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STRUCTURE MODIFICATION: EFFECT OF LIPOPHILIC, ELECTRONIC, AND STERIC PARAMETERS OF *N*-BENZOYL-*N′*-PHENYLTHIOUREA COMPOUNDS ON ANTIVIRAL ACTIVITY OF COVID-19 BY IN SILICO

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ABSTRACT

N-benzoyl-*N′*-phenylthiourea (BFTU) compound is similar to amprenavir derivatives in the urea compound, chloroquine in the -NH group, and the benzene ring, which is a potent antiviral. This study evaluated the effect of lipophilic, electronic, and steric parameters of the BFTU compound on the antiviral activity of Covid-19. In silico docking using Autodock 4.2 to confirm the activity and pkCSM webserver to predict bioavailability and toxicity. The SARS-CoV-2 receptor was binding pocket with the Protein Data Bank (PDB) code 6LU7. Two and three dimensions of BFTU were generated using Marvin Sketch 20.4 and UCSF Chimera. Steric parameters affected the antiviral activity more than lipophilic and electronic parameters. A linear relationship was obtained on lipophilic, steric, and electronic parameters on activity, and a non-linear was on bioavailability and toxicity. The best activity was predicted for the *N*-benzoyl-*N′*-2,4-dichloro-phenylthiourea compound with a docking score of -9.12 kcal/mol. BFTU compounds are more potent as antiviral activity of Covid-19 compare to the reference drugs.

Keywords: BFTU, Lipophilic, Electronic, Steric, In Silico, Covid-19.

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INTRODUCTION

Coronavirus Disease 2019 (COVID-19), a coronavirus derivative discovered at the end of 2019, is the cause of global-scaled respiratory diseases. This new variant from Wuhan is closely related to Severe Acute Respiratory Syndrome Corona Virus (SARS-CoV) and Middle East Respiratory Syndrome Corona Virus (MERS-CoV).[1,2] It will bind to the Angiotensin-Converting Enzyme 2 (ACE-2) receptor to enter human cells with an estimated incubation period of about 14 days.[3] The urea-based compound of amprenavir and its derivative are known to possess antiviral activity.[4,5] The similitude between *N*-benzoyl-*N′*-phenylthiourea (BFTU) with amprenavir and chloroquine arguably makes this compound potentially possess antiviral activity. Topliss modification on the aromatic ring of the BFTU compound can be used to design derivates that will affect the parameters of the physicochemical properties in the Hansch model, such as lipophilic, electronic, and steric parameters. Lipophilic parameters play a role in drug penetration into cell membranes, electronic parameters are in drug solubility in distribution, and steric parameters are related to the strength of drug interactions with receptors.[6-8] Calculated log P (ClogP) and Hansch constant (π) values are lipophilic parameters, σ Hammet and Etot are electronic parameters, as well as Calculated Molar Refractivity (CMR) and ES are steric parameters.[9] The effect of lipophilic, electronic, and steric parameters of BFTU compound and its derivatives on antiviral activity was observed using the reference drugs, including chloroquine, oseltamivir, hydroxychloroquine, remdesivir, and favipiravir. COVID main protease (PDB ID:6LU7), was used in this study for molecular docking.[10] The activity of BFTU compounds and their derivatives as COVID-19 antivirals will be carried out *in silico method* using the QSAR approach.

EXPERIMENTAL

Aspire ES 11 operated by Windows 10 Home, Intel® Celeron N3050 Dual-Core (1.6 GHz), 64-bit, hard disc drive 500 GB, and RAM 2 GB DDR3 were used to run the molecular docking process. In silico docking

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using Autodock 4.2 to predict activity, pkCSM through http://www.biosig.unimelb.edu.au/pkcsm/prediction to predict physicochemical, bioavailability, and toxicity properties, ProteinPlus through http://www.proteins.plus/ to observe the interaction of *N*-benzoyl-*N*′-phenylthiourea (BFTU) compound and its derivatives against SARS-CoV-2 receptor.

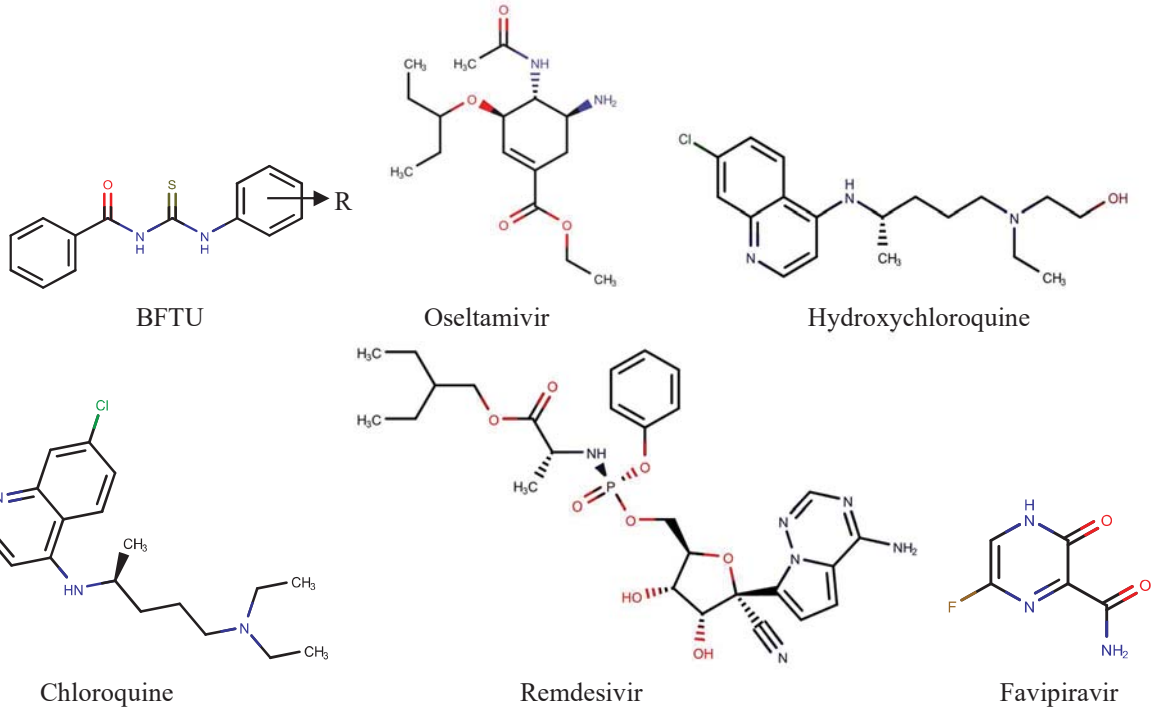

Fig.-1: Chemical Structure of BFTU, Oseltamivir, Hydroxychloroquine, Chloroquine, Remdesivir, and Favipiravir

The model of two and three dimensions of BFTU and its derivatives were optimized using Marvin Sketch 20.4 and UCSF Chimera. The SARS-CoV-2 receptor was obtained from http://www.rcsb.org/pdb with the Protein Data Bank (PDB) code 6LU7. Bioactive compounds, such as oseltamivir, hydroxychloroquine, chloroquine, remdesivir, and favipiravir were downloaded from http://www.pubchem.ncbi.nlm.nih.gov .[10-13]To determine the quantitative relationship between the physicochemical properties of BFTU compounds and its derivatives to their bioavailability, activity, and toxicity as antivirus through the IBM SPSS 24 statistical program.

RESULTS AND DISCUSSION

The Topliss approach on the BFTU compound resulted in 20 compounds with selected substituents, including H, 4-Cl, 3,4-diCl, 3-CF_3-4-Cl, 3-CF_3-4-NO_2, 4-CF_3, 4-Br, 4-I, 2,4-diCl, 4-NO_2, 3-Cl, 2-Cl, 2-OCH_3, 4-F, 4-$C(CH_3)_3$, 3-CF_3, 3,5-diCl, 4-OCH_3, 4-NH_2 and 4-OH.[9] Table-1 shows the value of intestinal absorption (human) of compounds 4-OCH_3-BFTU (18), 2-OCH_3-BFTU (13), and 4-F-BFTU (14) higher than the derivatives of other *N*-benzoyl-*N*′-phenylthiourea compounds and the reference drugs, so it can be predicted to have good bioavailability (F). The molecular docking process in this study used PDB ID: 6LU7, as a protein target which represents the main protease of SARS-Cov-2. This protein has native ligand of N-[(5-methylisoxazol-3-yl)carbonyl]alanyl-L-valyl-N~1~-((1R,2Z)-4-(benzyloxy)-4-oxo-1-{[(3R)-2-oxopyrrolidin-3-yl]methyl}but-2-enyl)-L-leucinamide (N3) with a value of Root Mean Square Deviation (RMSD) 2,13 Å, indicating acceptable reliability and validity.[14] The best docking score (DS) results were three compounds derived from BFTU, including 2,4-diCl-BFTU (9), 2-Cl-BFTU (12), and 4-$C(CH_3)_3$-BFTU (15), had a lower value than the reference drugs, including oseltamivir, hydroxychloroquine, chloroquine and favipiravir, but the docking score of remdesivir was lower. The lower the docking score, the more stable the bond that will be formed.[15] The result showed low Lethal Dose 50 (LD50) values for BFTU derivatives, 3-CF_3-4-Cl-BFTU (4), 3,4-diCl-BFTU (3), and 3,5-diCl-BFTU (17), the test compound was toxic and resulted in the death of the test animal.[16] The reference drugs, oseltamivir,

hydroxychloroquine, remdesivir, and favipiravir had a lower LD50 value, while the LD50 value of chloroquine was higher.

Table-1: Physicochemical Properties and *In Silico* Analysis of BFTU Compound, its Derivatives, and the Reference Drugs

Compounds	Physicochemical Properties						In Silico Analysis		
	Lipophilic Parameters		Electronic Parameters		Steric Parameters		Intestinal Absorption (Human) (Percent)	Docking Score (Kcal/mol)	Lethal Dose 50 (mol/kg)
	logP	Π	Etot	σ	MR	Es Taft			
(1) BFTU	3,56	0	-1,09	0	77,83	1,24	89,68	-7,84	2,436
(2) 4-Cl-BFTU	4,08	0,7	-3,37	0,23	82,63	0,27	88,30	-8,01	2,551
(3) 3,4-diCl-BFTU	4,6	1,25	2,63	0,52	87,43	0,54	88,02	-8,38	2,745*
(4) 3-CF_3- 4-Cl-BFTU	4,96	1,59	0,3	0,66	88,6	-0,89	85,03	-8,11	2,802*
(5) 3-CF_3-4-NO_2-BFTU	4,22	0,6	-4,35	1,21	89,37	-2,01	85,39	-8,30	2,689
(6) 4-CF_3-BFTU	4,45	0,88	23,92	0,54	83,8	-1,16	86,41	-7,74	2,725
(7) 4-Br-BFTU	4,36	0,86	-2,61	0,23	85,45	0,08	88,23	-8,26	2,555
(8) 4-I-BFTU	4,55	1,12	-1,91	0,18	91,19	-0,16	88,87	-8,51	2,531
(9) 2,4-diCl-BFTU	4,6	1,42	10,63	0,46	87,43	0,54	86,64	-9,12*	2,664
(10) 4-NO_2-BFTU	3,34	-0,28	5,09	0,78	83,4	-1,28	88,67	-8,37	2,618
(11) 3-Cl-BFTU	4,08	0,76	-4,76	0,37	82,63	0,27	88,94	-8,52	2,615
(12) 2-Cl-BFTU	4,08	0,71	18,64	0,23	82,63	0,27	88,02	-8,74*	2,562
(13) 2-OCH_3-BFTU	3,31	-0,02	10,83	-0,27	84,29	0,69	89,84*	-7,87	2,436
(14) 4-F-BFTU	3,7	0,14	-4,78	0,06	78,04	0,78	89,26*	-7,60	2,374
(15) 4-C(CH_3)$_3$-BFTU	5,19	1,98	12,73	-0,2	96,49	-1,54	87,51	-8,70*	2,584
(16) 3-CF_3-BFTU	4,45	0,88	18,44	0,43	83,8	-1,16	86,41	-7,75	2,725
(17) 3,5-diCl-BFTU	4,6	1,25	-14,12	0,75	87,43	0,52	87,74	-8,61	2,735*
(18) 4-OCH_3-BFTU	3,31	-0,04	-2,38	-0,27	84,29	0,69	90,75*	-8,06	2,437
(19) 4-NH_2-BFTU	2,78	-1,23	-16,02	-0,66	82,53	0,63	87,90	-8,19	2,154
(20) 4-OH-BFTU	3,28	-0,61	-12,25	-0,37	79,81	0,69	87,67	-8,17	2,017
(21) Oseltamivir	-	-	-	-	-	-	79,33	-7,07	2,467
(22) Hydroxychloroquine	-	-	-	-	-	-	88,98	-8,03	2,692
(23) Chloroquine	-	-	-	-	-	-	88,28	-7,84	2,805
(24) Remdesivir	-	-	-	-	-	-	64,20	-9,44	2,027
(25) Favipiravir	-	-	-	-	-	-	83,22	-5,38	2,008

Table-2 shows the interaction of the BFTU compound and its derivatives with the SARS-CoV-2 receptor, influenced by the type of bond involved, namely hydrogen bond and hydrophobicity. The ligand (N3) has hydrophobic bonds to the amino acids Leu4 dan Thr25, and hydrogen bonds to the amino acids Ala2, Phe140, Gly143, Cys145, His164, Met165, Glu166, Gln189, and Thr190. Based on the results of the study, it was found that the hydrophobic bond of the compound 2-OCH_3-BFTU (13) which binds to the amino

acids His164, Glu166, and Gln189 had the highest bond similarity with the comparison compound oseltamivir (His164, Glu166 dan Gln189), hydroxychloroquine and chloroquine (Glu166), remdesivir (Glu166 dan Gln189), so it can be predicted that these compounds have the same interactions with the reference drugs. Lipinski's Rule of Five is used to determine the physicochemical properties of a compound in penetrating cell membranes based on the following requirements: molecular weight less than 500 Da, log P value less than 5, number of hydrogen bond donors less than 5, and number of hydrogen bond acceptors less than 10.[17] BFTU compounds and its derivatives meet these requirements and are predicted to have the ability to penetrate cell membranes well so that more test compounds can bind to receptors.

Table-2: Ligand Interaction of BFTU Compound, its Derivatives, and the Reference Drugs

Compounds	Ligand Interaction
(1)	His164, Glu166
(2)	Glu166, Gln189
(3)	Gly143, Cys145
(4)	His164, Glu166, Gln189
(5)	Gly143, Glu166
(6)	Glu166, Gln189
(7)	Gly143, His164
(8)	His164, Gln189
(9)	His164, Glu166, Gln189
(10)	Met165, Gln192
(11)	Gln189
(12)	His164, Glu166
(13)	His164, Glu166, Gln189
(14)	-
(15)	Glu166, Gln189
(16)	-
(17)	His164
(18)	Gln189, Gln192
(19)	Glu166, Gln189
(20)	Gln192
(21)	Gly143, His164, Glu166, Gln189
(22)	Leu141, Glu166
(23)	Glu166
(24)	Cys145, Glu166, Arg188, Gln189
(25)	Phe140, His163

Correlation analysis using Pearson Correlation Matrix shows that there is a quantitative relationship between the physicochemical properties of BFTU compounds and their derivatives with lipophilic (ClogP dan π), electronic (σ Hammet dan Etot) and steric (CMR and ES) parameters on bioavailability, activity and toxicity as an antivirus for COVID-19. Regression analysis was performed on all test parameters using one parameter, two parameters, and three parameters. The results of the regression analysis showed that steric parameters affected the antiviral activity of COVID-19 compared to lipophilic and electronic parameters. The best similarity between the physicochemical properties of BFTU compound and its derivatives on bioavailability (F) = -0,905 π^2 + 0,659 π – 1,873 σ + 0,407 Es + 88,908 (n = 20, r = 0,799, SE = 0,98925, F = 6,604, Sig = 0,003), activity (DS) = 0,004 Etot – 0,050 MR – 4,036 (n = 20, r = 0,559, SE = 0,34083, F = 3,856, Sig = 0,042) and toxicity (LD50) = – 0,010 π^2 + 0,138 π - 0,234 σ + 2,418 (n = 20, r = 0,921, SE = 0,08459, F = 29,627, Sig = 0,000).

CONCLUSION

There is a linear relationship of steric and electronic properties of BFTU and its derivatives to activity prediction, the non-linear relationship of lipophilic, steric, and electronic properties to bioavailability

prediction, and the non-linear relationship of lipophilic and electronic properties to *in silico* toxicity prediction. The best Quantitative Structure-Activity Relationship (QSAR) equation can be used for the development of new antiviral drugs for COVID-19. The best compound against the SARS-CoV-2 receptor in this study was *N*-benzoyl-*N′*-2,4-dichloro-phenylthiourea.

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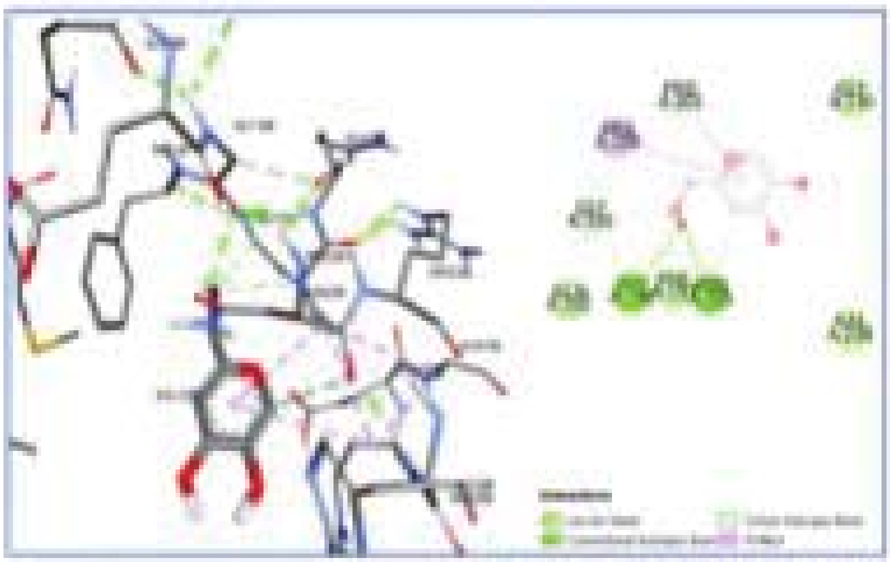

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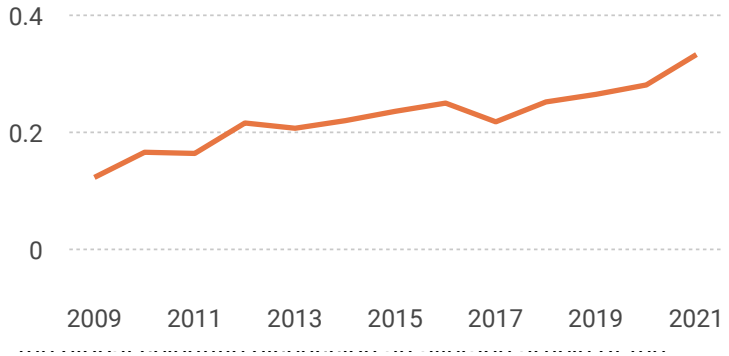

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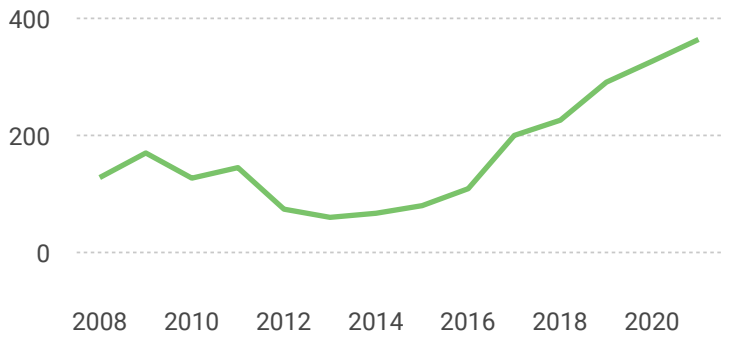

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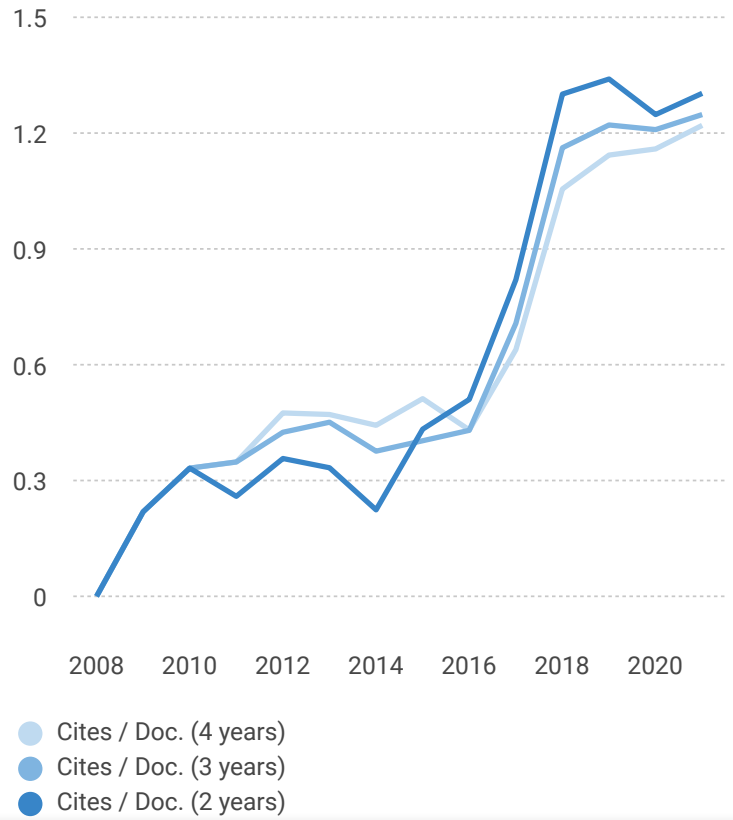

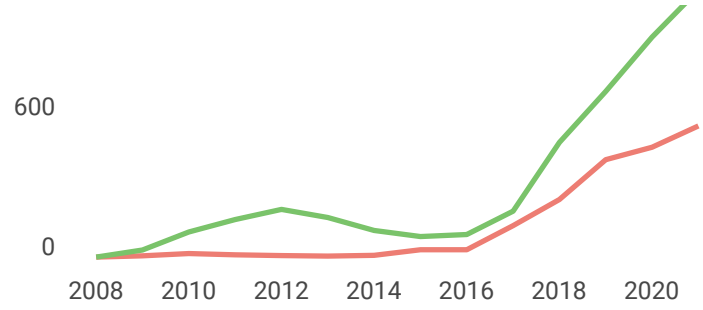

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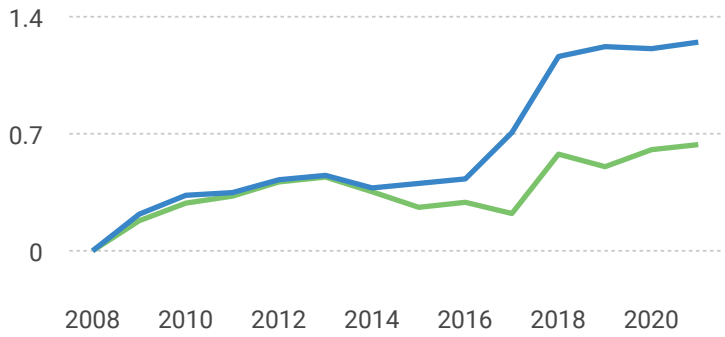

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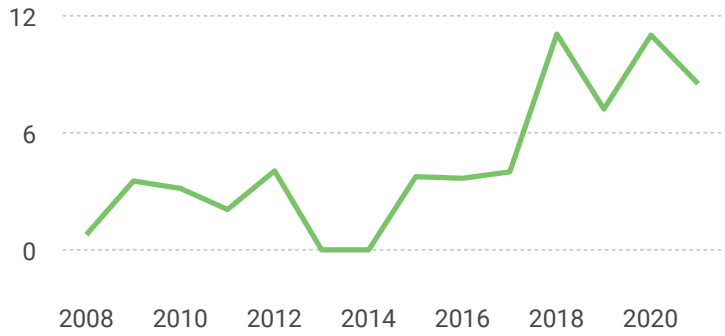

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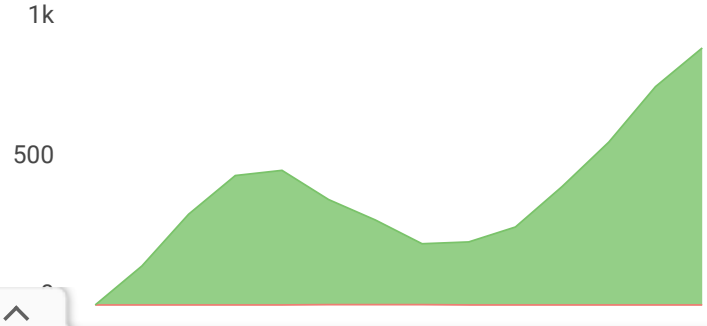

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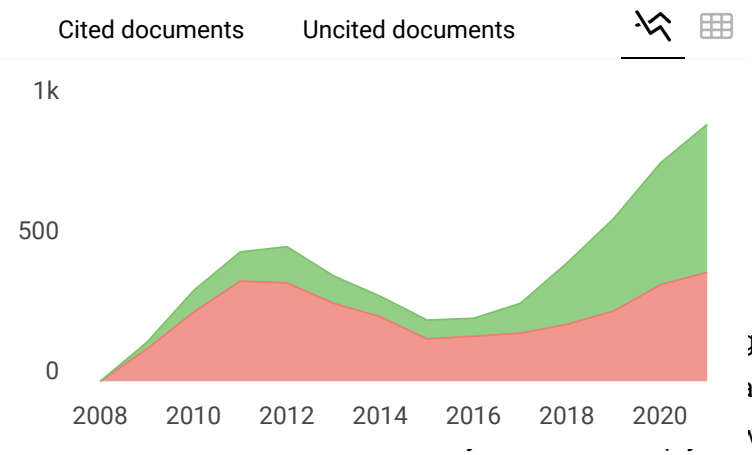

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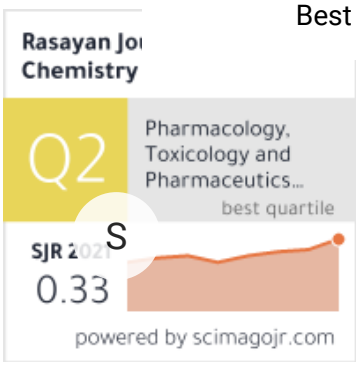

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