Yusuf Sert

List of Publications by Year in descending order

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93 papers	1,810 citations	331670 21 h-index	330143 37 g-index
93 all docs	93 docs citations	93 times ranked	966 citing authors

#	Article	IF	Citations
1	Discovery of sulfadrugâ€“pyrrole conjugates as carbonic anhydrase and acetylcholinesterase inhibitors. Archiv Der Pharmazie, 2022, 355, e2100242.	4.1	156
2	Corrosion inhibition of carbon steel in 1ÂM H2SO4 using new Azo Schiff compound: Electrochemical, gravimetric, adsorption, surface and DFT studies. Journal of Molecular Liquids, 2020, 315, 113690.	4.9	150
3	Synthesis, X-ray structure, vibrational spectroscopy, DFT, biological evaluation and molecular docking studies of (E)-Nâ€™-(4-(dimethylamino)benzylidene)-5-methyl-1H-pyrazole-3-carbohydrazide. Journal of Molecular Structure, 2020, 1219, 128541.	3.6	124
4	New Heterocyclic Compound as Carbon Steel Corrosion Inhibitor in 1 M H₂SO₄, High Efficiency at Low Concentration: Experimental and Theoretical Studies. Journal of Adhesion Science and Technology, 2023, 37, 525-547.	2.6	75
5	Synthesis and inhibition profiles of N-benzyl- and N-allyl aniline derivatives against carbonic anhydrase and acetylcholinesterase â€“ A molecular docking study. Arabian Journal of Chemistry, 2022, 15, 103645.	4.9	69
6	Molecular docking, Hirshfeld surface, structural, spectroscopic, electronic, NLO and thermodynamic analyses on novel hybrid compounds containing pyrazole and coumarin cores. Journal of Molecular Structure, 2018, 1171, 850-866.	3.6	68
7	Synthesis, spectrophotometric and DFT studies of new Triazole Schiff bases as selective naked-eye sensors for acetate anion. Supramolecular Chemistry, 2020, 32, 519-526.	1.2	66
8	Synthesis, structural, molecular docking and spectroscopic studies of (E)-N'-(4-methoxybenzylidene)-5-methyl-1H-pyrazole-3-carbohydrazide. Journal of Molecular Structure, 2021, 1225, 129072.	3.6	66
9	5-((1H-imidazol-1-yl)methyl)quinolin-8-ol as potential antiviral SARS-CoV-2 candidate: Synthesis, crystal structure, Hirshfeld surface analysis, DFT and molecular docking studies. Journal of Molecular Structure, 2021, 1232, 130005.	3.6	62
10	Quantum Computational Investigation of (E)-1-(4-methoxyphenyl)-5-methyl-Nâ€²-(3-phenoxybenzylidene)-1H-1,2,3-triazole-4-carbohydrazide. Molecules, 2022, 27, 2193.	3.8	50
11	Acesulfame based Co(II) complex: Synthesis, structural investigations, solvatochromism, Hirshfeld surface analysis and molecular docking studies. Polyhedron, 2022, 218, 115762.	2.2	50
12	Vibrational analysis of 4-chloro-3-nitrobenzonitrile by quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 107, 248-255.	3.9	46
13	Molecular structure, Hirshfeld surface analysis, spectroscopic (FT-IR, Laser-Raman, UVâ€“vis. and NMR), HOMO-LUMO and NBO investigations on N-(12-amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide. Journal of Molecular Structure, 2018, 1171, 696-705.	3.6	40
14	Synthesis, spectroscopic characterization, crystal structure, DFT, molecular docking and inÂvitro antibacterial potential of novel quinoline derivatives. Journal of Molecular Structure, 2020, 1209, 127940.	3.6	40
15	Experimental and computational study on molecular structure and vibrational analysis of a modified biomolecule: 5-Bromo-2â€²-deoxyuridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 92, 406-414.	3.9	35
16	Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, molecular docking studies and DFT calculations, and antioxidant activity of 2-oxo-1,2-dihydroquinoline-4-carboxylate derivatives. Journal of Molecular Structure, 2019, 1188, 255-268.	3.6	32
17	Synthesis, DFT Study, Molecular Docking and Drugâ€Likeness Analysis of the New Hydrazineâ€1â€Carbothioamide, Triazole and Thiadiazole Derivatives: Potential Inhibitors of HSP90. ChemistrySelect, 2021, 6, 5838-5846.	1.5	29
18	Role of the cluster deformations in explaining the exotic decay half-lives. European Physical Journal A, 2012, 48, 1.	2.5	26

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19	FT-IR, Laser-Raman spectra and quantum chemical calculations of methyl 4-(trifluoromethyl)-1H-pyrrole-3-carboxylate-A DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 122-130.	3.9	24
20	Vibrational frequency analysis, FT-IR and Laser-Raman spectra, DFT studies on ethyl (2E)-2-cyano-3-(4-methoxyphenyl)-acrylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 96-104.	3.9	23
21	Synthesis, dielectric properties, molecular docking and ADME studies of pyrrole-3-ones. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8655-8671.	3.5	23
22	Experimental (FT-IR, NMR and UV) and theoretical (M06-2X and DFT) investigation, and frequency estimation analyses on (E)-3-(4-bromo-5-methylthiophen-2-yl)acrylonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 502-511.	3.9	19
23	Spectroscopic Investigations and DFT Calculations on 3-(Diacetylamino)-2-ethyl-3H-quinazolin-4-one. Journal of Spectroscopy, 2016, 2016, 1-15.	1.3	19
24	Hirshfeld Surface analysis, spectroscopic, biological studies and molecular docking of (4E)-4-((naphthalen-2-yl)methyleneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpyrazol-5-one. Journal of Molecular Structure, 2020, 1202, 127315.	3.6	18
25	A new series of sulfa drugs containing pyrazolyl acylthiourea moiety: Synthesis, experimental and theoretical spectral characterization and molecular docking studies. Journal of Molecular Structure, 2020, 1204, 127479.	3.6	18
26	Vibrational frequency analysis, FT-IR, DFT and M06-2X studies on tert-Butyl N-(thiophen-2yl)carbamate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 46-53.	3.9	17
27	FT-IR and Raman vibrational analysis, B3LYP and M06-2X simulations of 4-bromomethyl-6-tert-butyl-2H-chromen-2-one. Journal of Molecular Structure, 2015, 1079, 194-202.	3.6	17
28	4â€[(1,â€‰3â€Dioxoisoindolinâ€2â€yl)methyl]benzenesulfonamide: Full Structural and Spectroscopic Characterization and Molecular Docking with Carbonic Anhydrase II. ChemistrySelect, 2018, 3, 10113-10124.	1.5	16
29	Utilization of pyrazole-perimidine hybrids bearing different substituents as corrosion inhibitors for 304 stainless steel in acidic media. Journal of Molecular Structure, 2022, 1262, 133025.	3.6	16
30	Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of a potential chemotherapeutic agent 6-(2-methylpropyl)-4-oxo-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 97-105.	3.9	15
31	Molecular Structure, DFT, Vibrational Spectra with Fluorescence Effect, Hirshfeld Surface, Docking Simulation and Antioxidant Activity of Thiazole Derivative. ChemistrySelect, 2019, 4, 4544-4558.	1.5	15
32	Vibrational spectroscopic studies of 3-hydroxyphenylboronic acid: molecular structure. Indian Journal of Physics, 2013, 87, 113-119.	1.8	14
33	Use of vibrational spectroscopy to study 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione: A combined theoretical and experimental approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 126, 280-290.	3.9	14
34	Experimental and computational study on molecular structure and vibrational analysis of an antihyperglycemic biomolecule: Gliclazide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 137-146.	3.9	14
35	Effect of intermolecular hydrogen bonding, vibrational analysis and molecular structure of 4-chlorobenzothioamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 130-136.	3.9	13
36	Synthesis, spectroscopic characterization, DFT, molecular docking and in vitro antibacterial potential of novel quinoline derivatives. Journal of Molecular Structure, 2021, 1246, 131217.	3.6	13

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37	Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of 2,3,4,5,6-Pentafluoro-trans-cinnamic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 119-126.	3.9	12
38	Vibrational spectroscopy (FT-IR and Laser-Raman) investigation, and computational (M06-2X and B3LYP) analysis on the structure of 4-(3-fluorophenyl)-1-(propan-2-ylidene)-thiosemicarbazone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 91-99.	3.9	12
39	Syntheses of N-substituted benzimidazolone derivatives: DFT calculations, Hirshfeld surface analysis, molecular docking studies and antibacterial activities. Journal of Molecular Structure, 2020, 1200, 127174.	3.6	12
40	Syntheses of novel 1,<scp>5â€benzodiazepine</scp> derivatives: Crystal structures, spectroscopic characterizations, Hirshfeld surface analyses, molecular docking studies, <scp>DFT</scp> calculations, corrosion inhibition anticipation, and antibacterial activities. Journal of Heterocyclic Chemistry, 2021, 58, 270-289.	2.6	12
41	New tetrazoles compounds incorporating galactose moiety: Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, molecular docking studies, DFT calculations and anti-corrosion property anticipation. Journal of Molecular Structure, 2022, 1247, 131300.	3.6	12
42	Adsorption of Cr(VI) from Aqueous Solutions Onto Raw and Acid-Activated ReÅŸadiye and HanÃ§Ä±lÄ± Clays. Spectroscopy Letters, 2010, 43, 68-78.	1.0	11
43	Theoretical and experimental spectroscopic studies, XPS analysis, dimer interaction energies and molecular docking study of 5-(adamantan-1-yl)-N-methyl-1,3,4-thiadiazol-2-amine. Journal of Physics and Chemistry of Solids, 2019, 135, 109091.	4.0	11
44	New alkyl (cyclohexyl) 2-oxo-1-(propâ€2-yn-1-yl)-1, 2-dihydroquinoline-4-carboxylates: Synthesis, crystal structure, spectroscopic characterization, hirshfeld surface analysis, molecular docking studies and DFT calculations. Journal of Molecular Structure, 2021, 1227, 129520.	3.6	11
45	Synthesis, Î±-Glucosidase Inhibition, Anticancer, DFT and Molecular Docking Investigations of Pyrazole Hydrazone Derivatives. Polycyclic Aromatic Compounds, 2023, 43, 5021-5040.	2.6	11
46	Conformational and vibrational analysis of 2-, 3- and 4-trifluoromethylbenzaldehyde by ab initio Hartreeâ€“Fock, density functional theory and Mollerâ€“Plesset pertubasyon theory calculations. Computational and Theoretical Chemistry, 2008, 861, 122-130.	1.5	9
47	The biomolecule, 2-[(2-methoxyl)sulfanyl]-4-(2-methylpropyl)-6-oxo-1,6-dihydropyrimidine-5-carbonitrile: FT-IR, Laser-Raman spectra and DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 126, 86-97.	3.9	9
48	Molecular docking, Hirshfeld surface analysis and spectroscopic investigations of 1-(adamantan-1-yl)-3-(4-fluorophenyl)thiourea: A potential bioactive agent. Chemical Physics Letters, 2019, 735, 136762.	2.6	9
49	Spectral, DFT/B3LYP and molecular docking analyses on ethyl 2-(5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)pent-4-enoate. Journal of Molecular Structure, 2020, 1206, 127680.	3.6	9
50	Structural and spectroscopic analysis of 3-[(4-phenylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione with experimental (FT-IR, Laser-Raman) techniques and ab initio calculations. Journal of Molecular Structure, 2014, 1076, 664-672.	3.6	8
51	Monomer spectroscopic analysis and dimer interaction energies on N-(4-methoxybenzoyl)-2-methylbenzenesulfonamide by experimental and theoretical approaches. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 142, 169-177.	3.9	8
52	Hirshfeld Surface, Molecular Docking Study, Spectroscopic Characterization and NLO Profile of 2â€Methoxyâ€4,6â€Diphenylnicotinonitrile. ChemistrySelect, 2019, 4, 9857-9870.	1.5	8
53	DFT, molecular docking and experimental FT-IR, laser-Raman, NMR and UV investigations on a potential anticancer agent containing triazole ring system. Journal of Molecular Structure, 2020, 1211, 128077.	3.6	8
54	Synthesis, characterization and vibrational spectra analysis of ethyl (2Z)-2-(2-amino-4-oxo-1,3-oxazol-5(4H)-ylidene)-3-oxo-3-phenylpropanoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 491-501.	3.9	7

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55	Effect of intermolecular hydrogen bonding, vibrational analysis and molecular structure of a biomolecule: 5-Hydroxymethyluracil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 41-46.	3.9	7
56	Theoretical and experimental investigations on vibrational and structural properties of tolazamide. Journal of Molecular Structure, 2015, 1095, 87-95.	3.6	7
57	Structural optimization and vibrational analysis of an antidiabetic drug: tolbutamide. Journal of Sulfur Chemistry, 2015, 36, 450-461.	2.0	7
58	Vibrational spectroscopy investigation using M06-2X and B3LYP methods analysis on the structure of 2-Trifluoromethyl-10H-benzo[4,5]-imidazo[1,2-a]pyrimidin-4-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 109-118.	3.9	6
59	Micro-Raman, Mid-IR, Far-IR and DFT studies on 2-[4-(4-Fluorobenzamido)phenyl]benzothiazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 414-421.	3.9	6
60	DFT, Molecular Docking and Drug-likeness Analysis: Acrylate molecule bearing perfluorinated pendant unit. Journal of Molecular Structure, 2021, 1244, 130940.	3.6	6
61	Molecular structures and vibrational spectra of 2-, 3-and 4-ethylpyridines and 2-, 3-and 4-vinylpyridines by density functional theory and ab initio Hartreeâ€“Fock calculations. Indian Journal of Physics, 2012, 86, 859-869.	1.8	5
62	Synthesis, spectroscopic and theoretical studies of ethyl (2E)-3-amino-2-({[(4-benzoyl-1,5-diphenyl-1H-pyrazol-3-yl)carbonyl]amino}carbonothioyl)but-2-enoate butanol solvate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 816-827.	3.9	5
63	FT-IR, Laser-Raman spectra and computational analysis of 5-Methyl-3-phenylisoxazole-4-carboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 145-155.	3.9	5
64	Synthesis, Vibrational Spectra, and DFT Simulations of 3-bromo-2-methyl-5-(4-nitrophenyl)thiophene. Journal of Applied Spectroscopy, 2017, 84, 888-899.	0.7	5
65	Spectroscopic (FT-IR, Laser-Raman and NMR) and conformational analysis on novel pyrazole Î²-keto ester compound. Journal of Molecular Structure, 2018, 1167, 280-293.	3.6	5
66	Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterization, and quantum computational evaluation of (E)-2-(((4-bromophenyl)imino)methyl)-6-methylphenol. Journal of Physics and Chemistry of Solids, 2020, 144, 109478.	4.0	5
67	Synthesis, Crystal structure, Hirshfeld surface analysis, Spectral characterizations and Quantum computational assessments of 1-hydroxy-3-methyl-11H-pyrido[2,1-b] quinazolin-11-one. Journal of Molecular Structure, 2021, , 131592.	3.6	5
68	Vibrational, Geometrical and HOMO/LUMO/MEP Analyses by Using DFT/B3LYP and DFT/M06-2X Methods: 3-Amino-1,2,4-triazole. Pamukkale University Journal of Engineering Sciences, 2018, 24, 1272-1277.	0.4	5
69	Synthesis, DFT study, molecular docking and drug-likeness analysis of the heteroaryl substituted new pregnenolone derivatives. Journal of Molecular Structure, 2022, 1260, 132818.	3.6	5
70	Vibrational spectroscopic investigation of p-, m- and o-nitrobenzonitrile by using Hartreeâ€“Fock and density functional theory. Indian Journal of Physics, 2013, 87, 809-818.	1.8	4
71	Synthesis, Experimental and Theoretical Characterization of Novel Pyrimidineâ€5â€Carboxamides. ChemistrySelect, 2019, 4, 4695-4708.	1.5	4
72	Synthesis, characterization and theoretical studies of novel sulfonamide-aldehydes derivatives having tautomeric forms. Organic Communications, 2019, 12, 176-187.	0.8	4

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73	Synthesis, molecular docking, molecular dynamics and evaluation of Drug-Likeness properties of the fused N-Formyl pyrazoline substituted new dehydroepiandrosterone derivatives. Journal of Biomolecular Structure and Dynamics, 2022, , 1-12.	3.5	4
74	Structure Elucidation, Hirshfeld Surface Analysis, Molecular Docking and Computational Studies of a Jahn-Teller Distorted Octahedral Cobalt (II) Complex with Saccharin Ligand. Polycyclic Aromatic Compounds, 2023, 43, 4396-4406.	2.6	4
75	Tautomeric, spectroscopic, electronic and NLO analyses of purpald (4-amino-3-hydrazino-5-mercapto-1,2,4-triazole). Materials Today Communications, 2022, 32, 103862.	1.9	4
76	A theoretical investigation of 9BeÂ+Â27Al reaction: phenomenological and microscopic model approximation. Indian Journal of Physics, 2015, 89, 1093-1100.	1.8	3
77	Experimental (FT-IR, Laser-Raman and NMR) and theoretical spectroscopic analysis of 3-[(N-methylanilino)methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3H)-thione. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750024.	1.8	3
78	Experimental (FT-IR, Laser-Raman and NMR) and theoretical comparative study on 2-benzylsulfanyl-4-pentyl-6-(phenylsulfanyl)pyrimidine-5-carbonitrile, a potential bioactive agent. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850035.	1.8	3
79	Experimental and Quantum Chemical Calculations of 2-Amino-4,5,6,7-Tetrahydrobenzo[b]Thiophene-3-Carbonitrile. Acta Physica Polonica A, 2017, 132, 1192-1199.	0.5	3
80	Oneâ€•step Synthesis of novel N1 â€•substituted benzimidazole derivatives: Experimental and theoretical investigations. Journal of Heterocyclic Chemistry, 0, , .	2.6	3
81	Ab Initio Hartree-Fock and Density Functional Theory Study on Molecular Structures, Energies, and Vibrational Frequencies of 2-Amino-3-, 4-, and 5-Nitropyridine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2010, 65, 107-112.	1.5	2
82	Experimental and theoretical investigations on structural, spectroscopic, electronic and thermodynamic properties of (adamantan-1-yl)(phenylsulfanyl)methanone. Journal of Molecular Structure, 2018, 1173, 596-607.	3.6	2
83	Combined experimental and theoretical investigations on a half-sandwich organometallic Os(II) complex. Journal of Molecular Structure, 2019, 1188, 86-98.	3.6	2
84	A research on structural vibrational, surface characterization of 2-methyl-3-{5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl}-4H-pyrido[1,2-a]pyrimidin-4-one hydrate: SCXRD, FT-IR, MEP, Hirshfeld and molecular docking studies. Journal of Molecular Structure, 2021, 1235, 130198.	3.6	2
85	Pyrazolylâ€Benzoxazinone Derivatives as Dual Hsp Inhibitors in Human Breast Cancer. ChemistrySelect, 2022, 7, .	1.5	2
86	Radial sensitivity of the optical model potentials for 4He+120Sn and 6He+120Sn. International Journal of Modern Physics E, 2016, 25, 1650071.	1.0	1
87	Spectroscopic investigation of 2-(4-benzoyl-1,5-diphenyl-1H-pyrazol-3-yl)-4H-naphto[2,3-d][1,3]oxazin-4-one molecule. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750039.	1.8	1
88	Structural, Spectroscopic, Electronic and Molecular Docking Studies on (11R,12â€...S)â€16â€Aminotetracyclo[6.6.2.0^{2,7}.0^{9,14}]hexadecaâ€2(7),3,5,9(14),10,12â€he ChemistrySelect, 2019, 4, 825-837.	1.5	1
89	Molecular docking and vibrational spectroscopy studies of (E)-Nâ€²-hydroxy-1,3-diphenyl-4,5-dihydro-1H-pyrazole-5-carboximidamide. Journal of Molecular Structure, 2019, 1184, 79-91.	3.6	1
90	Structural, spectral, electronic, and molecular docking investigations on N,N<scp>â€dimethyl</scp>â€2â€[(<scp>1E</scp>)â€{[(methylsulfanyl)methanethioyl]amino}imino)methyl]aniline. Journal of the Chinese Chemical Society, 2021, 68, 971-988.	1.4	1

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91	Synthesis, antiproliferative activity, molecular docking studies of hydrazone functionalised thioparabanic acid and rhodanine analogues. Phosphorus, Sulfur and Silicon and the Related Elements, 2022, 197, 918-926.	1.6	1
92	RADIAL SENSITIVITY OF THE ELASTIC SCATTERING AROUND THE COULOMB BARRIER ENERGIES FOR WEAKLY-BOUND AND HALO NUCLEI. Modern Physics Letters A, 2012, 27, 1250118.	1.2	0
93	Phenomenological and microscopic analysis of elastic scattering reactions: 9Be+27Al new results. Journal of the Korean Physical Society, 2015, 66, 748-753.	0.7	0