

STUDY OF THE BIOLOGICAL ACTIVITIES OF BIS-CARBAMATES OF THE MEE SERIES FOR THE AGRICULTURAL INDUSTRY

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ABSTRACT

This scientific work is devoted to the study of the biological activities of bis-carbamates of the MEE series for the agricultural industry. Virtual screenings were conducted online by the pass program. As a result, several activities with a high percentage of presence are predicted. The data obtained will help further studies of these compounds.

Keywords: Bis-carbamate, virtual, screening, structure, simulation, activity, biological, pharm, therapeutic, agriculture.

INTRODUCTION

Carbamates, or urethanes, are organic compounds derived from carbamic acid (carbonic acid amide). They are used on crops and in the home to kill cockroaches, ants, fleas, crickets, aphids, scale, whitefly, lace bugs and mealy bugs. Some carbamates control mosquitoes. Some carbamates have been found in groundwater at

levels high enough to cause concern [1]. In silico is a term for computer modeling (simulation) of an experiment, and it often studies biological activities [2]. Virtual screening of structural formulas based on "Structure-Activity" (SAR) relationship PASS Online computer prediction program to find directions of practical use of new substances. Conducted and studied more than 3500 species, including pharmacotherapeutic effects, biochemical mechanisms, toxicity, metabolism, gene expression modifiers, transporter-related activities, and other extrinsic activities with 95% accuracy [3]. The authors of this article synthesized bis-carbamates of the MEE series. The mechanism and parameters influencing the reaction have been studied [4-7,17]. The resulting product was studied in international chemical databases and classified according to the product range of foreign economic activity of the Republic of Uzbekistan [10,18]. Also, they were studied by spectral analysis methods and examined for acute toxicity [8,9,11,15,16,19]. Used as a plant biostimulator and corrosion inhibitor for metals and fuels [12-14]. We use N,N'-hexamethylene bis-[(o-cresolyl)-carbamate] i.e. MEE-1 and its derivatives as growth regulators (biostimulants) for various types of agricultural crops, including cotton, cotton, and cucumbers. Taking into account the possibility of application, we decided to study its other biological activities.

MATERIALS AND METHODS

Virtual screening of structural formulas based on "Structure-Activity" (SAR) relationship PASS Online <http://way2drug.com/PassOnline/predict.php> computer prediction program to find directions of practical use of new substances.

RESULTS AND DISCUSSIONS

Based on the obtained results, tables of potential activities for therapeutic and agricultural crops were compiled (Table 1).

Table 1

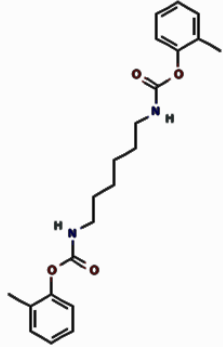
Availability of estimated biological activities of synthesized substances for agricultural crops - Pa (0.001-1000)

№	Faolliklar	MEE series compounds																	
		1	1a	1b	1v	1g	1d	2	2a	2b	2v	2g	2d	3	3a	3b	3v	3g	3d
1.	Anthelmintic (nematodes)	0,631	0,439	0,623	0,489	0,623	0,526	0,497	0,413	0,594	0,463	0,594	0,500	0,471	0,400	0,578	0,449	0,578	0,486
2.	Anthelmintic	0,485	0,194	0,342	0,334	0,342	0,313	0,440	0,188	0,329	0,322	0,329	0,302	0,424	0,193	0,340	0,333	0,340	0,307
3.	Acaricide	0,331	0,253	0,485	0,252	0,485	0,372	0,374	0,356	0,628	0,355	0,628	0,494	0,340	0,346	0,616	0,345	0,616	0,485
4.	Antifungal	0,379	-	0,186	0,177	0,273	-	0,357	-	0,183	0,174	0,270	-	0,325	-	0,187	0,178	0,274	-
5.	Insecticide	0,282	0,171	0,318	0,254	0,318	0,284	0,163	0,206	0,362	0,304	0,362	0,328	0,160	0,194	0,349	0,291	0,349	0,314
6.	Antiviral (picomavirus)	0,512	0,359	0,360	0,333	0,360	0,298	0,544	0,347	0,349	0,322	0,349	0,288	0,572	0,379	0,381	0,353	0,381	0,317
7.	Anti virus	0,227	-	0,156	0,173	-	-	0,240	-	-	0,161	-	-	0,253	-	-	0,160	-	-
8.	Antiseptic	-	0,147	0,298	0,146	0,527	0,231	-	0,188	0,347	0,187	0,600	0,260	-	0,152	0,303	0,151	0,535	0,240
9.	Against infection	0,275	0,223	0,438	0,269	0,560	0,268	0,338	0,254	0,488	0,303	0,615	0,302	0,328	0,246	0,475	0,295	0,602	0,288
10.	Antibiotic	0,191	-	-	-	0,097	-	0,176	-	-	-	-	-	0,174	-	-	-	0,099	-
11.	Against bacteria	0,366	-	0,150	-	0,173	-	0,327	-	-	-	0,217	-	0,326	-	-	-	0,232	-
12.	Antitoxic	0,327	-	0,226	0,287	0,226	0,182	0,341	-	0,257	0,317	0,257	0,214	0,332	-	0,252	0,311	0,252	0,208
13.	Antidote	0,350	0,192	0,298	0,288	0,298	0,233	0,362	0,200	0,307	0,298	0,307	0,241	0,349	0,214	0,324	0,314	0,324	0,249

Next Table 2 below shows the results of estimated biological activities of N,N'-hexamethylene bis-[(o-cresolyl)-carbamate], i.e. MEE-1 drug for agricultural crops:

Table 2

Estimated bioavailability of MEE-1 substance for agricultural crops

 <p>Structure of MEE-1</p>	Activities	Pa
	Anthelmintic (nematodes)	0,631
	Antihelminthic	0,485
	Acaricide	0,331
	Antifungal	0,379
	Insecticide	0,282
	Antiviral (picornavirus)	0,512
	Anti virus	0,227
	Antiseptic	-
	Against infection	0,275
	Antibiotic	0,191
	Against bacteria	0,366
	Antitoxic	0,327
	Antidote	0,350

According to predictions of Table 1, compound MEE-1 showed the highest result of 0.631 (63%) antihelminthic activity against nematodes and roundworms. The total anthelmintic activity of 0.485 (48%) showed the best result. Acaricidal activity was 0.331 (33%). The result of insecticidal activity was 0.282 (28%). 0.512 (51%) showed good activity against picornaviruses. Total antiviral activity was 0.227 (22%). Antiseptic activity was not determined. Anti-infective activity showed a result of 0.275 (27%). Antibiotic activity showed a satisfactory result of 0.191 (19%). 0.366 (37%) showed good antibacterial activity. Antitoxic activity showed a good result of 0.327 (32%). Antidote activity of 0.350 (35%) showed a good result.

CONCLUSION

In conclusion, it is advisable to check the activity of N,N'-hexamethylene bis-[(o-cresolyl)-carbamate] synthesized by us, which gave 50% higher results in practice. As you can see, the new bis-carbamate has a great contribution to the good growth, vigor and productivity of agricultural crops, and we believe that its practical application will greatly benefit the economy of our country.

REFERENCES:

1. American Conference of Governmental Industrial Hygienists (ACGIH). 2003. Guide to Occupational Exposure Values. Cincinnati, OH. <https://dhss.delaware.gov/dph/files/carbamfaq.pdf>
2. Emon N.U., Alam S, Rudra S., et al. Antidepressant, anxiolytic, antipyretic, and thrombolytic profiling of methanol extract of the aerial part of *Piper nigrum*: In vivo, in vitro, and in silico approaches. *Food Sci. Nutr.*, 2021, 9(2): 833-846.
3. Ochoa M.E., Farfán N., Labra-Vázquez P., et al. Synthesis, characterization and in silico screening of potential biological activity of 17 α -ethynyl-3 β , 17 β , 19-trihydroxyandrost-5-en acetylated derivatives. *Journal of Molecular Structure*, 2021, 1225: 129167.
4. Махсумов Абдухамид Гафурович, Абдукаримова Саида Абдужалиловна, Машаев Элдор Эргашвой Угли, and Азаматов Уткирбек Рашидович. "Синтез и свойства производного - N,N' quote -гексаметилен бис- [(орто-крезолило) -карбамата] и его применение" *Universum: химия и биология*, no. 10-2 (76), 2020, pp. 33-40.
5. Махсумов А.Г., Жагфаров Ф.Г., Арипджанов О.Ю., Машаев Э.Э., Азаматов У.Р. "Синтез и свойства производных мета-крезолило-карбаматов, их биологическая активность" *НефтеГазоХимия*, №3, 2022, 52-59 с. doi:10.24412/2310-8266-2022-3-52-59
6. Махсумов Абдухамид Гафурович, Машаев Элдор Эргашвой Угли, Холбоев Юсубжон Хакимович, Уразов Фируз Бахтиярович, and Зоҳиджонов Сирожиддин Аскаржон Угли. "N,N'–гексаметилен бис [(м-крезолило) -карбамат] и его физико-химические свойства" *Life Sciences and Agriculture*, no. 1 (9), 2022, pp. 7-11.
7. Maxsumov A.G., Mashayev E.E., Toshmatov D.A., Mirzaaxmedova M.A., Urazov F.B. N,N'-geksametilen bis-[(o-krezolilo)-karbamat]ning sintezi mexanizmi va xossalari // *Universal journal of academic and multidisciplinary research*. 2023. Vol.1, Issue 7, pp. 48-54. ISSN: 2992-8788 (E). RBIB-8.0
8. Maxsumov A.G., Mashayev E.E., Shapatov F.U., Azamatov O'R., Ismailov B.M. N, N'-geksametilen bis-[(o-, m-krezolilo)-karbamat] larning o'tkir toksikligini o'rganish // *Universal journal of medical and natural sciences*. 2023. Vol.1, Issue 7, pp. 53-61. ISSN: 2992-8826 (E). RBIB-8.0
9. Maxsumov A.G., Mashayev E.E., Shapatov F.U., Azamatov O'R., Ismailov B.M. N,N'-geksametilen bis-[(m-krezolilo)-karbamat]ning IQ-spektrlarini o'rganish // *Universal journal of technology and innovation*. 2023. Vol.1, Issue 7, pp. 164-171. ISSN: 2992-8842 (E). RBIB-8.0

10. Mashayev, E., Ismailov, B., Ergashev, J., Omonov, S., & Makhsumov, A. (2023). Research of N,N'-hexamethylene bis-[(o-cresolyl)-carbamate] in international chemicals databases. *B International Bulletin of Applied Science and Technology* (T. 3, Выпуск 11, сс. 397–401). Zenodo. <https://doi.org/10.5281/zenodo.10209951> ISSN: 2750-3402 (E). SJIF-6.904
11. Eldor Mashaev Ergashvoy ogli, Feruz Shapatov Utaganovich, & Bakhtiyar Kenjaev Ismatovich. (2023). In silico and in vivo study of acute toxicity of the substance of the MEE series. *Web of Medicine: Journal of Medicine, Practice and Nursing*, 1(8), 46–48. ISSN: 2938-3765 (E). SJIF-3.189
12. Eldor Mashaev, Bakhodir Mukhiddinov, Tursinay Kongratbaeva, and Nargiza Jovlieva, “Application of BIS-Carbamates of the MEE Series as Corrosion Inhibitors of Metal Equipment of Oil Refineries”, *AJEMA*, vol. 1, no. 10, pp. 57–59, Dec. 2023. ISSN: 2993-2637 (E). SJIF-5.512
13. E. E. Mashaev, A. G. Makhsumov, F. U. Shapatov “Study of the biostimulatory properties of MEE series bis-carbamates”, Vol. 2 No. 11 (2023): *International Journal of Agrobiotechnology and Veterinary Medicine*, pp. 1–4. ISSN: 2181-3450. RBIB-9.78
14. Eldor Mashaev, Utkirbek Azamatov, Abduhamid Makhsumov, and Boburbek Ismailov, “Synthesis and Study of Reducing the Corrosive Activity of Motor Fuels Using Additives of the MEE Series”, *AJEMA*, vol. 1, no. 10, pp. 75–78, Dec. 2023. ISSN: 2993-2637 (E). SJIF-5.512
15. Eldor Mashaev, Abduhamid Makhsumov, and Askar Parmanov, “Synthesis and spectral analysis of orthocresolylo carbamate”, *Best.Jour.Inno.Sci.Res.Dev.*, pp. 645–649, Dec. 2023. ISSN: 2835-3579 (E). SJIF-5.493
16. Eldor Mashaev, Husniddin Rahimov, Shoyunus Obidov, and Feruz Urazov, “Study of the Purity and Composition of the MEE-1 Molecule Using TLC and MS Spectroscopy”, *CAJMNS*, pp. 175-178, Dec. 2023. ISSN: 2660-4159. RBIB-10.84
17. Eldor Mashaev, Abduhamid Makhsumov, Sherbek Jo‘raqulov, “Synthesis Technology and Physicochemical Properties of Bis-Carbamate MEE-1”, *Euro.J.Ph.Ch.Ma.*, vol. 25, pp. 5–9, Dec. 2023. ISSN: 2795-7667 (E). SJIF-6.979
18. E.E. Mashaev, I.R. Asqarov, M.M. Xojimatov, and M.M. Muminjonov, “Classification of bis-carbamates of the MEE series based on the nomenclature of goods of foreign economic activity of the republic of Uzbekistan”, *JNCI*, vol. 42, no. 2, pp. 97–103, Dec. 2023. ISSN: 2181-368X
19. Eldor Mashaev, Abduhamid Makhsumov, Bahodir Fakhriddinov, Askar Parmanov. "Study of the structure of bis-carbamates of the MEE series using NMR and Mass spectral analysis methods" *Science and innovation*, vol. 2, no. 12, 2023, pp. 87-91. <https://doi.org/10.5281/zenodo.10360683> ISSN: 2181-3337 (P). SJIF- 5.608