

**ET36/2005 – Et. Unică/2005 – Lucrare în extenso**

Ministerul Educației și Cercetării  
Universitatea Tehnică din Cluj-Napoca  
Facultatea de Știința și Ingineria Materialelor  
Catedra de Chimie

Programul:	Cercetare de Excelență
Modul: II	Proiecte de Dezvoltare a Resurselor Umane pentru Cercetare
Tipul proiectului:	Proiecte de cercetare de excelență pentru tinerii cercetători
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Denumirea proiectului:	Investigații Structurale Integrate pe Compuși Biologic Activi
Etapa:	Unică/2005

***Lucrare în extenso***

***Cuprins***

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### ***Obiective și activități***

În cadrul proiectului *Investigații Structurale Integrate pe Compuși Biologic Activi*, pentru etapa unică a anului 2005 obiectivul planificat a fost *Elaborarea modelului de implementare soft și interfață online*, iar activitățile prevăzute a se desfășura au fost *Elaborare metodologie integrarea aplicațiilor complexe și Participări la manifestări științifice și dobândirea de competențe complementare*.

Activitățile au fost realizate și obiectivul planificat a fost atins.

### ***Activități și rezultate***

- Participări la manifestări științifice și dobândirea de competențe complementare:

În perioada 21-29 Octombrie 2005 s-a participat la 2 manifestări științifice la Washington D. C. desfășurate la *Hilton Washigton & Towers* și respectiv *Ronald Reagan Building & International Trade Center*.

1. S-a participat cu o lucrare științifică la Simpozionul *Biomedical and Health Informatics from Foundations to Applications to Policy* organizat de *American Informatics Medical Association* în perioada 22-26 Octombrie 2005 la Washington D. C., lucrare care a fost inclusă în extenso pe CD-ul de *Conference Proceedings*, paginile 66-70. Programul lucrărilor simpozionului la care s-a participat este parte integrantă a *lucrării în extenso* (anexa 1) aferente etapei unice / 2005 a proiectului *Investigații Structurale Integrate pe Compuși Biologic Activi*.
2. S-a participat la întrunirea anuală a asociației pentru industrie și investitori *2005 Mid-Atlantic Bio: The Conference for Industry and Investors* desfășurată în perioada 26-27 Octombrie 2005 la Washington D. C. pentru dobândirea competențelor complementare în domeniul transferului tehnologic și atragere a investitorilor din domeniul bioinformaticii, biochimiei și biotehnologiei. Programul lucrărilor întrunirii la care s-a participat este parte integrantă a *lucrării în extenso* (anexa 2) aferente etapei unice / 2005 a proiectului *Investigații Structurale Integrate pe Compuși Biologic Activi*.

- Elaborare metodologie integrarea aplicațiilor complexe:

A fost realizată metodologia pentru integrarea aplicațiilor complexe de investigații structurale integrate pe compuși biologic activi.

1. A fost realizată interfața online pentru predicția activității biologice pe clase de compuși chimici biologic activi și este la adresa URL:

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/sar/](http://vl.academicdirect.org/molecular_topology/mdf_findings/sar/)

Aplicația prezice activitatea biologică bazat pe un set școală și pe un set de modele structură-activitate ce folosesc familia de descriptori moleculari MDF pentru orice moleculă transmisă online aplicației de către utilizator în format HyperChem (HIN). Codul sursă al aplicației este parte integrantă a *lucrării în extenso* (anexa 3).

2. A fost realizată interfața online pentru calcularea oricărui membru al familiei de descriptori MDF (familia însumează un număr de 787968 membrii) și este la adresa URL:

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/j\\_mdf\\_demo.php](http://vl.academicdirect.org/molecular_topology/mdf_findings/j_mdf_demo.php)

Aplicația permite alegerea unui fișier conținând o moleculă cu activitate biologică în format HyperChem (HIN), alegerea unui operator de distanță, a unei proprietăți atomice, a unei formule de descriptor de interacțiune, a unui model de interacțiune, a unui criteriu de fragmentare, a unei formule de suprapunere moleculară globală, și a unui operator de linearizare în conformitate cu specificațiile metodei MDF SAR, și produce ca și rezultat întreg setul de calcule necesar pentru obținerea valorii descriptorului molecular membru al MDF ce corespunde alegerilor făcute, iar în final este redată valoarea numerică a acestuia pentru molecula aleasă. Codul sursă al aplicației și rezultatul obținut de aplicație pentru o moleculă școală este parte integrantă a *lucrării în extenso* (anexa 4 și anexa 5).

3. A fost realizată interfața online pentru analiza de predicție prin metoda leave-one-out și este la adresa URL:

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/loo/](http://vl.academicdirect.org/molecular_topology/mdf_findings/loo/)

Aplicația necesită transmiterea datelor într-un fișier în format HTML folosind un formular și formatul datelor trebuie să cuprindă: denumirile coloanelor, denumirile liniilor, variabilele independente – primul set de coloane, estimarea variabilei dependentă – următoarea coloană, variabila dependentă – următoarea coloană, variabila prezisă – ultima coloană. Aplicația calculează: numărul gradelor de libertate (Df), numărul

variabilelor modelului (Var), suma pătratelor de estimare (SSe), radical din suma pătratelor de estimare (QSSe), coeficientul de determinare în estimare ( $r_{2est}$ ), valoarea statistică Fisher pentru estimare ( $F_{est}$ ), valoarea probabilității de eșec al estimării calculată din valoarea statistică Fisher ( $p_{est}$ ), suma pătratelor de predicție (SSp), radical din suma pătratelor de predicție (QSSp), coeficientul de determinare în predicție ( $r_{2est}$ ), valoarea statistică Fisher pentru predicție ( $F_{pre}$ ), valoarea probabilității de eșec al predicției calculată din valoarea statistică Fisher ( $p_{pre}$ ), cu o limită de calcul a probabilităților de eșec în estimare și predicție de până la  $10^{-17}$ . Codul sursă al aplicației și rezultatul obținut de aplicație pentru un set școală este parte integrantă a lucrării în extenso (anexa 6 și anexa 7).

4. A fost realizată interfața online pentru realizarea experimentelor de predicție a activității biologice pe clase de compuși chimici folosind seturi școală și seturi test și este la adresa URL:

[http://vl.academicdirect.org/molecular\\_topology/qsar\\_qspr\\_s/](http://vl.academicdirect.org/molecular_topology/qsar_qspr_s/)

Aplicația permite efectuarea de experimente Training vs. Test. Pentru aceasta se folosește de datele obținute de modelul MDF SAR și salvează în format text, și conținând separat prin spațiu și rând nou următoarele informații: denumirile coloanelor, incluzând aici denumirile descriptorilor, valorile denumirilor moleculelor, descriptorilor calculați activitatea biologică estimată, măsurată și prezisă. Aplicația permite astfel alegerea fișierului de date, alegerea numărului de molecule în setul școală, generează partiția întregului set în sub-setul școală și sub-setul test (procedură repetabilă de oricâte ori, repartizare aleatoare), și produce următoarele rezultate: ecuația modelului MDF SAR calculată folosind metoda MLR combinată cu SSR din datele setului școală, calculează coeficientul de determinare al estimării, valoarea testului Fisher pentru estimare și a probabilității de a greși în estimare asociată valorii testului Fisher, face predicțiile pe setul test și afișează rezultatele, calculează

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coeficientul de determinare al predicției, valoarea testului Fisher pentru predicție și a probabilității de a greși în predicție asociată valorii testului Fisher. Codul sursă al aplicației și rezultatul obținut de aplicație pentru un set școală și un set test este parte integrantă a *lucrării în extenso* (anexa 8 și anexa 9).

### ***Valorificarea rezultatelor prin publicare***

- Rezultatele obținute din elaborarea metodologiei de integrare a aplicațiilor complexe pentru investigații structurale integrate pe compuși biologic activi au fost valorificate astfel:
  1. S-a elaborat metodologia de lucru pentru investigații structurale integrate pe clase de compuși biologic activi al cărui rezumat constitutiv a fost publicat în lucrarea: Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 1. Review of the Methodology*, *LEJPT*, Issue 6, p. 76-98, 2005, disponibilă la URL:  
<http://lori.academicdirect.org/articles/?id=45>
  2. S-a elaborat modelul statistic de evaluare a metodelor de estimare folosind ipoteza distribuției binomiale a datelor bazat pe o serie de criterii de evaluare iar rezultatele aplicării modelului pentru parametrul binomial „factor de risc” au fost comunicate la simpozionul: Sorana BOLBOACĂ, Lorentz JÄNTSCHI, *Binomial Distribution Sample Confidence Intervals Estimation for Positive and Negative Likelihood Ratio Medical Key Parameters*, *American Informatics Medical Association Annual Symposium on Biomedical and Health Informatics from Foundations to Applications to Policy*, Washington D.C., U.S.A., October 22-26, Conference Proceedings, p. 66-70, 2005, disponibilă la URL:  
<http://lori.academicdirect.org/conferences/?id=26>
  3. Fundamentarea teoretică fizico-chimică sub aspect termodinamic și de cinetică chimică ce stă la baza investigațiilor structurale integrate pe clase de compuși biologic activi a fost valorificată prin integrarea sa într-un capitol într-o carte: §12.2 *Caracterizarea matematică a reacțiilor complexe* (p. 189-216), *Cap. 12 Ecuații de viteză pentru reacțiile simple și complexe*, cartea Mihaela Ligia UNGUREȘAN, Lorentz JÄNTSCHI *Chimie fizică: termodinamică și cinetică chimică*, *Mediamira*, 292 p., 2005, disponibilă la cerere.
  4. Baza de date cuprinzând proprietățile atomice ale elementelor sistemului periodic al elementelor a fost și ea valorificată în lucrarea: Delia Maria

GLIGOR, Lorentz JÄNTSCHI, *Periodic System of Elements Database and Its Applications*, Oradea University Annals, Chemistry Fascicle, Issue 12, p. 180-194, 2005, disponibilă la URL:

<http://lori.academicdirect.org/articles/?id=49>

5. Elaborarea metodologiei de lucru pentru investigații structurale integrate pe clase de compuși biologic activi a permis aplicarea modelului MDF SAR pe câteva serii de compuși, iar rezultatele au fost valorificate astfel:

- Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 2. Insecticidal Activity of Neonicotinoid Compounds*, LJS, Issue 6, p. 78-85, 2005, disponibilă la URL:

<http://lori.academicdirect.org/articles/?id=46>

- Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 3. Antituberculosic Activity of some Polyhydroxyxanthenes*, LJS, Issue 7, p. 58-64, 2005, disponibilă la URL:

<http://lori.academicdirect.org/articles/?id=47>

- Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, *Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds*, LEJPT, Issue 7, 55-102, 2005, disponibilă la URL:

<http://lori.academicdirect.org/articles/?id=48>

6. O serie de lucrări au fost elaborate și trimise spre publicare astfel:

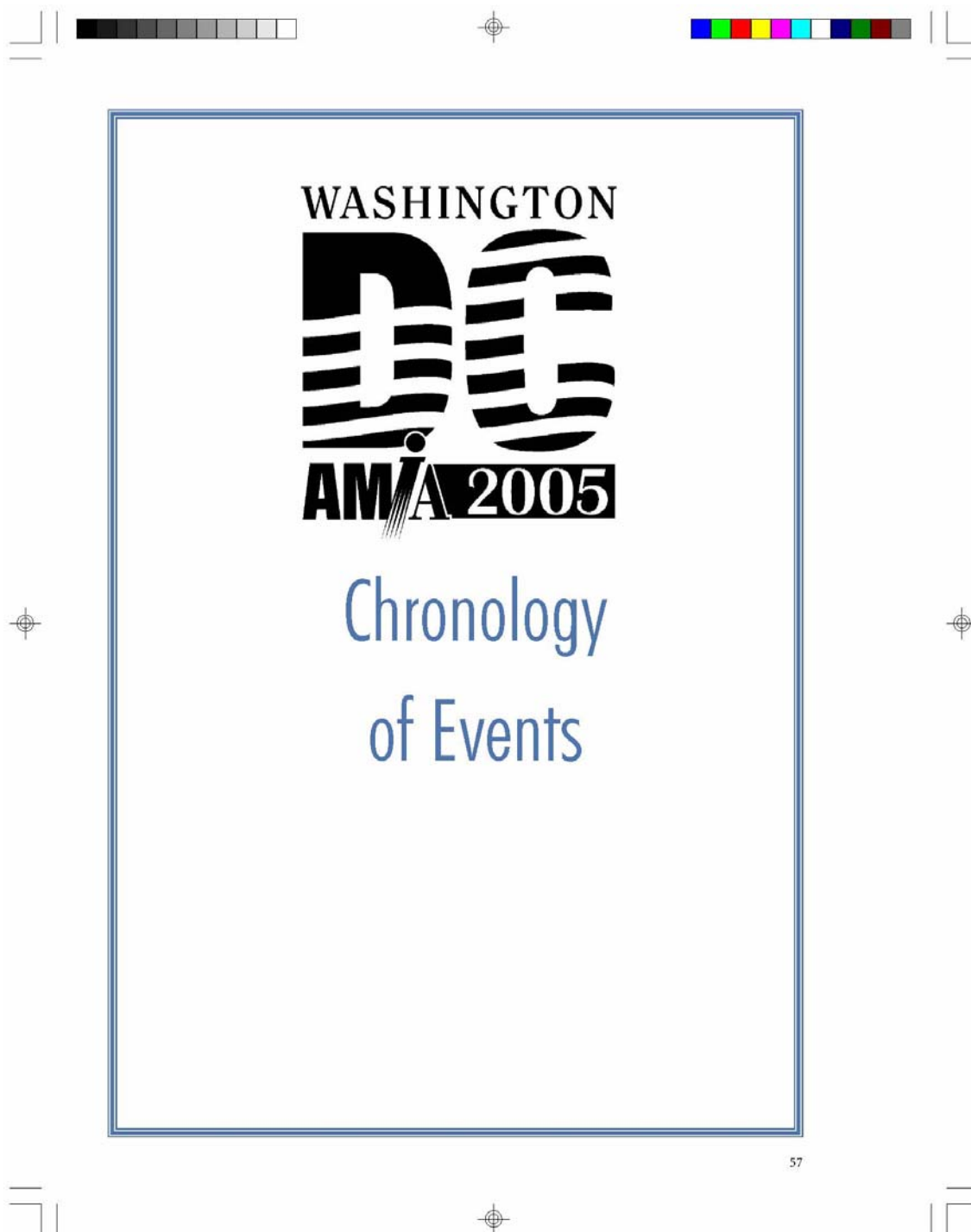
- Lorentz JÄNTSCHI, Camelia Claudia AVRAM, Sorana Daniela BOLBOACĂ, Mădălina Ana VĂLEANU, *Complex Applications Integration: Online Resources for Applied Research*, Applied Medical Informatics, - în curs de publicare în 2005;
- Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, *Molecular Descriptors Family on Structure Activity Relationships for Herbicidal*

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*Activity of a Substituted Triazines Class and Models Comparision,*  
Journal of Pesticide Sciences - acceptată spre publicare în 2005;

- Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, *QSARs on Anti-HIV-1 Potencies of HEPT and TIBO Derivatives by use of Molecular Descriptors Family*, Polish Journal of Chemistry - trimisă spre publicare în 2005, în curs de evaluare;
- Sorana Daniela BOLBOACĂ, Mădălina Ana VĂLEANU, Camelia Claudia AVRAM, Lorentz JÄNTSCHI, *Antioxidant Efficacy of 3-Indolyl Containing Compounds by Complex Information Integration*, Clujul Medical - trimisă spre publicare în 2005;
- Lucrările științifice publicate sunt parte integrantă a *lucrării în extenso* (anexa 10).

*Anexa 1. Programul și lucrările Simpozionului  
„Biomedical and Health Informatics from Foundations to Applications to Policy”*



**Saturday, October 22**

<b>7:00 a.m. - 7:00 p.m.</b>	<b>Registration Open</b>	<b>page 59</b>
<b>8:30 a.m. - 4:30 p.m.</b>	<b>Doctoral Consortium on Organizational Issues in Medical Informatics</b>	<b>page 59</b>
<b>8:30 a.m. - 4:30 p.m.</b>	<b>AMIA 2005 Nursing Informatics Symposium</b>	<b>page 59</b>
<b>8:30 a.m. - 4:30 p.m.</b>	<b>Full-day Tutorials</b>	<b>page 59</b>
	T01 Introduction to Biomedical and Health Informatics	
	T02 Terminologies and Classifications	
<b>8:30 a.m. - 12:00 p.m.</b>	<b>Half-day Tutorials</b>	<b>pages 59-62</b>
	T03 Building Bayesian Decision Support Systems	
	T04 A Primer on Health Level Seven (HL7)	
	T05 Using the Resources of the National Center for Biotechnology Information (NCBI)	
	T06 Natural Language Processing (NLP) in Biomedicine	
	T07 PACS - Digital Medical Image Management	
	T08 Information Security in Health Care: Process and Technology	
	T09 The eXtensible Markup Language (XML)	
	T10 Personal Health Records and E-health Portals	
<b>9:00 a.m. - 5:00 p.m.</b>	<b>AMIA Board of Directors Meeting</b>	<b>page 62</b>
<b>10:00 a.m. - 10:30 a.m.</b>	<b>Coffee Break</b>	<b>page 62</b>
<b>1:00 p.m. - 4:30 p.m.</b>	<b>Half-day Tutorials</b>	<b>pages 62-64</b>
	T11 Deriving Value from Your Electronic Health Record	
	T12 Applying Unified Modeling Language (UML) to Clinical Informatics	
	T13 Integration of Genomics, Biomedical and Clinical Databases	
	T14 Modeling, Designing, and Implementing ODBC Databases	
	T15 Human-computer Interaction for Biomedical Informatics	
	T16 Unified Medical Language System Overview (UMLS)	
	T17 Transforming and Visualizing Clinical Data for Clinical Research	
	T18A National Health Information Infrastructure (NHII) Overview: From A to Z	
<b>1:00 p.m. - 5:00 p.m.</b>	<b>Primary Care Informatics WG Special Event - Part 1</b>	<b>page 64</b>
<b>2:30 p.m. - 3:00 p.m.</b>	<b>Coffee Break</b>	<b>page 64</b>
<b>4:30 p.m. - 6:00 p.m.</b>	<b>Nursing Informatics Symposium Reception (for participants of the NI Symposium only)</b>	<b>page 64</b>
<b>5:00 p.m. - 6:00 p.m.</b>	<b>Primary Care Informatics WG Reception</b>	<b>page 64</b>
<b>5:30 p.m. - 7:30 p.m.</b>	<b>Alliance for Nursing Informatics (ANI) Governing Directors Dinner</b>	<b>page 64</b>
<b>6:30 p.m. - 7:00 p.m.</b>	<b>Ethical, Legal, and Social Issues WG Business Meeting</b>	<b>page 64</b>
<b>7:30 p.m. - 10:00 p.m.</b>	<b>Primary Care Informatics WG Business Meeting</b>	<b>page 64</b>
<b>7:30 p.m. - 10:00 p.m.</b>	<b>Leadership Dinner (by invitation)</b>	<b>page 64</b>
<b>7:30 p.m. - 10:00 p.m.</b>	<b>Workshops</b>	<b>pages 65-66</b>
	W01 Virtual Communities in Health Care	
	W02 Mountain Treks - Mole Hill Maneuvers: Traversing the Terrain	
	W03 Grants and Grantmaking in the Emerging Field of E-patients Studies	
	W04 Computer-based Patient-centered Monitoring: An Emerging Technology?	
	W05 Standards in Clinical Decision Support: Activities in Health Level Seven	
	W06 Ontological Foundations of Biomedical Terminology Systems	
	W07 Computer-assisted Coding: Current Practice and Future Directions	
	W08 Online Therapy: A New Medium for Psychotherapy	
	W09 Governance Models for Clinical Decision Support at Health Care Organizations	

Sunday, October 23		
7:00 a.m. - 7:00 p.m.	Registration Opens	page 68
7:00 a.m. - 12:00 p.m.	10x10 at OHSU - Special Session (for 10x10 students only)	page 68
8:00 a.m. - 12:00 p.m.	Primary Care Informatics WG Special Event - Part II	page 68
8:00 a.m. - 12:00 p.m.	Student Paper Competition	page 68
8:30 a.m. - 12:00 p.m.	<b>Half-day Tutorials</b>	<b>pages 68-71</b>
	T188 National Health Information Infrastructure (NHII) Overview: From A to Z	
	T19 Clinical Decision Support: A Practical Guide to Developing Your Program to Improve Outcomes	
	T20 EHR: Selection and Implementation	
	T21 The EHR and Patient Safety	
	T22 Design and Conduct of Evaluation Studies in Biomedical Informatics	
	T23 Discovering Knowledge: Data Mining	
	T24 Project Management: Implementing Systems on Time and with Budget	
	T25 Ontologies in Biomedicine	
	T26 Public Health for Informaticians	
	T27 Creating Employing Enterprise Data Repositories	
	T28 Evidence-based Nursing Knowledge - Content and System Design	
	T29 Simulation and Virtual Reality in Health Professions Education	
9:00 a.m. - 10:30 a.m.	<b>AMIA's Colloge of Informatics Executive Committee Meeting</b>	<b>page 71</b>
10:00 a.m. - 10:30 a.m.	<b>Coffee Break</b>	<b>page 71</b>
1:00 p.m. - 3:00 p.m.	<b>Opening Session and Keynote Presentation</b>	<b>page 71</b>
3:30 p.m. - 5:00 p.m.	<b>Scientific Sessions</b>	<b>pages 71-73</b>
	S01 Panel: Bioinformatics in Genomics/Medicine	Foundations
	S02 Papers: Linking Records and Standard Vocabularies	Foundations
	S03 Papers: Public Health and Biosurveillance Methods	Foundations
	S04 Papers: Concept Abstraction and Extraction	Foundations
	S05 Papers: Health Information Technology and Nursing Care	Applications
	S06 Papers: Electronic Health Record Development	Applications
	S07 Papers: Evaluation of Clinical Information Technology	Applications
	S08 Panel: Cognition Factors and Decision Making in Critical Care Environments	Applications
	S09 Panel: Enhancing the Safety of the Medication Management Process: Lessons from the Field	Applications
	S10 Panel: Integration of Patient Care and Clinical Research Systems: A Case for Interoperability	Applications
5:00 p.m. - 7:00 p.m.	<b>Welcome Reception - Exhibits Open</b>	<b>page 73</b>
7:00 p.m. - 10:00 p.m.	<b>AMIA's Colloge of Informatics Dinner and Induction of Fellows (by invitation)</b>	<b>page 73</b>
7:30 p.m. - 10:00 p.m.	<b>WG Business Meetings (Dental Informatics, Knowledge Discovery and Data Mining, Knowledge in Motion, and Student)</b>	<b>page 73</b>
7:30 p.m. - 10:00 p.m.	<b>Workshops</b>	<b>pages 73-75</b>
	W10 Integrating the Healthcare Enterprise (IHE): Standards, Interoperability, and the EHR	
	W11 Informatics Education for Clinical Researchers	
	W12 The Digital Human Project: Update on Biomedical Modeling and Simulation	
	W13 Strategies for Integrating Interdisciplinary Teams and Communication and Information to Improve Chronic Disease Management in Primary Care	
	W14 Electronic Health Technologies: Changing Patient-clinical Relationships	
	W15 The Education Steps Project: Exploring the Scientific Basis of Health Informatics and the Educational and Research Implications	

Monday, October 24		
7:00 a.m. - 8:15 a.m.	<b>Committee Meetings (Awards, Bylaws, Publications, and WG Steering)</b>	page 77
7:00 a.m. - 8:15 a.m.	<b>Sentillion Corporate Roundtable</b>	page 77
7:00 a.m. - 8:30 a.m.	<b>NIWG Leadership Meeting</b>	page 77
8:30 a.m. - 10:00 a.m.	<b>Semi-plenary Presentations</b>	page 77
	S11 National Centers for Biomedical Computing: Informatics Enabling Biomedical Research	Foundations
	S12 The Role of the Federal Government in Promoting Health Information Technology Adoption	Applications
10:00 a.m. - 2:00 p.m.	<b>Exhibit Hall Open</b>	page 77
10:00 a.m. - 10:30 a.m.	<b>Coffee Break</b>	page 77
10:00 a.m. - 2:00 p.m.	<b>Poster Session I Preview</b>	page 77
10:30 a.m. - 12:00 p.m.	<b>Scientific Sessions</b>	pages 77-80
	S14 Panel: The Changing Field of Informatics: Implications for Informatics Research Training in the US	Foundations
	S15 Papers: Natural Language Processing of Medical Free Text	Foundations
	S16 Papers: Data Mining	Foundations
	S17 Papers: Evaluation and Education Tools	Applications
	S18 Papers: Personal Health Records: Problems and Solutions	Applications
	S19 Papers: Using Information Technology to Support Clinical Research	Applications
	S20 Panel: CPOE Vendor Perspectives on Implementing CPOE	Applications
	S21 Panel: Advances in Nursing Terminology: A View from the Summit	Applications
	S22 Demonstrations: Emergency Response Systems	
	S23 Partnership in Innovation: Collaborative Technologies	
	S24 Late Breaking Policy Session: National Efforts to Advance a Children's Health Information Network	
12:00 p.m. - 1:30 p.m.	<b>CARING Luncheon (separate registration required) - sold out</b>	page 80
12:00 p.m. - 1:30 p.m.	<b>Meetings Committee Meeting</b>	page 80
12:30 p.m. - 1:30 p.m.	<b>AMIA's College of Informatics "Meet the Experts" Sessions</b>	page 80
1:45 p.m. - 3:15 p.m.	<b>Scientific Sessions</b>	pages 80-83
	S25 Panel: Towards Resource Sharing: Challenges and Opportunities for Imaging and Genomics Databases	Foundations
	S26 Papers: Health Care Informatics: Consumers and Users	Foundations
	S27 Papers: Semantic Issues in Clinical Guidelines	Foundations
	S28 Papers: Natural Language Processing Methods	Foundations
	S29 Papers: Disaster Management and Health Information Technology	Applications
	S30 Papers: Qualitative Inquiry to Improve Health Information Technology	Applications
	S31 Panel: Clinical Trial Registries and Publication: Controversy and Opportunity	Applications
	S32 Panel: Using IT Strategies to Generate Evidence-based Knowledge for Nursing Practice	Applications
	S33 Demonstrations: Integrated Information Technology Systems	
	S34 Partnerships in Innovation: Building Electronic Health Record Components	
	S35 Late Breaking Policy Session	
3:30 p.m. - 5:00 p.m.	<b>Clinical Trials WG Business Meeting</b>	page 83
3:30 p.m. - 5:00 p.m.	<b>Scientific Sessions</b>	pages 83-85
	S36 Panel: Towards Semantic Web for Life Sciences	Foundations
	S37 Papers: Temporal Modeling and Prediction	Foundations
	S38 Papers: Individual Differences and Individualized Care	Foundations
	S39 Papers: Formalizing and Analyzing Biomedical Concepts	Foundations
	S40 Papers: Clinical Vocabulary Issues	Applications
	S41 Papers: Clinical Decision Support	Applications
	S42 Papers: Sex, Drugs, and Other Risky Behaviors	Applications
	S43 Panel: Monolithic Systems Versus Best of Breed: State of the Debate in 2005	Applications
	S44 Panel: Prospects and Pitfalls of Patient-centered Information Technology	Applications
	S45 Demonstrations: Public Health Systems	
	S46 Late Breaking Policy Session: Reaching for Higher Ground-Expanding Continuity of Communications across Public and Private Sectors	
4:00 p.m. - 7:00 p.m.	<b>Exhibit Hall Open</b>	page 85
5:15 p.m. - 7:00 p.m.	<b>Poster Session I</b>	page 85
5:30 p.m. - 7:00 p.m.	<b>WG Business Meetings (Evaluation, Natural Language Processing, Open Source)</b>	page 85
5:30 p.m. - 8:30 p.m.	<b>Clinical Information Systems WG Business Meeting and Reception</b>	page 86
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	S48 Biomedical Informatics Year in Review	Both
	S49 Realizing the Financial Benefits of Electronic Health Records: What Do the Data Show?	Applications
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	S51 Papers: Mapping Between Ontologies	Foundations
	S52 Papers: Evaluation Methods	Foundations
	S53 Papers: Practical Issues in Building a Health Information Infrastructure	Applications
	S54 Papers: Integrating Decision Support and Order Entry	Applications
	S55 Papers: Health Information for Consumers	Applications
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	S57 Panel: Deployment of the Vista Free and Open Source EHR/EMR Software Stack	Applications
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	S60 Demonstrations: Systems Supporting Research	
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	S70 Panel: Disaster Informatics: Next Generation Internet Systems for the Point of the Spear	Applications
	S71 Demonstrations: Knowledge and Information Representation	
	S72 Late Breaking Policy Session: Report from the President's Commission on Systemic Interoperability	
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	S77 Papers: Electronic Health Records Around the World	Applications
	S78 Papers: Interactions Between Humans and Computers	Applications
	S79 Panel: Informatics Support for Personal Health Management	Applications
	S80 Panel: Virtual Patients in Maintenance of Certification	Applications
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**Anexa 2. Programul lucrărilor întrunirii**

**2005 Mid-Atlantic Bio: The Conference for Industry and Investors**

**Day 1: Wednesday, October 26**

*Track Sponsor (Amphitheater) – Maryland TEDCO*

*Track Sponsor (Polaris) – Greater Williamsburg Partnership*

<b>8:30 am - 7:00 pm</b>	<b>Exhibit Hall Open</b>
<b>9:00 am - 11:00 am</b>	<p><b>Pre-conference Workshops</b></p> <p><b>Capital-Raising for Bioentrepreneurs</b>  Identifying and tapping into the right sources of capital for your company’s current stage of product development is an ongoing challenge for every management team. This workshop will provide practical advice covering the entire spectrum of financing needs, from seed funding to public offerings, from those who have been there/done that.</p> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Ryan Schwarz, Managing Director, The Carlyle Group</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• M. James Barrett, Ph.D., New Enterprise Associates</li> <li>• Elizabeth Good, Managing Director, Maryland Venture Fund</li> <li>• Peter Gibson, Comerica Bank</li> <li>• Richard H Osgood, Chairman, Pacific Growth Equities</li> </ul> <p><b>Innovative Tools to Facilitate Bioscience Research</b>  Cutting-edge bioscience research, whether in industry or academia, relies heavily on the development of new devices, methods, and instruments that take advantage of new technologies to generate data more quickly, more reliably, and with greater precision. This workshop will present some of the latest advances in research tools and analysis methods and their applications toward improving public health.</p> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Maciek Sasinowski, Ph.D., CEO, Incogen, Inc.</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Richard Drake, Ph.D., Associate Director, Center for Biomedical Proteomics, Eastern Virginia Medical School</li> <li>• William Cooke, Professor, Dept. of Physics, College of William and Mary</li> <li>• James Lazar, VP Research, Marligen Biosciences, Inc.</li> <li>• Heng Zhu, Ph.D., Asst. Professor, Dept. of Pharmacology &amp; HiT Center, Johns Hopkins School of Medicine</li> </ul> <p><b>Basics of Biotech</b>  Biotechnology is rapidly changing the way patients are treated for disease, farmers grow their crops and emergency response personnel detect airborne toxins. Presented by BioTech Primer, Inc., this workshop will provide an overview of all things biotech, tailored to individuals without an extensive scientific background. Familiarize yourself with the industry sectors and explore the applications within each sector. Discover how stem cells, tissue engineering, biosensors and other biotech innovations are becoming a part of your everyday life.</p> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Stacey Franklin, Vice President, Biotech Primer, Inc.</li> </ul> <p><b>Instructor</b></p> <ul style="list-style-type: none"> <li>• Collins Jones, Ph.D., Instructor and Scientific Advisor, Biotech Primer, Inc.</li> </ul>
<b>11:15 am - 12:30 pm</b>	<b>Plenary Session – Keynote Address</b> <b>Host</b>

	<ul style="list-style-type: none"> <li>• Bruce Robertson, Ph.D., Managing Director, H.I.G. Ventures</li> </ul> <p><b>Introduction</b></p> <ul style="list-style-type: none"> <li>• James Richardson, President, Alexandria Real Estate Equities</li> </ul> <p><b>Keynote Address</b></p> <ul style="list-style-type: none"> <li>• George Poste, DVM, PH.D., DSc, Director, Arizona Biodesign Institute, Arizona State University</li> </ul>
<b>12:30 pm - 2:00 pm</b>	<b>Lunch (in Exhibit Hall)</b>
<b>2:00 pm - 3:30 pm</b>	<p><b>Concurrent Sessions</b></p> <p><b>Investor Sessions IA, IB</b> Six selected companies will make their case for financing to the investor community.</p> <p><b>Should Venture-Backed Companies be Eligible for SBIR Funding?</b> The Federal government's SBIR program has become an important source of research funding for early-stage bioscience companies. However, many contend that small companies that are majority-owned by institutional venture capital investors should no longer be eligible to apply for these awards. The speakers in this session will examine the issue from both sides of the fence, sharing their well-reasoned justifications for supporting each position. Attendees will learn why even the smallest bioscience companies need to pay attention to public policy debates - they can't afford not to.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Douglas M. Duncan, County Executive, Montgomery County, Maryland</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Michael Rosenwald, Biotech Reporter, Washington Post</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Douglas A. Doerfler, Ph.D., President &amp; CEO, MaxCyte, Inc.</li> <li>• Gerard J. McGarrity, Ph.D., President &amp; CEO, Intronn, Inc.</li> <li>• Barry Michael, B.A. Michael Consulting, LLC</li> <li>• Maciek Sasinowski, Ph.D., Chief Executive Officer, INCOGEN, Inc.</li> <li>• Mary Woolley, President &amp; CEO, Research! America</li> </ul> <p><b>Clinical Development Resources</b> The clinical development process for new medicines is a complex, costly and time-consuming endeavor, but there are myriad resources available to assist companies in this daunting effort. This session will focus on each phase of clinical development, and highlight some of the institutions and programs that can assist companies with trial management, patient recruitment, data analysis, etc.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Jerry Coughter, Ph.D., Director, Life Sciences Management, George Mason University</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• G. Stephen DeCherney, MD, President, Clinical Development Services Americas, Quintiles Transnational</li> <li>• Patricia Lovell Hoare, LLB, Head of International Regulatory Affairs, Chiltern International Limited</li> <li>• Thomas Thorpe, President, Afton Scientific, Inc.</li> <li>• Zobair M. Younossi, MD, Co-Director, GMU-Inova Translational Research Centers</li> </ul>
<b>3:30 pm - 4:00 pm</b>	<b>Break (Refreshments in Exhibit Hall)</b>
<b>4:00 pm - 5:30 pm</b>	<p><b>Concurrent sessions</b></p> <p>Investor Sessions IIA, IIB Six selected companies will make their case for financing to the investor community.</p>

	<p><b>Outsourcing – Making it Work to Your Advantage</b>                  Outsourcing to CROs has been traditionally used to acquire services and expertise rather than assuming the responsibility and expense of maintaining in-house staff. Some smaller companies are, in fact, “virtual” companies that outsource most or all aspects of product development. More recently, companies are conducting clinical trials outside the US to take advantage of lower labor costs to determine preliminary efficacy of products. This session will review the pros (cost, experience, staffing) and cons (control, management logistics) of outsourcing research, development and manufacturing services and how to leverage it to your advantage.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Mark McNamee, Ph.D., Provost, Virginia Tech</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Neil J. Campbell, Chairman and CEO, Mosaigen, Inc.</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Stephen J. Trevisan, President &amp; CEO, Accelovance</li> <li>• Magid Abou-Gharbia, Ph.D., Senior VP and Head, Chemical &amp; Screening Sciences, Wyeth Drug Discovery &amp; Development</li> <li>• Ann Orth, Ph.D., Director of Research Products, FMC Corporation</li> <li>• Gary Pekoe, Ph.D., President &amp; CEO, Arkios BioDevelopment</li> </ul> <p><b>How the Aging Population Will Affect the Market for New Health Care Products</b>                  As people are living ever longer and healthier lives, the mix of products that will be needed to sustain them will change. As the baby boomers continue to “mature,” the size of the market for “geriatric” medicines will increase dramatically over the next 20-30 years. The speakers in this session will examine these trends, and discuss what they should mean for the product development decisions companies are making today.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Christopher Yochim, Associate Director Global Discovery, AstraZeneca</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Louis F. Rossiter, Ph.D., Director of Research, Center of Excellence in Aging and Geriatric Health, College of William &amp; Mary</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• John F. Beary III, M.D., Medical Director, Arthritis Research Worldwide Clinical Development &amp; Medical Affairs, P&amp;G Pharmaceuticals</li> <li>• C. Randal Mills, President &amp; CEO, Osiris Therapeutics, Inc.</li> </ul>
<p>5:30 pm - 7:00 pm</p>	<p><b>General Reception (in Exhibit Hall)</b></p>
<p><b>Day 2: Thursday, October 27</b>  <i>Track Sponsor (Polaris) - Harvest Bank</i></p>	
<p>7:00 am - 8:30 am</p>	<p><b>Continental Breakfast (in Exhibit Hall)</b></p>
<p>8:30 am - 9:30 am</p>	<p><b>Opening Plenary Session</b>  <b>Host</b></p> <ul style="list-style-type: none"> <li>• Edward M. Rudnic, Ph.D., President &amp; CEO, Advancis Pharmaceutical Corp.</li> </ul> <p><b>Plenary Address</b></p> <ul style="list-style-type: none"> <li>• Julie McHugh, President, Centocor, Inc.</li> </ul>
<p>9:30 am - 10:45 am</p>	<p><b>Concurrent Sessions</b>  <b>Confronting Obesity: A Scientific, Business and Public Health Challenge</b>                  This session will take an in-depth look at one of the key therapeutic areas being addressed by today’s biopharmaceutical industry. Obesity clearly leads to numerous health problems, and is a major contributor to the spiraling cost of medical care. What have we learned about the physiology underlying obesity, and what does this suggest about the</p>

	<p>potential for developing commercial treatments? Where is the market opportunity, i.e. who is going to pay for anti-obesity drugs, and how much will they be willing to spend?</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Shawn M. Lofstrom, Ph.D., Director of Research, Sloan Biotechnology Industry Center, University of Maryland College Park</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Richard Atkinson, M.D., President, Obetech, LLC</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Sanjiv Arora, Director, Cargill Ventures</li> <li>• Morgan Downey, Executive Director &amp; CEO, American Obesity Association</li> <li>• Mir Imran, Founder and Chairman, IntraPace</li> <li>• John Jason Mullins, CEO, ZPRO Pharmaceutical, Inc.</li> </ul> <p><b>Is Partnering Becoming a Business Imperative?</b>                  What are the business and legal strategies that lead to successful development and commercialization of new biotech products? How do you seize collaborative opportunities in the development and commercialization process? The panel will discuss the pros and cons of different partnering strategies for companies at different stages of development.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Pace Lochte, Director, Virginia Gateway, Office of the VP for Research and Graduate Studies, University of Virginia</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Morrie Ruffin, Executive VP, Business Development &amp; Emerging Companies, Biotechnology Industry Organization</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• H. Casey Logan, Manager, Corporate Business Development, Eli Lilly &amp; Co.</li> <li>• Vincent J. Miles, Ph.D., Sr. VP, Business Development, Alnylam Pharmaceuticals, Inc.</li> <li>• Eric Richman, VP, Business Development &amp; Strategic Planning, Pharmathene, Inc.</li> </ul> <p><b>Hype vs. Reality – Will Investor Dollars Follow the Latest Trends?</b>                  Biodefense. Nanobiotechnology. Stem Cells. These buzzwords are familiar to much of the general public, so they must be the hot areas for bioscience investment. Right? Maybe not. This session will take another look at areas like these - from the investor perspective. What will help investors decide where to place their bets going forward?</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• René Salas, Mid-Atlantic Area Leader, Life Sciences, Ernst &amp; Young</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Alex Orfinger, Publisher, Washington Business Journal</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Linda Powers, Managing Director, Toucan Capital Corp.</li> <li>• Joseph Grzyb, CEO, Reactive NanoTechnologies, Inc.</li> <li>• Sydney J. Ulvick, Ph.D., In-Q-Tel</li> </ul>
<p><b>10:45 am - 11:15 am</b></p>	<p><b>Break (in Exhibit Hall)</b></p>
<p><b>11:15 am – 12:30 pm</b></p>	<p><b>Concurrent Sessions</b></p> <p><b>Finding the Right Way Out: Exit Strategies for Today's Markets</b>                  Going public offers biotech companies liquidity for their investors and much-needed cash for development programs. But is it worth it? Recent IPOs have lacked the investor enthusiasm and valuation of old, so is it time to consider a different option? The panel will discuss the pros and cons of going public, mergers and acquisitions and other “exit</p>

	<p>strategies”. The perspectives of venture capitalists, biotech companies and other stakeholders will be presented.</p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Claude Nash, Ph.D., VP, Research and Development, UMBI</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Lawrence Alleva, Partner, PriceWaterhouseCoopers</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• William Bertrand, Jr., VP &amp; General Counsel, MedImmune, Inc.</li> <li>• C. Boyd Clarke, Chairman &amp; CEO, Neose Technologies, Inc.</li> <li>• Krish S. Krishnan, CFO &amp; COO, New River Pharmaceuticals, Inc.</li> </ul> <p><b>Personalized Medicine: What Will It Mean for the Future of Drug Development?</b></p> <p>The new genomic era of medicine is likely to lead to significant changes in the economic realities on which drug development is based. Have we seen the end of blockbuster medicines with huge potential markets? Are theranostic products the wave of the future? Will smaller niche markets mean less incentive to develop follow-on biologics? This session will look ahead to a future of highly personalized medical treatments.</p> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• J. Brian Munroe, President, Personalized Medicine Coalition and Vice President, Government Relations &amp; Public Policy, Millennium Pharmaceuticals, Inc.</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Lance A. Liotta, MD, Ph.D., Co-Director, Center for Applied Proteomics &amp; Molecular Medicine, George Mason University</li> <li>• Richard S. Bakalar, MD, CMO, Information Based Medicine EBO IBM Healthcare &amp; Life Sciences</li> <li>• Donald Abraham, Ph.D., Director, Institute for Structure Biology &amp; Drug Discovery, Virginia Commonwealth University</li> </ul> <p><b>Building the Right Management Team for a Successful Bioscience Company</b></p> <p>This session will present ways to identify the optimum composition of a management team which is aligned with the corporate mission and strategic focus. In addition, thought leaders will contribute their perspective of developing the management team's vision and creativity which is the differentiator between good companies and successful companies.</p> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Jonathan Aberman, Managing Director, Amplifier Venture Partners</li> </ul> <p><b>Panelists</b></p> <ul style="list-style-type: none"> <li>• Arthur M. Mandell, President &amp; CEO, Collective Therapeutics, Inc.</li> <li>• Don Rainey, Venture Partner, Intersouth Partners</li> <li>• James K Leslie, Sr. Vice President, Kincannon &amp; Reed</li> <li>• Bruce Robertson, Ph.D., Managing Director, H.I.G. Ventures</li> </ul>
<p>12:30 pm – 2:00 pm</p>	<p><b>Plenary and Closing Luncheon: Building a Sustainable Bioscience Company – The CEO Perspective</b></p> <p><b>Host</b></p> <ul style="list-style-type: none"> <li>• Henry N. Wixon, Senior Partner, Wilmer Cutler Pickering Hale Dorr</li> </ul> <p><b>Moderator</b></p> <ul style="list-style-type: none"> <li>• Geoffrey Allan, Ph.D., President, CEO &amp; Chairman, Insmid Inc.</li> </ul> <p><b>Speakers</b></p> <ul style="list-style-type: none"> <li>• David M. Mott, CEO, MedImmune, Inc.</li> <li>• H. Thomas Watkins, President &amp; CEO, Human Genome Sciences, Inc.</li> </ul>

Anexa 3. Codul sursă al aplicației

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/sar/](http://vl.academicdirect.org/molecular_topology/mdf_findings/sar/)

*index.php*

```

<?
$b="";
if(!array_key_exists("file",$_GET)){
$a=explode("\n",ls *.sql res/);
unset($a[0]);
unset($a[count($a)]);
?>
Predict activity based on <UL><li> a learning set and<LI>a set of previous obtained MDF SAR models for<li>any molecule
submitted as HIN file by the user.</UL><BR>
<table align='right' style='background-color:#2e215f; color:#f6f1b0;'>
<tr>
<td>
© November 2005, <A HREF='http://lori.academicdirect.org' Target='_blank' Style='color:#f6f1b0;'>Lorentz
JÄNTSCHI</A>
</table>
<BR>
Learning set:
<form method='get' action='<? echo($_SERVER["PHP_SELF"]); ?>'>
<select name='file'>
<?
foreach($a as $v) {
list($v,$w)=explode(".sql",$v,2);
echo("<option value='".$v.">".$v);
}
?>
</select>
<input type='submit'>
</form>
<?
die();
}else{
if(file_exists("res/".$_GET["file"].".sql"))
$b=file_get_contents("res/".$_GET["file"].".sql");
}
if(!$b)die("no data");
unset($a);
$a=explode("\r\n",$b);
unset($b);
for($i=0;$i<count($a);$i++){
list($b,$a[$i])=explode("INSERT INTO `molecular_topology` VALUES (","",$a[$i],2);
list($a[$i],$b)=explode(")","",$a[$i],2);
$b=explode("","",$a[$i]);
$a[$i]=trim($b[1]);
unset($b);
$b=explode("",$a[$i]);
$a[$i]=trim($b[1]);
unset($b);
$b=explode("y=",$a[$i]);
$a[$i]=$b[1];
unset($b);
}
?>
Predictor's equation:
<form method='post' enctype='multipart/form-data' action='mdf_predictor.php'>
<select name='equation'>
<?
foreach($a as $v){
echo("<option value='".$v.">".$v);
}
?>

```

```
}  
?>  
</select>  
<BR>  
<BR>  
<BR>  
<BR>  
<BR>  
<BR>  
Molecule:<BR>  
HIN file:  
<input type='file' name='file'>  
<input type='submit'>  
</form>
```

### ***mdf\_predictor.php***

```
<?  
if(!$ _POST["equation"])die("no data");  
$a=explode("+",$ _POST["equation"]);  
$coef[0]=$a[0];  
$name[0]="";  
for($i=1;$i<count($a);$i++){  
    list($name[$i],$coef[$i])=explode("*",$a[$i]);  
}  
$file_name=$ _FILES["file"]["name"];  
$file_data=file_get_contents($ _FILES["file"]["tmp_name"]);  
if(strpos($file_data,"H H")>0)die("<pre>\r\n".$file_data."\r\n<font color='red'><b>You must withdraw Hydrogen's from  
structure for MDF calculation.\r\n</b></font></pre>");  
echo("<b>Molecule file name:</b><UL><LI>".$file_name."</UL>");  
include("mdf_functions.php");  
include("mdf_predictus.php");  
class m_c {  
    var $a;//number of atoms  
    var $b;//number of bonds  
    var $atom;//molecule structure  
    var $prop;//property structure  
    var $dist;//distances structure  
    var $e;//seed  
    var $f;//forcefield  
    var $m;//molecule number  
    var $p;//paths structure  
    var $s;//sys  
    var $v;//view  
    function m_c() {  
        $this->a=0;$this->b=0;$this->p[0][0][0]=0;//atomul 0, calea 0, varful 0 e 0  
    }  
}  
class fragments {  
    var $a;//number of atoms  
    var $f;//fragments structure  
    var $d;//substructura de distanta  
    function fragments(&$mol){!!!!!!!!!!!!de implementat cu foreach  
        $this->a=$mol->a;  
        foreach ($mol->atom as $atom_i){fiecare varf i  
            foreach ($mol->atom as $atom_j){fiecare varf j  
                $this->f[0][$atom_i[0]][$atom_j[0]][0]=$atom_i[0];  
            }//primul varf - implicit  
            $this->f[0][$atom_i[0]][$atom_i[0]][0]=0;  
        }//genereaza fragmentele minimale - ok  
    }  
}  
class models {
```

## ET36/2005 – Et. Unică/2005 – Lucrare in extenso

```
var $m_t; var $m_d; var $m_s; var $fty; var $pty; var $dty; var $smo; var $lty;
function models(&$poo){
  $this->m_t = array("mMDP","CHMEGQ","DdOoPpQqJjKkLlVvEwWfFfSsTt","RrMmDd");
  $this->m_d[0]="pr2m_".strpos($this->m_t[2],$poo["Df"]);
  $this->m_s[0]="prf_dmr_".strpos($this->m_t[3],$poo["Im"]);
  $this->fty=strpos($this->m_t[0],$poo["Fc"]);
  $this->pty=strpos($this->m_t[1],$poo["Ap"]);
  $this->dty=strpos("gt",$poo["Do"]);
  $this->smo=strpos("mMmNSPsAaBbGgFfHhIi",$poo["Sf"]);
  $this->lty=strpos("IiAaLl",$poo["Lo"]);
  $this->m_t = array($poo["Fc"],$poo["Ap"],$poo["Df"],$poo["Im"]);
}
}
$M = new m_c;
read_mol_new($M,$file_data,"z_atom_data.txt");
tree_mol($M,$tv);
$f = new fragments($M);
gen_f_max($f,$M);
gen_f_sdi($f,$M);
gen_f_fdi($f,$M,$tv);
unset($f->d);

//echo("<pre>");
//echo("POST data: ");
//print_r($_POST);
//echo("Molecule's data: ");
//unset($M->dist);
//unset($M->v);
//print_r($M);

echo("<b>Predictor's equation:</b><UL><LI>".$_POST["equation"]."</UL>");
echo("<b>MDF Members:</b><UL>");
$Sval_sum=$coef[0];
for($i=1;$i<count($Name);$i++){
  $post["Do"] = $Name[$i][6];
  $post["Ap"] = $Name[$i][5];
  $post["Df"] = $Name[$i][4];
  $post["Im"] = $Name[$i][3];
  $post["Fc"] = $Name[$i][2];
  $post["Sf"] = $Name[$i][1];
  $post["Lo"] = $Name[$i][0];
  $model = new models($post);
  $afisa=af_f_pf($f,$M,$model);
  echo("<LI>".$afisa);
  list($tmp,$Sval)=explode("=", $afisa);
  $Sval_sum += $coef[$i]*$Sval;
}
echo("</UL>");
echo("<b>Predicted activity:</b><UL><LI>");
echo($Sval_sum."</UL>");
unset($M);
unset($tv);
unset($f);
?>
```

### mdf\_predictus.php

```
<?
function af_f_pf(&$frag,&$mol,&$md){
  $contor=0;
  $tip_f=$md->fty;//tip de fragment (4)
  $tip_p=$md->pty;//tip de proprietate (6)
  $md_d_c=$md->m_d[0];//tip de descriptor (24)
```

## ET36/2005 – Et. Unică/2005 – Lucrare in extenso

```
$md_i_c=$md->m_s[0];//tip de interactiune (6)
$f_cnt=0;
foreach ($mol->atom as $atom_i){//fiecare varf i
  $i=$atom_i[0];
  foreach ($mol->atom as $atom_j){//fiecare varf j
    $varf=$atom_j[0];
    if($i==$varf) continue;
    if(!is_array($frag->f[$tip_f][$i][$varf][0]))
      $fragment[0]=$frag->f[$tip_f][$i][$varf];
    else
      $fragment=$frag->f[$tip_f][$i][$varf];
    for($fr_i=0;$fr_i<count($fragment);$fr_i++){
      $tmpp = $md_i_c($tip_p,$md_d_c,$varf,$fragment[$fr_i],$mol);
      $p_array[0][$f_cnt]=$tmpp[0];//gt
      $p_array[1][$f_cnt]=$tmpp[1];
      $f_cnt++;
    }
  }
}
}
}
$afisa="";//$afisa="Fragments: ".$f_cnt."\r\n"; $afisa="Fragmental properties: ".print_r($p_array[$md->dty],TRUE);
$na_fprop="";
$na_fprop=$md->m_t[0].$md->m_t[3].$md->m_t[2].$md->m_t[1];
$afisa.=af_cumul($contor,$mol->a,$mol->b,$p_array,$na_fprop,$md->dty,$md->smo,$md->lty);
unset($p_array);
unset($frag);
unset($mol);
return $afisa;
}
}
}
//genereaza si afiseaza proprietatile fragmentale
function af_cumul(&$contor,$nr_at,$nr_bo,&$p_array,&$na_fprop,$dty,$smo,$lty){
  $metric="gt";
  $nr_frags=count($p_array[0]);
  for($tip_x=$dty;$tip_x<$dty+1;$tip_x++){
    $sum=0; $prd=1; $isu=0;
    $max=-1e100; $max_a=0; $min=1e100; $min_a=1e100;
    $nr_fprop=0;
    for($tip_y=0;$tip_y<$nr_frags;$tip_y++){
      if(!$p_array[$tip_x][$tip_y]) continue;
      if(!is_finite($p_array[$tip_x][$tip_y]))continue;
      $nr_fprop++;
      $sum += $p_array[$tip_x][$tip_y];
      $prd *= $p_array[$tip_x][$tip_y];
      $isu += 1/$p_array[$tip_x][$tip_y];
      if($p_array[$tip_x][$tip_y]>$max) $max=$p_array[$tip_x][$tip_y];
      if(abs($p_array[$tip_x][$tip_y])>$max_a) $max_a=abs($p_array[$tip_x][$tip_y]);
      if($p_array[$tip_x][$tip_y]<$min) $min=$p_array[$tip_x][$tip_y];
      if(abs($p_array[$tip_x][$tip_y])<$min_a) $min_a=abs($p_array[$tip_x][$tip_y]);
    }
    if($max===-1e100) $max=(float)"INF";
    $v[0]=$max;//max property
    $af[0]="m".$na_fprop.$metric[$tip_x];
    $v[1]=$max_a;//max_a property
    $af[1]="M".$na_fprop.$metric[$tip_x];
    if($min==1e100) $min=(float)"INF";
    $v[2]=$min;//min property
    $af[2]="n".$na_fprop.$metric[$tip_x];
    if($min_a==1e100) $min_a=(float)"INF";
    $v[3]=$min_a;//min_a property
    $af[3]="N".$na_fprop.$metric[$tip_x];
    $v[4]=$sum;//sum property
    $af[4]="S".$na_fprop.$metric[$tip_x];
    $v[5]=$prd;//product property
    $af[5]="P".$na_fprop.$metric[$tip_x];
    if($isu)
      $v[6]=1/$isu;//harmonic sum property
```

*ET36/2005 – Et. Unică/2005 – Lucrare in extenso*

```
else $v[6]=(float)"INF";
$af[6]="s".$na_fprop.$metric[$tip_x];
if($nr_fprop)
  $v[7]=$sum/$nr_fprop;//average mean property for valid fragments
else $v[7]=(float)"INF";
$af[7]="A".$na_fprop.$metric[$tip_x];
$v[8]=$sum/$nr_frags;//average mean property for all fragments
$af[8]="a".$na_fprop.$metric[$tip_x];
$v[9]=$sum/$nr_at;//average mean property for all fragments
$af[9]="B".$na_fprop.$metric[$tip_x];
$v[10]=$sum/$nr_bo;//average mean property for all fragments
$af[10]="b".$na_fprop.$metric[$tip_x];
if($nr_fprop)
  $v[11]=pow(abs($prd),1/$nr_fprop);//geometric mean property for valid fragments - without sign
else $v[11]=1;
$af[11]="G".$na_fprop.$metric[$tip_x];
$v[12]=pow(abs($prd),1/$nr_frags);//geometric mean property fragments - without sign
$af[12]="g".$na_fprop.$metric[$tip_x];
$v[13]=pow(abs($prd),1/$nr_at);//geometric mean property fragments - without sign
$af[13]="F".$na_fprop.$metric[$tip_x];
$v[14]=pow(abs($prd),1/$nr_bo);//geometric mean property fragments - without sign
$af[14]="f".$na_fprop.$metric[$tip_x];
if($isu)
  $v[15]=$nr_fprop/$isu;//harmonic mean property for valid fragments
else $v[15]=(float)"INF";
$af[15]="H".$na_fprop.$metric[$tip_x];
if($isu)
  $v[16]=$nr_frags/$isu;//harmonic mean property for valid fragments
else $v[16]=(float)"INF";
$af[16]="h".$na_fprop.$metric[$tip_x];
if($isu)
  $v[17]=$nr_at/$isu;//harmonic mean property for valid fragments
else $v[17]=(float)"INF";
$af[17]="I".$na_fprop.$metric[$tip_x];
if($isu)
  $v[18]=$nr_bo/$isu;//harmonic mean property for valid fragments
else $v[18]=(float)"INF";
$af[18]="i".$na_fprop.$metric[$tip_x];
}
$ret="";//$ret = $af[$smo]." = ".$v[$smo]."\r\n";
if($lty==0){
  $ret = "I".$af[$smo]." = ".$v[$smo]."\r\n";
}
if($lty==1){
  $ret = "i".$af[$smo]." = "(1/$v[$smo])."\r\n";
}
if($lty==2){
  $ret = "A".$af[$smo]." = "(abs($v[$smo]))."\r\n";
}
if($lty==3){
  $ret = "a".$af[$smo]." = "(abs(1/$v[$smo]))."\r\n";
}
if($lty==4){
  $ret = "L".$af[$smo]." = "(log(abs($v[$smo]))).\r\n";
}
if($lty==5){
  $ret = "l".$af[$smo]." = "(log($v[$smo]))."\r\n";
}
return $ret;
}
?>
```

Anexa 4. Codul sursă al aplicației

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/j\\_mdf\\_demo.php](http://vl.academicdirect.org/molecular_topology/mdf_findings/j_mdf_demo.php)

```

<?
if(!array_key_exists("hin",$_POST)){
$a='ls -l demo/';
$b=explode("\n",$a);
unset($b[count($b)-1]);
unset($a);
echo("MDF Demo Calculator");
echo("<form method='post' action='".$_SERVER["PHP_SELF"].">");
echo("<table border='1'><tr>");
echo("<td>Molecule filename:<BR><select name='hin'>");
for($i=0;$i<count($b);$i++){
    echo("<option value='".$b[$i]."'>".$b[$i]);
}
echo("</select>");
echo("<td>Distance operator:<BR><select name='Do'>");
echo("<option value='t'>Topological distance, t");
echo("<option value='g'>Geometrical distance, g");
echo("</select>");
echo("<td>Atomic property:<BR><select name='Ap'>");
echo("<option value='C'>Cardinality, C");
echo("<option value='H'>Count of directly bounded hydrogen's, H");
echo("<option value='M'>Relative atomic mass, M");
echo("<option value='E'>Atomic electronegativity, E");
echo("<option value='G'>Group electronegativity, G");
echo("<option value='Q'>Partial charge, Q");
echo("</select>");
echo("</table><table border='1'><tr>");
echo("<td>Descriptor (of interaction) formula:<BR><select name='Df'>");
echo("<option value='D'>Distance, `D` = d");
echo("<option value='d'>Inverted distance, `d` = 1/d");
echo("<option value='O'>First atom's property, `O` = p1");
echo("<option value='o'>Inverted O, `o` = 1/p1");
echo("<option value='P'>Product of atomic properties, `P` = p1p2");
echo("<option value='p'>Inverted P, `p` = 1/p1p2");
echo("<option value='Q'>Squared P, `Q` = p1p2^1/2");
echo("<option value='q'>Inverted Q, `q` = 1/p1p2^1/2");
echo("<option value='J'>First atom's Property multiplied by distance, `J` = p1d");
echo("<option value='j'>Inverted J, `j` = 1/p1d");
echo("<option value='K'>Product of atomic properties and distance, `K` = p1p2d");
echo("<option value='k'>Inverted K, `k` = 1/p1p2d");
echo("<option value='L'>Product of distance and squared atomic properties, `L` = d(p1p2)^1/2");
echo("<option value='l'>Inverted L, `l` = 1/p1p2d");
echo("<option value='V'>First atom's property potential, `V` = p1/d");
echo("<option value='E'>First atom's property field, `E` = p1/d^2");
echo("<option value='W'>First atom's property work, `W` = p1^2/d");
echo("<option value='w'>Properties work, `w` = p1p2/d");
echo("<option value='F'>First atom's property force, `F` = p1^2/d^2");
echo("<option value='f'>Properties force, `f` = p1p2/d^2");
echo("<option value='S'>First atom's property weak nuclear force, `S` = p1^2/d^3");
echo("<option value='s'>Properties weak nuclear force, `s` = p1p2/d^3");
echo("<option value='T'>First atom's property strong nuclear force, `T` = p1^2/d^4");
echo("<option value='t'>Properties strong nuclear force, `t` = p1p2/d^4");
echo("</select>");
echo("<td>Interaction model:<BR><select name='Im'>");
echo("<option value='R'>Rare model and resultant relative to fragment's head, R");
echo("<option value='r'>Rare model and resultant relative to conventional origin, r");
echo("<option value='M'>Medium model and resultant relative to fragment's head, M");
echo("<option value='m'>Medium model and resultant relative to conventional origin, m");
echo("<option value='D'>Dense model and resultant relative to fragment's head, D");
echo("<option value='d'>Dense model and resultant relative to conventional origin, d");

```

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```
echo("</select>");
echo("</table><table border='1'><tr>");
echo("<td>Fragmentation criteria:<BR><select name='Fc'>");
echo("<option value='m'>Minimal fragments, m");
echo("<option value='M'>Maximal fragments, M");
echo("<option value='D'>Szedged distance based fragments, D");
echo("<option value='P'>Cluj path based fragments, P");
echo("</select>");
echo("<td>Molecular overall superposing formula:<BR><select name='Sf'>");
echo("<option value='m'>Cond., smallest, m");
echo("<option value='M'>Cond., highest, M");
echo("<option value='n'>Cond., smallest absolute, n");
echo("<option value='N'>Cond., highest absolute, N");
echo("<option value='S'>Avg., sum, S");
echo("<option value='A'>Avg., average, A");
echo("<option value='a'>Avg., S/count(fragments), a");
echo("<option value='B'>Avg., Avg.(Avg./atom)/count(atoms), B");
echo("<option value='b'>Avg., S/count(bonds), b");
echo("<option value='P'>Geom., product, P");
echo("<option value='G'>Geom., mean, G");
echo("<option value='g'>Geom., P^1/count(fragments), g");
echo("<option value='F'>Geom., Geom.(Geom./atom)/count(atoms), F");
echo("<option value='f'>Geom., P^1/count(bonds), f");
echo("<option value='s'>Harm., sum, s");
echo("<option value='H'>Harm., mean, H");
echo("<option value='h'>Harm., s/count(fragments), h");
echo("<option value='I'>Harm., Harm.(Harm./atom)/count(atoms), I");
echo("<option value='i'>Harm., s/count(bonds), i");
echo("</select>");
echo("<td>Linearization operator:<BR><select name='Lo'>");
echo("<option value='I'>Identity (no change), I");
echo("<option value='i'>Inversed I, i");
echo("<option value='A'>Absolute I, A");
echo("<option value='a'>Inversed A, a");
echo("<option value='L'>Logarithm of A, L");
echo("<option value='l'>Logarithm of I, l");
echo("</select>");
echo("</table><center><input type='submit'></center></form>");
} else {
include 'f_mdf_functions.php';
class m_c {
var $a;//number of atoms
var $b;//number of bonds
var $atom;//molecule structure
var $prop;//property structure
var $dist;//distances structure
var $e;//seed
var $f;//forcefield
var $m;//molecule number
var $p;//paths structure
var $s;//sys
var $v;//view
function m_c(){
$this->a=0;$this->b=0;$this->p[0][0][0]=0;//atomul 0, calea 0, varful 0 e 0
}
}
class fragments {
var $a;//number of atoms
var $f;//fragments structure
var $d;//substructura de distanta
function fragments(&$mol){!!!!!!!!!!!!de implementat cu foreach
$this->a=$mol->a;
foreach ($mol->atom as $atom_i){//fiecare varf i
foreach ($mol->atom as $atom_j){//fiecare varf j
```

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```
$this->f[0][$atom_i[0]][$atom_j[0]][0]=$atom_i[0];
} //primul varf - implicit
$this->f[0][$atom_i[0]][$atom_i[0]][0]=0;
} //genereaza fragmentele minimale - ok
}
}
class models{
var $m_t; var $m_d; var $m_s; var $fty; var $pty; var $dty; var $smo; var $lty;
function models(){
$this->m_t = array("mMDP","CHMEGQ","DdOoPpQqJjKkLlVvWwFfSsTt","RrMmDd");
$this->m_d[0]="pr2m_".strpos($this->m_t[2],$ _POST["Df"]);
$this->m_s[0]="prf_dmr_".strpos($this->m_t[3],$ _POST["Im"]);
$this->fty=strpos($this->m_t[0],$ _POST["Fc"]);
$this->pty=strpos($this->m_t[1],$ _POST["Ap"]);
$this->dty=strpos("gt",$ _POST["Do"]);
$this->smo=strpos("mMmNSPsAaBbGgFfHhIi",$ _POST["Sf"]);
$this->lty=strpos("IiAaLl",$ _POST["Lo"]);
$this->m_t = array($ _POST["Fc"],$ _POST["Ap"],$ _POST["Df"],$ _POST["Im"]);
}
}
$b=$ _POST["hin"];
$model = new models;
$m = new m_c;
read_mol($m,"demo".$b,"z_atom_data.txt");
tree_mol($m,$tv);
$f = new fragments($m);
gen_f_max($f,$m);
gen_f_sdi($f,$m);
gen_f_fdi($f,$m,$tv);
unset($f->d);
$afisa=af_f_pf($f,$m,$model);
echo("<pre>");
echo("POST data: ");
print_r($ _POST);
echo("Molecule's data: ");
unset($m->dist);
unset($m->v);
print_r($m);
echo("Fragments tree structure: ");
print_r($f->f[$model->fty]);
echo($afisa);
unset($m);
unset($tv);
unset($f);
}
function af_f_pf(&$frag,&$mol,&$md){
$contor=0;
$stip_f=$md->fty;//tip de fragment (4)
$stip_p=$md->pty;//tip de proprietate (6)
$md_d_c=$md->m_d[0];//tip de descriptor (24)
$md_i_c=$md->m_s[0];//tip de interactiune (6)
$f_cnt=0;
foreach ($mol->atom as $atom_i){fiecare varf i
$si=$atom_i[0];
foreach ($mol->atom as $atom_j){fiecare varf j
$svarf=$atom_j[0];
if($i==$svarf) continue;
if(!is_array($frag->f[$stip_f][$si][$svarf][0]))
$fragment[0]=$frag->f[$stip_f][$si][$svarf];
else
$fragment=$frag->f[$stip_f][$si][$svarf];
for($fr_i=0;$fr_i<count($fragment);$fr_i++){
$tmpp = $md_i_c($stip_p,$md_d_c,$svarf,$fragment[$fr_i],$mol);
$sp_array[0][$f_cnt]=$tmpp[0];//gt
```

```

    $p_array[1][$f_cnt]=$tmpp[1];
    $f_cnt++;
  }
}
}
$afisa="Fragments: ".$f_cnt."\n";
$afisa="Fragmental properties: ".print_r($p_array[$smd->dti],TRUE);
$na_fprop="";
$na_fprop=$smd->m_t[0].$smd->m_t[3].$smd->m_t[2].$smd->m_t[1];
$afisa=af_cumul($contor,$mol->a,$mol->b,$p_array,$na_fprop,$smd->dti,$smd->smo,$smd->lty);
unset($p_array);
unset($frag);
unset($mol);
return $afisa;
} //genereaza si afiseaza proprietatile fragmentale
function af_cumul(&$contor,$nr_at,$nr_bo,&$p_array,&$na_fprop,$sdydy,$smo,$lty){
  $metric="gt";
  $nr_frags=count($p_array[0]);
  for($stip_x=$sdydy;$stip_x<$sdydy+1;$stip_x++){
    $sum=0;
    $prd=1;
    $isu=0;
    $max=-1e100;
    $max_a=0;
    $min=1e100;
    $min_a=1e100;
    $nr_fprop=0;
    for($stip_y=0;$stip_y<$nr_frags;$stip_y++){
      if(!$p_array[$stip_x][$stip_y]) continue;
      if(!is_finite($p_array[$stip_x][$stip_y]))continue;
      $nr_fprop++;
      $sum += $p_array[$stip_x][$stip_y];
      $prd *= $p_array[$stip_x][$stip_y];
      $isu += 1/$p_array[$stip_x][$stip_y];
      if($p_array[$stip_x][$stip_y]>$max) $max=$p_array[$stip_x][$stip_y];
      if(abs($p_array[$stip_x][$stip_y])>$max_a) $max_a=abs($p_array[$stip_x][$stip_y]);
      if($p_array[$stip_x][$stip_y]<$min) $min=$p_array[$stip_x][$stip_y];
      if(abs($p_array[$stip_x][$stip_y])<$min_a) $min_a=abs($p_array[$stip_x][$stip_y]);
    }
    if($max===-1e100) $max=(float)"INF";
    $v[0]=$max;//max property
    $af[0]="m".$na_fprop.$metric[$stip_x];
    $v[1]=$max_a;//max_a property
    $af[1]="M".$na_fprop.$metric[$stip_x];
    if($min===1e100) $min=(float)"INF";
    $v[2]=$min;//min property
    $af[2]="n".$na_fprop.$metric[$stip_x];
    if($min_a===1e100) $min_a=(float)"INF";
    $v[3]=$min_a;//min_a property
    $af[3]="N".$na_fprop.$metric[$stip_x];
    $v[4]=$sum;//sum property
    $af[4]="S".$na_fprop.$metric[$stip_x];
    $v[5]=$prd;//product property
    $af[5]="P".$na_fprop.$metric[$stip_x];
    if($isu)
      $v[6]=1/$isu;//harmonic sum property
    else
      $v[6]=(float)"INF";
    $af[6]="s".$na_fprop.$metric[$stip_x];
    if($nr_fprop)
      $v[7]=$sum/$nr_fprop;//average mean property for valid fragments
    else
      $v[7]=(float)"INF";
    $af[7]="A".$na_fprop.$metric[$stip_x];
  }
}

```

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```
$v[8]=$sum/$nr_frags;//average mean property for all fragments
$af[8]="a".$na_fprop.$metric[$tip_x];
$v[9]=$sum/$nr_at;//average mean property for all fragments
$af[9]="B".$na_fprop.$metric[$tip_x];
$v[10]=$sum/$nr_bo;//average mean property for all fragments
$af[10]="b".$na_fprop.$metric[$tip_x];
if($nr_fprop)
  $v[11]=pow(abs($prd),1/$nr_fprop);//geometric mean property for valid fragments - without sign
else
  $v[11]=1;
$af[11]="G".$na_fprop.$metric[$tip_x];
$v[12]=pow(abs($prd),1/$nr_frags);//geometric mean property fragments - without sign
$af[12]="g".$na_fprop.$metric[$tip_x];
$v[13]=pow(abs($prd),1/$nr_at);//geometric mean property fragments - without sign
$af[13]="F".$na_fprop.$metric[$tip_x];
$v[14]=pow(abs($prd),1/$nr_bo);//geometric mean property fragments - without sign
$af[14]="f".$na_fprop.$metric[$tip_x];
if($isu)
  $v[15]=$nr_fprop/$isu;//harmonic mean property for valid fragments
else
  $v[15]=(float)"INF";
$af[15]="H".$na_fprop.$metric[$tip_x];
if($isu)
  $v[16]=$nr_frags/$isu;//harmonic mean property for valid fragments
else
  $v[16]=(float)"INF";
$af[16]="h".$na_fprop.$metric[$tip_x];
if($isu)
  $v[17]=$nr_at/$isu;//harmonic mean property for valid fragments
else
  $v[17]=(float)"INF";
$af[17]="I".$na_fprop.$metric[$tip_x];
if($isu)
  $v[18]=$nr_bo/$isu;//harmonic mean property for valid fragments
else
  $v[18]=(float)"INF";
$af[18]="i".$na_fprop.$metric[$tip_x];
}
$ret = $af[$smo]. " = ".$v[$smo]. "\r\n";
if($lty==0){
  $ret .= "I".$af[$smo]. " = ".$v[$smo]. "\r\n";
}
if($lty==1){
  $ret .= "i".$af[$smo]. " = "(1/$v[$smo]). "\r\n";
}
if($lty==2){
  $ret .= "A".$af[$smo]. " = "(abs($v[$smo])). "\r\n";
}
if($lty==3){
  $ret .= "a".$af[$smo]. " = "(abs(1/$v[$smo])). "\r\n";
}
if($lty==4){
  $ret .= "L".$af[$smo]. " = "(log(abs($v[$smo])). "\r\n";
}
if($lty==5){
  $ret .= "I".$af[$smo]. " = "(log($v[$smo])). "\r\n";
}
return $ret;
}
?>
```

Anexa 5. Rezultatul obținut de aplicație pentru o moleculă școală

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/j\\_mdf\\_demo.php](http://vl.academicdirect.org/molecular_topology/mdf_findings/j_mdf_demo.php)

POST data: Array

```
(
  [hin] => 01_mr1001.hin
  [Do] => t
  [Ap] => C
  [Df] => D
  [Im] => R
  [Fc] => m
  [Sf] => m
  [Lo] => I
)
```

Molecule's data: m\_c Object

```
(
  [a] => 9
  [b] => 9
  [atom] => Array
    (
      [1] => Array
        (
          [0] => 1
          [1] => -
          [2] => C
          [3] => C4
          [4] => -
          [5] => -0.1095657
          [6] => 0.4318282
          [7] => 0.6380987
          [8] => 2.849884
          [9] => 1
          [10] => 2
          [11] => 1
        )
      [2] => Array
        (
          [0] => 2
          [1] => -
          [2] => C
        )
    )
)
```

```
[3] => C4
[4] => -
[5] => 0.5250869
[6] => -0.2941397
[7] => 0.1247597
[8] => 1.592484
[9] => 3
[10] => 1
[11] => 1
[12] => 3
[13] => 1
[14] => 7
[15] => 1
)

[3] => Array
(
  [0] => 3
  [1] => -
  [2] => C
  [3] => C4
  [4] => -
  [5] => -0.0686326
  [6] => -0.2920918
  [7] => -1.415741
  [8] => 1.596032
  [9] => 2
  [10] => 2
  [11] => 1
  [12] => 4
  [13] => 1
)

[4] => Array
(
  [0] => 4
  [1] => -
  [2] => C
  [3] => C4
  [4] => -
  [5] => 0.4661818
  [6] => -1.039482
  [7] => -1.962821
  [8] => 0.3649576
  [9] => 2
  [10] => 3
  [11] => 1
  [12] => 5
  [13] => 1
)

[5] => Array
(
  [0] => 5
  [1] => -
  [2] => O
  [3] => O2
  [4] => -
  [5] => -0.9945602
  [6] => -0.3896529
  [7] => -1.532219
  [8] => -0.8337278
  [9] => 2
  [10] => 4
  [11] => 1
)
```

```
[12] => 6
[13] => 1
)
[6] => Array
(
  [0] => 6
  [1] => -
  [2] => P
  [3] => P5
  [4] => -
  [5] => 1.883921
  [6] => -0.5882888
  [7] => 0.2352459
  [8] => -1.032513
  [9] => 3
  [10] => 5
  [11] => 1
  [12] => 7
  [13] => 1
  [14] => 8
  [15] => 1
)
[7] => Array
(
  [0] => 7
  [1] => -
  [2] => O
  [3] => O2
  [4] => -
  [5] => -1.095338
  [6] => 0.3748803
  [7] => 0.6139225
  [8] => 0.4270911
  [9] => 2
  [10] => 6
  [11] => 1
  [12] => 2
  [13] => 1
)
[8] => Array
(
  [0] => 8
  [1] => -
  [2] => O
  [3] => O2
  [4] => -
  [5] => -1.019472
  [6] => 0.6156649
  [7] => 1.142236
  [8] => -1.997664
  [9] => 2
  [10] => 6
  [11] => 1
  [12] => 9
  [13] => 1
)
[9] => Array
(
  [0] => 9
  [1] => -
  [2] => C
```

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```
[3] => C4
[4] => -
[5] => 0.4202826
[6] => 0.2612277
[7] => 2.5274
[8] => -2.022074
[9] => 1
[10] => 8
[11] => 1
)
)
[prop] => Array
(
  [1] => Array
  (
    [0] => 1
    [1] => 4
    [2] => 12
    [3] => 2.746
    [4] => 2.6296707827796
    [5] => -0.1095657
  )
  [2] => Array
  (
    [0] => 1
    [1] => 2
    [2] => 12
    [3] => 2.746
    [4] => 2.6678890531654
    [5] => 0.5250869
  )
  [3] => Array
  (
    [0] => 1
    [1] => 3
    [2] => 12
    [3] => 2.746
    [4] => 2.6423489837131
    [5] => -0.0686326
  )
  [4] => Array
  (
    [0] => 1
    [1] => 3
    [2] => 12
    [3] => 2.746
    [4] => 2.6423489837131
    [5] => 0.4661818
  )
  [5] => Array
  (
    [0] => 1
    [1] => 1
    [2] => 15.99491464
    [3] => 3.654
    [4] => 3.654
    [5] => -0.9945602
  )
)
```

```
[6] => Array
(
  [0] => 1
  [1] => 1
  [2] => 30.9737634
  [3] => 2.515
  [4] => 2.515
  [5] => 1.883921
)

[7] => Array
(
  [0] => 1
  [1] => 1
  [2] => 15.99491464
  [3] => 3.654
  [4] => 3.654
  [5] => -1.095338
)

[8] => Array
(
  [0] => 1
  [1] => 1
  [2] => 15.99491464
  [3] => 3.654
  [4] => 3.654
  [5] => -1.019472
)

[9] => Array
(
  [0] => 1
  [1] => 4
  [2] => 12
  [3] => 2.746
  [4] => 2.6296707827796
  [5] => 0.4202826
)

)

[e] => seed 0
[f] => forcefield mm+
[m] => mol 1
[s] => sys 0 0 1
)
Fragments tree structure: Array
(
  [1] => Array
  (
    [1] => Array
    (
      [0] => 0
    )

    [2] => Array
    (
      [0] => 1
    )

    [3] => Array
    (
      [0] => 1
    )
  )
)
```

```
[4] => Array
  (
    [0] => 1
  )

[5] => Array
  (
    [0] => 1
  )

[6] => Array
  (
    [0] => 1
  )

[7] => Array
  (
    [0] => 1
  )

[8] => Array
  (
    [0] => 1
  )

[9] => Array
  (
    [0] => 1
  )
)

[2] => Array
  (
    [1] => Array
      (
        [0] => 2
      )

    [2] => Array
      (
        [0] => 0
      )

    [3] => Array
      (
        [0] => 2
      )

    [4] => Array
      (
        [0] => 2
      )

    [5] => Array
      (
        [0] => 2
      )

    [6] => Array
      (
        [0] => 2
      )
  )
```

*ET36/2005 – Et. Unică/2005 – Lucrare in extenso*

```
[7] => Array
  (
    [0] => 2
  )

[8] => Array
  (
    [0] => 2
  )

[9] => Array
  (
    [0] => 2
  )
)

[3] => Array
  (
    [1] => Array
      (
        [0] => 3
      )

    [2] => Array
      (
        [0] => 3
      )

    [3] => Array
      (
        [0] => 0
      )

    [4] => Array
      (
        [0] => 3
      )

    [5] => Array
      (
        [0] => 3
      )

    [6] => Array
      (
        [0] => 3
      )

    [7] => Array
      (
        [0] => 3
      )

    [8] => Array
      (
        [0] => 3
      )

    [9] => Array
      (
        [0] => 3
      )
  )
)
```

```
[4] => Array
(
    [1] => Array
        (
            [0] => 4
        )
    [2] => Array
        (
            [0] => 4
        )
    [3] => Array
        (
            [0] => 4
        )
    [4] => Array
        (
            [0] => 0
        )
    [5] => Array
        (
            [0] => 4
        )
    [6] => Array
        (
            [0] => 4
        )
    [7] => Array
        (
            [0] => 4
        )
    [8] => Array
        (
            [0] => 4
        )
    [9] => Array
        (
            [0] => 4
        )
)

[5] => Array
(
    [1] => Array
        (
            [0] => 5
        )
    [2] => Array
        (
            [0] => 5
        )
    [3] => Array
        (
            [0] => 5
        )
)
```

```
    )  
    [4] => Array  
    (    [0] => 5  
    )  
    [5] => Array  
    (    [0] => 0  
    )  
    [6] => Array  
    (    [0] => 5  
    )  
    [7] => Array  
    (    [0] => 5  
    )  
    [8] => Array  
    (    [0] => 5  
    )  
    [9] => Array  
    (    [0] => 5  
    )  
    )  
[6] => Array  
    (    [1] => Array  
    (    [0] => 6  
    )  
    [2] => Array  
    (    [0] => 6  
    )  
    [3] => Array  
    (    [0] => 6  
    )  
    [4] => Array  
    (    [0] => 6  
    )  
    [5] => Array  
    (    [0] => 6  
    )  
    [6] => Array  
    (    [0] => 0  
    )
```

```
[7] => Array
(
    [0] => 6
)

[8] => Array
(
    [0] => 6
)

[9] => Array
(
    [0] => 6
)
)

[7] => Array
(
    [1] => Array
    (
        [0] => 7
    )

    [2] => Array
    (
        [0] => 7
    )

    [3] => Array
    (
        [0] => 7
    )

    [4] => Array
    (
        [0] => 7
    )

    [5] => Array
    (
        [0] => 7
    )

    [6] => Array
    (
        [0] => 7
    )

    [7] => Array
    (
        [0] => 0
    )

    [8] => Array
    (
        [0] => 7
    )

    [9] => Array
    (
        [0] => 7
    )
)
```

*ET36/2005 – Et. Unică/2005 – Lucrare in extenso*

```
)  
[8] => Array  
(  
  [1] => Array  
  (  
    [0] => 8  
  )  
  
  [2] => Array  
  (  
    [0] => 8  
  )  
  
  [3] => Array  
  (  
    [0] => 8  
  )  
  
  [4] => Array  
  (  
    [0] => 8  
  )  
  
  [5] => Array  
  (  
    [0] => 8  
  )  
  
  [6] => Array  
  (  
    [0] => 8  
  )  
  
  [7] => Array  
  (  
    [0] => 8  
  )  
  
  [8] => Array  
  (  
    [0] => 0  
  )  
  
  [9] => Array  
  (  
    [0] => 8  
  )  
  
)  
[9] => Array  
(  
  [1] => Array  
  (  
    [0] => 9  
  )  
  
  [2] => Array  
  (  
    [0] => 9  
  )  
  
  [3] => Array  
  (  
    [0] => 9  
  )  
  
)
```

*ET36/2005 – Et. Unică/2005 – Lucrare in extenso*

```
        [0] => 9
      )
    [4] => Array
      (
        [0] => 9
      )
    [5] => Array
      (
        [0] => 9
      )
    [6] => Array
      (
        [0] => 9
      )
    [7] => Array
      (
        [0] => 9
      )
    [8] => Array
      (
        [0] => 9
      )
    [9] => Array
      (
        [0] => 0
      )
  )
```

)

**Fragments: 72**

**Fragmental properties: Array**

(

```
[0] => -7.11111111111111
[1] => -7.11111111111111
[2] => -7.11111111111111
[3] => -7.11111111111111
[4] => -7.11111111111111
[5] => -7.11111111111111
[6] => -7.11111111111111
[7] => -7.11111111111111
[8] => -7.88888888888889
[9] => -7.88888888888889
[10] => -7.88888888888889
[11] => -7.88888888888889
[12] => -7.88888888888889
[13] => -7.88888888888889
[14] => -7.88888888888889
[15] => -7.88888888888889
[16] => -7.55555555555556
[17] => -7.55555555555556
[18] => -7.55555555555556
[19] => -7.55555555555556
[20] => -7.55555555555556
[21] => -7.55555555555556
[22] => -7.55555555555556
[23] => -7.55555555555556
[24] => -7.66666666666667
[25] => -7.66666666666667
```

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[26] => -7.6666666666667  
[27] => -7.6666666666667  
[28] => -7.6666666666667  
[29] => -7.6666666666667  
[30] => -7.6666666666667  
[31] => -7.6666666666667  
[32] => -7.7777777777778  
[33] => -7.7777777777778  
[34] => -7.7777777777778  
[35] => -7.7777777777778  
[36] => -7.7777777777778  
[37] => -7.7777777777778  
[38] => -7.7777777777778  
[39] => -7.7777777777778  
[40] => -8.1111111111111  
[41] => -8.1111111111111  
[42] => -8.1111111111111  
[43] => -8.1111111111111  
[44] => -8.1111111111111  
[45] => -8.1111111111111  
[46] => -8.1111111111111  
[47] => -8.1111111111111  
[48] => -8  
[49] => -8  
[50] => -8  
[51] => -8  
[52] => -8  
[53] => -8  
[54] => -8  
[55] => -8  
[56] => -7.5555555555556  
[57] => -7.5555555555556  
[58] => -7.5555555555556  
[59] => -7.5555555555556  
[60] => -7.5555555555556  
[61] => -7.5555555555556  
[62] => -7.5555555555556  
[63] => -7.5555555555556  
[64] => -6.7777777777778  
[65] => -6.7777777777778  
[66] => -6.7777777777778  
[67] => -6.7777777777778  
[68] => -6.7777777777778  
[69] => -6.7777777777778  
[70] => -6.7777777777778  
[71] => -6.7777777777778

)

**mmRDCt** = -6.7777777777778

**ImmRDCt** = -6.7777777777778

## Anexa 6. Codul sursă al aplicației

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/loo/](http://vl.academicdirect.org/molecular_topology/mdf_findings/loo/)

### *index.php*

Leave one out analysis require a tabulated data in html format as input data with followings:

```
<UL>
<LI>column labels;
<LI>row labels;
<LI>independent variables - first set of columns;
<LI>estimated dependent variable - following column;
<LI>dependent variable;
<LI>predicted variable - last column;
</UL>
<form method='post' enctype='multipart/form-data' action='do.php'>
<input type='file' name='file'>
<input type='submit'>
</form>
<table align='right' style='background-color:#2e215f; color:#f6f1b0;'>
<tr>
<td>
© November 2005, <A href='http://lori.academicdirect.org' Target='_blank' Style='color:#f6f1b0;'>Lorentz
JÄNTSCHI</A>
</td>
</tr>
<BR>
<BR>
Data example:
<?
echo(file_get_contents("mysql_query_php_Triazines.htm"));
highlight_file("mysql_query_php_Triazines.htm");
?>
```

### *functions.php*

```
<?
include("statistics/FDistribution.php");
function m1(&$v){
$rez=0;
$n=count($v);
for($i=0;$i<$n;$i++)
$rez+=$v[$i];
return $rez/$n;
}
function m2(&$v,&$u){
$rez=0;
$n=count($v);
for($i=0;$i<$n;$i++)
$rez+=$v[$i]*$u[$i];
return $rez/$n;
}
function coef_r(&$y1,&$y2){
$m1=m1($y1);
$dy2=m2($y1,$y1)-$m1*$m1;
$m2=m1($y2);
$mxy=m2($y1,$y2);
$m2x=$m1*$m2;
$m2y=m2($y2,$y2);
$dx2=$m2y-$m2x;
$r2=pow($mxy-$m1*$m2,2)/($dx2*$dy2);
return $r2;
}
function coef_F(&$y1,&$y2,$df_r){
```

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```
$my1=m1($y1);
$T_SS=0;
for($i=0;$i<count($y1);$i++)
  $T_SS+=pow($y1[$i]-$my1,2);
$E_SS=0;
for($i=0;$i<count($y1);$i++)
  $E_SS+=pow($y1[$i]-$y2[$i],2);
$R_SS=$T_SS-$E_SS;
$T_df=count($y1)-1;
$R_df=$df_r;
$E_df=$T_df*$R_df;
if(!$R_df)die();
if(!$E_SS)die();
$F=$R_SS*$E_df/$R_df/$E_SS;
return $F;
}
function coef_pF($df_r,$df_t,$F){
  $Fd = new FDistribution($df_r,$df_t-$df_r);
  return 1.0 - $Fd->CDF($F);
}
?>
```

### do.php

```
<?
include("functions.php");
$a=strip_tags(file_get_contents($_FILES['file']['tmp_name']),"<tr><td>");
$b=explode("<TR>",$a);
echo("<table border=1>");
for($i=1;$i<count($b);$i++){
  $b[$i]=explode("<TD>",$b[$i]);
}
for($i=1;$i<count($b);$i++){
  for($j=1;$j<count($b[$i]);$j++){
    $b[$i][$j]=trim($b[$i][$j]);
  }
}
for($i=1;$i<count($b);$i++){
  echo("\r\n<tr>");
  for($j=1;$j<count($b[$i]);$j++){
    echo("<td>".$b[$i][$j]);
  }
}
echo("\r\n</table>");
$df=count($b)-count($b[1])+2;
echo("Df = ".$df."<BR>\r\n");
$var=count($b[1])-5;
echo("Var = ".$var."<BR>\r\n");

$ssp=0;
$sse=0;
for($i=1;$i<count($b);$i++){
  $ssp+=pow($b[$i][count($b[1])-2]-$b[$i][count($b[1])-1],2);
  $sse+=pow($b[$i][count($b[1])-2]-$b[$i][count($b[1])-3],2);
  $y_mas[] = $b[$i][count($b[1])-2];
  $y_est[] = $b[$i][count($b[1])-3];
  $y_pre[] = $b[$i][count($b[1])-1];
}
array_shift($y_mas);
array_shift($y_est);
array_shift($y_pre);

echo("<b>Estimated:</b><br>");
```

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```
echo("Sse = ".$sse."<BR>\r\n");
$sse /= $df;
$sse = pow($sse,0.5);
echo("QSSe = ".$sse."<BR>\r\n");
echo("r2est = ".coef_r($y_mas,$y_est)."<BR>\r\n");
$cFe = coef_F($y_mas,$y_est,$var);
echo("Fest = ".$cFe."<BR>\r\n");
$pest=coef_pF($var,$df+$var,$cFe);
if($pest==0) $pest="<1e-17";
echo("p_est = ".$pest."<BR>\r\n");
echo("<b>Predicted:</b><br>");
echo("SSp = ".$ssp."<BR>\r\n");
$ssp /= $df;
$ssp = pow($ssp,0.5);
echo("QSSp = ".$ssp."<BR>\r\n");
echo("r2pre = ".coef_r($y_mas,$y_pre)."<BR>\r\n");
$cFp = coef_F($y_mas,$y_pre,$var);
echo("Fpre = ".$cFp."<BR>\r\n");
$ppre=coef_pF($var,$df+$var,$cFp);
if($ppre==0) $ppre="<1e-17";
echo("p_pre = ".$ppre."<BR>\r\n");
?>
```

Anexa 7. Rezultatul obținut de aplicație pentru un set școală

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/loo/](http://vl.academicdirect.org/molecular_topology/mdf_findings/loo/)

http://vl.academicdirect.org/molecular\_topology/mdf\_findings/loo/

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Mail

Address http://vl.academicdirect.org/molecular\_topology/mdf\_findings/sar/

Google Search PageRank 7 blocked Check

Predict activity based on

- a learning set and
- a set of previous obtained MDF SAR models for
- any molecule submitted as HIN file by the user.

Learning set:

26449t Submit Query

http://vl.academicdirect.org/molecular\_topology/mdf\_findings/sar/index

File Edit View Favorites Tools Help

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Address http://vl.academicdirect.org/molecular\_topology/mdf\_findings/sar/index.php?file=26449t

Google Search PageRank 7 blocked Check AutoLink

Predictor's equation:

-19.112864129011363+IHPDOQg\*2.317497007317971+IsMRKGg\*19.343096061022083

Molecule:

HIN file: C:\01\_Bromobenzene.hi Browse... Submit Query

http://vl.academicdirect.org/molecular\_topology/mdf\_findings/sar/mdf\_predictor.p

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Mail

Address http://vl.academicdirect.org/molecular\_topology/mdf\_findings/sar/mdf\_predictor.php

Google Search PageRank 7 blocked Check AutoLink AutoFill Op

Molecule file name:

- 01\_Bromobenzene.hin

Predictor's equation:

- -19.112864129011363+IHPDOQg\*2.317497007317971+IsMRKGg\*19.343096061022083

MDF Members:

- IHPDOQg = -2.3176387046408
- IsMRKGg = 1.8367105404093

Predicted activity:

- 11.043683528368

## Anexa 8. Codul sursă al aplicației

[http://vl.academicdirect.org/molecular\\_topology/qsar\\_qspr\\_s/](http://vl.academicdirect.org/molecular_topology/qsar_qspr_s/)

### *index.php*

```
<h1>
Training vs. Test Experiment
</h1>
Please select a data file from the list of available data.
<BR>
The experiment will performe a random split of experimental data in two sets: "trainig set" and "test set".
<BR>
The QSAR/QSPR model are calculate using the data from training set.
<BR>
The obtained QSAR equation are apply then on both sets, in order to calculate statistical parameters.
<BR>
<?
$a='ls -al *.txt';
$b=explode("\n",$a);
?>
<form method='post' action='select.php'>
<table width='50%'>
<tr>
<td>
<select name='select'>
<?
for($i=0;$i<count($b);$i++){
    $c=explode(" ",$b[$i]);
    $d=$c[count($c)-1];
    if($d) echo("<option value=\"$.d.\">$.d);
}
?>
</select>
<td>
<input type='submit'>
</table>
</form>
```

### *select.php*

```
<?
include 'functions.php';
get_all_data("select",$_POST,$e);
?>
<table border=0>
<tr>
<td>
<form method='post' action='query.php'>
You selected:
<BR>
Set file:
<select name='select'>
<option value='<? echo($_POST['select']); ?>' selected><? echo($_POST['select']); ?>
</select>
<BR>
<BR>
Please select:
<BR>
Training set count:
<select name='test'>
<?
for($i=count($e[0])-1;$i<count($e);$i++){
```

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```
echo("<option value='".Si."'");
if($i==(int)((count($e[0])+count($e))/2)) echo(" selected ");
echo(">".Si);
}
?>
</select>
<BR>
<BR>
<input type='submit'>
</form>
<td>
<?
af($e,"");
?>
</table>
```

### ***query.php***

```
<?
include 'functions.php';
get_all_data("select",$_POST,$e);
?>
Please make <font color='green'>refresh</font> to generate other sets lists.
<BR>
<table border=0>
<tr>
<td>
<form method='post' action='result.php'>
Set file:
<select name='select'>
<option value='<? echo($_POST['select']); ?>' selected><? echo($_POST['select']); ?>
</select>
<BR>
<BR>
Training set count:
<select name='test'>
<option value='<? echo($_POST['test']); ?>' selected><? echo($_POST['test']); ?>
</select>
<?
for($i=0;$i<$_POST['test'];$i++){
do {
$ok=0;
$trs[$i]=rand(1,count($e)-1);
for($j=0;$j<count($trs)-1;$j++)
if($trs[$j]==$trs[$i]){
$ok=1;
break;
}
}while($ok);
}
for($i=1;$i<count($e);$i++)
$f[$i]=$i;
for($i=0;$i<count($trs);$i++){
unset($f[$trs[$i]]);
$trs[$i]=$e[$trs[$i]][0];
}
$str_s=implode(" ",$trs);
foreach($f as $kf=> $vf)
$f[$kf]=$e[$vf][0];
$str_s=implode(" ",$f);
?>
<BR>
<BR>
```

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Training set list:

```
<BR>
<textarea name='training' rows='5' cols='30'>
<?
echo($tr_s);
?>
</textarea>
<BR>
<BR>
Test set list:
<BR>
<textarea name='rest' rows='5' cols='30'>
<?
echo($te_s);
?>
</textarea>
<BR>
<BR>
<input type='submit'>
</form>
<td>
<?
af($e,"");
?>
</table>
```

### result.php

```
<?
include 'functions.php';
include 'mlr.php';
get_all_data("select",$ _POST,$e);
echo("Set file: ".$ _POST['select']."<BR>");
echo("Training set count: ".$ _POST['test']."<BR>");
echo("Training set: ".$ _POST['training']."<BR>");
echo("Test set: ".$ _POST['rest']."<BR>");//af($e,"All set:");
$tra=explode(" ",$ _POST['training']);
$tes=explode(" ",$ _POST['rest']);
sub_test($tra,$e,$t_tra);
sub_test($tes,$e,$t_tes);
af($t_tra,"Training set data:");
echo("QSAR/QSPR: ");
for($i=1;$i<count($t_tra[0])-1;$i++){
  $t[$i-1]=$t_tra[0][$i];
  for($j=1;$j<count($t_tra);$j++){
    $x[$i-1][$j-1]=$t_tra[$j][$i];
  }
  for($j=1;$j<count($t_tra);$j++){
    $y[$j-1]=$t_tra[$j][count($t_tra[0])-1];
  }
  get_coefs($y,$x,$c);
  for($j=0;$j<count($c);$j++){
    $c[$j]=spalare($c[$j]);//echo($c[$j]." ");
  }
  echo(put_coef_ind($c,$t,"EST")."<BR>");
  calc_eq_1($c,$x,$y_pred);
  echo("Coefficient of determination r<sup>2</sup> = ".coef_r($y,$y_pred)."<BR>");
  $coef_F=coef_F($y,$y_pred,count($c)-1);
  echo("Fisher test value F = ".spalare($coef_F)."<BR>");
  $coef_pF=coef_pF(count($c)-1,count($y)-1,$coef_F);
  echo("Probability of wrong (from F) p<sub>F</sub> = ".sprintf("%1.5f",$coef_pF*100)."% (".$coef_pF)."<BR>");
  for($i=1;$i<count($t_tes[0])-1;$i++){
    $tt[$i-1]=$t_tes[0][$i];
    for($j=1;$j<count($t_tes);$j++){
      $xx[$i-1][$j-1]=$t_tes[$j][$i];
    }
  }
}
```

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```
}
for($j=1;$j<count($t_les);$j++)
  $yy[$j-1]=$t_les[$j][count($t_les[0])-1];
if(count($t_les)>1){
  af($t_les,"Test set data:");
  calc_eq_1($c,$xx,$yy_pred);
  echo("Coefficient of determination  $r^2$  = ".coef_r($yy,$yy_pred)."<BR>");
  $coef_F=coef_F($yy,$yy_pred,count($c)-1);
  echo("Fisher test value F = ".spalare($coef_F)."<BR>");
  $coef_pF=coef_pF(count($c)-1,count($yy)-1,$coef_F);
  echo("Probability of wrong (from F)  $p <sub>F</sub>$  = ".sprintf("%1.5f",$coef_pF*100)."% (".$coef_pF)."<BR>");
} else echo("You selected all data in training set, thus no Test set data here.<BR>");
?>
```

### functions.php

```
<?
function get_all_data($text,&$tab,&$e){
  if(!array_key_exists($text,$tab)) die("no select");
  $a=file_get_contents($tab[$text]);
  $b=explode("\r\n",$a);
  for($j=0,$i=0;$i<count($b);$i++)
    if(!$b[$i]) continue; else
      $c[$j++]=explode(" ",$b[$i]);
  for($i=0;$i<count($c);$i++)
    for($k=0,$j=0;$j<count($c[$i]);$j++)
      if(!$c[$i][$j]) continue; else
        $d[$i][$k++]=$c[$i][$j];
  for($i=0;$i<count($d);$i++){
    for($j=0;$j<count($d[$i])-2;$j++)
      $e[$i][$j]=$d[$i][$j];
    $e[$i][count($d[$i])-3]=$d[$i][count($d[$i])-2];
  }
}
function af(&$e,$msg){
  if($msg) echo($msg."<BR>");
}
?>
<table border=1>
<?
for($i=0;$i<count($e);$i++){
  echo("<tr>");
  for($j=0;$j<count($e[$i]);$j++)
    echo("<td>".$e[$i][$j]);
}
?>
</table>
<?
}
}
?>
```

### mlr.php

```
<?
include 'statistics/FDistribution.php';
function m1(&$v){
  $rez=0;
  $n=count($v);
  for($i=0;$i<$n;$i++)
    $rez+=$v[$i];
  return $rez/$n;
}
function m2(&$v,&$u){
```

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```
$rez=0;
$n=count($v);
for($i=0;$i<$n;$i++)
  $rez+=$v[$i]*$u[$i];
return $rez/$n;
}
function get_coefs(&$y,&$x,&$b){
$b[0] = m1($y);//x[ind][mol]
$a[0][0] = 1.0;
for($k=1;$k<=count($x);$k++){
  $a[0][$k] = m1($x[$k-1]);
  $a[$k][0] = $a[0][$k];
  $a[$k][$k] = m2($x[$k-1],$x[$k-1]);
  $b[$k] = m2($x[$k-1],$y);
  for($l=$k+1;$l<=count($x);$l++){
    $a[$k][$l] = m2($x[$k-1],$x[$l-1]);
    $a[$l][$k] = $a[$k][$l];
  }
}
$a[0][0] = gauss($b,$a);
}
function gauss(&$b,&$a){
for($i=0;$i<count($a);$i++){
  $m=$i;//caut max in coloana
  for($j=$i+1;$j<count($a);$j++)
    if(abs($a[$i][$j])>abs($a[$i][$m]))$m=$j;
  if($a[$i][$m]==0)return -1;
  if($m != $i){inlocuiesc linii
    $tmp=$b[$m];$b[$m]=$b[$i];$b[$i]=$tmp;
    for($j=0;$j<count($a);$j++){
      $tmp=$a[$m][$j];$a[$m][$j]=$a[$i][$j];$a[$i][$j]=$tmp;
    }
  }
  if(!abs($a[$i][$i])) return -1;
  for($j=$i+1;$j<count($a);$j++)//impart linie
    $a[$i][$j]/=$a[$i][$i];
  $b[$i]/=$a[$i][$i];
  $a[$i][$i]=1;
  for($j=$i+1;$j<count($a);$j++){//fac 0 sub diagonala
    $b[$j]-=$a[$j][$i]*$b[$i];
    for($k=count($a)-1;$k>$i;$k--){
      $a[$j][$k]-=$a[$j][$i]*$a[$i][$k];
    }
  }
  for($i=count($a)-1;$i>0;$i--)// fac 0 peste diagonala
    for($j=$i-1;$j>=0;$j--){
      $b[$j]-=$a[$j][$i]*$b[$i];
    }
  return 1;
}
function calc_eq(&$coef,&$val,&$rez){//predictie pentru fiecare molecula
for($i=0;$i<count($val[1]);$i++){//a cata molecula
  $rez[$i]=$coef[0];
  for($j=1;$j<count($coef);$j++){//al catelea indice si coeficient
    $rez[$i]+=$coef[$j]*$val[$j][$i];
  }
  $rez[$i]=spalare($rez[$i]);
}
}
function calc_eq_1(&$coef,&$val,&$rez){//predictie pentru fiecare molecula
for($i=0;$i<count($val[0]);$i++){//a cata molecula
  $rez[$i]=$coef[0];
  for($j=1;$j<count($coef);$j++){//al catelea indice si coeficient
    $rez[$i]+=$coef[$j]*$val[$j-1][$i];
  }
}
```

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```
$rez[$i]=spalare($rez[$i]);
}
}

function new_y(&$y_old,&$x_old,&$y_new){//x[ind][mol]
$cate=count($x_old[1]);
$cati=count($x_old);
for($i=0;$i<$cate;$i++){
$rest[0]=exclude_i($i,$y_old,$y_new_i);
for($j=1;$j<=$cati;$j++){
$rest[$j-1]=exclude_i($i,$x_old[$j],$x_new_i[$j-1]);
get_coefs($y_new_i,$x_new_i,$c_new);
calc_1v($c_new,$rest,$y_new[$i]);//predicție pentru o molecula
}
}
function calc_1v(&$coef,&$val,&$rez){//predicție pentru o molecula
$rez=$coef[0];
for($j=1;$j<count($coef);$j++){//al catelea indice si coeficient
$rez+=$coef[$j]*$val[$j-1];
}
$rez=spalare($rez);
}
function exclude_i($i,&$data,&$new_data){
for($j=0;$j<$i;$j++)
$new_data[$j]=$data[$j];
for($j=$i+1;$j<count($data);$j++)
$new_data[$j-1]=$data[$j];
return $data[$i];
}
function spalare($value){
if(!is_finite($value))
return (float)"INF";
$log_cifre=log(abs($value),10);
if($log_cifre<0) $cifre=(int)$log_cifre;
if($log_cifre>0) $cifre=(int)($log_cifre+1);
$new2value=((int)($value*pow(10,5-$cifre)))*pow(10,-4);
$new3value=$new2value."e".($cifre-1);
if(($cifre>0)&&($cifre<6)) $new3value=sprintf("%.5-$cifre."f",$new3value);
return $new3value;
}
function sub_test(&$list,&$data,&$out){
$out[0]=$data[0];
for($i=0;$i<count($list);$i++)
for($j=1;$j<count($data);$j++){
if($list[$i]==$data[$j][0]){
$out[$i+1]=$data[$j];
break;
}
}
}
function coef_r(&$y1,&$y2){
$my1=m1($y1);
$dy2=m2($y1,$y1)-$my1*$my1;
$mx1=m1($y2);
$mx2=m2($y2,$y1);
$mx1=$mx1*$mx1;
$mx2=m2($y2,$y2);
$dx2=$mx2-$mx1;
$sr2=pow($mx2-$mx1*$my1.2)/($dx2*$dy2);
return $sr2." (n = ".count($y1).)";
}
function coef_F(&$y1,&$y2,$df_r){
$my1=m1($y1);
$T_SS=0;
for($i=0;$i<count($y1);$i++)
```

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```
$T_SS+=pow($y1[$i]-$my1,2);
$E_SS=0;
for($i=0;$i<count($y1);$i++)
  $E_SS+=pow($y1[$i]-$y2[$i],2);
$R_SS=$T_SS-$E_SS;
$T_df=count($y1)-1;
$R_df=$df_r;
$E_df=$T_df-$R_df;
if(!$R_df)die();
if(!$E_SS)die();
$F=$R_SS*$E_df/$R_df/$E_SS;
return $F;
}
function coef_pF($df_r,$df_t,$F){
  $Fd = new FDistribution($df_r,$df_t-$df_r);
  return 1.0 - $Fd->CDF($F);
}
function put_coef_ind(&$coef,&$indx,$msg){
  $seq="Y ".$msg." = ".$coef[0];
  for($i=1;$i<count($coef);$i++){
    $seq.=" ".$coef[$i]."*".$indx[$i-1];
  }
  return $seq;
}
?>
```

Anexa 9. Rezultatul obținut de aplicație pentru un set școală și un set test

[http://vl.academicdirect.org/molecular\\_topology/qsar\\_qspr\\_s/](http://vl.academicdirect.org/molecular_topology/qsar_qspr_s/)

**Training vs. Test Experiment**

Please select a data file from the list of available data.  
 The experiment will perform a random split of experimental data in two sets: "trainig set" and "test set".  
 The QSAR/QSPR model are calculate using the data from training set.  
 The obtained QSAR equation are apply then on both sets, in order to calculate statistical parameters.

26449t.txt Submit Query

You selected:  
 Set file: 26449t.txt

Please select:  
 Training set count: 7

Mol	lHPDOQg	IsMRKGg	Y
x01	-1.0441	1.1824	1.33
x02	-6.5994e-1	1.1361	1.33
x03	-9.491e-1	1.1687	1.33
x04	-5.9172e-1	1.1609	2
x05	-5.8128e-1	1.1260	1.33
x06	-5.7953e-1	1.1107	1
x07	-4.8518e-1	1.0622	0.33
x08	-4.8318e-1	1.0802	0.67
x09	-7.4112e-1	1.0940	0.33
x10	-6.9026e-1	1.1423	1.33

Submit Query

Please make refresh to generate other sets lists.  
 Set file: 26449t.txt

Training set count: 7

Training set list:  
 x10 x03 x04 x01 x09 x05 x02

Test set list:  
 x06 x07 x08

Mol	lHPDOQg	IsMRKGg	Y
x01	-1.0441	1.1824	1.33
x02	-6.5994e-1	1.1361	1.33
x03	-9.491e-1	1.1687	1.33
x04	-5.9172e-1	1.1609	2
x05	-5.8128e-1	1.1260	1.33
x06	-5.7953e-1	1.1107	1
x07	-4.8518e-1	1.0622	0.33
x08	-4.8318e-1	1.0802	0.67
x09	-7.4112e-1	1.0940	0.33
x10	-6.9026e-1	1.1423	1.33

Submit Query

http://vl.academicdirect.org/molecular\_topology/qsar\_qspr\_s/

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Back Forward Stop Home Search Favorites Refresh Print

Address http://vl.academicdirect.org/molecular\_topology/qsar\_qspr\_s/result.php

Google Search PageRank 7 blocked Check

Set file: 26449t.txt  
 Training set count: 7  
 Training set: x10 x03 x04 x01 x09 x05 x02  
 Test set: x06 x07 x08  
 Training set data:

Mol	IHPDOQg	IsMRKGg	Y
x10	-6.9026e-1	1.1423	1.33
x03	-9.491e-1	1.1687	1.33
x04	-5.9172e-1	1.1609	2
x01	-1.0441	1.1824	1.33
x09	-7.4112e-1	1.0940	0.33
x05	-5.8128e-1	1.1260	1.33
x02	-6.5994e-1	1.1361	1.33

QSAR/QSPR:  $Y\_EST = -19.373 + 2.3295 * IHPDOQg + 19.579 * IsMRKGg$   
 Coefficient of determination  $r^2 = 0.99658072544657$  (n = 7)  
 Fisher test value F = 582.75  
 Probability of wrong (from F)  $p_F = 0.00117\%$  (1.1698107642233E-05)

Test set data:

Mol	IHPDOQg	IsMRKGg	Y
x06	-5.7953e-1	1.1107	1
x07	-4.8518e-1	1.0622	0.33
x08	-4.8318e-1	1.0802	0.67

Coefficient of determination  $r^2 = 0.99956211139332$  (n = 3)  
 Fisher test value F = 0e-1  
 The degrees of freedom must be greater than zero.

**Anexa 10. Lucrările științifice publicate**

**– sunt disponibile online –**

1. Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 1. Review of the Methodology*, LEJPT, Issue 6, p. 76-98, 2005  
<http://lori.academicdirect.org/articles/?id=45>, **24 pagini**
2. Sorana BOLBOACĂ, Lorentz JÄNTSCHI, *Binomial Distribution Sample Confidence Intervals Estimation for Positive and Negative Likelihood Ratio Medical Key Parameters*, American Informatics Medical Association Annual Symposium on Biomedical and Health Informatics from Foundations to Applications to Policy, Washington D.C., U.S.A., October 22-26, Conference Proceedings, p. 66-70, 2005  
<http://lori.academicdirect.org/conferences/?id=26>, **5 pagini**
3. Delia Maria GLIGOR, Lorentz JÄNTSCHI, *Periodic System of Elements Database and Its Applications*, Oradea University Annals, Chemistry Fascicle, Issue 12, p. 180-194, 2005  
<http://lori.academicdirect.org/articles/?id=49>, **15 pagini**
4. Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 2. Insecticidal Activity of Neonicotinoid Compounds*, LJS, Issue 6, p. 78-85, 2005  
<http://lori.academicdirect.org/articles/?id=46>, **8 pagini**
5. Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI, *Molecular Descriptors Family on Structure Activity Relationships 3. Antituberculous Activity of some Polyhydroxyxanthenes*, LJS, Issue 7, p. 58-64, 2005  
<http://lori.academicdirect.org/articles/?id=47>, **7 pagini**
6. Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, *Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds*, LEJPT, Issue 7, 55-102, 2005  
<http://lori.academicdirect.org/articles/?id=48>, **48 pagini**

Cluj-Napoca,  
la 28.11.2005

Director temă ET36/2005,  
Șef. L. Dr., Ing. Lorentz JÄNTSCHI

<http://lori.academicdirect.org>