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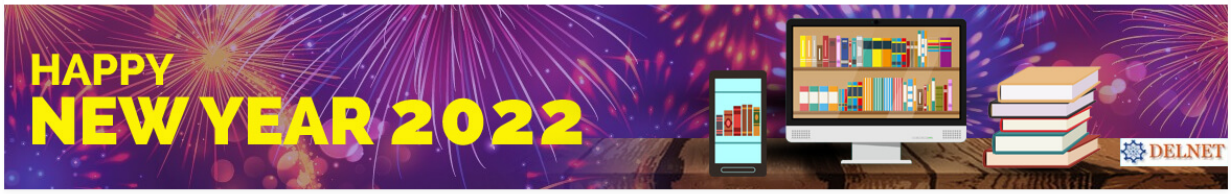

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Design, Synthesis and Characterization of Novel Sulfonamides Derivatives as Anticancer Agent Targeting EGFR TK, and Development of New Methods of Synthesis by Microwave Irradiation

Souad Akili[1], Djamila Ben Hadda[2], Yaser Bitar[1], Amir Balash[3], Mustapha Fawaz Chehna[1*]

[1]Department Quality Control and Pharmaceutical Chemistry, Faculty of Pharmacy, University of Aleppo, Aleppo, Syria.

[2]Department Quality Control and Pharmaceutical Chemistry, Faculty of Pharmacy, Ebla Private University, Aleppo, Syria.

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Abstract

Some novel sulfonamide-derivatives were designed to develop novel kinase inhibitors. The molecular docking study was performed for the designed compounds against epidermal growth factor kinase receptor T790M/L858R (TMLR) (PDB ID: 5EDQ) to identify new drug candidates for treating cancer. Binding free energy was calculated by Molegro virtual docker (MVD) to select the most promising hits. The corresponding docking score values into EGFR (TMLR) of 4b gave the best energy docking -147.213 Kcal/mol. And some of the designed sulfonamide derivatives have been synthesized by conventional method in addition to a microwave-assisted method of synthesis. The reaction of an amino group-containing drug; sulfamethoxazole and sulfanilamide with carbonyl group in benzoyl chloride and phthalic acid in basic media, generated a series of sulfonamide derivatives. The structures of all the synthesized compounds were well characterized by Mass spectrometry (MS), Infrared spectroscopy (IR), ^{1}H nuclear magnetic resonance (^{1}H NMR), ^{13}C nuclear magnetic resonance (^{13}C NMR) and elemental analysis. After obtaining experimental data regarding the yield and the time taken for the synthesis by both the approaches, conventional and microwave-assisted method, it was shown that the microwave-assisted method gave higher yield with shorter time and higher temperature compared to conventional heating methods.

Keywords

Sulfonamide, Anticancer, EGFR, TMLR, 5EDQ, Molegro Virtual Docker, Sul-famethoxazole, Sulfanilamide, Microwave

Akili, S. , Ben Hadda, D. , Bitar, Y. , Balash, A. and Fawaz Chehna, M. (2021) Design, Synthesis and Characterization of Novel Sulfonamides Derivatives as Anticancer Agent Targeting EGFR TK, and Development of New Methods of Synthesis by Microwave Irradiation. *International Journal of Organic Chemistry*, **11**, 199-223. doi: 10.4236/ijoc.2021.114014.

1. Introduction

Cancer is a worldwide health problem and the most deadly disease in humans [1] [2], and it is considered the second leading cause of mortality after cardiovascular diseases [2]. There are several methods for the treatment of cancer such as Surgery, Chemotherapy, Hormonal therapy, Immunotherapy [3] [4], and Phototherapy [5]. Today, anticancer chemotherapy is still the main method applied in the treatment of cancer [6]. Chemotherapy drugs include antitumor antibiotics, anti-metabolites, mitotic inhibitors, hormonal therapies. Cancer chemotherapy offers a unique advantage: it can treat the entire body, even the cells that may have escaped from the primary tumor [4] [7].

Among the wide range of compounds tested as potential anticancer agents, derivatives of sulfonamide have attracted reasonable attention [8].

The compounds which contain SO_2NH_2 functional group are called sulfonamides. The general formula of sulfonamides is RSO_2NH_2 [9] (Figure 1).

Sulfa drugs are amphoteric, they have pKa 4.79 to 8.56 and act as weak organic acids. They are weakly soluble in water, their solubility is increased at alkaline pH. The lipophilicity of the N_1 group has the largest effect on protein binding [10]. Sulfonamide derivatives comprise an important class of drugs with diverse biological applications [11]. Over 30 drugs containing this functional group are in clinical use, including antihypertensive, antibacterial, antiprotozoal, antifungal, anti-inflammatory, non-peptidic vasopressin receptor antagonists, translation initiation inhibitors, rheumatoid arthritis, antimalarial, anti-leishmanial, anti-thyroid, Antidepressant [10] [11] [12], hypoglycemics, anticonvulsants [13], diuretic, receptor tyrosine kinase inhibitors, and antipsychotics [1]. They are also used to treat ulcerative colitis, urinary, intestinal, and ophthalmic infections [14]. Recently, sulfonamides have been used as anti-cancer, anti-viral, and anti-HIV [15] [16], and in Alzheimer's disease [13].

Epidermal growth factor receptor (EGFR) is a member of the tyrosine kinase family and is usually overexpressed in several types of cancer, such as non-small-cell lung cancer, breast, esophageal, head, cervical, and neck cancer [17] [18]. The TMLR (T790M/L858R) mutation, the L858R mutation is located in the tyrosine kinase domain of EGFR in exon 2 and

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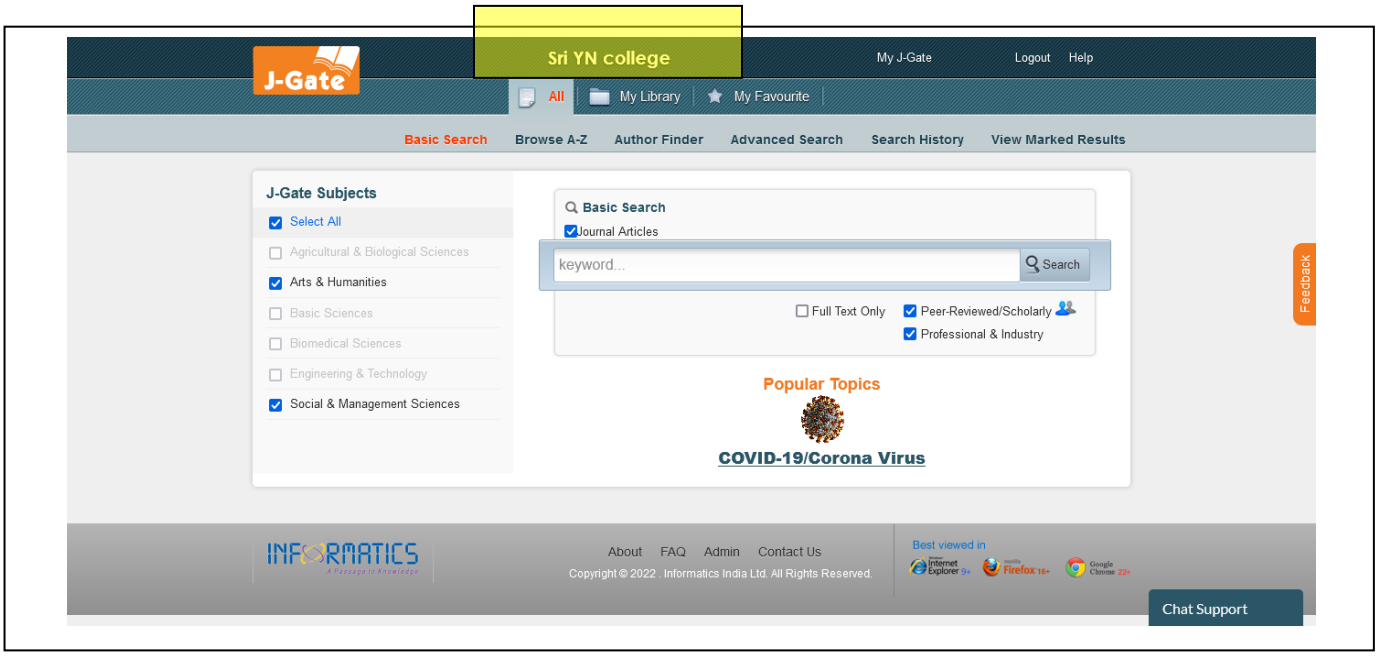
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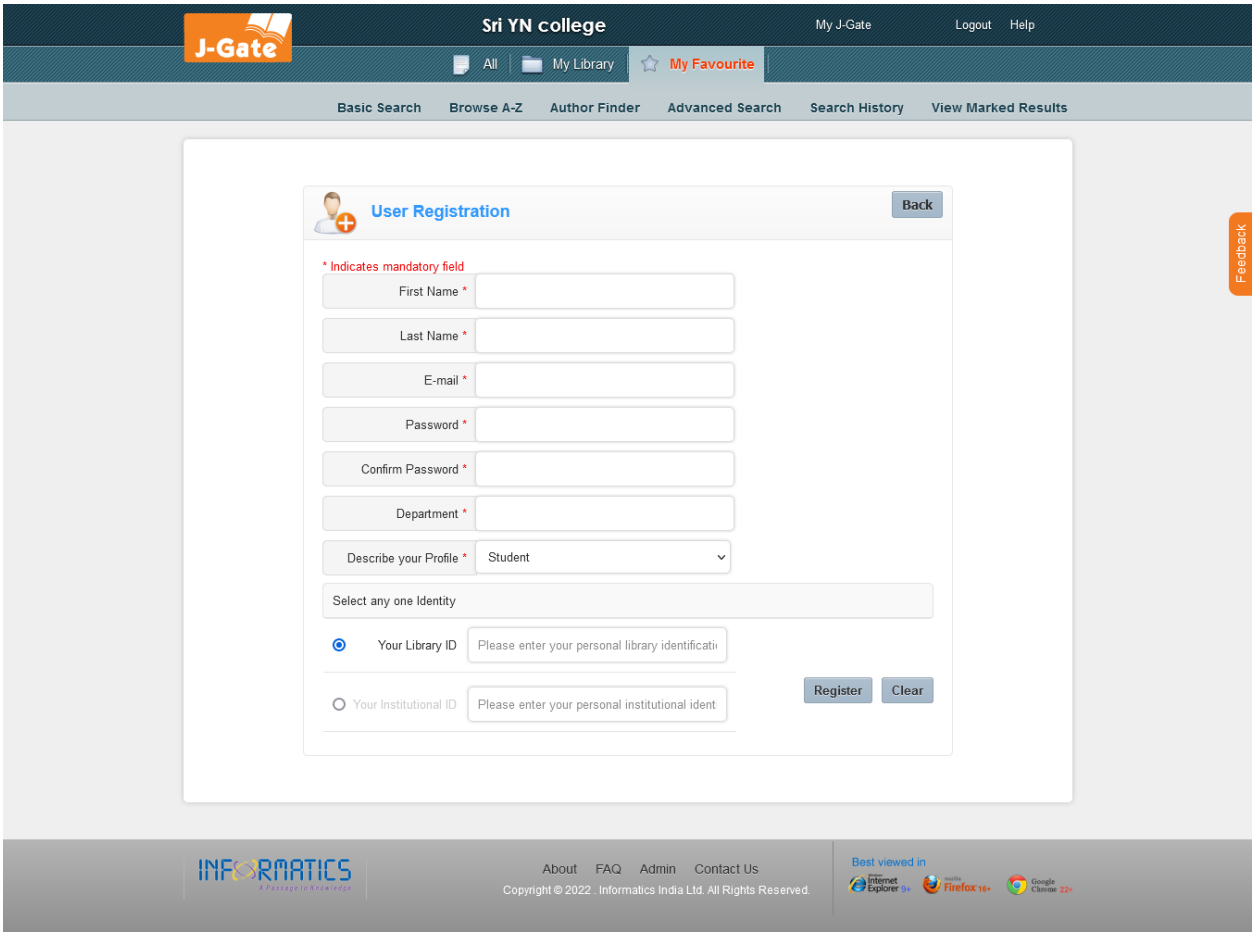

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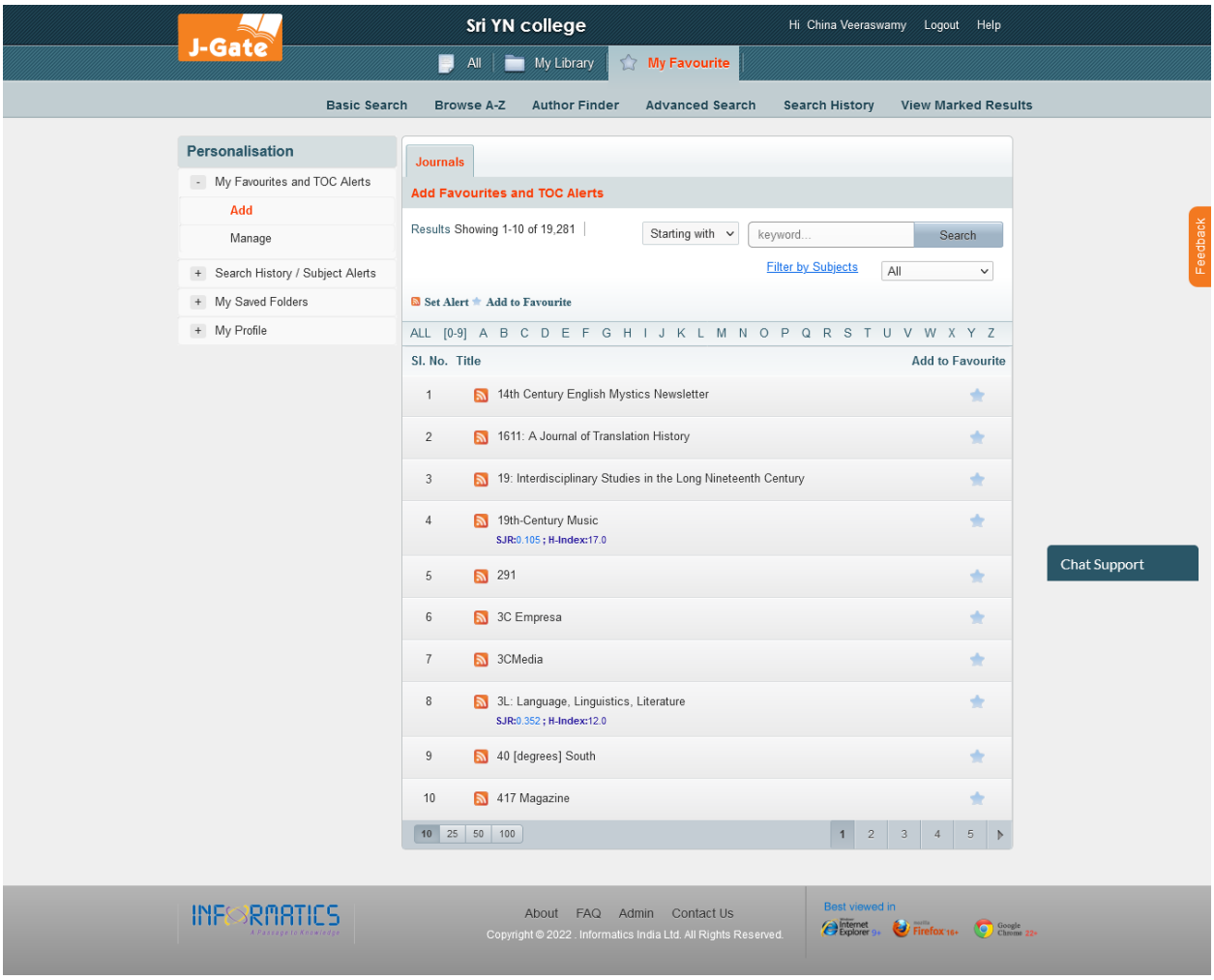

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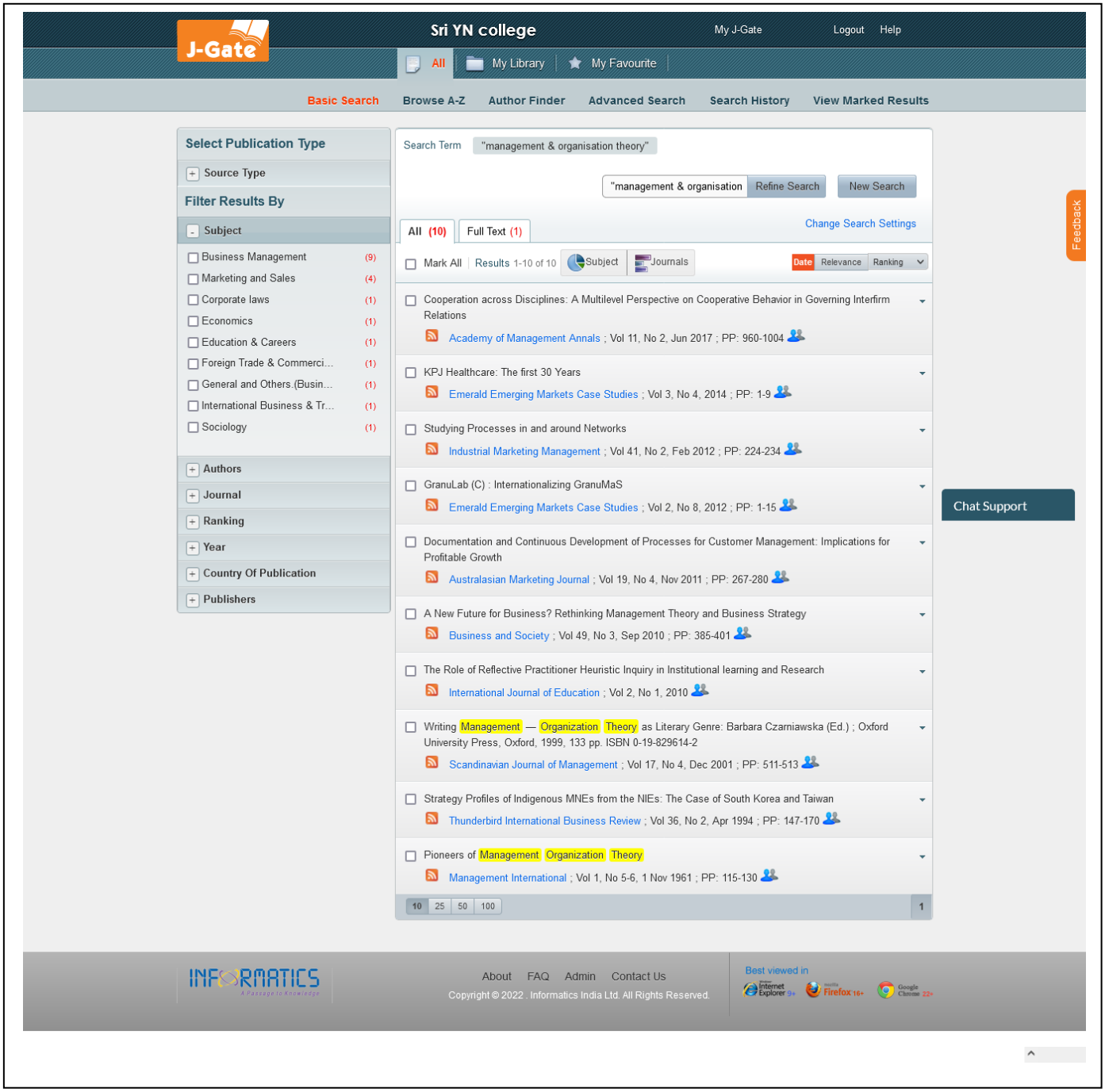

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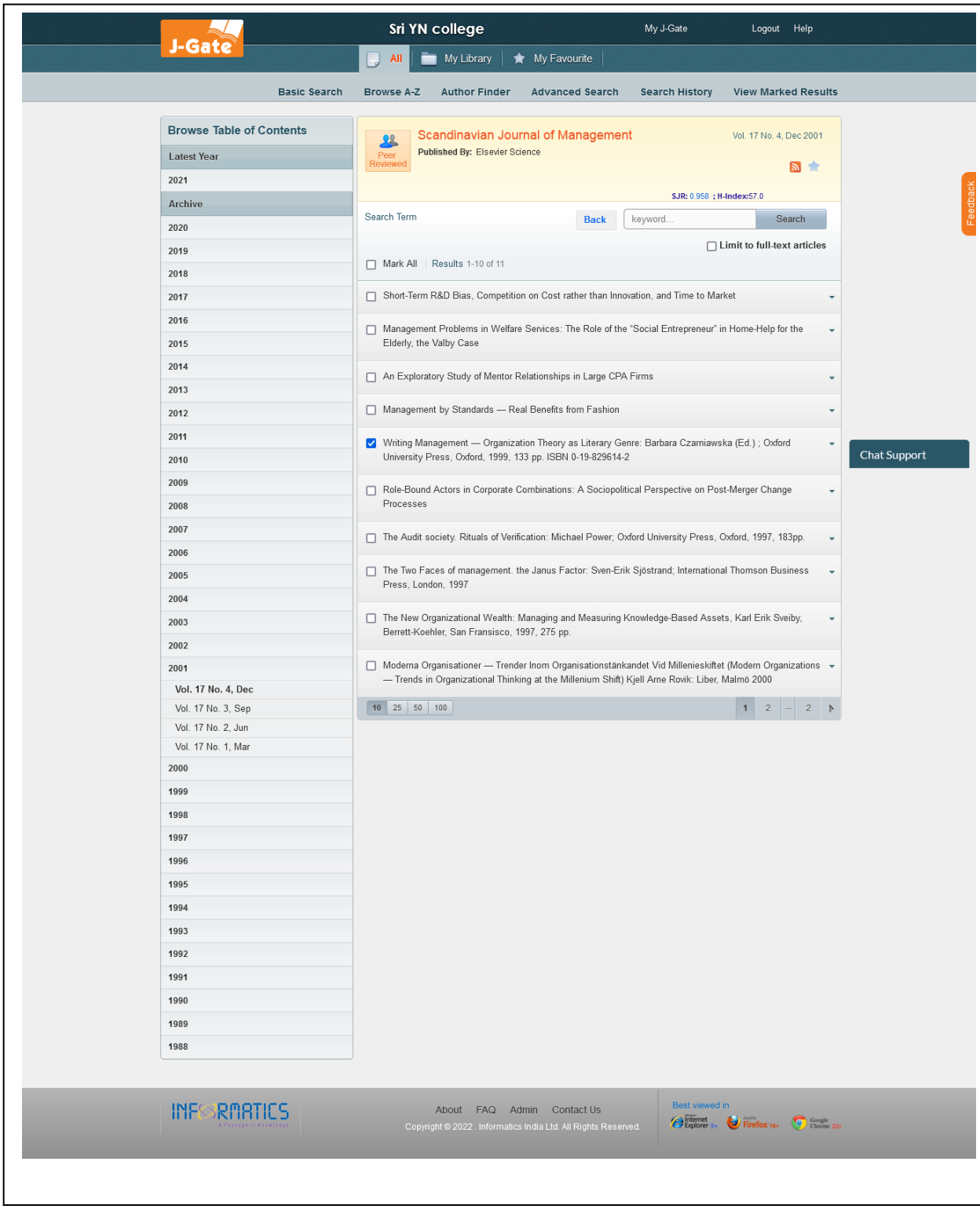

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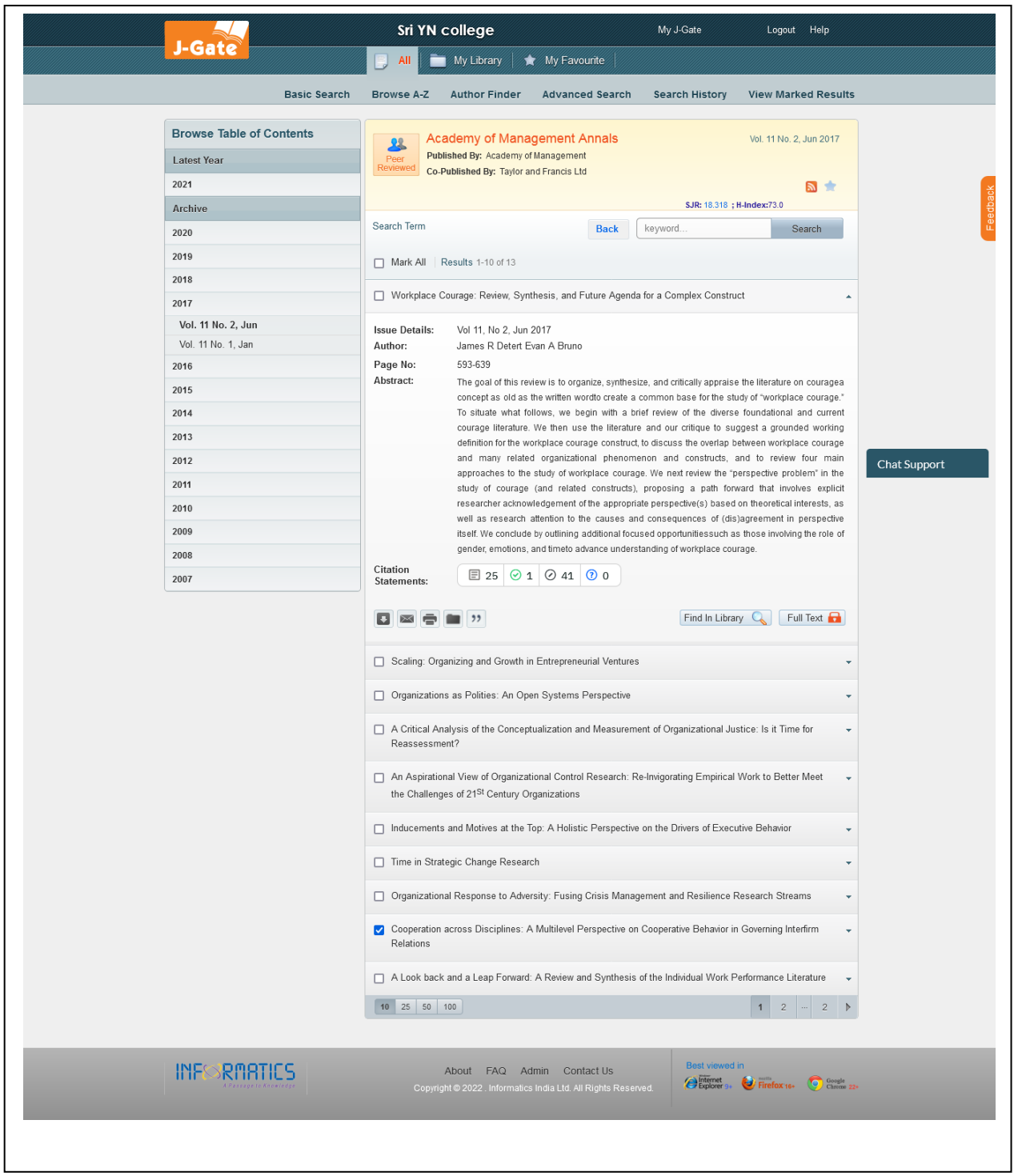

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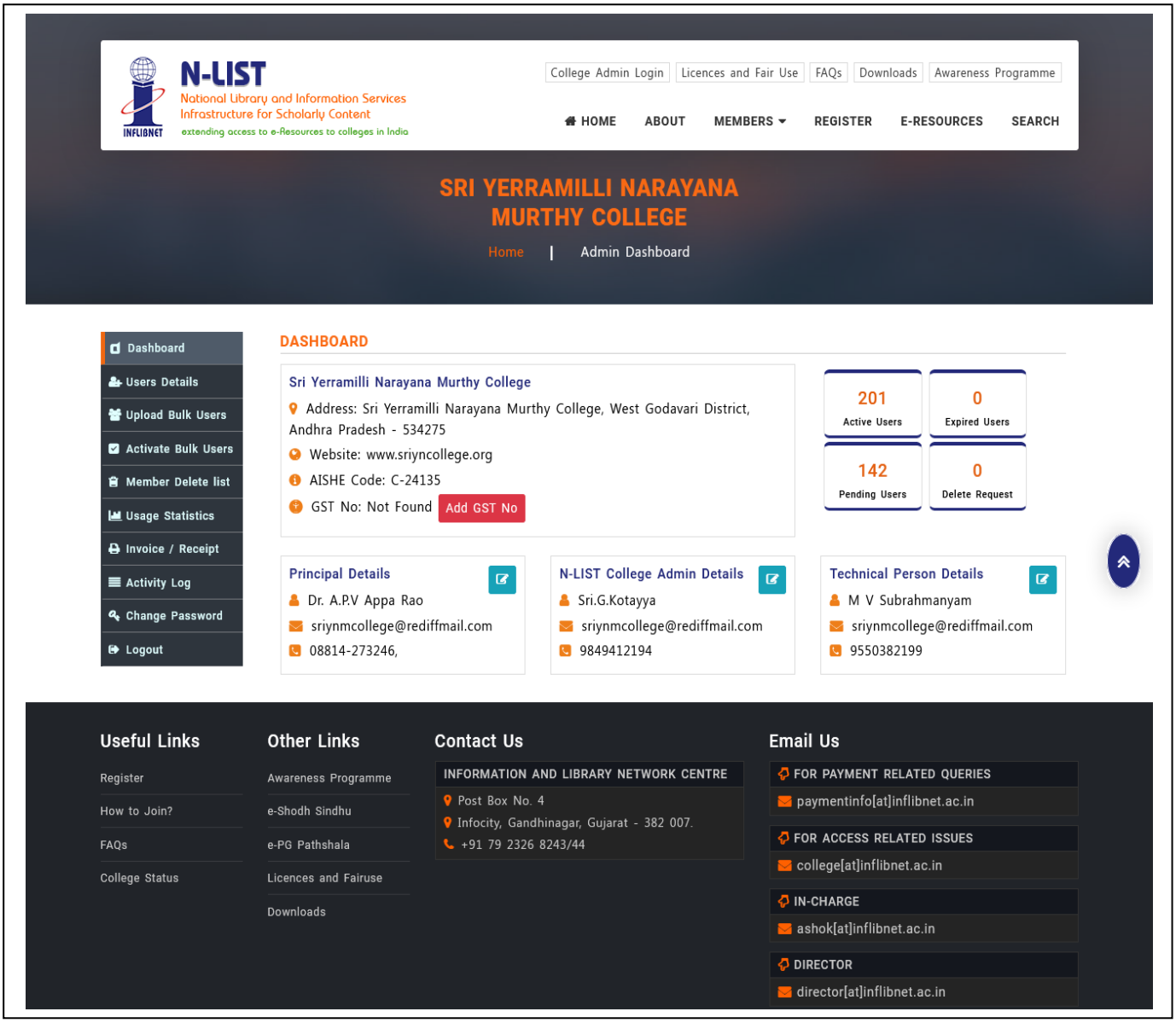
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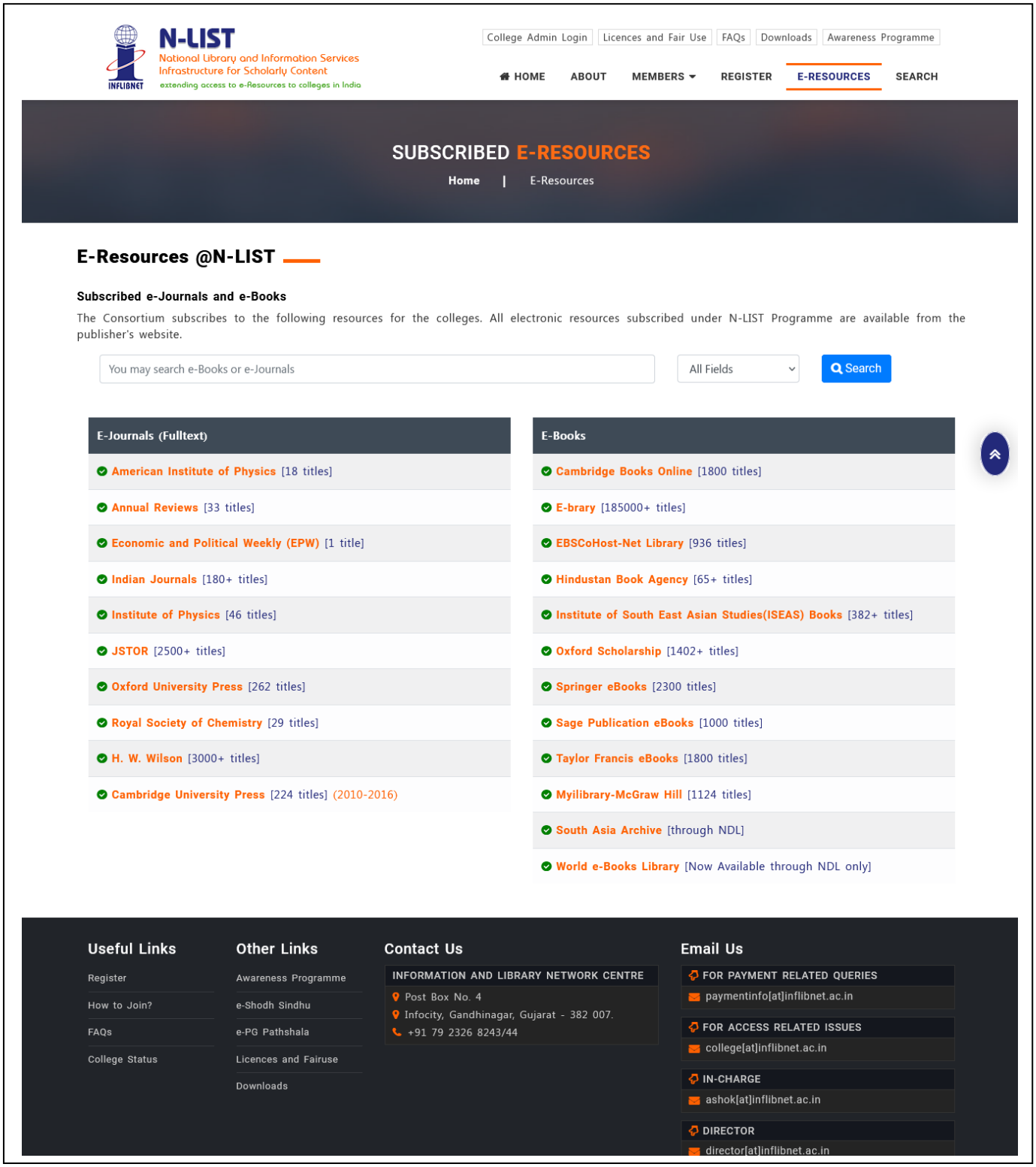

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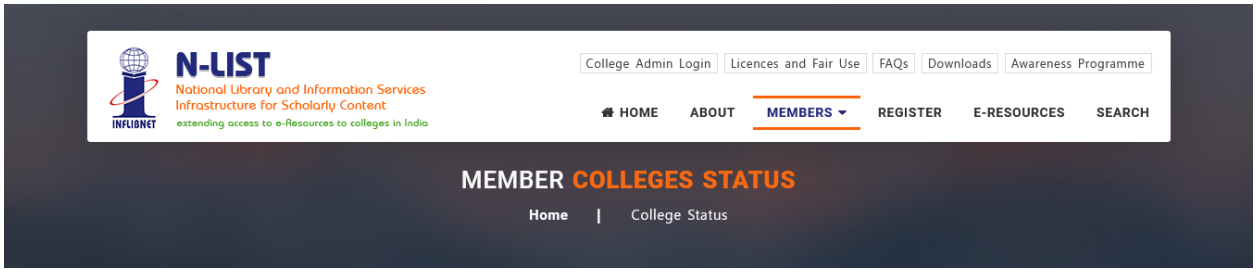

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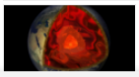

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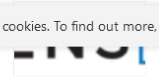

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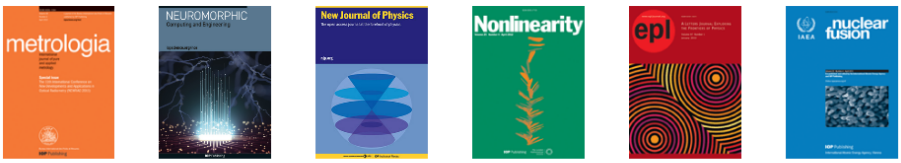

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