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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].
-diaqua [MVP+20]. -diketones [AV20]. -LIO [SDK20]. -phenyl [AS20].
-pyrazine-M [MH20]. -thymine [SSS+20].

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

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].

Absolute [SZLD20]. **Absorption** [AS20]. **Accelerating** [GCL⁺20]. **Accessible** [GCL⁺20, VCL20]. **accurate** [CSWW20, WD20]. **acetato** [MVP⁺20]. **Acetylene** [OOY20]. **acid** [HPG20, ODL20, OE20, PRH20, WGKG20]. **acid-catalyzed** [PRH20]. **actinide** [SDK20]. **Activated** [WLZM20]. **Activation** [BWM20, MKSS20, SLR⁺20, DZL⁺20, LA20]. **Active** [VDK⁺20, HL20]. **activities** [YFS20]. **activity** [SS20]. **Acylation** [CD20]. **adapted** [OE20]. **additive** [KYM20]. **additivity** [PB20]. **Adsorption** [GGK20]. **aeruginosa** [VDK⁺20]. **Affinity** [dSBFdAJ20]. **Ag** [MH20]. **agent** [SDK20]. **aggregate** [RDS⁺20]. **AI** [AS20]. **Alchemical** [Min20]. **AlGDock** [Min20]. **algebra** [GJMPVR⁺20]. **Algorithm** [WSL⁺20, SS20]. **alkali** [ODL20]. **Alkyne** [WLZM20]. **Alkynes** [JFZ⁺20, TYZ20]. **all-atom** [LKM20, WGKG20]. **Allosteric** [BSL20]. **along** [CG20]. **AMgF** [SL20]. **amine** [HPG20]. **amino** [ODL20]. **Ammonia** [MFC20]. **ammonium** [ODL20]. **AMOEBa** [PLP⁺20]. **Amorphous** [XZZ⁺20]. **Analyses** [SLR⁺20]. **Analysis** [AD20, KUNT20, MH20, CSP20, CB20, HL20, JMK⁺20, JRS20, MT20b, ZGZC20]. **analytic** [BSF20]. **Analytical** [VCL20]. **Analyze** [dSBFdAJ20]. **analyzing** [HPG20]. **Anion** [LJ20, XAD20]. **Anion-Ring** [LJ20]. **Anionic** [PT20]. **Anisotropic** [ZGZ⁺20, AYO20]. **anomaly** [XCJ20]. **Anti** [KUNT20]. **Anti-Human** [KUNT20]. **Antibodies** [KUNT20]. **antiporter** [WSV20]. **antitumor** [PRH20]. **Application** [GJMPB⁺20, XAD20, AAe20, YBS⁺20]. **Applications** [SHM⁺20, IYI⁺20]. **applied** [KCGK20]. **Approach** [PWW20, SBG20, SB20, ASW20, IYI⁺20, OSHT20, PW20, STR20, VCL20]. **approaches** [AV20]. **approximation** [YW20]. **Approximations** [HFPS20, BSF20]. **AQUA** [LGD⁺20]. **AQUA-MER** [LGD⁺20]. **aqueous** [LGD⁺20]. **Area** [GCL⁺20, VCL20]. **aromatic** [APS20, ODL20]. **art** [BSF20]. **artifacts** [ÖLP⁺20]. **Artificial** [QB20]. **Aspartate** [HPG20]. **asplatin** [PPSP20]. **assembly** [PRH20]. **Assessment** [SK20, SB20, ZRSST20]. **assisted** [AV20]. **atom** [LKM20, WGKG20]. **Atomistic** [GOY20, HZG⁺20, SL20]. **atoms** [AKN⁺20, CSGVF⁺20, OE20].

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

B [DZL⁺20]. **Backbone** [CLS⁺20]. **BAND** [LPP20]. **Based** [DBE20, AV20, BAO⁺20, GJMPVR⁺20, GJMPB⁺20, MT20b, OE20, PW20, SM20, ZFRM20]. **Basis** [YXGZ20, SM20]. **bath** [CQSG20]. **Bel** [ZXD20b, ZXD20a]. **benchmark** [OMC⁺20]. **Benchmarking** [XZ20]. **Benoit** [IBL20]. **bent** [WG20]. **benzene** [XCJ20]. **between** [CTBB20, HYA⁺20, Min20]. **bile** [WGKG20]. **Binding** [GOY20, MXM20, Min20, NNT⁺20, SZLD20, dSBFdAJ20, CSP20, HGF20, IYI⁺20, ÖLP⁺20, SWF⁺20, SSO⁺20]. **Biological** [AWID⁺20, SS20]. **biology** [IBL20]. **Biomolecules** [WZZ⁺20, ZGZC20]. **biosystems** [GUCCR20]. **birthday** [IBL20]. **bis** [YFS20]. **block** [AR20]. **Boltzmann** [XAD20]. **Bond** [LR20, AV20, HL20, SSS⁺20, XCJ20]. **bonding** [AV20, BGS⁺20, MVP⁺20]. **bonds** [CB20, WG20]. **Born** [GCL⁺20]. **both** [KCF⁺20, PRH20]. **boundary** [YAO20]. **Br** [GGK20]. **Breakdown** [AD20]. **Breaking** [LR20]. **brevicompectum** [HYA⁺20]. **Bridging** [HZG⁺20]. **Building** [AD20].

C [LR20, ZFRM20, DZL⁺20, DSC20]. **cage** [DSC20, GGK20]. **CAI** [ZXD20a]. **CAI** [ZXD20b]. **calculate** [SS20]. **Calculation** [Sán20, CSWW20, ÖLP⁺20, VCL20, YBS⁺20]. **Calculations** [DBE20, MXM20, Min20, EK20, FV20, FB20, KL20, QLC⁺20, SWF⁺20]. **Calibration** [DPSG20]. **camptothecin** [PRH20]. **canonical** [GGK20].

Carbon

[ZXD20a, APS20, AKN⁺20, CTBB20, GPEK⁺20, ZSD⁺20, ZXD20b]. **carboxylation** [JMK⁺20]. **Carlo** [GGK20, KCGK20]. **carrier** [ZGZ⁺20]. **case** [OSHT20]. **catalysis** [JRS20]. **catalytic** [YFS20]. **catalyzed** [HYA⁺20, PRH20]. **Cation** [LJ20, ODL20]. **Cavity** [GRN20]. **CBS** [CSWW20, SK20]. **CC3** [GGK20]. **CC3-R** [GGK20]. **CCSD** [CSWW20]. **CCSDT** [SK20]. **Celebrating** [IBL20]. **cells** [AYO20]. **CEPA/1** [Sán20]. **CH** [dCVARN20, SLR⁺20, dCVARN20]. **chains** [ODL20]. **changes** [ÖLP⁺20]. **channel** [LA20, XAD20]. **Chaperone** [VDK⁺20]. **character** [BGS⁺20]. **Characterization** [PT20, GPEK⁺20]. **Charge** [GRN20, CB20, KCGK20, ÖLP⁺20, OMC⁺20, PLP⁺20, ZGZ⁺20]. **charged** [HPG20]. **CHARMM** [KYM20, QLC⁺20]. **CHARMM-GUI** [QLC⁺20]. **Chem** [MT20a]. **Chemical** [AWID⁺20, MSL⁺20, OOO20, VAL20, CB20, HGF20, Pil20, TTDT20]. **chemistry** [SDK20]. **chiral** [GJMPVR⁺20]. **Cholesterol** [Ban20]. **Cis** [YXGZ20]. **Cis-Azobenzene** [YXGZ20]. **CI** [GGK20, SLR⁺20, WSV20]. **cleavage** [JRS20]. **Cluster** [BLP20, WZZ⁺20, BSF20, STR20]. **cluster-continuum** [STR20]. **Clusters** [MFC20, DZL⁺20]. **CO** [WLZM20, DZL⁺20, AR20]. **Coarse** [MT20a, WSL⁺20, WZZ⁺20, MT19]. **Coarse-Grained** [MT20a, WSL⁺20, WZZ⁺20, MT19]. **Code** [SHM⁺20]. **codelivery** [PRH20]. **Coelenterazine** [GOY20]. **Coenzyme** [CWZD20].

Colorings [Bal20]. **Combining** [WSL⁺20]. **compared** [WD20]. **Comparison** [SK20]. **compatible** [PLP⁺20]. **Complete** [HL20]. **complex** [KL20, OE20, SWF⁺20]. **complexation** [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]. **Computations** [Bal20, BSF20]. **Computing** [GJMPVR⁺20]. **condition** [MT20b, YAO20]. **configurational** [BAO⁺20]. **conformational** [SS20, STR20, WSV20, ZGZC20]. **conical** [AIV20]. **consistent** [CQSG20, PW20]. **constant** [SSS⁺20]. **constants** [dCVARN20]. **construction** [ZFRM20]. **Contact** [CLS⁺20]. **Contacts** [MKSS20]. **containing** [CTBB20, ZGZ⁺20]. **Continuum** [BBK20, STR20]. **contracted** [SM20]. **contribution** [Sán20]. **convergence** [MT20b]. **Coordinate** [AD20]. **Coordination** [MVP⁺20]. **Core** [NRH⁺20, Pil20]. **Core-Substituted** [NRH⁺20]. **corrected** [CTBB20, HCS⁺20]. **Correcting** [ÖLP⁺20]. **correction** [ASW20]. **correction-scaling** [ASW20]. **Corrections** [HFPS20]. **correlation** [PW20, Sán20, SSO⁺20]. **correlations** [AS20, YW20]. **corrole** [ASL⁺20]. **COSMO** [VAL20]. **COSMO-RS** [VAL20]. **costly** [CSWW20]. **Coulomb** [CQSG20]. **coumarin** [ZRSST20]. **coumarin-schiff** [ZRSST20]. **Counterion** [SLR⁺20]. **Coupled** [BWM20, BSF20, WGKG20, XCJ20]. **coupled-cluster** [BSF20]. **coupling** [DZL⁺20]. **Covalent** [AWID⁺20]. **Cover** [Ano20a, Ano20n, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m]. **Cp** [WLZM20]. **CR** [WLZM20]. **creating** [LKM20]. **Criegee** [SK20]. **Critical** [SB20, MT20b]. **crystal** [RDS⁺20]. **Crystalline** [HZG⁺20]. **Cs** [SL20]. **Cu** [MH20, AD20]. **cupric** [XZZ⁺20]. **Current** [BSL20]. **Current-Flow** [BSL20]. **cyclization** [TYZ20]. **cyclopropane** [WG20].

D [SS20, dCVARN20]. **Data** [SK20, XZ20]. **databases** [LGD⁺20]. **DD** [CD20]. **DD-peptidase** [CD20]. **deacylation** [CD20]. **decomposition** [AV20, MT20b]. **decomposition-based** [MT20b]. **decorporation** [SDK20]. **Deep** [LPP20]. **DEER** [QLC⁺20]. **defects** [CTBB20, GPEK⁺20]. **Deformation** [FMFG20]. **densities** [Pil20]. **Density** [BBK20, CWZD20, FMFG20, SK20, YXGZ20, APS20, BSF20, CQSG20, CTBB20, DZL⁺20, FB20, HCS⁺20, IYI⁺20, 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]. **Derivatives** [GRN20]. **Description** [BLP20, HRT⁺20, XCJ20]. **descriptors** [GJMPVR⁺20]. **designs** [YBS⁺20]. **details** [TYZ20]. **Determination** [NNT⁺20]. **determines** [HYA⁺20]. **Determining** [WZZ⁺20]. **Development** [WSL⁺20]. **devices** [AMF⁺20]. **DFT** [FV20, SB20, WD20, ZRSST20].

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, HPG20]. **Direct** [FMFG20, YW20]. **Directing** [AD20]. **directions** [YAO20]. **Disentanglement** [CB20]. **dispersion** [CTBB20]. **dispersion-corrected** [CTBB20]. **displacement** [CB20]. **distance** [QLC⁺20]. **Distributed** [GJMPVR⁺20]. **distribution** [QLC⁺20]. **DLPNO** [Sán20]. **DLPNO-CEPA** [Sán20]. **DLPNO-CEPA/1** [Sán20]. **DNA** [HKS20]. **do** [GUCCR20, ZGZC20]. **Dock** [Min20]. **Docking** [XZ20, BAO⁺20]. **DOI** [MT20a]. **Domain** [PT20, PW20]. **Domain-based** [PW20]. **doped** [DZL⁺20]. **Double** [FV20, OMC⁺20]. **Doubles** [HFPS20]. **downregulation** [CSP20]. **drive** [RLR⁺20]. **driven** [AIV20]. **Drude** [KYM20, LJ20, ODL20]. **drugs** [PRH20]. **Dual** [YW20]. **Dual-hybrid** [YW20]. **due** [ÖLP⁺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** [JFZ⁺20, SLR⁺20, dCVARN20]. **Efficient** [CSGVF⁺20, MT20b]. **elacestrant** [CSP20]. **Electric** [SHM⁺20]. **electride** [DSC20]. **electrocatalysts** [AR20]. **electron** [SS20, SSO⁺20]. **electronic** [AMF⁺20, OSHT20, STB⁺20]. **electrostatic** [AS20, ÖLP⁺20]. **Electrostatics** [HRT⁺20]. **Elementometalation** [WLZM20]. **embrittlement** [ZFRM20]. **emission** [AS20, FB20]. **Empirical** [LJ20]. **Encapsulation** [DSC20]. **Encoding** [GJMPB⁺20]. **End** [MXM20]. **End-Point** [MXM20]. **Energetics** [HHL⁺20, WGKG20]. **Energies** [BBK20, FMFG20, HFPS20, MFC20, NRH⁺20, HCS⁺20, ÖLP⁺20]. **Energy** [GRN20, LPP20, MXM20, Min20, NNT⁺20, SZLD20, AV20, CSGVF⁺20, CSWW20, CSP20, MSL⁺20, Sán20, SSS⁺20, YBS⁺20]. **Enhanced** [FMFG20, MH20]. **ensemble** [QLC⁺20]. **enter** [APS20]. **Enumeration** [SZLD20]. **environment** [KCF⁺20]. **Enzymatic** [SHM⁺20]. **enzyme** [DPSG20]. **equations** [MT20b]. **Erratum** [MT20a]. **estrogen** [CSP20]. **Evaluation** [PRH20, VAL20, SSS⁺20]. **events** [RLR⁺20]. **Evolution** [MM20, CG20]. **Exchange** [BBK20, SEZ20, YW20]. **Excitation** [HFPS20, HCS⁺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** [QLC⁺20]. **Factors** [AD20]. **fail** [JRS20]. **fail-safe** [JRS20]. **Fast** [YAO20, AYO20]. **Fe** [ZFRM20]. **Fe-C** [ZFRM20]. **Features** [SHM⁺20].

FePS [EK20]. **Fermi** [ASW20]. **FFLUX** [HRT⁺20]. **FFParam** [KYM20].
FGFR3 [MKSS20]. **Field**
 [BAC20, LJ20, WSL⁺20, KYM20, ODL20, PLP⁺20]. **Fields**
 [SHM⁺20, AMF⁺20]. **Fields-Features** [SHM⁺20]. **First** [DBE20, EK20].
First-Principles [DBE20, EK20]. **fitted** [BSF20]. **fitting** [CQSG20]. **Five**
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Fragmentation [AKN⁺20]. **Framework** [GRN20, LPP20, GUCCR20]. **Free**
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 [GUCCR20]. **function** [AV20, SWF⁺20]. **function-based** [AV20].
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 [BSF20, VCL20]. **Grained** [MT20a, WSL⁺20, WZZ⁺20, MT19]. **grand**
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GRP1 [PT20]. **GUI** [QLC⁺20]. **Guided** [CLS⁺20].

H [LR20, WSV20, dCVARN20]. **H/D** [dCVARN20]. **halogen** [CB20].
Hartree [BBK20]. **heat** [BAO⁺20]. **heat-shock** [BAO⁺20]. **Hedgehog**
 [Ban20]. **helices** [VCL20]. **helium** [BGS⁺20]. **Helix** [MKSS20]. **heme**
 [SWF⁺20]. **Heterolytic** [LR20]. **Hf** [DBE20]. **Hg** [SSS⁺20]. **High**
 [KUNT20, BSF20]. **high-level** [BSF20]. **Higher** [HFPS20]. **Highly**
 [JFZ⁺20]. **histogram** [MT20b]. **Hoff** [ZXD20b, ZXD20a]. **Hoff/Le**
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 [SDK20]. **Hopping** [YXGZ20]. **Human** [KUNT20]. **hybrid**
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Hydrocyanation [JFZ⁺20]. **hydrogen** [AV20, CB20, ZFRM20].

Hydrostatic [SL20]. **hydroxychromones** [AIV20]. **hydroxylation** [HYA⁺20]. **hydroxyquinolinato** [AS20]. **Hypercube** [Bal20]. **Hyperplanes** [Bal20].

II [AD20, SSS⁺20]. **III** [AS20]. **Image** [Ano20a, Ano20n, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m]. **imino** [YFS20]. **immersive** [MSL⁺20]. **Immunodeficiency** [KUNT20]. **implementation** [CSGVF⁺20, OMC⁺20]. **Implicit** [GCL⁺20]. **Importance** [HKSW20]. **improbability** [RLR⁺20]. **Improved** [BBK20, LJ20]. **Improving** [FB20]. **increase** [LKM20]. **Indexes** [WZZ⁺20]. **Induced** [QB20, EK20]. **Information** [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]. **infrared** [GPEK⁺20]. **inhibitor** [BAO⁺20]. **Initio** [SK20, VAL20]. **inner** [Sán20]. **inner-shell** [Sán20]. **Insight** [JFZ⁺20]. **Insights** [ASL⁺20, GOY20]. **insulator** [EK20]. **insulator-to-metal** [EK20]. **Integrated** [VDK⁺20]. **integration** [KCGK20]. **interacting** [CSGVF⁺20, OE20]. **Interaction** [KUNT20, PT20, ASW20, CSWW20]. **Interactions** [BWM20, LJ20, CTBB20, HPG20, ODL20, OE20, YW20]. **interatomic** [ZFRM20]. **intercalation** [HKSW20]. **interesting** [HPG20]. **Intermediates** [SK20]. **Intermolecular** [OOY20]. **Internal** [WZZ⁺20]. **Interplay** [HYA⁺20, ZRSST20]. **Interpolation** [WSL⁺20]. **intersection** [AIV20]. **intramolecular** [AIV20]. **Intrinsic** [AD20]. **inversion** [SWF⁺20]. **Investigating** [BSL20]. **Investigation** [CSP20, HL20, SS20]. **Involving** [SK20]. **Iodine** [ASL⁺20]. **Ion** [SLR⁺20, HPG20, JRS20, LA20, XAD20]. **Ion-Pair** [SLR⁺20]. **Ionic** [VAL20, XAD20]. **ions** [ODL20, SDK20]. **Ir** [DZL⁺20]. **Irreducible** [Bal20]. **Isoelectronic** [ZXD20a, ZXD20b]. **Isolation** [BLP20]. **isomerase** [DPSG20]. **isotope** [JMK⁺20, dCVARN20]. **Issue** [Ano20a, Ano20n, Ano20o, Ano20p, Ano20q, Ano20r, Ano20s, Ano20t, Ano20u, Ano20b, Ano20c, Ano20d, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, 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 [JMK⁺20, dCVARN20]. **Kinetics** [SK20, CD20]. **Kohn** [HCS⁺20]. **Koopmans** [GX20].

L536S [CSP20]. **Laplacian** [TTDT20]. **Large** [MFC20]. **Large-Sized** [MFC20]. **Late** [PWW20]. **Leading** [AD20]. **Learning** [LPP20, YFS20]. **length** [MVP⁺20]. **less** [CSWW20]. **level** [BSF20]. **Lewis** [OE20]. **library**

[RDS⁺20]. **Lif** [VDK⁺20]. **Ligand** [Ban20, JFZ⁺20, MXM20, NNT⁺20, AAe20, 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].

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 [QB20]. **Matrix** [BLP20]. **MD** [SSS⁺20]. **MDMS** [Zac20].
Me [SDK20, WLZM20]. **Me-3** [SDK20]. **Mechanical** [SL20, AAe20, 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** [LGD⁺20]. **metadynamics** [PPSP20]. **Metal** [HHL⁺20, PWW20, AR20, EK20, TYZ20, YFS20]. **metal-free** [TYZ20].
metal/ [AR20]. **methane** [DZL⁺20]. **Method** [QB20, AKN⁺20, AYO20, IYI⁺20, MT20b, SS20, YAO20]. **Methods** [AWID⁺20, KUNT20, SK20, ASW20, BSF20, GUCCR20, 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, LJ20, SHM⁺20, GUCCR20, LGD⁺20]. **models** [CTBB20, PLP⁺20]. **Modification** [AWID⁺20, Ban20]. **modified** [XAD20].
Modulation [ZSD⁺20]. **Molecular** [FMFG20, GJMPB⁺20, GGK20, 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, GGK20, KYM20, SSO⁺20, VCL20]. **Møller** [CSGVF⁺20, Sán20]. **Møller-Plesset** [CSGVF⁺20, Sán20]. **moments** [BSF20]. **Mono** [ZXD20b, ZXD20a]. **Mono-silicon** [ZXD20b, ZXD20a].
monooxygenase [HYA⁺20]. **Monte** [GGK20, KCGK20]. **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].

NADP [CWZD20]. **NADPH** [CWZD20]. **named** [SS20]. **nanotube** [APS20, CTBB20]. **Nanotubes** [DBE20, VCL20]. **Naphthalene** [NRH⁺20]. **Natural** [KL20, CB20, MH20, PW20]. **Nature** [MVP⁺20]. **NCF** [OE20]. **net** [ÖLP⁺20]. **net-charge** [ÖLP⁺20]. **Network** [BSL20]. **neutral** [BGS⁺20]. **Neutralizing** [KUNT20]. **Newton** [MT20b]. **Newton-Raphson** [MT20b]. **Newton-Raphson/singular** [MT20b]. **Next** [AMF⁺20]. **Next-generation** [AMF⁺20]. **NH** [OE20, SLR⁺20]. **nitrogen** [XZZ⁺20]. **NMR** [TTDT20]. **NN** [LPP20]. **noncovalent** [CSWW20, CTBB20, OE20, YW20]. **Noniterative** [HFPS20]. **nonlocal** [YW20]. **Nonredundant** [XZ20]. **novel** [SS20]. **nuclear** [VCL20]. **nucleobases** [CTBB20]. **number** [MT20b]. **numbers** [ASW20].

O [SWF⁺20, TYZ20]. **Obelin** [GOY20]. **occupation** [ASW20]. **OCOH** [dCVARN20]. **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]. **orbitals** [FV20, KL20, MH20]. **order** [CSGVF⁺20, GX20, Sán20, YW20]. **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** [AYO20, CSGVF⁺20]. **Path** [SZLD20]. **pathway** [HL20]. **pathways** [CG20]. **penicillin** [CD20]. **PepPro** [XZ20]. **peptidase** [CD20]. **Peptide** [XZ20]. **Peptide-Protein** [XZ20]. **Performance** [BBK20, NRH⁺20, PB20, LKM20]. **Performing** [Zac20]. **Periodic** [SDK20, YAO20]. **permeability** [ZSD⁺20]. **perspective** [PPSP20]. **Perturbation** [NNT⁺20, AAe20, GX20, MH20, OE20, Sán20, YBS⁺20]. **PH** [PT20, SSS⁺20]. **Phase** [HFPS20, YW20]. **phenyl** [AS20]. **Phonons** [DBE20]. **phosphate** [DPSG20]. **phosphoborane** [STB⁺20]. **phosphoglucose** [DPSG20]. **phosphorus** [ASL⁺20]. **photochemical** [CG20]. **photodynamic** [ASL⁺20]. **Photoisomerization** [YXGZ20]. **Photoprotein** [GOY20]. **photosensitizers** [ASL⁺20]. **pistol** [JRS20]. **pK** [PWW20]. **planewave** [SM20]. **Plasticity** [AD20]. **Plesset** [CSGVF⁺20, Sán20]. **Point** [MXM20, BSF20]. **Poisson** [XAD20]. **Polarizable** [HRT⁺20, LJ20, KYM20, ODL20]. **polarization** [SSO⁺20]. **polyatomic** [SSO⁺20]. **Polyethyleneimine** [BAC20]. **Polyethylenimine** [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, AAe20, 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**
 [BGS⁺20]. **projection** [VCL20]. **promenades** [MSL⁺20]. **Properties**
 [DBE20, GOY20, HZG⁺20, SL20, SB20, AS20, STB⁺20, WSV20]. **Protein**
 [BWM20, BSL20, CLS⁺20, MXM20, SZLD20, XZ20, BAO⁺20, KCGK20,
 SEZ20, WGKG20]. **Protein-Ligand** [MXM20]. **Protein-Protein** [BSL20].
Proteins [HHL⁺20, LJ20, KCF⁺20]. **Proton** [MFC20, AIV20]. **Protonated**
 [BAC20]. **Pseudodiagonalization** [SM20]. **Pseudodiagonalization-based**
 [SM20]. **Pseudomonas** [VDK⁺20]. **Pt** [DZL⁺20, PPSP20]. **puzzling**
 [XCJ20]. **pyrazine** [MH20]. **PyRETIS** [RLR⁺20]. **pyridine** [YFS20].

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, OYO20, Pil20, CSGVF⁺20, GPEK⁺20, HKSW20, OE20].
quaternary [ODL20]. **QuBiLS** [GJMPVR⁺20]. **QuBiLS-MIDAS**
 [GJMPVR⁺20].

R [GGK20, LR20]. **R-C** [LR20]. **R61** [CD20]. **Raman** [GPEK⁺20, MH20].
Random [HFPS20, YW20]. **Range** [BBK20, HCS⁺20]. **Raphson/singular**
 [MT20b]. **rapid** [MT20b]. **rare** [RLR⁺20]. **Ras** [MM20]. **rate** [dCVARN20].
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].
replica [SEZ20]. **Representation** [WZZ⁺20]. **Representations**
 [Bal20, SBG20]. **repulsive** [SEZ20]. **Resolving** [XCJ20]. **resonance** [AV20].
resonance-assisted [AV20]. **resource** [LGD⁺20]. **responsive** [KCF⁺20].
restrained [QLC⁺20]. **restrained-ensemble** [QLC⁺20]. **Restrains**
 [MXM20]. **reveals** [JRS20]. **Review** [ZFRM20]. **revisited** [SWF⁺20].
riboswitches [AAe20]. **ribozyme** [JRS20]. **Rigid** [Min20]. **Ring** [LJ20].
RNA [AAe20]. **Role** [MKSS20]. **Roux** [IBL20]. **RS** [VAL20]. **RubisCO**
 [JMK⁺20].

S [DBE20, SLR⁺20, PWW20]. **safe** [JRS20]. **same** [Sán20]. **same-spin** [Sán20]. **Sampling** [FMFG20, SSS⁺20, STR20, ZGZC20]. **scale** [BGS⁺20, RDS⁺20]. **scaled** [Sán20]. **scaling** [ASW20, SEZ20]. **scattering** [MH20]. **Scheme** [BSL20, GRN20, MT20b, STR20]. **schiff** [ZRSST20]. **scoring** [AMF⁺20]. **scramblase** [KCF⁺20]. **screened** [YW20]. **screening** [AR20]. **search** [BAO⁺20]. **second** [CSGVF⁺20, GX20, Sán20, YW20]. **second-order** [CSGVF⁺20, GX20, Sán20, YW20]. **Secondary** [AD20, AAe20, JRS20]. **selenium** [ZGZ⁺20]. **selenium-containing** [ZGZ⁺20]. **self** [ASW20, CQSG20, PRH20]. **self-assembly** [PRH20]. **self-consistent** [CQSG20]. **self-interaction** [ASW20]. **semiconductor** [ZGZ⁺20]. **Semiempirical** [GUCCR20]. **sensor** [ZRSST20]. **Separated** [BBK20]. **separation** [WG20]. **sequential** [GGK20]. **server** [LGD⁺20]. **Set** [XZ20, YXGZ20]. **Sham** [HCS⁺20]. **Shavitt** [SBG20]. **shell** [Sán20]. **shift** [TTDT20]. **shock** [BAO⁺20]. **side** [ODL20]. **Silicon** [HZG⁺20, GPEK⁺20, ZXD20b, ZXD20a]. **similar** [HGF20]. **Simplex** [WSL⁺20]. **Simulating** [LA20]. **Simulation** [HZG⁺20, NNT⁺20, SL20, CSP20, KCGK20]. **Simulations** [SZLD20, Zac20, GKG20, LKM20, QLC⁺20, WGKG20]. **Singlet** [HFPS20]. **singular** [MT20b]. **Site** [VDK⁺20, DPSG20, PLP⁺20]. **sites** [HGF20, LKM20]. **size** [HKS⁺20, XAD20]. **size-modified** [XAD20]. **Sized** [MFC20]. **Slater** [FV20]. **Small** [LPP20, KYM20]. **Smoothed** [GJMPB⁺20]. **Software** [Zac20, GJMPVR⁺20]. **Solute** [GRN20]. **solutions** [SSS⁺20]. **Solvation** [GRN20, MFC20]. **Solvent** [BBK20, FMFG20, GCL⁺20, SLR⁺20, VCL20, XAD20]. **solvent-accessible** [VCL20]. **Some** [QB20]. **sp** [AKN⁺20]. **space** [BAO⁺20, HL20]. **speciation** [LGD⁺20]. **species** [XAD20]. **Spectra** [CWZD20, GPEK⁺20]. **Spectroscopy** [BLP20, FB20]. **Spherical** [GJMPB⁺20]. **Spin** [IYI⁺20, SWF⁺20, HYA⁺20, QLC⁺20, Sán20, XCJ20]. **spin-coupled** [XCJ20]. **Spin-flip** [IYI⁺20]. **Spin-inversion** [SWF⁺20]. **spin-pair** [QLC⁺20]. **splitting** [OSHT20]. **SPOT** [CLS⁺20]. **SPOT-Fold** [CLS⁺20]. **Stability** [STB⁺20, VAL20, PB20]. **Standalone** [KYM20]. **State** [BWM20, BSF20, AIV20, KL20, OSHT20, WD20, ZRSST20, dCVARN20]. **State-of-the-art** [BSF20]. **states** [CG20, HYA⁺20, OMC⁺20, RDS⁺20]. **Statistical** [AAe20]. **steels** [ZFRM20]. **stereographic** [VCL20]. **Stereoselectivity** [WLZM20]. **Steric** [VDK⁺20]. **stone** [CTBB20]. **stone-wales** [CTBB20]. **storage** [WG20]. **Strain** [SLR⁺20]. **strength** [MVP⁺20]. **Streptomyces** [CD20]. **Structural** [SL20]. **Structure** [CLS⁺20, XZ20, AAe20, AYO20, HGF20]. **Structures** [CWZD20, HZG⁺20]. **Studies** [CWZD20, HKS⁺20, ZFRM20]. **Study** [JFZ⁺20, APS20, CTBB20, DZL⁺20, OE20, PRH20, RDS⁺20, SSS⁺20, WG20]. **Substituted** [NRH⁺20, ASL⁺20]. **Substitutional** [GPEK⁺20]. **substrates** [KCF⁺20]. **Superfamily** [MM20]. **supported** [DZL⁺20]. **Surface** [GCL⁺20, MH20, YXGZ20, VCL20]. **Surface-enhanced** [MH20]. **surfaces** [MSL⁺20, VCL20]. **swarms** [LA20]. **symmetry** [OE20].

symmetry-adapted [OE20]. **synergistic** [PRH20]. **System** [HHL⁺20]. **Systematic** [KUNT20, STR20]. **Systems** [LR20, WG20, YAO20].

T [CSWW20]. **Taba** [dSBFdAJ20]. **TaH** [WLZM20]. **tailoring** [AV20]. **TD** [WD20]. **TDDFT** [NRH⁺20]. **Technique** [WSL⁺20]. **tensor** [GJMPVR⁺20]. **Terminal** [JFZ⁺20, MKSS20]. **tetrahydrodibenzazosines** [SS20]. **tetrakis** [MVP⁺20]. **tetravalent** [SDK20]. **Tf** [TYZ20]. **TGR5** [WGKG20]. **theorem** [GX20]. **Theoretical** [JMK⁺20, PRH20]. **Theory** [IYI⁺20, SK20, YXGZ20, APS20, ASL⁺20, CTBB20, DZL⁺20, FB20, GX20, HCS⁺20, MH20, OE20, OMC⁺20, SDK20, SWF⁺20, Sán20, dCVARN20]. **therapy** [ASL⁺20]. **thermal** [GGK20]. **Thermodynamic** [DBE20, SZLD20, KCGK20]. **Thermodynamics** [SK20]. **Thiols** [AWID⁺20]. **Three** [PLP⁺20, YAO20]. **three-dimensional** [YAO20]. **Three-site** [PLP⁺20]. **thymine** [SSS⁺20]. **tight** [IYI⁺20, Pil20]. **tight-binding** [IYI⁺20]. **Time** [YXGZ20, FB20, IYI⁺20, OMC⁺20]. **Time-Dependent** [YXGZ20, FB20, IYI⁺20, OMC⁺20]. **TITAN** [SHM⁺20]. **TMEM16** [KCF⁺20]. **Tool** [dSBFdAJ20, LKM20, ZGZC20]. **topology** [MVP⁺20, Pil20]. **trajectories** [LA20]. **Trajectory** [OSHT20, YXGZ20, ZGZC20]. **transfer** [AIV20, KCGK20, OMC⁺20]. **Transition** [PWW20, AR20, EK20, KL20, dCVARN20]. **Transition-Metal** [PWW20]. **Transmembrane** [MKSS20]. **Transport** [HHL⁺20, WSV20, ZGZ⁺20]. **tree** [AYO20]. **trends** [SDK20]. **Trichoderma** [HYA⁺20]. **Triplet** [HFPS20]. **tris** [AS20]. **tropolone** [OSHT20]. **truncated** [GJMPVR⁺20]. **Truncation** [GJMPB⁺20]. **Tuning** [BBK20]. **tunneling** [OSHT20]. **two** [HYA⁺20, KL20, STB⁺20, YAO20]. **two-component** [KL20]. **two-dimensional** [STB⁺20]. **type** [FV20, KUNT20]. **Type-1** [KUNT20].

U [SB20]. **umbrella** [SSS⁺20]. **Unitary** [SBG20]. **Units** [AD20, GCL⁺20]. **Unlocking** [GUCCR20]. **Unprecedented** [JFZ⁺20]. **updated** [MT20b]. **uranyl** [PB20]. **useful** [ZGZC20]. **Using** [GCL⁺20, KUNT20, LJ20, VAL20, WZZ⁺20, AV20, BSL20, BSF20, CQSG20, LA20, SEZ20]. **UV** [CWZD20]. **UV-Vis** [CWZD20].

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