A Complete Bibliography of Publications in
Journal of Computational Chemistry:
2020–2029

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04 June 2020
Version 1.02

Title word cross-reference

4 [SS20]. 5 [AS20, SDK20]. + [CWZD20, LR20, WSV20]. ~ [WSV20]. 2
[AKN+20]. 2+ [JRS20, ZRSST20]. 3 [TTDT20]. 10 [LR20]. 2
[AR20, DSC20, DBE20, GGK20, MH20, SWF+20, TYZ20, WLZM20]. 20
[LR20]. 2 [SLR+20]. 3 [EK20, OE20, SLR+20, SL20, WLZM20, dCVARN20].
4 [ZXD20b, ZXD20a]. 450 [HYA+20]. 60 [DSC20]. a [PWW20]. N [SLR+20]. α
[CSP20]. β [AV20]. · [OE20, OE20]. μ [MVP+20]. p [AR20]. π
[AV20, LJ20, ODL20]. σ [AV20].

-acetato [MVP+20]. -Based [DBE20]. -block [AR20]. -dependent [JRS20].
-pyrazine-M [MH20]. -thymine [SSS+20].

/CBS [CSWW20, SK20]. /H [WSV20].

1
1 [KUNT20, Sán20]. 10.1002/jcc.25747 [MT20a].

2 [RLR+20, SLR+20]. 2-HOPO [SDK20].

40 [MT20a].

6-lutidine [TYZ20]. 60th [IBL20].

7D [Bal20]. 7D-Hypercube [Bal20].

8-hydroxyquinolinato [AS20].

= [AS20, MH20, SL20].

augmented [Pil20]. Avoids [SZLD20]. azide [XZZ+20]. Azobenzene [YXGZ20].

Colorings [Bal20]. Combining [WSL+20], compared [WD20].
Comparison [SK20], compatible [PLP+20]. Complete [HL20], complex [KL20, OE20, SWF+20], complexion [SDK20]. Complexes [AD20, BGS+20, ASL+20, AS20, MVP+20, PB20, SEZ20, YFS20].
component [KL20], components [AV20], composite [PW20], compound [EK20]. Compounds [SL20], comprehensive [PRH20], compressed [XZZ+20]. Comput [MT20a], Computational [AD20, AR20, GOY20, XZ20, WG20].
Computing [GJMPVR+20], condition [MT20b, YAO20]. configu
Computational [AD20, AR20, GOY20, XZ20, WG20]. Computations [Bal20, BSF20].
coupling [DG20]. Covalent [AWID+20]. Cover [Ano20a, Ano20n, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20v, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20n, Ano20o, Ano20, Ano20k, Ano20l, Ano20m].
dependent [YXGZ20, MH20, OE20, OMC+20, SDK20, SWF+20]. density-fitted [BSF20]. Depend [BWM20]. Dependence [YXGZ20, MH20].
Dependent [YXGZ20, FB20, IYI+20, JRS20, OMC+20, XAD20]. Derivation [FMFG20].
DFT/MRCI [ZRSST20]. dianionic [DPSG20]. diaqua [MVP+20].
dichromium [MVP+20]. dicopper [MVP+20]. Diimides [NRH+20].
diketones [AV20]. dimensional [STB+20, YAO20]. Dimerization
[WGKG20]. Dioxide [SB20, ZSD+20]. dipole [BSF20, HP20]. Direct
[FMFG20, YW20]. Directing [AD20]. directions [YAO20].
Disentanglement [CB20]. dispersion [CTBB20]. dispersion-corrected
[CTBB20]. displacement [CB20]. distance [QLC+20]. Distributed
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DLPNO-CEPA [San20]. DLPNO-CEPA/1 [San20]. DNA [HKSW20]. do
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[DSZ+20]. Double [FV20, OMC+20]. Doubles [HP20]. downregulation
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drugs [PRH20]. Dual [YW20]. Dual-hybrid [YW20]. due [OLP+20].
dynamic [BAO+20]. dynamically [MT20b]. Dynamics
[FMFG20, HHL+20, KUNT20, YXGZ20, Zac20, BAO+20, CSP20, GGK20, JRS20, LKM20, OSHT20, QLC+20, WSV20, ZFRM20].

E-fields [AMF+20]. Effect [AD20, GRN20, JMK+20, PRH20]. Effects
[CFZ+20, SLR+20, dCVARN20]. Efficient [CSGVF+20, MT20b].
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[AMF+20, OSHT20, STB+20]. electrostatic [AS20, OLP+20].
Electrostatics [HRT+20]. Elementometalation [WLZM20].
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Encapsulation [DSC20]. Encoding [GJMPB+20]. End [MXM20].
End-Point [MXM20]. Energetics [HHL+20, WGKG20].
Energies [BBK20, FMFG20, HP20, MFC20, NRH+20, HCS+20, OLP+20].
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Enhanced [FMFG20, MH20]. ensemble [QLC+20]. enter [APS20]. Enumeration
[SZLD20]. environment [KCF+20]. Enzymatic [SHM+20]. enzyme
[DSG20]. equations [MT20b]. Erratum [MT20a]. estrogen [CS20].
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[MM20, CG20]. Exchange [BBK20, SEZ20, YW20]. Excitation
[HP20, HSC+20, NRH+20]. Excited [AIV20, CG20, KL20, OSHT20, OMC+20, RDS+20, WD20, ZRSST20].
Excited-state [AIV20, WD20, ZRSST20]. Exhaustive [BAO+20, SZLD20].
Exploration [OOY20, SDK20]. Exploring [MSL+20]. expressed [HCS+20].
Extended [GX20]. Extension [AYO20].

F [GGK20]. Facilitates [VDK+20]. Facilitating [Zac20]. facilitator
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Hydrostatic [SL20]. hydroxycromones [AIV20]. hydroxylation
Hyperplanes [Bal20].

[YFS20]. Immerse [MSL20]. Immunodeficiency [KUNT20].
Improving [FB20]. Increase [LKM20]. Indexes [WZZ20]. Implicit
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[KUNT20, PT20, ASW20, CSWW20]. Interactions
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intramolecular [AIV20]. Intrinsic [AD20]. inversion [SWF20].
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[SK20]. Iodine [ASL20]. Ion [SLR20, HPG20, JRS20, LA20, XAD20].
Ionom-Pair [SLR20]. Ionic [VAL20, XAD20]. ions [ODL20, SDK20]. Ir
[DZL20]. Irreducible [Bal20]. Isoelectronic [ZXD20a, ZXD20b].
Isolation [BLP20]. isomerase [DPSG20]. isoctope [JMK20, dCVARN20].
Issue [Ano20a, Ano20b, Ano20c, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20v, Ano20w, Ano20x, Ano20y, Ano20z, Ano20-27, Ano20-28, Ano20-29, Ano20-30, Ano20-31, Ano20-32, Ano20-33, Ano20-34, Ano20-35, Ano20-36, Ano20-37, Ano20-38, Ano20-39]. IV
[PPSP20].

J [MT20a]. jcc.25747 [MT20a].

kinetic [JMK20, dCVARN20]. Kinetics [SK20, CD20]. Kohn [HCS20].
Koopmans [GCX20].

L536S [CSP20]. Laplacian [TTDT20]. Large [MFC20]. Large-Sized
[MFC20]. Late [PWW20]. Leading [AD20]. Learning [LPP20, YFS20].
length [MVP20]. less [CSWW20]. level [BSF20]. Lewis [OE20]. library
**Ligand**
- [RDS+20], Lif [VDK+20].
- [Ban20, JFZ+20, MMX20, NNT+20, AAc20, HGF20, ÖLP+20].

**Ligand-Binding**
- [NNT+20, HGF20].
- Ligands [Min20, SZLD20].
- LIO [SDK20].
- Lipase [VDK+20].
- lipids [KCF+20].
- Liquids [VAL20].
- Local [WSV20, PW20].
- Lone [TTDT20].
- Long [BBK20, HCS+20].
- Long-range [BBK20, HCS+20].
- Löwdin [ASW20].
- lutidine [TYZ20].

**Methods**
- M [AS20, MH20, AS20, MH20], machine [YFS20].
- Macroscale [HZG+20].
- Mannose [KUNT20].
- Map [CLS+20].
- mapping [TTDT20].
- Martini [MT20a, BAC20, MT19].
- material [GGK20].
- materials [ZGZ+20].
- Mathematical [QZB20].
- Matrix [BLP20].
- MD [SSS+20].
- MDMS [Zac20].
- Me [SDK20, WLZM20].
- Me-3 [SDK20].
- Mechanical [SL20, AAc20, GPEK+20, HKSW20].
- Mechanism [Ban20, CWZD20, WLZM20, CD20, CSP20, PPSP20].
- mechanisms [LA20, SWF+20].
- Mechanistic [JFZ+20, TYZ20].
- mechanistically [KCF+20].
- mediated [TYZ20].
- Membership [GJMPB+20].
- Membrane [BWM20, FMFG20, HHL+20, KCF+20, VDK+20, IBL20, ZSD+20].
- Membrane-Integrated [VDK+20].
- Membranes [PT20].
- mer [HHL+20, LGD+20].
- mercury [LDG+20].
- metadynamics [PPSP20].
- Metal [HHL+20, PW20, AR20, EK20, TYZ20, YFS20].
- metal-free [TYZ20].

**Model**
- [QZB20, AKN+20, AYO20, 1Y+20, MT20b, SS20, YAO20].
- Methods [AWID+20, KUNT20, SK20, AS20, BSF20, GUCR20, PW20, PB20].
- methotrexate [PRH20].
- methotrexate-camptothecin [PRH20].
- Mg [DSC20, JRS20, ZRSST20].
- Microscale [HZG+20].
- Microscopic [PT20].
- microsolvation [STR20].
- MIDAS [GJMPVR+20].
- Minimal [HHL+20].
- minimizing [YBS+20].
- MkVsites [LKM20].
- MM [SSS+20].
- Model [GCL+20, HRT+20, MT20a, SSS+20, CQSG20, HKSW20, HPG20, MT19, SWF+20, SSO+20, VAL20, XAD20].
- Modeling [AWID+20, BLP20, Li20, SM+20, GUCR20, LGD+20].
- models [CTBB20, PLP+20].
- Modification [AWID+20, Ban20].
- modified [XAD20].

**Modification**
- [ZSD+20].
- Molecular [FMFG20, GJMPB+20, GKG20, GCL+20, JRS20, KUNT20, YXGZ20, Zac20, AV20, AKN+20, AS20, AMF+20, BAO+20, CSP20, GJMPVR+20, HGF20, LKM20, OSHT20, QLC+20, RDS+20, ZFRM20].
- Molecules [LPP20, APS20, BGS+20, FB20, GGG20, KYM20, SSO+20, VCL20].
- Moller [CSGVF+20, Sán20].
- Moller-Plesset [CSGVF+20, Sán20].
- moments [BSF20].
- Mono [ZX20, ZXD20a].
- Mono-silicon [ZX20, ZXD20a].
- monooxygenderase [HYA+20].
- Monte [GGK20, KCG20].
- MRCI [ZRSST20].
- multicanonical [BAO+20].
- multicore [GJMPVR+20].
- Multilinear [WSL+20].
- Multiple [SZLD20, XAD20].
- Multipolar [HRT+20].
- multipole [AYO20, YAO20].
- multiscale [LGD+20].
- mutant [CSP20].

**N**
- [DZL+20, MKSS20].
- N-co-doped [DZL+20].
- N-Terminal [MKSS20].
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[APS20, CTBB20]. Nanotubes [DBE20, VCL20]. Naphthalene [NRH+20].
Natural [KL20, CB20, MH20, PW20]. Nature [MVP+20]. NCF [OE20].
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[BGS+20]. Neutralizing [KUNT20]. Newton [MT20b]. Newton-Raphson
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NMR [TTDT20]. NN [LPP20]. noncovalent
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nucleobases [CTBB20]. number [MT20b]. numbers [ASW20].

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d[CVARN20]. on-the-fly [OSHT20]. Opening [VDK+20]. oppositely
[HPG20]. optical [STB+20]. Optimal [WZZ+20, YBS+20]. Optimization
[LPP20, MT20b, SM20]. optoelectronic [ZGZ+20]. Orbital
[AD20, BBK20, KUNT20, AKN+20, ASW20, CB20, HCS+20, PW20].
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Organic [LPP20, FB20, GGK20, ZGZ+20]. organophosphorus [TYZ20].
Origin [EK20]. Origins [JFZ+20]. orthogonal [CB20]. Other [FMFG20].
Oversampling [NNT+20]. Oxidation [CWZD20]. oxide [TYZ20].
Oxidized [CWZD20]. Oxygen [GOY20, HL20]. oxygen-oxygen [HL20].

P [HYA+20]. package [KYM20]. Paddlewheel [AD20]. Pair
[SLR+20, HPG20, PW20, QLC+20]. pairs [TTDT20]. pairwise [YBS+20].
parameters [LKM20]. parametrization [KYM20]. partition
Peptide-Protein [XZ20]. Performance [BBK20, NRH+20, PB20, LKM20].
Performing [Zac20]. Periodic [SDK20, YAO20]. permeability [ZSD+20].
perspective [PPSP20]. Perturbation
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[PPW20]. planewave [SM20]. Plasticity [AD20]. Plesset
[CSGVF+20, Sán20]. Point [MXM20, BSF20]. Poisson [XAD20].
Polarizable [HRT+20, LJ20, KJM20, ODL20]. polarization [SSO+20].
polyatomic [SSO+20]. Polyethyleneimine [BAC20]. Polyethyleneimine
[MT20a, MT19]. polymerization [XZZ+20]. polymers [VCL20]. porous
[GGK20]. Poses [SZLD20]. Positron [SSO+20]. possible [ASL+20].
potential [AS20, MSL+20, SDK20, SSO+20]. potential-energy [MSL+20].
potentials [ZFRM20]. Predicted [CLS+20]. Predicting [APS20, PB20].
Prediction [CLS+20, GOY20, LPP20, PWW20, SEZ20, SB20, YFS20, AAc20, YBS+20].
predictive [FB20], prefer [APS20], preparation [QLC+20], Pressure [SL20, EK20], pressure-induced [EK20].
Principles [DBE20, EK20].
Probing [WG20]. Process [WLZM20, PRH20, WG20]. Processing [GCL+20], prodrug [PRH20, PPSP20], profiles [SSS+20], Progress [DBE20, GOY20, HZG+20, SL20, SB20, AS20, STB+20, WSV20].
Properties [BWM20, BSL20, CLS+20, MXM20, SZLD20, XZ20, BAO+20, KCGK20, SEZ20, WGKG20]. Protein-Ligand [MXM20]. Protein-Protein [BSL20]. Proteins [HHL+20, LJ20, KCF+20].
Q [SK20],QM [PWW20, SSS+20]. QM/MM [SSS+20]. QM/QM [PWW20]. QSAR [SS20]. QTAIM [AMF+20]. quality [FB20].
quantifying [IBL20]. Quantitative [AV20, BGS+20]. Quantum [AWID+20, OOY20, Pil20, CSGVF+20, GPEK+20, HKSW20, OE20].
quaternary [ODL20]. QuBiLS [GJMPVR+20]. QuBiLS-MIDAS [GJMPVR+20].
ray [FB20]. Rb [SL20]. RC \(\equiv\) [WLZM20]. R \(\equiv\) [WLZM20]. Reaction [QB20, SLR+20, CG20, CD20, HL20, SSS+20, TYZ20].
Reactions [OOY20, SK20, dCVARN20]. Reactivity [SHM+20, VAL20]. reality [MSL+20]. Reasoning [QB20]. Receptor [BWM20, CSP20, WGKG20].
receptor- [CSP20]. Receptor-Membrane [BWM20]. Receptors [Min20].
recognition [DPSG20]. Recognizing [HGF20]. Record [HZG+20].
rectangular [AYO20]. reduction [AR20, PPSP20]. Regioselective [JFZ+20]. Regioselectivity [JFZ+20], regulating [WSV20], relativistic [SDK20]. release [GGK20, PRH20]. Replacement [ZXD20a, ZXD20b].
resonance-assisted [AV20]. resource [LGD+20]. responsive [KCF+20].


Waals [EK20, YW20]. wales [CTBB20]. Water [HRT+20, MM20, PLP+20].
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X [FB20]. X-ray [FB20].

Zr [DBE20].

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