chromatography/mass spectrometry data. *Journal of Mass Spectrometry*, 48(2), 234-242. (IF= 2.379, Ranking = 14/44, 31%, Category: Spectroscopy)
26. Tsai, D. M., Kang, J. J., Lee, S. S., Wang, S. Y., Tsai, I. L., Chen, G. Y., Liao, H. W., Li, W.C., Kuo, C.H., & Tseng, Y. J.* (2013). Metabolomic analysis of complex Chinese remedies: examples of induced nephrotoxicity in the mouse from a series of remedies containing aristolochic acid. *Evidence-Based Complementary and Alternative Medicine*, 2013. (IF =1.88, Ranking = 7/24, 29%, Category: Integrative & Complementary Medicine)
27. Shao, C. Y., Chen, S. Z., Su, B. H., Tseng, Y. J.*, Esposito, E. X., & Hopfinger, A. J. (2013). Dependence of QSAR models on the selection of trial descriptor sets: a demonstration using nanotoxicity endpoints of decorated nanotubes. *Journal of chemical information and modeling*, 53(1), 142-158. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
28. Wang, K. C., Wang, S. Y., Kuo, C. H., & Tseng, Y. J.* (2012). Distribution-based classification method for baseline correction of metabolomic 1D proton nuclear magnetic resonance spectra. *Analytical chemistry*, 85(2), 1231-1239. (IF=5.636, Ranking = 4/74, 5%, Category: Chemistry, Analytical)
29. Wang, S. Y., Kuo, C. H., & Tseng, Y. J.* (2012). Batch Normalizer: a fast total abundance regression calibration method to simultaneously adjust batch and injection order effects in liquid chromatography/time-of-flight mass spectrometry-based metabolomics data and comparison with current calibration methods. *Analytical chemistry*, 85(2), 1037-1046. (IF=5.636, Ranking = 4/74, 5%, Category: Chemistry, Analytical)
30. Jansen, J. M., Amaro, R. E., Cornell, W., Tseng, Y. J., & Walters, W. P. (2012). Computational chemistry and drug discovery: a call to action. *Future medicinal chemistry*, 4(15), 1893-1896. (IF = 3.744, Ranking = 8/59, 13%, Category: Chemistry, Medicinal)
31. Jansen, J. M., Cornell, W., Tseng, Y. J.*, & Amaro, R. E. (2012). Teach–Discover–Treat (TDT): Collaborative computational drug discovery for neglected diseases. *Journal of Molecular Graphics and Modelling*, 38, 360-362.

(IF = 1.722, Ranking = 36/102, 35%, Category: Computer Science, Interdisciplinary Applications)

32. Su, B. H., Tu, Y. S., Esposito, E. X., & Tseng, Y. J.* (2012). Predictive toxicology modeling: protocols for exploring hERG classification and *Tetrahymena pyriformis* end point predictions. *Journal of chemical information and modeling*, 52(6), 1660-1673. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
33. Kuo, C. H., Wang, K. C., Tian, T. F., Tsai, M. H., Chiung, Y. M., Hsieh, C. M., Tsai, S. J., Wang, S. Y., Tsai, D. M., Huang, C.C., & Tseng, Y. J.* (2012). Metabolomic characterization of laborers exposed to welding fumes. *Chemical research in toxicology*, 25(3), 676-686. (IF =3.529, Ranking = 10/59, 16%, Category: Chemistry, Medicinal)
34. Tseng, Y. J., Hopfinger, A. J., & Esposito, E. X. (2012). The great descriptor melting pot: mixing descriptors for the common good of QSAR models. *Journal of computer-aided molecular design*, 26(1), 39-43. (IF =2.99, Ranking = 12/102, 11%, Category: Computer Science, Interdisciplinary Applications)
35. Lin, F. Y., & Tseng, Y. J.* (2011). Structure-based fragment hopping for lead optimization using predocked fragment database. *Journal of chemical information and modeling*, 51(7), 1703-1715. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
36. Shen, M. Y., Su, B. H., Esposito, E. X., Hopfinger, A. J., & Tseng, Y. J.* (2011). A comprehensive support vector machine binary hERG classification model based on extensive but biased end point hERG data sets. *Chemical research in toxicology*, 24(6), 934-949. (IF =3.529, Ranking = 10/59, 16%, Category: Chemistry, Medicinal)
37. Wang, S. Y., Ho, T. J., Kuo, C. H., & Tseng, Y. J.* (2010). Chromaligner: a web server for chromatogram alignment. *Bioinformatics*, 26(18), 2338-2339. (IF = 4.981, Ranking = 3/57, 5%, Category: Mathematical & Computational Biology)
38. Su, B. H., Shen, M. Y., Esposito, E. X., Hopfinger, A. J., & Tseng, Y. J.* (2010). In silico binary classification QSAR models based on 4D-fingerprints and MOE descriptors for prediction of hERG blockage. *Journal of chemical information and modeling*, 50(7), 1304-1318. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
39. Kuo, C. H., Lee, C. W., Lin, S. C., Tsai, I. L., Lee, S. S., Tseng, Y. J., ... & Wei-Chu, L. (2010). Rapid determination of aristolochic acids I and II in herbal

products and biological samples by ultra-high-pressure liquid chromatography–tandem mass spectrometry. *Talanta*, 80(5), 1672-1680. (IF =3.545, Ranking = 11/74, 14%, Category: Chemistry, Analytical)

40. Zheng, T., Hopfinger, A. J., Esposito, E. X., Liu, J., & Tseng, Y. J.* (2008). Membrane-Interaction Quantitative Structure– Activity Relationship (MI-QSAR) Analyses of Skin Penetration Enhancers. *Journal of chemical information and modeling*, 48(6), 1238-1256. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
41. Liu, J., Kern, P. S., Gerberick, G. F., Santos-Filho, O. A., Esposito, E. X., Hopfinger, A. J., & Tseng, Y. J.* (2008). Categorical QSAR models for skin sensitization based on local lymph node assay measures and both ground and excited state 4D-fingerprint descriptors. *Journal of computer-aided molecular design*, 22(6-7), 345-366. (IF =2.99, Ranking = 12/102, 11%, Category: Computer Science, Interdisciplinary Applications)
42. Iyer, M., Zheng, T., Hopfinger, A. J., & Tseng, Y. J.* (2007). QSAR analyses of skin penetration enhancers. *Journal of chemical information and modeling*, 47(3), 1130-1149. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
43. Li, Y., Pan, D., Liu, J., Kern, P. S., Gerberick, G. F., Hopfinger, A. J., & Tseng, Y. J.* (2007). Categorical QSAR models for skin sensitization based upon local lymph node assay classification measures Part 2: 4D-Fingerprint three-state and two-2-state logistic regression models. *Toxicological sciences*, 99(2), 532-544. (IF =3.854, Ranking = 11/88, 12%, Category: Toxicology)
44. Iyer, M., Zheng, T., Hopfinger, A. J., & Tseng, Y. J.* (2007). QSAR analyses of skin penetration enhancers. *Journal of chemical information and modeling*, 47(3), 1130-1149. (IF =3.738, Ranking = 7/139, 5%, Category: Computer science, Information systems)
45. Iyer, M., Tseng, Y. J., Senese, C. L., Liu, J., & Hopfinger, A. J. (2007). Prediction and mechanistic interpretation of human oral drug absorption using MI-QSAR analysis. *Molecular pharmaceuticals*, 4(2), 218-231. (IF =4.384, Ranking = 29/255, 11%, Category: Pharmacology & Pharmacy)
46. Li, Y., Tseng, Y. J., Pan, D., Liu, J., Kern, P. S., Gerberick, G. F., & Hopfinger, A. J. (2007). 4D-fingerprint categorical QSAR models for skin sensitization based on the classification of local lymph node assay measures. *Chemical research in toxicology*, 20(1), 114-128. (IF =3.529, Ranking = 10/59, 16%, Category: Chemistry, Medicinal)

47. Senese, C. L., Duca, J., Pan, D., Hopfinger, A. J., & Tseng, Y. J.* (2004). 4D-fingerprints, universal QSAR and QSPR descriptors. *Journal of chemical information and computer sciences*, 44(5), 1526-1539. (IF =4.34, Ranking = 3/100, 3%, Category: Computer Science, Interdisciplinary Applications)
48. Pan, D., Liu, J., Senese, C., Hopfinger, A. J., & Tseng, Y. J.* (2004). Characterization of a ligand-receptor binding event using receptor-dependent four-dimensional quantitative structure-activity relationship analysis. *Journal of medicinal chemistry*, 47(12), 3075-3088. (IF =5.48, Ranking = 3/58, 5%, Category: Chemistry, Medicinal)
49. Liu, J., Pan, D., Tseng, Y. J., & Hopfinger, A. J. (2003). 4D-QSAR analysis of a series of antifungal p450 inhibitors and 3D-pharmacophore comparisons as a function of alignment. *Journal of chemical information and computer sciences*, 43(6), 2170-2179. (IF =4.34, Ranking = 3/100, 3%, Category: Computer Science, Interdisciplinary Applications)
50. Senese, C. L., Duca, J., Pan, D., Hopfinger, A. J., & Tseng, Y. J.*. (2004). 4D-fingerprints, universal QSAR and QSPR descriptors. *Journal of chemical information and computer sciences*, 44(5), 1526-1539. (IF =4.34, Ranking = 3/100, 3%, Category: Computer Science, Interdisciplinary Applications)
51. Pan, D., Tseng, Y. J., & Hopfinger, A. J. (2003). Quantitative structure-based design: formalism and application of receptor-dependent RD-4D-QSAR analysis to a set of glucose analogue inhibitors of glycogen phosphorylase. *Journal of chemical information and computer sciences*, 43(5), 1591-1607. (IF =4.34, Ranking = 3/100, 3%, Category: Computer Science, Interdisciplinary Applications)
52. Duca, J. S., Tseng, Y. F., & Hopfinger, A. J. (2001). 4D-QSPR analysis and virtual screening in materials science. *Advanced Materials*, 13(22), 1713 (IF =17.49, Ranking = 2/139, 1%, Category: Chemistry, Physical)
53. Hopfinger, A. J., Vankatarangan, P., Tseng, Y.F., Wang, S., Duca, J. S. (2000) Evaluation of alignment dependence in 3D-QSAR model construction using 4D-QSAR analysis. *Internet Journal of Chemistry* 3(9-11)

Conference papers

1. Tzeng, T. H., Kuo, C. Y., Wang, S. Y., Huang, P. K., Kuo, P. H., Huang, Y. M., Tseng, Y. J.*, Tian, W. C., Lee, S. C., & Lu, S. S.. 21.5 A portable micro gas chromatography system for volatile compounds detection with 15ppb of sensitivity, IEEE International Solid-State Circuits Conference, San Francisco, California, Feb. 22-26. 2015

2. Shao, C. Y., Su, B. H., Tu, Y.S., Lin, C., Lin, O. A., Tseng, Y. J.*, CypRules: A rule-based P450 inhibition prediction server, 248th ACS National Meeting & Exposition, San Francisco, California, Aug. 10-14. 2014
3. Wang, S. Y., Kuo, C. H., Tseng, Y. J.*, An ion trace detection algorithm to extract pure ion chromatogram to improve untargeted peak detection quality for LC/TOF-MS-based metabolomics data, 10th International conference of the Metabolomics Society, Tsuruoka, Japan, June 26-29, 2014
4. Tsai, D. M., Kuo, C. H., Tseng, Y. J.*, Strategy of UPLC/MS-based Targeted Metabolomics, 10th International conference of the Metabolomics Society, Tsuruoka, Japan, June 26-29, 2014
5. Tan, C. E., Chung, Y. Y., Tseng, Y. J.*, IDMass: GC/MS Data Management and Analyzes Software for Metabolomics Studies, 10th International conference of the Metabolomics Society, Tsuruoka, Japan, June 26-29, 2014
6. Lin, S. W., Kang, W. Y., Lin, D. T., Lee, J., Wu, F. L., Chen, C. L. Tseng, Y. J.*, Comparison of warfarin therapy clinical outcomes following implementation of an automated mobile phone-based critical laboratory value text alert system, Translational Bioinformatics Conference, Seoul, Korea, October 2-4, 2013
7. Tseng, Y. J.*, BaselineCorrector: A distribution-based classification method for baseline correction of metabolomic 1D proton nuclear magnetic resonance spectra, 246th ACS National Meeting & Exposition, Indianapolis, Indiana, September 8-12, 2013
8. Tseng, Y. J.*, GAME: Gpu accelerated mixture elucidator 246th ACS National Meeting & Exposition, Indianapolis, Indiana, September 8-12, 2013
9. Tseng, Y. J.*, "Drug discovery through Teach-Discover-Treat initiative, 246th ACS National Meeting & Exposition, Indianapolis, Indiana, September 8-12, 2013
10. Wang, S. Y., Wu, M. S., Kuo, C. H., Liao, W. C., Tseng, Y. J.*, Metabolomics study of metabolite changes in the serum of morbidly obese patients after the gastric bypass surgery, 4th AOMSC & 10th TSMS Annual Conference, TICC, Taipei, Taiwan, July 10-12, 2013
11. Tsai, D. M., Chen, G. Y., Kuo, C. H., Tseng, Y. J.*, Development of a hydrophilic interaction chromatography coupled with mass spectrometry method for metabolomic analysis, 4th AOMSC & 10th TSMS Annual Conference, TICC, Taipei, Taiwan, July 10-12, 2013

12. Kuo, P. H., Chang, N. W., Kuo, C. H., Tseng, Y. J.*, Metabolomic analysis of exhaled breath condensates (EBC) in healthy volunteers and patients with chronic obstructive pulmonary disease (COPD) and bronchiectasis, 4th AOMSC & 10th TSMS Annual Conference, TICC, Taipei, Taiwan, July 10-12, 2013
13. Wang, S. Y., Tseng, Y. J.*, BN server: a web-based service for LC/TOFMS-based metabolomics data normalization and statistical analysis, 9th International conference of the Metabolomics Society, SECC, Glasgow, Scotland, July 1-4, 2013
14. Chung, Y. Y, Kuo, C. H., Tseng, Y. J.*, Noise reduction of GC/TOF-MS using spectrum domain baseline removal and chromatogram segment filtering, 9th Annual Conference of the Metabolomics Society, SECC, Glasgow, Scotland, July 1- 4, 2013
15. Kuo, T. C., Tsai, D. M., Kuo, H. C., Kuo, C. H., Tseng, Y. J., Establish Targeted Lipidomics Workflow Using TIPick, 9th International Conference of the Metabolomics Society, SECC, Glasgow, Scotland, July 1-4, 2013
16. Chang, N. W., Kuo, C. H., Tseng, Y. J., Metabolomics characterisation of Angelica species by comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GCxGC-TOFMS), 9th International conference of the Metabolomics Society, SECC, Glasgow, Scotland, July 1-4, 2013
17. Liu, J. W., Kuo, C. H., Tseng, Y. J.*, The Retention Time Alignment for non-targeted LC/MS analysis Using Kernel Density Estimation with a Novel Bandwidth Estimator, 9th International conference of the Metabolomics Society, SECC, Glasgow, Scotland, July 1-4, 2013
18. Hsu, K. H., Tseng, Y. J.*, A new approach of traditional Chinese medicine taxonomy: using marker ingredients as bases, 245th ACS National Meeting & Exposition, New Orleans, Louisiana, April 7-11, 2013
19. Shao, C. Y., Tseng, Y. J.*, Exploration of mechanism between nanotoxicity and protein targets: QSAR models using nanotoxicity endpoints of decorated nanotubes, 245th ACS National Meeting & Exposition, New Orleans, Louisiana, April 7-11, 2013
20. Tu, Y. S., Harn, Y. C., Shen, M. Y., Tseng, Y. J.*, Classification tree and random forest based prediction models on molecular autofluorescence, 245th ACS National Meeting & Exposition, New Orleans, Louisiana, April 7-11, 2013

21. Tseng, Y. J.*, LeadOp: Structure-based fragment hopping for lead optimization using pre-docked fragment database, 244th ACS National Meeting & Exposition, Philadelphia, Pennsylvania, August 19-23, 2012. (Invited talk, Drug Discovery Symposium)
22. Chen, S. Z., Tseng, Y. J.*, Predictive toxicity protocol for cell-viability high throughput data, 244th ACS National Meeting & Exposition, Philadelphia, Pennsylvania, August 19-23, 2012
23. Tseng, Y. J.*, Kuo, C. H., Yang, W. Q., Wang, S. Y., Metabolic Signatures Associated with the Progression of Breast Cancer by Ultra High Pressure Liquid Chromatography Time-of-Flight Mass Spectrometry, 8th International conference of the Metabolomics Society, Washington D.C., June 25-28, 2012
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