



## لیست پوسترهای پنجمین سمینار کمومتریکس ایران

### Poster session 1 Wednesday 15:50 -17:00

کد مقاله	عنوان مقاله	ارایه دهنده
1003	Investigating the effect of constraints on the accuracy of the area of feasible solutions for the real datasets with an improved cost function of the polygon inflation algorithm	رحیم دوست مژدهی، نهال
1005	Simultaneous determination of cationic dyes from aqueous solution using first-order derivative spectrophotometry	بگتاش، مریم
1006	Design of potent aromatase inhibitors through pharmacophore hybridization: QM/MM and docking study	اسدی، پروین
1007	Multivariate calibration methods for simultaneous multicomponent determination of two synthetic dyes in fruit juice samples	رحمانیان، رضا
1012	Estimating complicated baselines in analytical signals by iterative training of Bayesian regularized artificial neural networks	کنگی نژاد، عاطفه
1014	QSAR modeling of Sphingosine kinase inhibitors using multivariate adaptive regression spline and projection based regression techniques	نی بند، مرضیه سادات
1016	Study of anti-cancer activity of parthenin derivatives using support vector regression and molecular docking	گرکانی نژاد، زهرا
1017	In silico prediction of cutaneous penetration rate of some chemicals from their molecular structural descriptors	به گزین، سیده مژگان
1019	3D QSAR prediction of molecular flux through polydimethylsiloxane membranes using CoMFA and CoMSIA methodology	به گزین، سیده مژگان
1020	Developing a support vector machine based QSPR model for prediction of half-life of some herbicides	سامقانی، کبری
1021	Modeling and prediction of adsorption behavior of nanotubes	حیدری، افسانه
1022	Novel application of the CORAL software to model Cellular Uptake of Magnetofluorescent Nanoparticles in Pancreatic Cancer Cells	ملک زاده، هانیه
1024	Selective extraction and determination of urinary nickel in foundry workers with the aid of a novel magnetic ion imprinted polymer nanoparticles and experimental design methodology	جلیلیان، نیلوفر



1025	Characterization of Teucrium Polium Essential Oil component by GC-MS analysis using MCR and PARAFAC methods	نیک پور، حمیدرضا
1028	Development of New Interfaces for Performing Chemometric Methods in Portable Instruments and Smartphones	شایع، حمیدرضا
1029	Partial least squares multicalibration method as an alternative and improved method for the simultaneous determination of montelukast, fexofenadine and cetirizine in pharmaceutical tablets and biological sample	نیکو، سید محمد
1031	Application of experimental design as chemometrics tool for optimization of new coupling of ultrasound assisted and reverse phase- dispersive liquid-liquid microextraction before high performance liquid chromatography for the sensitive determination of vitamin A in oil samples	فارسی مدان، سحر
1032	Chemometric optimization of ultrasound-assisted dispersive liquid-liquid microextraction based on solidification of floating organic droplets for determination of sertraline and citalopram in human serum by high performance liquid chromatography	فارسی مدان، سحر
1033	Potential of modified ionic liquid cold-induced aggregation dispersive liquid-liquid microextraction and central composite design for simultaneous preconcentration and determination of lead and cadmium in food and water samples	سعیدزاده امیری، نصیبه
1034	Characterization and classification of Iranian honeys based on physicochemical properties and antioxidant activities, with chemometrics approach	مولودیان، حمید
1035	Investigation of the effect of various gravitational-constant functions on the feature selection performance of GSA: A QSAR study of antiprotozoal activity of benzyl phenyl ether diamidine derivatives	باغگلی، طیبه
1037	Implementing partial knowledge based on Duality	توکلی، الناز
1038	Gaussian apodization evolving factor analysis as a novel method for curve resolution of gas chromatography-mass spectrometry datasets and precise local rank detection	امیر حسین علی نوری
1040	Identification of potential antioxidant compounds in Walnut ( <i>Juglans regia</i> L.) leaves extract by linear multivariate calibration techniques and HPLC-DAD-MS	معصوم، سعید
1044	Potentiality of independent component regression in assessment of the peaks responsible for antioxidant activity of Thyme using gas chromatography-mass spectrometry technique	معصوم، سعید
1045	Advantage of multivariate calibration methods to introduce carbon dots as a novel pH sensor	براتی، علی

1046	An Approach to Determine Accurate Model Parameters of Buffered Chemical Processes	مسرور سعادت ابادی، محمد جواد
1047	Chemometrical study of spectral curve fitting constraint on self-modeling curve resolution methods	خدادادی، سمیه
1048	Sargassum Glaucescens for the removal of Methylen blue, Crystal Violet and Safranin in ternary system by artificial neural network modeling, Plackett–Burman design and response surface analysis	ناطقى، اشرف
1051	Comparison of discriminatory power from soft-modeling methods coupled with multivariate pattern recognition technique for the identification of similar compounds	کاظمی، داود
1055	Simultaneous optimization of dispersive micro-solid-phase extraction of acidic and basic pollutants with the aid of desirability function	اصغری نژاد، علی اکبر
1056	Is There Possible to Compare Biological Potency and Features of Colloidal Silver Nanoparticles Applied in Different Culturing Media?	میرزاجانی دمنه، فاطمه
1057	Application of random forest (RF) for the modeling of Anti-HIV activity of some dibenzyle pyridinon derivatives, as HIV-1 integrase inhibitor, using group contribution descriptors	عسلی، عطیه
1059	Chemometrics-assisted excitation-emission fluorescence analytical data for rapid and selective determination of optical brighteners in the presence of uncalibrated interferences	محسنی کیا، عاطفه
1060	Evaluation of physical properties and antioxidant activity of some Iranian herbhones and classified by PCA and HCA chemometric method	صادقی نژاد، نگار
1061	Simultaneous determination of paracetamol, diphenhydramine and dextromethorphan in pharmaceutical preparations using multivariate calibration 1	نیکو، سید محسن
1062	QSAR modeling of binding affinity of some serotonin receptor antagonists using docking derived molecular descriptors	بهرامی، هنگامه
1063	Spectrophotometric multicomponent analysis of a ternary and a quaternary mixture in human urine samples by analyzing first order data using MCR-ALS.	قاسم زاده، بهار
1064	Determination of acidity constants of cinnamic acid derivatives using two rank annihilation factor analysis (TRAFA)	زارعی، طاهره
1065	Fourier transform infrared spectroscopy coupled with multivariate classification methods to identify adulterated infant formula powder with Melamine and Cyanuric Acid	شیخی زاده، ساحله



## Poster session 2

### Thursday 9:50-11:00

1068	Standard Addition Method Coupled with Principal Component Analysis for Quantitative Study of Real Samples Using Spectroscopic Data	غفاری، مهدیه
1070	Useing net analyte signal for determination of acidity constants caffiec acid in multivariate spectrophotometric analysis systems	زارعی، طاهره
1071	Geographical origin identification of Iranain soil samples by ICP-MS and ICP-OES elemental analysis by chemometrics methods	ویسه، سمیه
1072	Flotation-assisted homogeneous liquid-liquid microextraction and inductively coupled plasma-mass spectrometry for determination of thorium based on Box-Behnken Design	ویسه، سمیه
1075	Visualization of error propagation and one-factor at-a-time local sensitivity analysis concepts	رستمی، اکرم
1076	Pharmacophore-based virtual screening and toxicity risk analysis for identifying novel MPS1 inhibitors	نظر شده، المیرا
1077	Evaluation of electrochemical process variables for removal of basic yellow 28 using a central composite design	روحانی مقدم، مسعود
1078	Experimental design and multiple response optimization for decolorization of acid blue 25 using electrochemical treatment	روحانی مقدم، مسعود
1079	Mean centering of ratio spectra for colorimetric recognition of morphine using melamine modified gold nanoprobe	محسنی، نعیمه
1080	Determination of Ofloxacin in human plasma using dispersive liquid-liquid microextraction combined with spectrofluorimetry with the aid of box-behnken design	اسدیان، فرح
1081	Rapid chromatographic analysis of selected UV filters and parabens in sunscreen products exploiting second-order calibration methods	شکاری، نفیسه
1082	An efficient chemometric strategy based on wavelet transform for preprocessing of multi-capillary column – electronic nose data	علی نوری، امیرحسین
1084	Multi-element analysis of hair samples by ICP-MS and classification using chemometrics methods	صدری، نرگس
1085	Principal component analysis and K-nearest neighbor clustering for classification of soil samples via ICP-MS in Maygan salt lake	ربیعی، محبوبه

1086	A method for rapid screening of interactions of pharmacologically active compounds with bovine serum albumin by chemometrics methods	منوچهری، فیروزه
1087	Application of vortex – assisted dispersive liquid–liquid microextraction coupled with spectrofluorimetry for determination of aspirin in human urine by response surface methodology	تمیجی، زهرا
1088	Box-behnken experimental design based optimization technique in head space-solid-phase microextraction–gas chromatography/mass spectrometry for simultaneous determination of BTEX in Urine.	رحمانی، مهدی
1089	Box-behnken experimental design (BBD) for optimization instrumental parameters effects for powder coating particle size	رحمانی، مهدی
1092	Quality control of standard saffron samples from food colorant adulteration using chemometrics analysis of transmittance FT-IR spectra	کریمی، صادق
1093	Chemometrics assisted of ultrasonic emulsification–microextraction for simultaneous spectrophotometric determination of Cobalt, Nickel and Copper	درودی، زهره
1094	Simultaneous spectrophotometric determination of oxytetracycline, tetracycline and doxycycline in milk and honey samples. Comparison PLS and PARAFAC	درودی، زهره
1095	Quantitative Nanostructure–Activity Relationship (QNAR) modeling for the cellular uptake of magnetofluorescent engineered nanoparticles in pancreatic cancer cells	پهلوان یلی، زهرا
1096	Bee algorithm as a descriptor selection in QSAR study of $\beta$ -site amyloid precursor protein cleaving enzyme1 (BACE1) inhibitors	لیلی اخوندی
1097	Evaluation of long-heating kinetic process of edible oils using ATR-FTIR and chemometrics tools	محبوبی فر، مرجان
1098	Spectrophotometric determination of acidity constant of Cinnamic acid using rank annihilation factor analysis (RAFA)	عباس دادرس
1100	QSPR Approaches to Elucidate the Stability Constants between $\beta$ -Cyclodextrin and some Organic Compounds: Docking Based 3D Conformer	میررحیمی، فرشته السادات
1101	Probing and identification of the solute effects on the methanol–water association by chemometrics methods	شجاعی فرد، زهرا
1102	The study of pre-concentration and determination of some phthalates in plastic containers by using QuEChERS method and high performance liquid chromatography	اقوامی، بنفشه
1103	Application of Extended ratio subtraction and simultaneous ratio subtraction methods for determination of Toluidine Blue and Methyl violet in their binary mixture	زاهدنیا، زهرا



1104	Classification of <i>Mentha piperita</i> accessions according to their antioxidant activity	ایزدیان، پریسا
1105	3D-QSAR Studies for Prediction of Graphene Dispersibility in Diverse Organic Solvents	میررحیمی، فرشته السادات
1106	QSAR study of pyrazole sulfonamide derivatives, a potent inhibitor of trypanosoma brucei N-myristoyltransferase (TbNMT) using bee algorithm	علیزاده فرد، وحید
1110	MIA for a QSAR study of inhibitory activity of CCB with using WT and GA for pixel processing	اکرمی، احمد
1113	Determination of Enantiomer Excess of Some Amino Acids Using Fluorescence Spectroscopy and Multivariate Curve Resolution Analysis	نقاشیان حقیقی، آزاده
1115	Multiset analysis of ATR-FT-IR and synchronous fluorescence spectra by multivariate curve resolution analysis to study the hydrogen-bond disruption in Ethylene Glycol-water binary mixtures	طالبانپوریات، الهه
1116	Odor Visualization and Discrimination of Herbal Distillates Using a Colorimetric Sensor Array	بردبار، محمد مهدی
1117	The complexity of molecular docking and need for chemometrics: studying drug resistance in HIV-1 protease as an example	مبارکی، نبی الله
1119	Investigation of the interaction between adenosine and DNA G-quadruplex by fluorescence resonance energy transfer and molecular modeling	پشته شیرانی، مرضیه
1120	Infrared spectrometric evaluation of carbon nanotube sulfonation process	محمدی، مهسا
1122	Tabu search as a descriptor selection in QSAR study of 1,5- diheteroaryl penta-1,4-dien-3-ones: a class of promising curcumin-based anti-cancer agents	تیموری، مریم

### Poster session 3

#### Thursday 15:50-17:00

1123	The Effect of Acetylation on Lysine Residues on the Structure and Dynamics of TDP-43	رضایی مخوری، فرحناز
1124	QSAR Study of tri-substituted 1,2,4-triazoles as inhibitors of the annexin A2-S100A10 protein using the multiple linear regression model	محمد رضایی، وحید



1127	Diagnosis of brain glioma using near-infrared micro-spectroscopy comparing partial least squares discriminant analysis and target factor analysis	مونا خورانی
1128	Spectroscopic study on the interaction of 5, 10, 15, 20-Tetrakis(4-([1,10] Phenanthroline[5,6-f]imidazol-2 yl) benzen) porphyrin with DNA by means of chemometric methods	عالیشاه، رقیه
1129	Improvement of the patial least squares model for simultaneous determination of dyes by Orthogonal signal correction	صبا احمدی
1132	Study of human prostate anticancer activity of novel arylpiperazines using genetic algorithm and adaptive neuro-fuzzy inference system	اکرمی، مهناز
1133	Application of mean centering of ratio spectra for dye degradation study using Fenton reaction	مرتضی بهرام
1134	Target transformation fitting for simultaneous dye degradation using Fenton reaction	مرتضی بهرام
1135	Application of Central Composite Design for Optimization of Coacervative Extraction of Cu (II) Using Anionic Surfactant	محسنی، نعیمه
1136	Elicitation of the most important structural properties of volatiles affecting electroantennogram responses in Aphis fabae; a QSPR approach	بیک نژاد، داود
1138	Structural analysis of ZSM-5 nano zeolite by diffuse reflectance near-infrared spectrometry and chemometrics	امانی، شهین
1139	Simultaneous quantification of triphenylmethane dyes using three-way data analysis	بیات، مهرنوش
1140	Multivariate curve resolution-alternating least squares assisted voltammetry for simultaneous determination of non-steroidal anti-inflammatory drugs	سعیدی نژاد، فائزه
1142	Spectrophotometric determination of oxazepam in drug and biological samples by parallel factor analysis	سمیه یادگاری
1144	Simultaneous determination of drospirenone and ethinyl estradiol by spectrophotometric method using partial least square and support vector regression	رحیمی فراهانی، سعیده
1145	Prediction of the acidity number of edible oils during long heating procedure using chemometrics tools based on FTIR-ATR results	محبوبی فر، مرجان
1148	Chemometric approach to optimization of micellar liquid chromatographic separation of some natural anthraquinone dyes	رمضانی مقدم، امیر
1149	Spectrophotometric simultaneous determination of Cobalt, Copper and Nickel using pH gradient Flow injection analysisand MCR-ALS	سید جمال صادقی

1151	Evaluation of partial least squares-discriminant analysis for classification of gas chromatography fingerprints of saffron	علی اکبرزاده، غزاله
1152	Prediction of photolysis half-lives of dihydroindolizines by genetic algorithm-multiple linear regression (GA-MLR)	بیک نژاد، داود
1153	Quantitative Structure-Electrochemistry Relationship in Non-aqueous Solutions: On the Reduction Potential of Anthraquinone Derivatives in Organic phase	یوسفی نژاد، سعید
1154	Design and evaluation of a novel Bismuth optical sensor by using PC-ANN application	حبیب الله خواجه شریفی
1155	Simultaneous determination of anionic dyes from aqueous solution using partial least square regression	بگتاش، مریم
1156	Competitive Biosorption of Safranin, Malachite green and Januse green B in ternary system by Sargassumilicifolium: Application of artificial neural network modeling and Taguchi L16 orthogonal array design	خدابخشی، مینا
1157	Multivariate optimization and determination of Hg(II) content in aqueous samples after preconcentration with modified graphene oxide	امیری، نیره
1159	Metal-dependent activity of the 8-17 DNase studied by resolution of rank deficient multi-way fluorescence data	زهره شمالی
1160	Application of machine learning methods in classification and pattern recognition of Carbonic anhydrase (CA) inhibitors	انتظاری هروی، یگانه
1161	Principal Component Analysis of Molecular Dynamics Trajectories on Unbound and Agonist-Bound Dopamine D2	هوشمند، شبنم
1162	Dispersive liquid-liquid microextraction based on solidification of organic drop with central composite design for the determination of 5-hydroxymethyl-2-furfural using high-performance liquid chromatography	شیری، فرشته
1163	Simultaneous Spectrophotometric determination of Cysteine and Ascorbic acid using Cu(OH) <sub>2</sub> /CuO Nanowires and Parallel Factor Analysis	کوهساریان، مریم
1164	Gene expression classification (tumor or non-tumor) using wavelet based feature extraction method	زهرا حیدری
1166	Using QSAR calculation of Indol derivatives and 7-azaindoles for the treatment of Multiple Sclerosis(MS)	موسوی، سیده مریم
1167	Using QSAR calculation of amid derivatives for the treatment of Parkinson's disease	نظیری، مولود
1169	Comparison of Cadmium-induced toxicity in ionic and nano forms applying <sup>1</sup> HNMR based Metabolomics analysis	خوشکام، مریم





1171

A review on the application of chemometrics methods in the field of industrial lubricants

یوسفیان، آیدا



# لیست سخنرانی های پنجمین سمینار کموتریکس ایران

نام و نام خانوادگی	عنوان سخنرانی	شماره
اکبری لاکه، مهسا	An Investigation on Meaning and Reliability of Local Rank Constraint in Self-Modeling Curve Resolution of Chemical Data	1015
سامقانی، کبری	3D-QSAR studies of the inhibition efficiency of phenolic herbicides on photosynthesis by using CoMFA and CoMSIA	1018
حیدری، افسانه	A theoretical approach to model and predict the adsorption coefficients of some small aromatic molecules on carbon nanotube	1013
احمدوند، محمد	A systematic study on the effect of noise and shift on multivariate figures of merit of second-order calibration algorithms	1030
ایزدیان، پرینا	Metabolite profiling and chemometric classification of two varieties of Ocimum basilicum medicinal plant	1036
بیرامی سلطان، سمیرا	Analytical view on uniqueness	1043
پرستار شهری، هادی	How to Expand the Use of Independent Component Analysis in Analytical Chemistry?	1053
امیدی کیا، نعمت الله	Direct Triadic Decomposition	1058
رستمی، اکرم	Using global and local sensitivity analysis for variable sorting and selection	1074
رشوند، معصومه	Investigation of a sewage treatment plant for removal of selective pharmaceutical and personal care products using HPLC-DAD and second-order calibration	1108
صابری دهکردی، زینب	Design and construct a small fluoremeter with a smartphone as the detector associated with image processing	1111
مانی ورنوسفاد رانی، احمد	What is in Chemometrics for Chemoinformatics: Validating Classical Relativity in Chemical Space	1121



1126	Introducing of invasive weed optimization as a new variable selection method	شیخی زاده، ساحله
1146	Challenges in drug discovery and development	خیامیان، تقی
1147	Influence of bonded-phase density in chiral chromatography via molecular simulation	آقای، الهام
1158	Computational Chemogenomics: an emerging strategy for rapid target and drug discovery	قرقانی، سجاد
1165	Quantitative Nanostructure Activity Relationship Modeling (Nano-QSAR)	صلاحی نژاد، مریم
1168	Identification of potential antimicrobial and antioxidant constituents in some medicinal herbs using hephenated chromatograrhic methods and multivariate calibration techniques	معصوم، سعید
1170	Present and future of QSAR	فاطمی، محمدحسین
1172	Geochemometrics	نیازی، علی
1173	Multi-way assisted chromatographic methodologies for analysing highly complex samples	وثوق، مریم
1174	Calculation of Feasible Bands for Visualizing the Constraint Effects in Soft Modeling Methods	عبداللهی، حمید
1175	Defining the Applicability Domain for Classification Models by Hedging Predictions	K. Baumann
1176	Applications of Particle swarm optimization in chemometrics	Federico Marini
1177	Chemometrics and chemistry	Marcel Maeder
1178	Novel feature selection methods and CAIS resolution software	موسوی، مهدی
1150	Quantitative sequence activity relationship of bitter tasting threshold peptides: a comparison study between some two-way and three-way modeling methods	یوسفی نژاد، سعید