N Sundaraganesan

List of Publications by Year
in descending order

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102 papers	4,257 citations	101543 36 h-index	118850 62 g-index
102 all docs	102 docs citations	102 times ranked	3276 citing authors

#	Article	IF	Citations
1	FT-Raman and FT-IR spectra, vibrational assignments and density functional studies of 5-bromo-2-nitropyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2995-3001.	3.9	388
2	The spectroscopic (FT-IR, FT-IR gas phase, FT-Raman and UV) and NBO analysis of 4-Hydroxypiperidine by density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 941-952.	3.9	279
3	FTIR and Raman studies on benzimidazole. Spectrochimica Acta Part A: Molecular Spectroscopy, 1991, 47, 1111-1115.	0.1	176
4	FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 4-N,Nâ€²-dimethylamino pyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 898-906.	3.9	144
5	FT-Raman and FT-IR spectra, ab initio and density functional studies of 2-amino-4,5-difluorobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 287-297.	3.9	116
6	Molecular structure, vibrational, UV and NBO analysis of 4-chloro-7-nitrobenzofurazan by DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1162-1170.	3.9	116
7	Comparison of experimental and ab initio HF and DFT vibrational spectra of benzimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 628-635.	3.9	112
8	FT-IR, FT-Raman, NMR and UVâ€“vis spectra, vibrational assignments and DFT calculations of 4-butyl benzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 179-189.	3.9	105
9	FTIR, FT-Raman spectra and ab initio DFT vibrational analysis of 2-bromo-4-methyl-phenylamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 740-751.	3.9	101
10	Molecular structure, anharmonic vibrational frequencies and NBO analysis of naphthalene acetic acid by density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 612-619.	3.9	92
11	Molecular structure, spectroscopic studies and first-order molecular hyperpolarizabilities of ferulic acid by density functional study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 312-323.	3.9	88
12	FTIR, FT-Raman spectra and ab initio, DFT vibrational analysis of 2,4-dinitrophenylhydrazine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 17-27.	3.9	85
13	Experimental FTIR, FT-IR (gas phase), FT-Raman and NMR spectra, hyperpolarizability studies and DFT calculations of 3,5-dimethylpyrazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 788-797.	3.9	84
14	FT-IR, FT-Raman, NMR spectra and DFT calculations on 4-chloro-N-methylaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1523-1529.	3.9	83
15	Molecular structure and vibrational spectra of 3-chloro-4-fluoro benzonitrile by ab initio HF and density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1134-1139.	3.9	80
16	Molecular structure, vibrational spectroscopic, first-order hyperpolarizability and HOMO, LUMO studies of 2-aminobenzimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 184-195.	3.9	74
17	Molecular structure, vibrational spectroscopic, firstâ€order hyperpolarizability and HOMO, LUMO studies of 3â€hydroxyâ€2â€naphthoic acid hydrazide. Journal of Raman Spectroscopy, 2010, 41, 53-62.	2.5	69
18	Molecular structure, spectroscopic (FTIR, FTIR gas phase, FTâ€Raman) firstâ€order hyperpolarizability and HOMOâ€“LUMO analysis of 4â€methoxyâ€2â€methyl benzoic acid. Journal of Raman Spectroscopy, 2010, 41, 1369-1378.	2.5	68

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19	DFT, FT-Raman, FT-IR and FT-NMR studies of 4-phenylimidazole. Journal of Molecular Structure, 2011, 990, 14-20.	3.6	67
20	FT-IR, FT-Raman spectra and ab initio HF, DFT vibrational analysis of 2,3-difluoro phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 561-566.	3.9	61
21	Vibrational spectra and fundamental structural assignments from HF and DFT calculations of methyl benzoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 771-777.	3.9	57
22	Molecular structure, vibrational spectra and DFT molecular orbital calculations (TD-DFT and NMR) of the antiproliferative drug Methotrexate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 264-275.	3.9	55
23	Vibrational spectra, assignments and normal coordinate analysis of 3-aminobenzyl alcohol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2511-2517.	3.9	51
24	Vibrational spectra and assignments of 5-amino-2-chlorobenzoic acid by ab initio Hartreeâ€“Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 381-388.	3.9	49
25	The spectroscopic FT-IR gas phase, FT-IR, FT-Raman, polarizabilities analysis of Naphthoic acid by density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 704-713.	3.9	48
26	Vibrational spectroscopic study and NBO analysis on bis(4-amino-5-mercapto-1,2,4-triazol-3-yl) methane using DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 877-884.	3.9	48
27	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 3-aminobenzotrifluoride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 214-224.	3.9	47
28	FT-IR, FT-Raman spectra and ab initio HF, DFT vibrational analysis of p-chlorobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 871-879.	3.9	47
29	Spectroscopic (FTIR, FT-Raman, NMR and UV) and molecular structure investigations of 1,5-diphenylpenta-1,4-dien-3-one: A combined experimental and theoretical study. Journal of Molecular Structure, 2012, 1030, 191-203.	3.6	47
30	Synthesis, structural, spectral (FTIR, FT-Raman, UV, NMR), NBO and first order hyperpolarizability analysis of N-phenylbenzenesulfonamide by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 417-431.	3.9	47
31	Molecular structure and vibrational spectra of indole and 5-aminoindole by density functional theory and ab initio Hartreeâ€“Fock calculations. Computational and Theoretical Chemistry, 2008, 850, 84-93.	1.5	45
32	Molecular structure and vibrational spectra of 2-amino-5-methyl pyridine and 2-amino-6-methyl pyridine by density functional methods. Journal of Molecular Structure, 2008, 891, 284-291.	3.6	45
33	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 2-amino-4,6-dimethoxypyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 1186-1196.	3.9	44
34	The spectroscopic (FTIR, FT-Raman, NMR and UV), first-order hyperpolarizability and HOMOâ€“LUMO analysis of methylboronic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 92, 67-77.	3.9	43
35	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of butylated hydroxy toluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 562-569.	3.9	42
36	The spectroscopic (FTIR, FT-Raman, UV and NMR), first-order hyperpolarizability and HOMOâ€“LUMO analysis of 4-amino-5-chloro-2-methoxybenzoic acid. Journal of Molecular Structure, 2012, 1024, 1-12.	3.6	41

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37	FTIR, FT-Raman spectra and ab initio DFT vibrational analysis of 2-amino-5-chloropyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 586-594.	3.9	39
38	Molecular structure, vibrational spectra, NMR and UV spectral analysis of sulfamethoxazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 1-10.	3.9	37
39	Experimental and theoretical investigation of the molecular and electronic structure of anticancer drug camptothecin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1058-1067.	3.9	36
40	Density functional study on the molecular structure, infrared and Raman spectra, and vibrational assignment for 4-thiocarbamoylpyridine. Journal of Molecular Structure, 2006, 791, 70-76.	3.6	35
41	Vibrational spectra and quantum chemical calculations of 3,4-diaminobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 376-383.	3.9	33
42	Molecular structure and vibrational spectroscopic studies of Chrysin using HF and Density Functional Theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 87, 67-76.	3.9	33
43	FTIR, FT-Raman spectra and ab initio DFT vibrational analysis of 2,4-dichloro-6-nitrophenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 1053-1062.	3.9	32
44	Vibrational spectra, assignments and normal coordinate calculation of acrylamide. Talanta, 2001, 54, 233-241.	5.5	31
45	FT-IR, FT-Raman spectra and ab initio DFT vibrational analysis of p-bromophenoxyacetic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 773-780.	3.9	31
46	The spectroscopic properties of anticancer drug Apigenin investigated by using DFT calculations, FT-IR, FT-Raman and NMR analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 86-99.	3.9	30
47	VIBRATIONAL DYNAMICS AND POTENTIAL ENERGY DISTRIBUTION OF TWO WELL-KNOWN NEUROTRANSMITTER RECEPTORS: TYRAMINE AND DOPAMINE HYDROCHLORIDE. Journal of Theoretical and Computational Chemistry, 2009, 08, 433-450.	1.8	29
48	The spectroscopic (FT-IR, FT-Raman), NCA, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of l-cysteine by ab inito HF and density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1515-1524.	3.9	29
49	FT-Raman and FTIR spectra, assignments and ab initio calculations of 2-aminobenzyl alcohol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 377-385.	3.9	28
50	Molecular structure, vibrational spectroscopic studies and NBO analysis of the 3,5â€dichlorophenylboronic acid molecule by the density functional method. Journal of Raman Spectroscopy, 2010, 41, 1379-1387.	2.5	28
51	X-ray crystallography characterization, vibrational spectroscopy, NMR spectra and quantum chemical DFT/HF study of N,Nâ€²-di(2-methoxyphenyl)formamidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 182-190.	3.9	27
52	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 3,4-dimethylbenzaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 680-687.	3.9	26
53	Vibrational spectra and assignments of 3-aminobenzyl alcohol by ab initio Hartreeâ€“Fock and density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 198-204.	3.9	26
54	Anharmonic vibrational analysis of 3,4-diaminopyridine and 3-aminopyridine by density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 502-512.	3.9	26

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55	Spectral and structural studies of the anti-cancer drug Flutamide by density functional theoretical method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 604-613.	3.9	25
56	Molecular structure and vibrational spectra of 4-phenylsemicarbazide by density functional method. Journal of Molecular Structure, 2011, 994, 379-386.	3.6	23
57	Molecular structure and vibrational spectra of Irinotecan: A density functional theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 1-6.	3.9	22
58	FT-IR, FT-Raman, dispersive Raman, NMR spectroscopic studies and NBO analysis of 2-Bromo-1H-Benzimidazol by density functional method. Journal of Molecular Structure, 2015, 1081, 506-518.	3.6	21
59	Vibrational spectra and assignments of 2-amino-5-iodopyridine by ab initio Hartreeâ€“Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 830-836.	3.9	20
60	Molecular structure, vibrational spectra and NBO analysis of phenylisothiocyanate by density functional method. Computational and Theoretical Chemistry, 2008, 863, 44-49.	1.5	20
61	Harmonic analysis of vibrations of morpholine-4-ylmethylthiourea: A DFT, midinfrared and Raman spectral study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 996-1002.	3.9	20
62	FT-IR, FT-Raman, NMR spectra, density functional computations of the vibrational assignments (for) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 of Molecular Structure, 2014, 1063, 192-202.	3.6	19
63	FT-IR, FT-Raman spectra and quantum chemical calculations of 3,4-dimethoxyaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 50-59.	3.9	18
64	Molecular structure, vibrational spectra and HOMO, LUMO analysis of 4-piperidone by density functional theory andab initioHartreeâ€“Fock calculations. Molecular Simulation, 2009, 35, 705-713.	2.0	18
65	Experimental and theoretical spectroscopic studies of anticancer drug rosmarinic acid using HF and density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 340-351.	3.9	18
66	The spectroscopic (FT-IR, FT-Raman, UV and NMR) first order hyperpolarizability and HOMOâ€“LUMO analysis of dansyl chloride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 234-244.	3.9	18
67	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular conformational analysis of 2,5-di-tert-butyl-hydroquinone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 165-174.	3.9	17
68	Vibrational spectral and quantum chemical investigations of tert-butyl-hydroquinone. Journal of Molecular Structure, 2012, 1012, 168-176.	3.6	17
69	FT-IR, FT-Raman spectra and quantum chemical calculations of some chloro substituted phenoxy acetic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 430-438.	3.9	16
70	Molecular structure, vibrational spectroscopic, first order hyperpolarizability and HOMOâ€“LUMO studies of 7-amino-8-oxo-3-vinyl-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 660-669.	3.9	16
71	Vibrational spectra, assignments and normal coordinate analysis of 2-amino-5-bromopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1113-1118.	3.9	15
72	FT-Raman and FT-IR spectra, ab initio and density functional studies of 3,4-dichlorobenzyl alcohol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 826-832.	3.9	15

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73	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 5-amino-o-cresol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 619-625.	3.9	15
74	Synthesis, X-ray crystallography characterization, vibrational spectroscopic, molecular electrostatic potential maps, thermodynamic properties studies of N,Nâ€²-di(p-thiazole)formamidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 88-95.	3.9	15
75	FT-IR, FT-Raman spectra and DFT vibrational analysis of 2-aminobiphenyl. Molecular Simulation, 2008, 34, 277-287.	2.0	13
76	Structural, vibrational (FT-IR and FT-Raman) and UVâ€“Vis spectral analysis of 1-phenyl-3-(1,2,3-thiadiazol-5-yl)urea by DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 331-340.	3.9	12
77	Synthesis and spectroscopic characterization on 4-(2,5-di-2-thienyl-1H-pyrrol-1-yl) benzoic acid: A DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 8-17.	3.9	12
78	Synthesis, structural and spectral analysis of (E)-Nâ€²-(4-Methoxybenzylidene)pyridine-3-carbohydrazide dihydrate by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 1123-1136.	3.9	11
79	Spectra, electronic structure and molecular docking investigations on 3-(phenyl(p-tolylamino)methyl)naphthalen-2-ol â€“ An experimental and computational approach. Journal of Molecular Structure, 2017, 1135, 53-66.	3.6	11
80	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 2-amino-5-methylphenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 550-558.	3.9	10
81	Spectral analysis, vibrational assignments, NBO analysis, NMR, UVâ€“Vis, hyperpolarizability analysis of 2-aminofluorene by Density Functional Theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 211-221.	3.9	10
82	Spectroscopic and molecular structure investigations of 9-vinylcarbazole by DFT and ab initio method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 690-699.	3.9	10
83	Synthesis, molecular structure, quantum chemical analysis, spectroscopic and molecular docking studies of N-(Morpholinomethyl) succinimide using DFT method. Journal of Molecular Structure, 2019, 1175, 609-623.	3.6	10
84	Vibrational spectra, UV and NMR, first order hyperpolarizability and HOMOâ€“LUMO analysis of 2-amino-4-chloro-6-methylpyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 811-824.	3.9	9
85	Molecular structure and spectroscopic (FT-IR, FT-Raman,¹³C,¹H NMR and UV) studies of 3,4-dihydroxy-<scp>l</scp>-phenylalanine using density functional theory. Molecular Simulation, 2012, 38, 987-1000.	2.0	9
86	The infrared, Raman, NMR and UV spectra, ab initio calculations and spectral assignments of 2-amino-4-chloro-6-methoxypyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 451-459.	3.9	9
87	Vibrational and structural observations upon 3-((1H-benzo[d]imidazol-1-yl)methyl)naphthalen-2-ol from spectral and DFT computing approaches. Journal of Molecular Structure, 2016, 1112, 33-44.	3.6	9
88	Aggregation properties and structural studies of anticancer drug Irinotecan in DMSO solution based on NMR measurements. Journal of Molecular Structure, 2012, 1013, 26-35.	3.6	7
89	Conformational analysis, molecular structure, spectroscopic, NBO, reactivity descriptors, wavefunction and molecular docking investigations of 5,6-dimethoxy-1-indanone: A potential anti Alzheimer's agent. Heliyon, 2022, 8, e08821.	3.2	7
90	Spectroscopic (FTIR, FT-Raman, NMR and UV) and molecular structure investigations of 1,5-diphenylpenta-2,4-dien-1-one: a combined experimental and theoretical approach. Molecular Simulation, 2013, 39, 330-349.	2.0	6

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91	Molecular structure, vibrational spectra and first-order hyperpolarisability analysis of 2-amino-6-nitrobenzothiazole by DFT method. Molecular Simulation, 2013, 39, 1052-1064.	2.0	6
92	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra, molecular geometry, conformational stability and some molecular properties of 1-Bromo-2,3-dimethoxynaphthalene. Journal of Molecular Structure, 2014, 1074, 51-61.	3.6	6
93	Synthesis, spectroscopic, computational and molecular docking studies of 1-(pyridin-2-yl amino)methyl napthalene-2-ol. Journal of Molecular Structure, 2019, 1197, 417-429.	3.6	6
94	Structural, vibrational, electronic and NMR spectral analysis of 3-chloro-6-methoxypyridazine by DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 36-45.	3.9	5
95	Synthesis and Raman spectroscopic investigation of a new selfâ€assembly monolayer material 4â€[Nâ€phenylâ€Nâ€(3â€methylphenyl)â€amino]â€benzoic acid for organic lightâ€emitting devices. Journal of Raman Spectroscopy, 2011, 42, 1682-1689.	2.5	3
96	Molecular structure and vibrational spectra of alpha-benzoinoxime by density functional method. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 116, 187-195.	0.6	3
97	FT-IR, FT-Raman, UVâ€“Visible, NMR, DFT and molecular docking investigation of 1-(phenyl (piperidin-1-yl)) Tj ETQq1 1 0.784314 rgBT /C	2.0	3
98	Vibrational analysis of deoxy-andrographolide using MM/QM methods. Spectroscopy, 2007, 21, 279-292.	0.8	1
99	Synthesis, Characterization, Spectroscopic, DFT and Molecular Docking Studies of 3-(3,4-Dihydroxyphenyl)-1-Phenyl-3-(Phenylamino)Propan-1-One. Polycyclic Aromatic Compounds, 2020, , 1-21.	2.6	1
100	Molecular structure and vibrational spectra of 4-nitrobenzylchloride byab initioHartreeâ€“Fock and density functional methods. Molecular Simulation, 2008, 34, 619-630.	2.0	0
101	Structural and vibrational spectroscopic analysis of anticancer drug mitotane using DFT method; a comparative study of its parent structure. Journal of Molecular Structure, 2015, 1086, 73-85.	3.6	0
102	Pharmacophore based virtual screening, molecular docking and density functional theory approaches to discover the potent beta-amyloid precursor protein (B-APP) inhibitor. AIP Conference Proceedings, 2019, , .	0.4	0