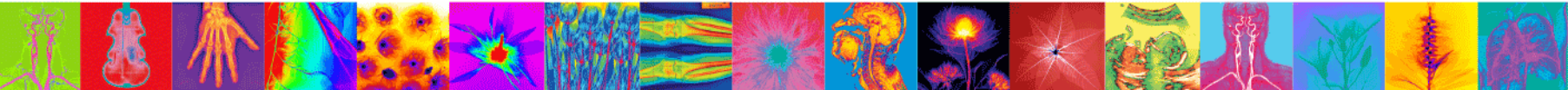


**Digital technologies from pharmaceutical company's perspective – Bracco SpA**

*Alessandro Maiocchi – Innovation hub – Bracco SpA*

Bracco Group Presentation



# Digitalization & AI for the Pharma Industry

- ❑ What types of AI applications are currently in use in the pharmaceutical industry?
- ❑ What tangible results has AI driven in pharma?
- ❑ Are there any common trends among these innovation efforts? How could these trends affect the future of pharmaceuticals?

## The Pharma Industry Value Chain



A study from **MIT** has found that only **13.8%** of drugs successfully pass clinical trials. Furthermore, a company can expect to pay between **\$161 million to \$2 billion** for any drug to complete the entire clinical trials process and get FDA approval.

C.H. WONG, K.W. SIAH, ANDREW W. LO Biostatistics (2019) 20, 2, pp. 273–286





# AI in Drug Discovery (1/2)

## Machine Learning for Pharmaceutical Discovery and Synthesis Consortium

This group is a collaboration between the pharmaceutical and biotechnology industries and MIT. The goal of the collaborative efforts is to facilitate the design of useful software for the automation of small molecule discovery and synthesis.

### Members



### Chemical Science



#### EDGE ARTICLE

View Article Online  
View Journal | View Issue

Check for updates

#### A graph-convolutional neural network model for the prediction of chemical reactivity†

Cite this: Chem. Sci., 2019, 10, 370

All publication charges for this article have been paid for by the Royal Society of Chemistry

Connor W. Coley,<sup>a</sup> Wengong Jin,<sup>b</sup> Luke Rogers,<sup>a</sup> Timothy F. Jamison,<sup>b,c</sup> Tommi S. Jaakkola,<sup>b</sup> William H. Green,<sup>b</sup> Regina Barzilay<sup>a,b</sup> and Klavs F. Jensen<sup>a,b\*</sup>

This is an open access article published under an ACS AuthorChoice License, which permits copying and redistribution of the article or any adaptations for non-commercial purposes.



Research Article

Cite This: ACS Cent. Sci. 2018, 4, 1465–1476

http://pubs.acs.org/journal/acscii

ACS  
central  
science

#### Using Machine Learning To Predict Suitable Conditions for Organic Reactions

Hanyu Gao,<sup>a</sup> Thomas J. Struble,<sup>a</sup> Connor W. Coley,<sup>a</sup> Yuran Wang, William H. Green,<sup>a</sup> and Klavs F. Jensen<sup>a\*</sup>

Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts

Article

Cite This: Acc. Chem. Res. 2018, 51, 1281–1289

pubs.acs.org/accounts

ACCOUNTS  
of chemical research

#### Machine Learning in Computer-Aided Synthesis Planning

Connor W. Coley,<sup>a</sup> William H. Green,<sup>a,\*</sup> and Klavs F. Jensen<sup>a,\*</sup>

Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts

#### Predicting Organic Reaction Outcomes with Weisfeiler-Lehman Network

Wengong Jin<sup>1</sup>, Connor W. Coley<sup>1</sup>, Regina Barzilay<sup>1</sup>, Tommi Jaakkola<sup>1</sup>

<sup>1</sup>Computer Science and Artificial Intelligence Lab, MIT

<sup>2</sup>Department of Chemical Engineering, MIT

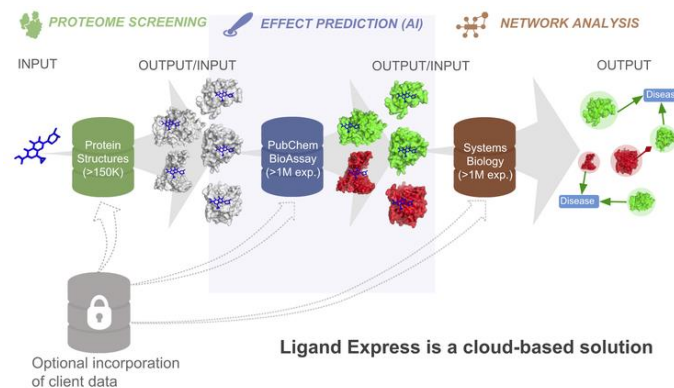
†{wengong,regina,tommi}@csail.mit.edu, †ccooley@mit.edu



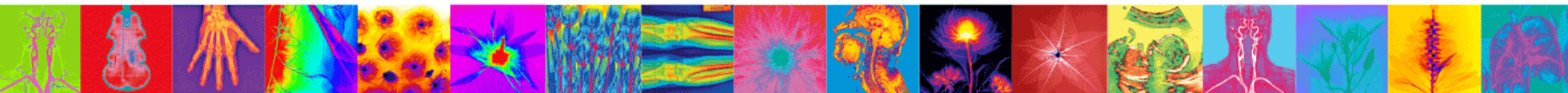
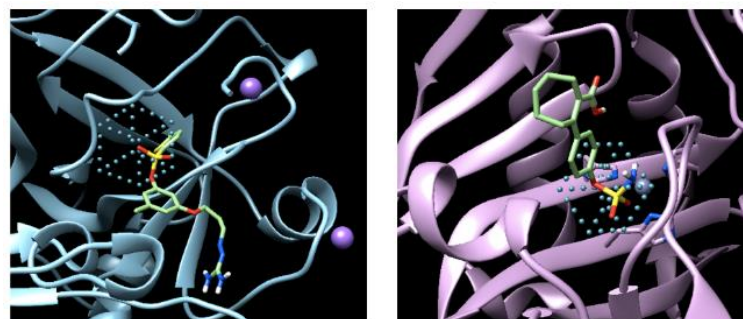
# AI in Drug Discovery (2/2)

**Drug Discovery:** scientific efforts towards the identification of molecules that could potentially be developed into a new drug

Cyclica is a biotechnology company that combines biophysics and AI to discover drugs faster, safer, and cheaper. They have partnered with Bayer to create an AI-augmented integrated network of cloud-based technologies



Atomwise developed AtomNet technology, a deep learning neural network application for structure-based drug design and discovery.



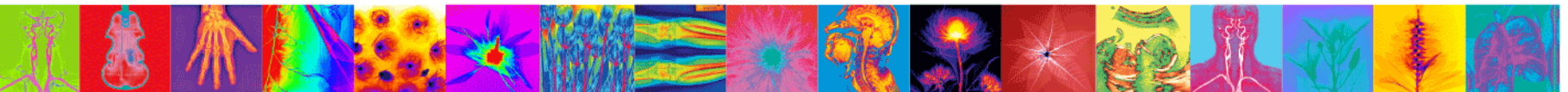
# AI in Drug Development

---

**Drug Development:** Scientific efforts towards the identification of molecules that could potentially be developed into a new drug

Clinical Development: where AI has been used:

- a) Identification, screening and engagements of patients for clinical trials (IBM Watson, Brite Health)
- b) optimizing drug dosage at an individual level (CURATE.AI)
- c) drug adherence in clinical trials (AI.CURE)
- d) Analyse clinical trial operations (Mc Kinsey's Quantum Black)



# AI in Clinical Applications

---

## Mining Medical Records

### Google Deepmind Health:

Google Deepmind is able to process hundreds of thousands of medical information within minutes. Google is cooperating with the Moorfields Eye Hospital NHS Foundation Trust to improve eye treatment.

### IBM Watson :

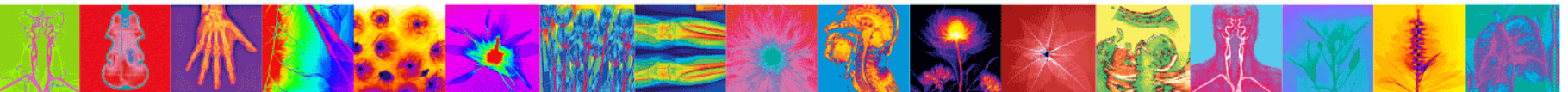
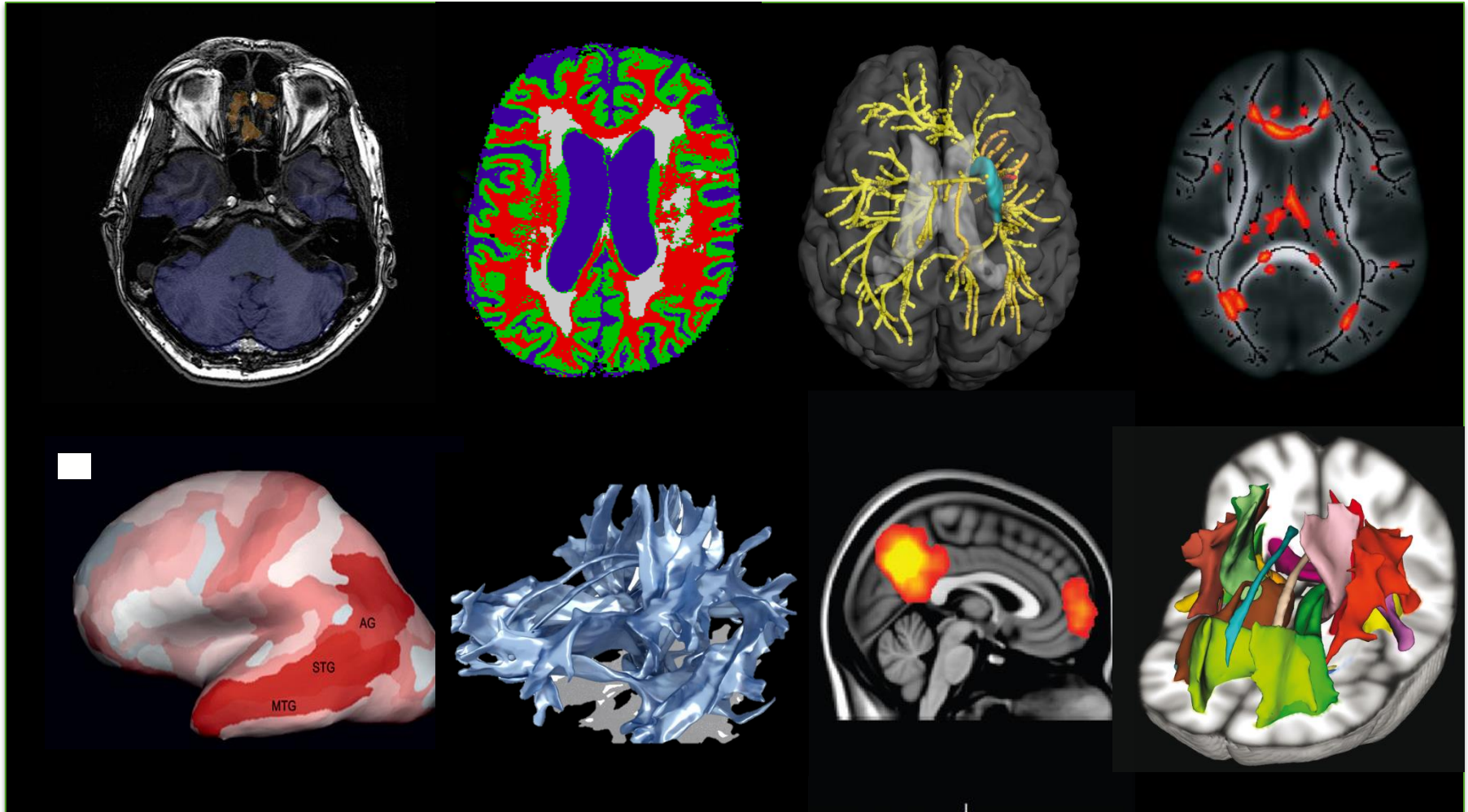
IBM Watson Health offer a suite of products and services which help physicians to make more informed and accurate decisions faster and to cull new insights from electronic medical records (EMR).





# AI in Clinical Applications

## Extraction of “Invisible” Biomarkers





# AI in Clinical Applications: Radiology

Radiology

## Radiomics Based on Adapted Diffusion Kurtosis Imaging Helps to Clarify Most Mammographic Findings Suspicious for Cancer<sup>1</sup>

Sebastian Bickelhaupt, MD\*  
Paul Ferdinand Jaeger, MSc\*  
Franklin Edward Lee, PhD†‡

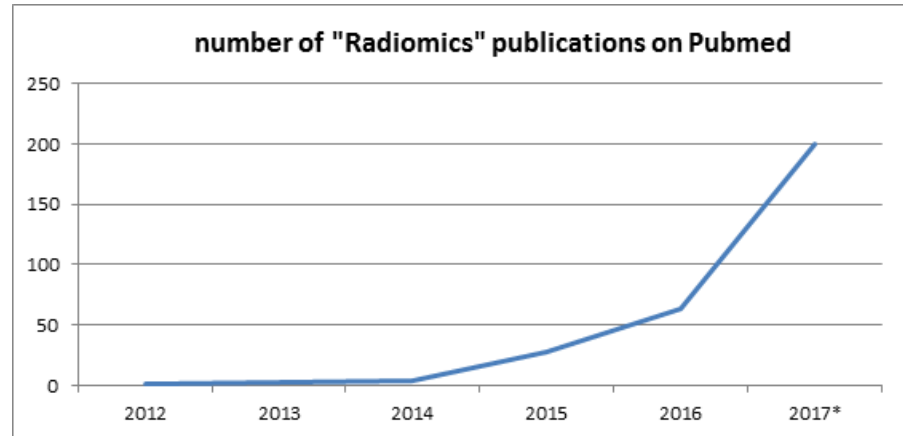
**Purpose:** To evaluate a radiomics model of Breast Imaging Reporting and Data System (BI-RADS) 4 and 5 breast lesions

ORIGINAL RESEARCH ■ BREAST IMAGING

Abdominal Radiology

© This is a U.S. Government work and not under copyright protection in the US; foreign copyright protection may apply 2018

Abdom Radiol (2018)  
https://doi.org/10.1007/s00261-018-1660-7



## Radiomics and radiogenomics of prostate cancer

Clayton P. Smith,<sup>1,2</sup> Marcin Czarniecki,<sup>1</sup> Sherif Mehrlivand,<sup>1,3,4</sup> Radka Stoyanova,<sup>5</sup>  
Peter L. Choyke,<sup>1</sup> Stephanie Harmon,<sup>6</sup> and Baris Turkbey<sup>6</sup>

npj | Breast Cancer

www.nature.com/npjbcancer  
All rights reserved 2374-4677/16

ARTICLE OPEN

### Quantitative MRI radiomics in the prediction of molecular classifications of breast cancer subtypes in the TCGA/TCIA data set

Hui Li<sup>1,12</sup>, Yitan Zhu<sup>2,12</sup>, Elizabeth S Burnside<sup>3</sup>, Erich Huang<sup>4</sup>, Karen Drukker<sup>1</sup>, Katherine A Hoadley<sup>5</sup>, Cheng Fan<sup>1</sup>, Suzanne D Conzen<sup>6</sup>, Margarita Zuley<sup>7</sup>, Jose M Net<sup>8</sup>, Elizabeth Sutton<sup>9</sup>, Gary J Whitman<sup>10</sup>, Elizabeth Morris<sup>9</sup>, Charles M Perou<sup>11</sup>, Yuan Ji<sup>2,11</sup> and Maryellen L Giger<sup>1</sup>

## SCIENTIFIC REPORTS

### OPEN Precision Radiology: Predicting longevity using feature engineering and deep learning methods in a radiomics framework

Received: 8 December 2016  
Accepted: 6 April 2017  
Published online: 10 May 2017

Luke Oakden-Rayner<sup>1,2</sup>, Gustavo Carneiro<sup>3</sup>, Taryn Bessen<sup>1</sup>, Jacinto C. Nascimento<sup>4</sup>, Andrew P. Bradley<sup>5</sup> & Lyle J. Palmer<sup>6</sup>

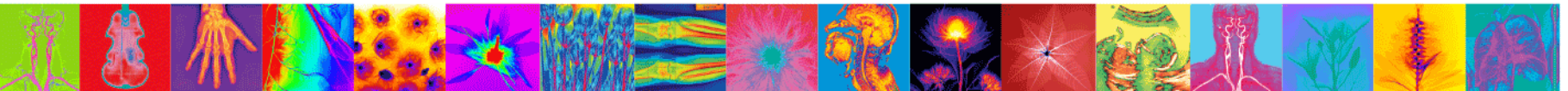
IEEE Access

Date of publication xxxx 00, 0000, date of current version xxxx 00, 0000.  
Digital Object Identifier 10.1109/ACCESS.2017.2691

### Deep radiomic analysis of MRI related to Alzheimer's disease

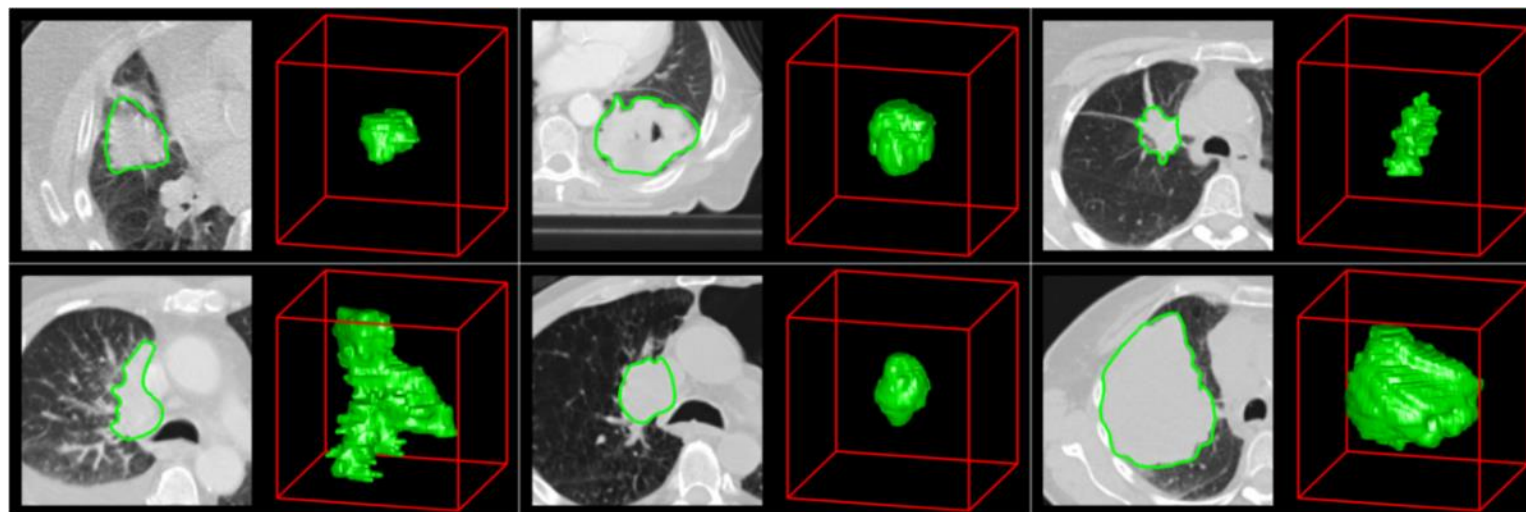
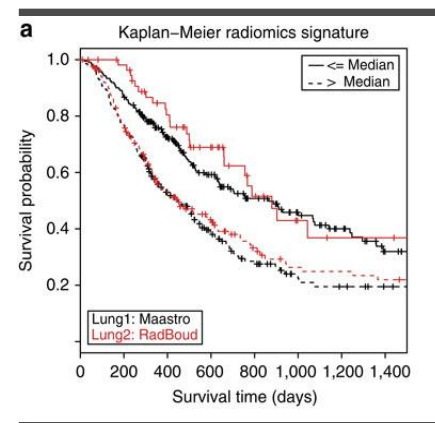
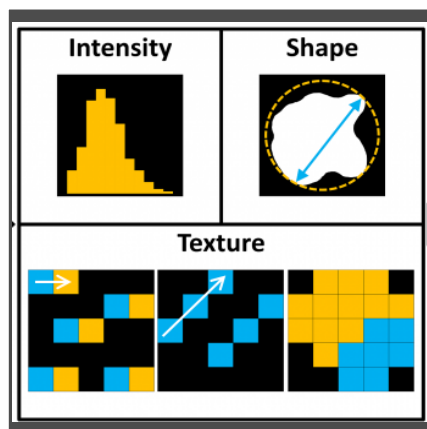
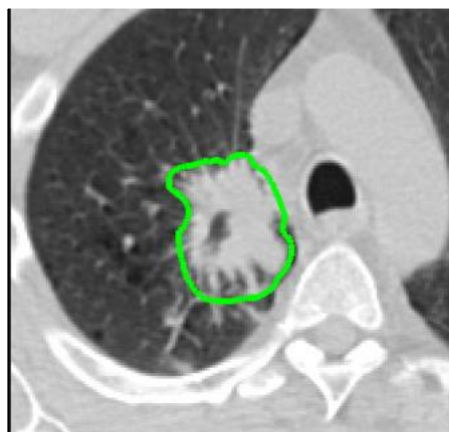
AHMAD CHADDAD<sup>1,3</sup>, CHRISTIAN DESROSIER<sup>2</sup>, TAMIM NIAZI<sup>3</sup>

<sup>1</sup>Department of Automated Manufacturing Engineering, Ecole de technologie supérieure, Montreal, QC, Canada  
<sup>2</sup>Department of Software and IT Engineering, Ecole de technologie supérieure, Montreal, QC, Canada  
<sup>3</sup>Department of Radiation Oncology, McGill University, Montreal, QC, Canada



# A.I. + Radiology = Radiomics

## Quantification of Imaging Phenotype



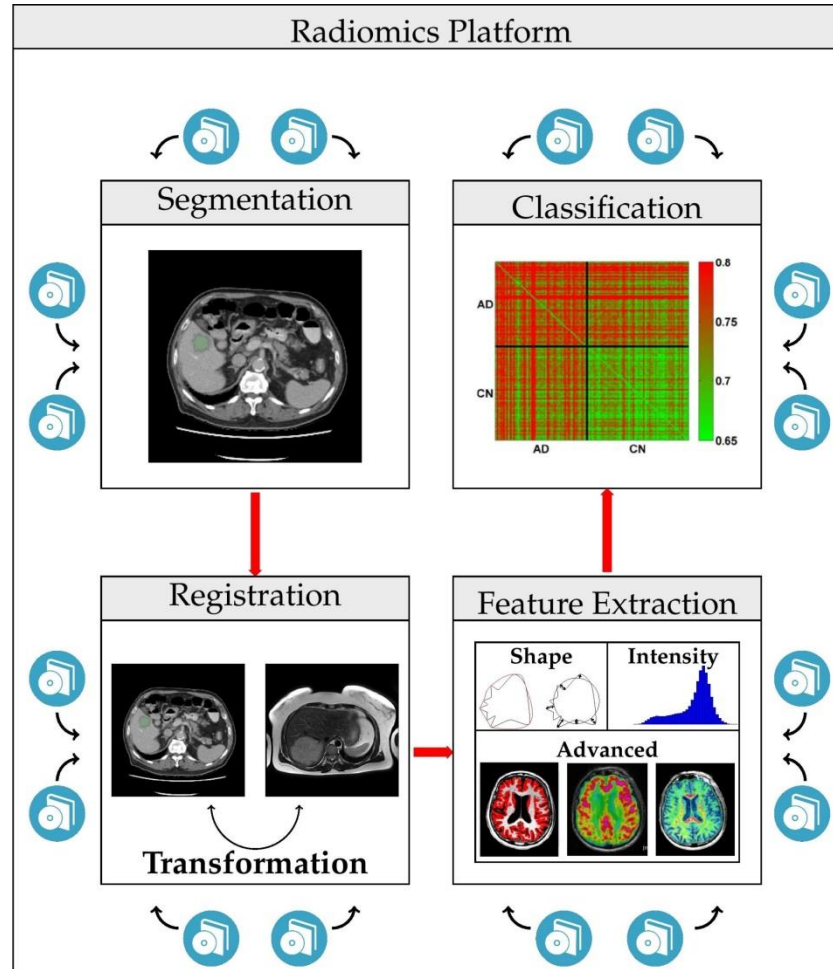
# Multiparametric Radiomics Platform

Online Multiparametric Database

Lung PET      Liver CT

Head Desmoid T1-weighted MR      Liver T2-weighted MR

Brain T1-Weighted MR      Mammogram



Predictions

- Genetic Mutations
- Tumor Phenotype
- Therapy Response
- Patient Prognosis
- Dementia Diagnosis

Quantitative maps



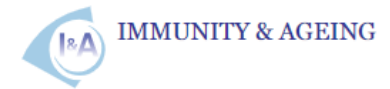


IEEE International Conference on Bioinformatics and Biomedicine  
3-6 December 2018, Madrid

## Radiomics for Predicting CyberKnife response in acoustic neuroma: a pilot study

Natascha Claudia D'Amico<sup>\*‡</sup>, Rosa Sicilia<sup>†‡</sup>, Ermanno Cordelli<sup>†</sup>,  
Isa Bossi Zanetti<sup>§‡</sup>, Giancarlo Beltramo<sup>§</sup>, Deborah Fazzini<sup>\*‡</sup>, Giuseppe  
<sup>\*</sup>Imaging Department, Centro Diagnostico Italiano  
<sup>†</sup>Unit of Computer Systems and Bioinformatics, Department of Engineering  
<sup>‡</sup>Joint Laboratory on Precision Medicine and E  
Università Campus Bio-Medico di Roma - Centro Diagnostico Italiano  
<sup>§</sup>Cyberknife Department, Centro Diagnostico Italiano  
<sup>¶</sup>Bracco Imaging S.p.A., Milan, Italy

Grossi *Immunity & Ageing* 2010, 7(Suppl 1):S3  
<http://www.immunityageing.com/content/7/751/S3>



PROCEEDINGS

Open Access

## Artificial Adaptive Systems and predictive medicine: a revolutionary paradigm shift

Enzo Grossi



A new radiomics approach to predict the evolution of PI-RADS score 3/5 prostate areas in multiparametric MR

N.C. D'Amico, E. Grossi, G. Valbusa, A. Malasevski, G. Cardone, S. Papa



Centro Diagnostico Italiano, Milan, Italy.  
Bracco Imaging S.p.A



# Conclusion

---

Many fear that robots, A.I., and automation, in general, will take their jobs without alternatives. The same anxieties emerged in healthcare about artificial intelligence taking the place of radiologists, robots surpassing the skills of surgeons, or taking jobs in pharma.

## That is not true !!!

Physicians should accept technology understanding and using it continuing to take the final decision about their patients

Physicians will work more efficiently at the interface with patients, supporting and guiding them towards the fighting against their own disease.

