Reunião do Grupo de Física Atômica e Molecular
Colisões de elétrons e pósitrons por moléculas

Márcio H. F. Bettega
17/08/2018

GFAM (UFPR):

Márcio Henrique Franco Bettega (P)
Sergio d'Almeida Sanchez (P)
Alessandra de Souza Barbosa (P)
Giseli Maria Moreira (D)
Letícia da Silva Maioli (D)
Rafael de Oliveira Lima (D)
Murilo de Oliveira Silva (M)
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Luiz Vitorino dos Santos Dalagnol (IC)
Raul Vinícius Basso Morás (IC)

Thiago Corrêa de Freitas (C)
Diego Farago Pastega (C)

Matheus Bacigalupo Kiataki (retorna em 2019)

Espalhamento de elétrons:

Temas e sistemas de interesse:

Piridina - microssolvatação (Letícia)
Cianoamina - dissociação e microssolvatação (Letícia)
Sevoflurano, r-isoflurano, r-isoflurano e halotano - elástico, espectro de ressonâncias, comparação com os dados experimentais da UNL e com os resultados teóricos do IAM-SCAR.
Tiofeno - excitação eletrônica (Giseli)
Halogenetos - elástico, espectro de ressonâncias e mínimo RT (Matheus)
Radiossensibilizadores - estado ligado (lei empírica de escala), elástico, espectro de ressonâncias (Murilo)
Fluoro e clorobenzenos - estado ligado (lei empírica de escala), elástico, espectro de ressonâncias (Vitorino)
Radiossensibilizadores - estrutura eletrônica (Cesar)
Halouracilas - estrutura eletrônica (Raul)
Cubano - elástico, espectro de ressonâncias (Thiago)

Versão do SMC - serial X paralelo

Versão do GAMESS - agosto de 2018, compilado pela Giseli

Espalhamento de pósitrons:

Temas e sistemas de interesse:

Benzeno, tetrahidrofurano e piridina - elástico (Alessandra)
Piridina - microssolvatação (Letícia)
Pirazina - elástico (Giseli)
Hidrocarbonetos - elástico, efeito isômero (Giseli)
Álcoois - elástico, efeito isômero (Giseli)
? - excitação eletrônica (Rafael)
Radiossensibilizadores - elástico (Murilo)

Trends in Pharmacological Sciences

Feature Review

Cancer Radiosensitizers

Hao Wang,[1,5] Xiaoyu Mu,[2,5] Hua He,[3] and Xiao-Dong Zhang[2,4,*]

Radiotherapy (RT) is a mainstay treatment for many types of cancer, although it is still a large challenge to enhance radiation damage to tumor tissue and reduce side effects to healthy tissue. Radiosensitizers are promising agents that enhance injury to tumor tissue by accelerating DNA damage and producing free radicals. Several strategies have been exploited to develop highly effective and low-toxicity radiosensitizers. In this review, we highlight recent progress on radiosensitizers, including small molecules, macromolecules, and nanomaterials. First, small molecules are reviewed based on free radicals, pseudosubstrates, and other mechanisms. Second, nanomaterials, such as nanometallic materials, especially gold-based materials that have flexible surface engineering and favorable kinetic properties, have emerged as promising radiosensitizers. Finally, emerging macromolecules have shown significant advantages in RT because these molecules can be combined with biological therapy as well as drug delivery. Further research on the mechanisms of radioresistance and multidisciplinary approaches will accelerate the development of radiosensitizers.

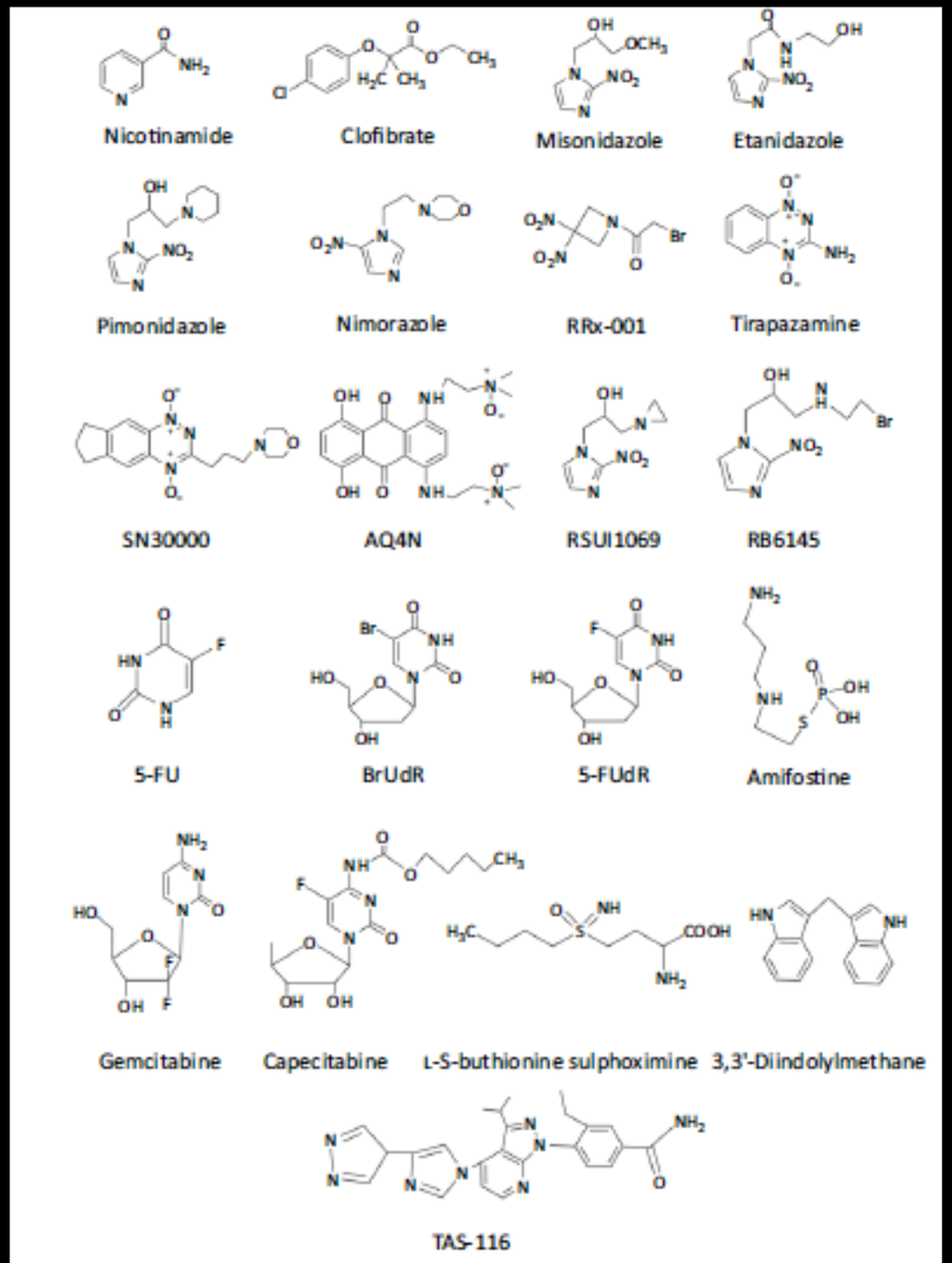

Figure 2. Molecular Structures of Some Representative Small-Molecule Radiosensitizers Discussed in This Paper. Nicotinamide and Clofibrate are for promoting oxygenation. Misonidazole is the prototype of 2-nitroimidazoles, which is followed by the modified structures of Etanidazole and Pimonidazole. Nimorazole, a 5-nitro imidazole, is now recommended for use clinically in Denmark. RRx-001, a dinitro compound, is evaluated in clinical trials. Tirapazamine, SN30000, and AQ4N are hypoxia-specific cytotoxins, and RSU1069 and RB6145 are multifunctional. These structures revealed the directions in this field at early stage. In addition, other types of small molecules were exhibited here, such as pseudosubstrates (5-FU, BrUdR, 5-FUdR, Gemcitabine, Capecitabine), depletor of reductant (L-S-buthionine sulfoximine), drugs influencing the pathways (TAS-116), and radioprotectants (DIM, Amifostine). Abbreviations: 5-FU, 5-fluorouracil; 5-FUdR, fluorodeoxyuridine; BrUdR, bromodeoxyuridine; DIM, 3,3′-diindolylmethane.

APPLIED PHYSICS REVIEWS 5, 021302 (2018)

APPLIED PHYSICS REVIEWS

Effective and absolute cross sections for low-energy (1-30 eV) electron interactions with condensed biomolecules

Yi Zheng[1,a)] and Léon Sanche[2]
[1]Research Institute of Photocatalysis, State Key Laboratory of Photocatalysis on Energy and Environment, Fuzhou University, Fuzhou 350116, People's Republic of China
[2]Group in the Radiation Sciences, Faculty of Medicine and Health Sciences, Université de Sherbrooke, Sherbrooke, Quebec J1H 5N4, Canada

Positron Scattering from Molecules: An Experimental Cross Section Compilation for Positron Transport Studies and Benchmarking Theory

M J BrungerS J BuckmanK Ratnavelu

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Topical Review

Electron scattering from molecules and molecular aggregates of biological relevance

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Seminários:

- 24/08 - Alessandra - Aplicações do SMC no espalhamento de elétrons por moléculas (Sala PE04, 13h30min)
- 31/08 - Alessandra - Aplicações do SMC no espalhamento de pósitrons por moléculas (Sala PE04, 13h30min)
- 14/09 - Giseli - artigo de revisão do Sanche
- 21/09 - Murilo - artigo dos radiossensibilizadores já mostrando alguns resultados de cálculos de estrutura eletrônica
- 28/09 - Marcio - como gerar os parâmetros dos pseudopotenciais de BHS
- 05/10 - Marcio - como gerar funções de base para os pseudopotenciais de BHS
- 19/10 - Letícia - artigo de revisão Jimena/Sylwia
- 26/10 - Sergio - artigo de revisão Brunger/Buckman/Ratnavelu
- 09/11 - Cesar - radiossensibilizadores
- 16/11 - Vitorino - fluoro e clorobenzenos

Seminários:

Sala - responsabilidade da Profa. Dra. Alessandra

Café colonial - responsabilidade de Sergio, Giseli e Letícia